Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 10:56 PM EDT

PDB ID	:	1D4C / pdb_00001d4c
Title	:	CRYSTAL STRUCTURE OF THE UNCOMPLEXED FORM OF THE FLAVOCYTOCHROME C FUMARATE REDUCTASE OF SHEWANELLA PUTREFACIENS STRAIN MR-1
Authors	:	Leys, D.; Tsapin, A.S.; Meyer, T.E.; Cusanovich, M.A.; Van Beeumen, J.J.
Deposited on	:	1999-10-03
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

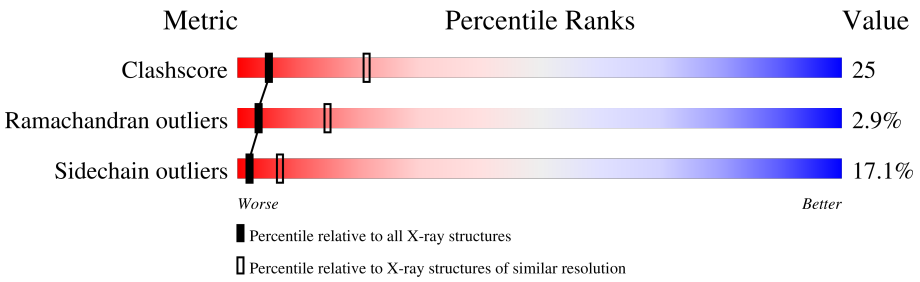
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	572	34% 44% 17% •
1	B	572	36% 44% 16% • •
1	C	572	34% 43% 19% • •
1	D	572	38% 43% 16% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEC	A	601	X	-	-	-
2	HEC	A	602	X	-	-	-
2	HEC	A	603	X	-	-	-
2	HEC	A	604	X	-	-	-
2	HEC	B	601	X	-	-	-
2	HEC	B	602	X	-	-	-
2	HEC	B	603	X	-	-	-
2	HEC	B	604	X	-	-	-
2	HEC	C	601	X	-	-	-
2	HEC	C	602	X	-	-	-
2	HEC	C	603	X	-	-	-
2	HEC	C	604	X	-	-	-
2	HEC	D	601	X	-	-	-
2	HEC	D	602	X	-	-	-
2	HEC	D	604	X	-	-	-
3	FAD	A	600	X	-	-	-
3	FAD	B	700	X	-	-	-
3	FAD	C	800	X	-	-	-
3	FAD	D	900	X	-	-	-

2 Entry composition (i)

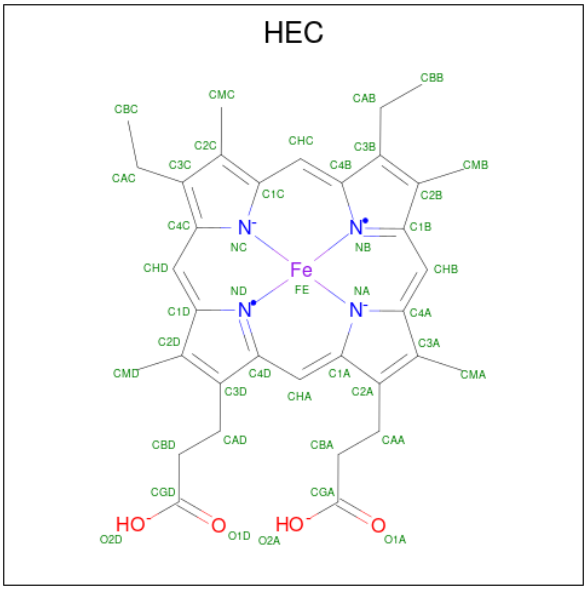
There are 5 unique types of molecules in this entry. The entry contains 17470 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called FLAVOCYTOCHROME C FUMARATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	570	4124	2562	736	807	19	0	0	0
1	B	566	4093	2542	731	801	19	0	0	0
1	C	568	4099	2546	733	801	19	0	0	0
1	D	570	4113	2553	734	807	19	0	0	0

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
2	A	1	43	34	1	4	4	0	0

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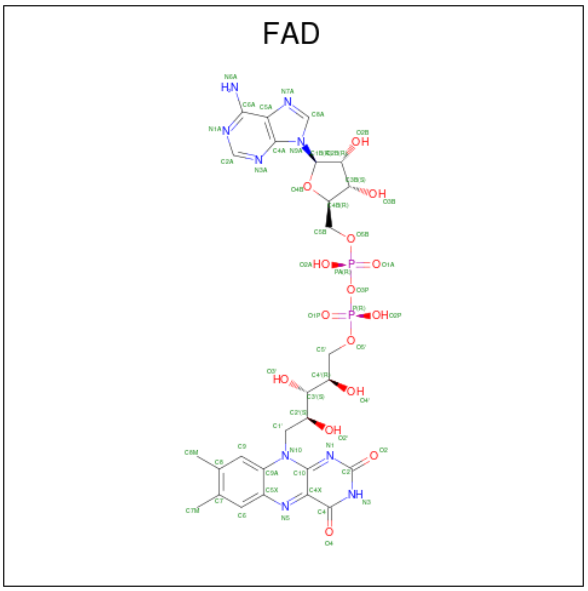
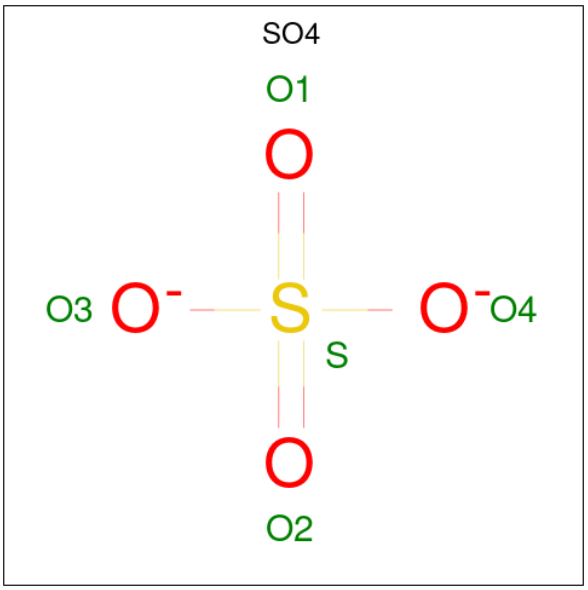
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	D	1	43	34	1	4	4	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	B	1	5	4	1	0	0
			Total	O	S		
4	C	1	5	4	1	0	0
			Total	O	S		
4	D	1	5	4	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	48	48	48	0	0
			Total	O		
5	B	29	29	29	0	0
			Total	O		
5	C	30	30	30	0	0
			Total	O		
5	D	19	19	19	0	0

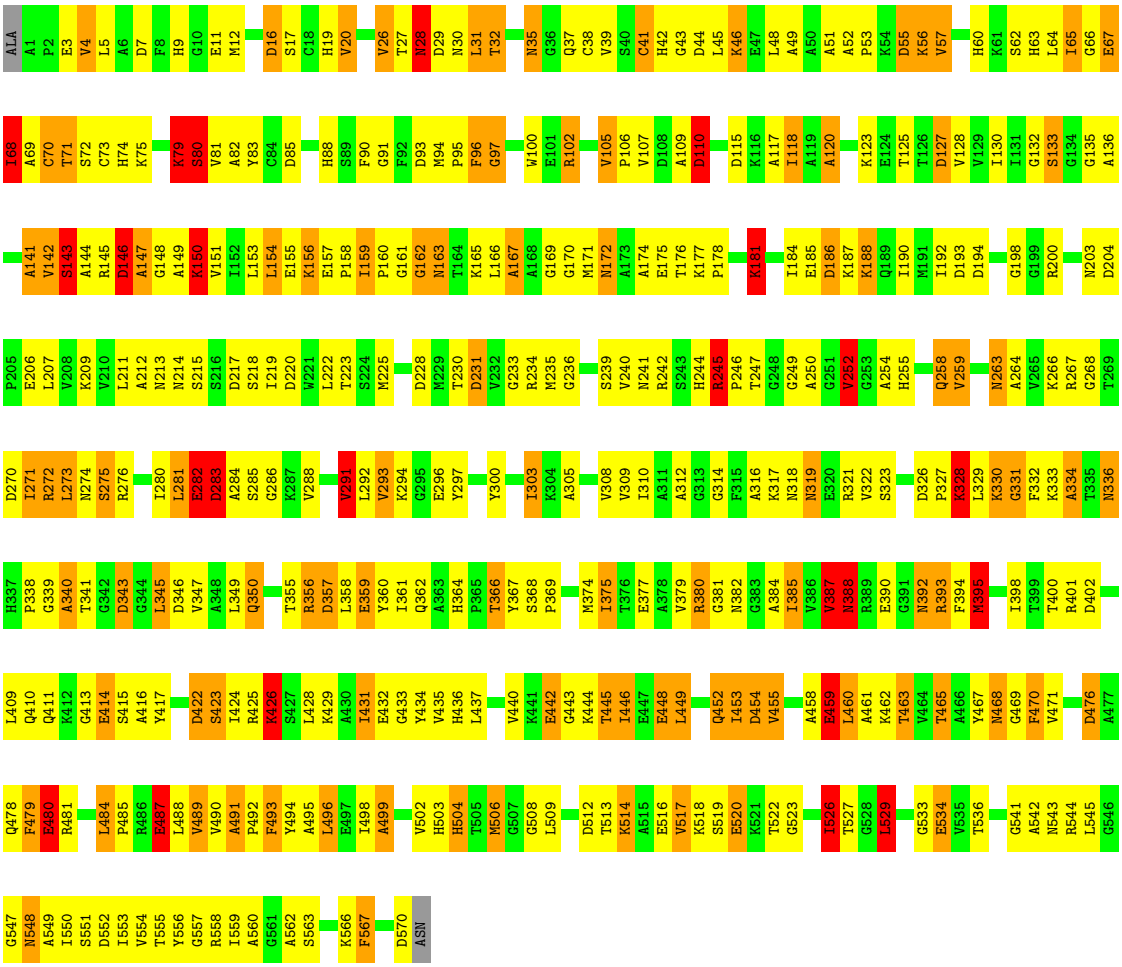
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

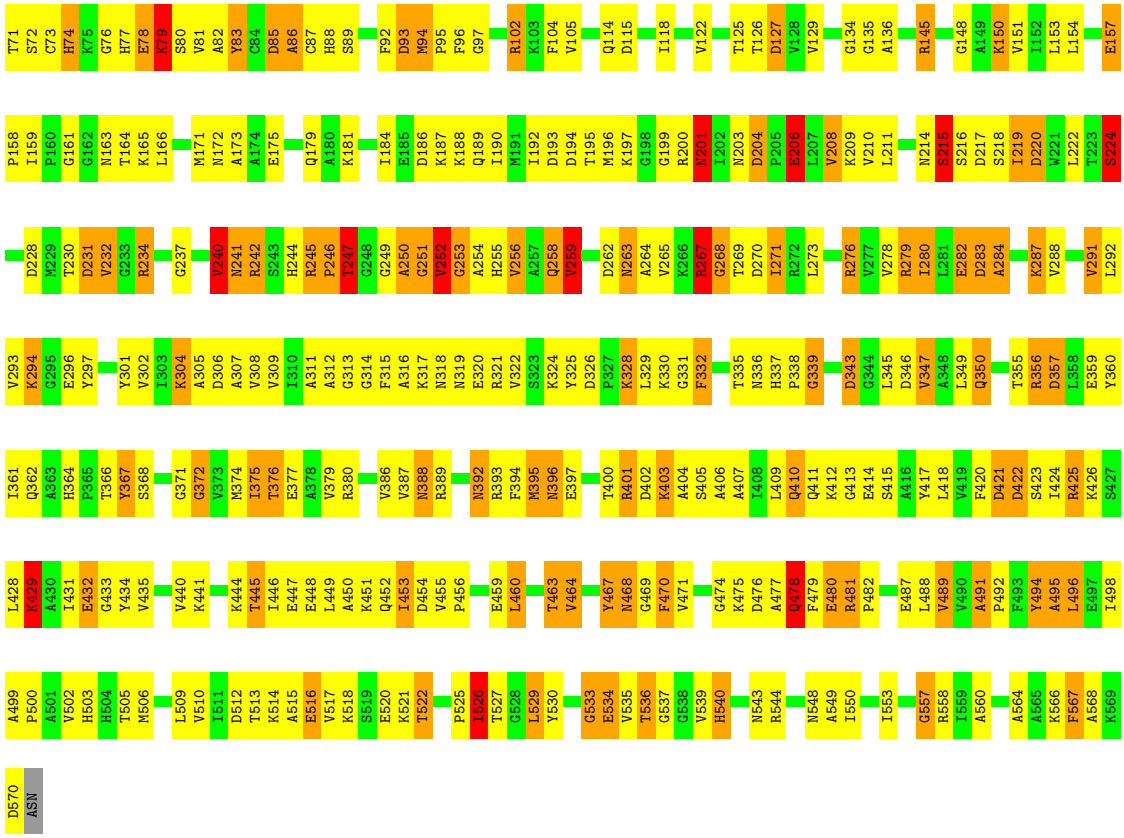
• Molecule 1: FLAVOCYTOCHROME C FUMARATE REDUCTASE

Chain A: 34% 44% 17% •



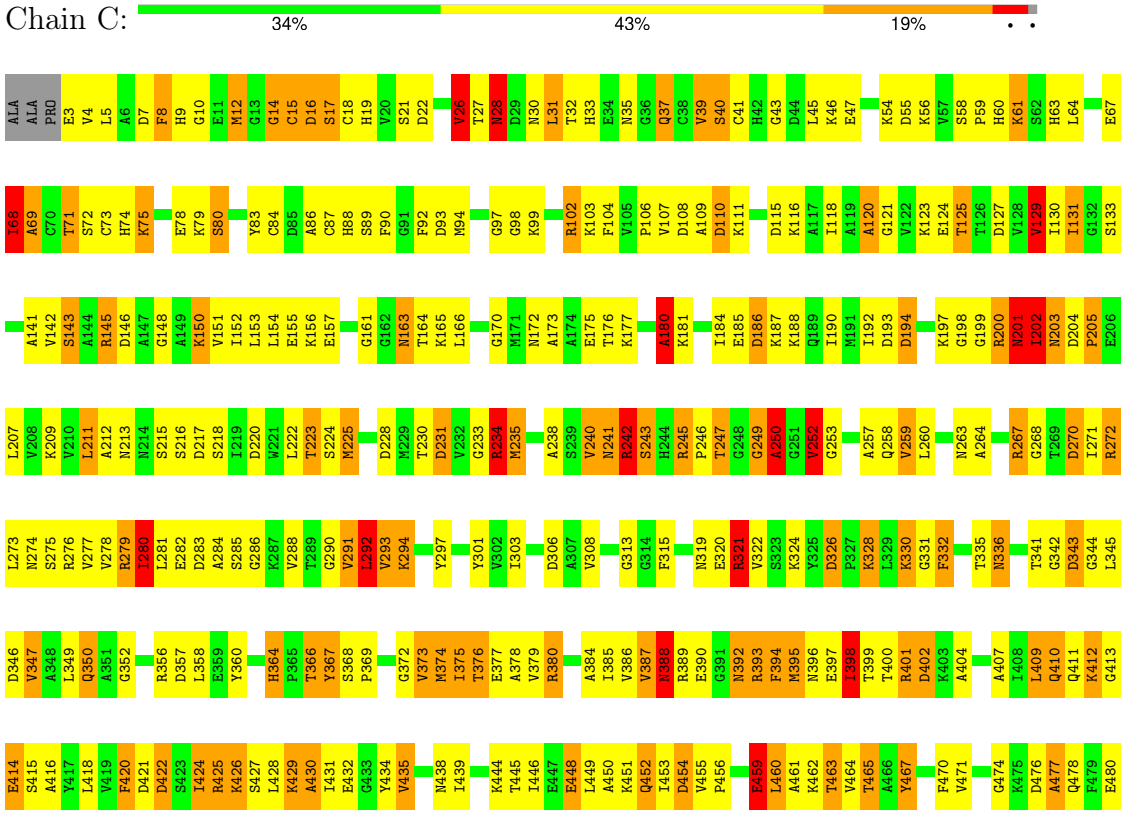
• Molecule 1: FLAVOCYTOCHROME C FUMARATE REDUCTASE

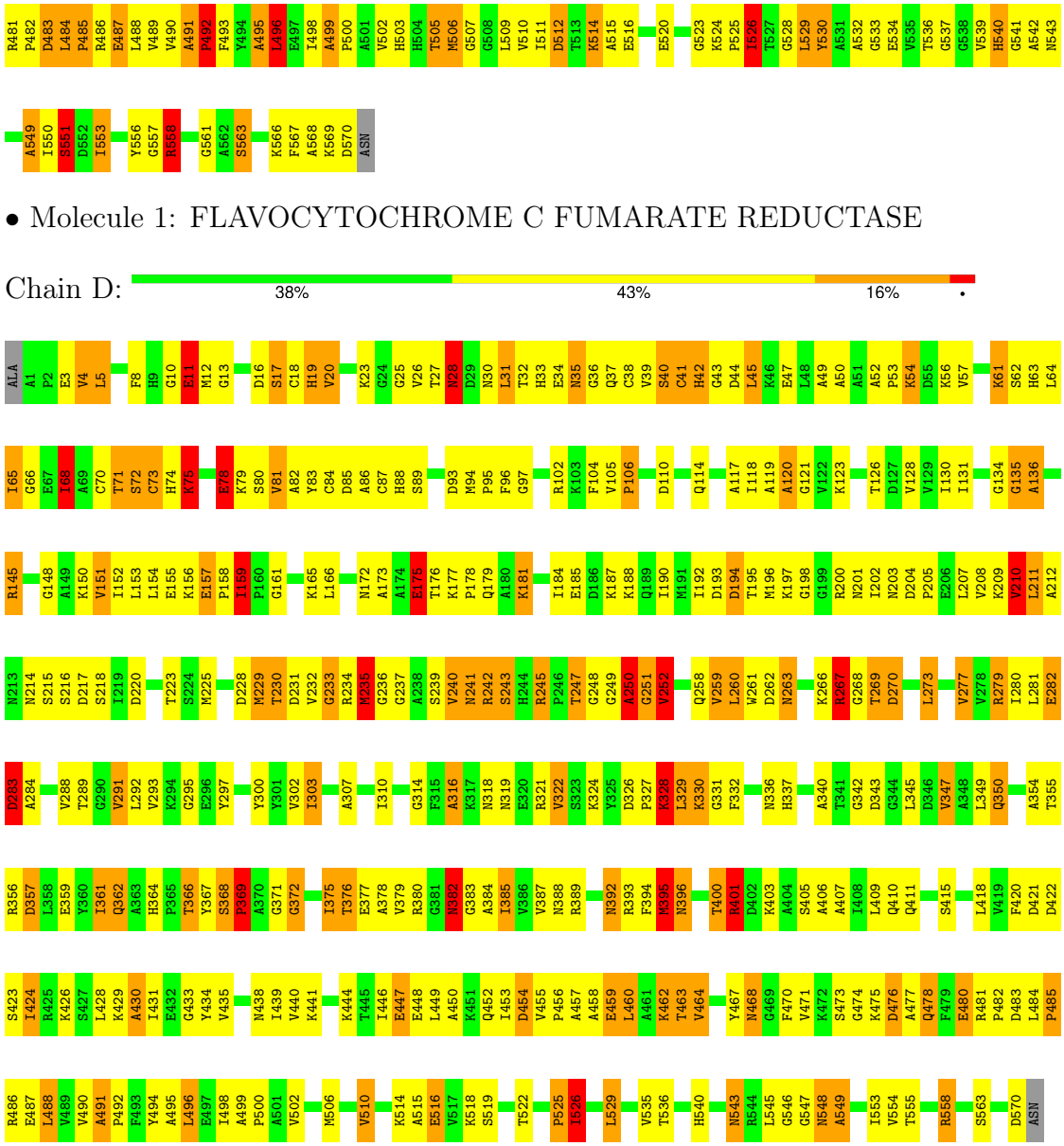
Chain B: 36% 44% 16% • •



- Molecule 1: FLAVOCYTOCHROME C FUMARATE REDUCTASE

Chain C:





• Molecule 1: FLAVOCYTOCHROME C FUMARATE REDUCTASE

Chain D:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	109.69Å 216.36Å 112.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90	Depositor
% Data completeness (in resolution range)	93.7 (15.00-2.90)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.210 , 0.300	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17470	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, SO4, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.01	1/4192 (0.0%)	2.68	353/5683 (6.2%)
1	B	0.97	15/4159 (0.4%)	2.52	288/5637 (5.1%)
1	C	0.93	3/4166 (0.1%)	2.56	322/5649 (5.7%)
1	D	0.84	1/4179 (0.0%)	2.44	251/5665 (4.4%)
All	All	0.94	20/16696 (0.1%)	2.55	1214/22634 (5.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	3
1	D	0	2
All	All	0	10

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	476	ASP	CG-OD1	10.26	1.44	1.25
1	B	475	LYS	C-O	10.05	1.36	1.23
1	C	477	ALA	C-O	9.29	1.35	1.24
1	B	477	ALA	N-CA	7.39	1.55	1.46
1	B	469	GLY	N-CA	7.25	1.55	1.45
1	B	468	ASN	C-O	7.21	1.32	1.24
1	B	468	ASN	CG-OD1	6.85	1.36	1.23
1	B	478	GLN	N-CA	6.77	1.54	1.46
1	D	468	ASN	CG-ND2	6.12	1.46	1.33
1	B	476	ASP	CG-OD2	5.86	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	480	GLU	CD-OE1	5.84	1.36	1.25
1	B	474	GLY	CA-C	5.77	1.58	1.51
1	A	267	ARG	CD-NE	-5.59	1.38	1.46
1	C	459	GLU	CD-OE1	5.54	1.35	1.25
1	B	469	GLY	C-N	5.51	1.41	1.33
1	B	247	THR	N-CA	-5.17	1.39	1.46
1	C	459	GLU	CD-OE2	5.11	1.35	1.25
1	B	268	GLY	N-CA	5.08	1.52	1.45
1	B	251	GLY	N-CA	-5.07	1.38	1.45
1	B	476	ASP	C-N	5.04	1.40	1.33

All (1214) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	245	ARG	CD-NE-CZ	28.45	164.23	124.40
1	D	491	ALA	CA-C-O	-25.02	100.19	119.46
1	C	491	ALA	CA-C-O	-23.99	95.97	119.24
1	B	570	ASP	CA-CB-CG	23.53	136.13	112.60
1	A	267	ARG	CD-NE-CZ	23.43	157.20	124.40
1	D	401	ARG	CD-NE-CZ	21.28	154.19	124.40
1	A	491	ALA	CA-C-O	-19.91	100.00	119.51
1	A	281	LEU	CA-C-N	19.13	157.03	121.06
1	A	281	LEU	C-N-CA	19.13	157.03	121.06
1	B	491	ALA	CA-C-O	-18.86	102.03	119.75
1	B	356	ARG	CD-NE-CZ	18.59	150.43	124.40
1	C	267	ARG	CD-NE-CZ	18.36	150.10	124.40
1	B	246	PRO	CA-C-N	18.07	156.06	121.54
1	B	246	PRO	C-N-CA	18.07	156.06	121.54
1	A	7	ASP	CA-CB-CG	17.71	130.31	112.60
1	C	392	ASN	CA-CB-CG	17.01	129.61	112.60
1	B	145	ARG	CD-NE-CZ	16.17	147.04	124.40
1	D	281	LEU	CA-C-N	16.02	147.99	121.39
1	D	281	LEU	C-N-CA	16.02	147.99	121.39
1	B	468	ASN	OD1-CG-ND2	15.82	138.42	122.60
1	C	477	ALA	CA-C-O	-15.59	102.05	119.97
1	A	558	ARG	CG-CD-NE	14.77	144.50	112.00
1	A	283	ASP	CA-CB-CG	14.65	127.25	112.60
1	A	245	ARG	CB-CG-CD	14.40	144.42	111.30
1	C	332	PHE	CA-CB-CG	14.32	128.12	113.80
1	D	185	GLU	CA-CB-CG	14.24	142.58	114.10
1	C	16	ASP	CA-CB-CG	14.24	126.84	112.60
1	D	283	ASP	CA-CB-CG	14.24	126.84	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	102	ARG	NE-CZ-NH2	14.18	131.97	119.20
1	B	252	VAL	N-CA-CB	14.16	125.49	110.62
1	C	328	LYS	CA-CB-CG	14.02	142.13	114.10
1	B	11	GLU	CB-CG-CD	13.63	135.78	112.60
1	A	93	ASP	CA-CB-CG	-13.38	99.22	112.60
1	A	319	ASN	CA-CB-CG	13.31	125.91	112.60
1	C	110	ASP	CA-CB-CG	12.94	125.54	112.60
1	D	396	ASN	CA-CB-CG	12.81	125.41	112.60
1	A	380	ARG	NE-CZ-NH2	12.54	130.49	119.20
1	A	558	ARG	NE-CZ-NH2	12.45	130.40	119.20
1	B	246	PRO	CA-C-O	12.35	136.13	121.31
1	C	543	ASN	OD1-CG-ND2	12.25	134.85	122.60
1	D	382	ASN	CA-CB-CG	12.14	124.74	112.60
1	A	186	ASP	CA-CB-CG	12.11	124.71	112.60
1	D	176	THR	CA-C-N	11.89	134.52	119.78
1	D	176	THR	C-N-CA	11.89	134.52	119.78
1	B	343	ASP	CA-CB-CG	11.79	124.39	112.60
1	C	401	ARG	CD-NE-CZ	11.74	140.83	124.40
1	B	267	ARG	CA-C-O	-11.67	109.75	122.01
1	C	506	MET	CA-C-O	-11.55	108.54	120.90
1	B	16	ASP	CA-CB-CG	11.49	124.09	112.60
1	B	474	GLY	O-C-N	11.24	134.00	122.54
1	D	262	ASP	CA-CB-CG	11.23	123.83	112.60
1	C	156	LYS	CA-CB-CG	11.22	136.55	114.10
1	B	4	VAL	N-CA-CB	11.17	129.68	111.36
1	B	470	PHE	N-CA-C	-11.15	99.13	111.28
1	B	250	ALA	CA-C-N	10.98	142.93	121.41
1	B	250	ALA	C-N-CA	10.98	142.93	121.41
1	B	270	ASP	CA-CB-CG	10.96	123.56	112.60
1	B	220	ASP	CA-CB-CG	10.91	123.51	112.60
1	C	102	ARG	CD-NE-CZ	10.89	139.65	124.40
1	D	492	PRO	N-CA-CB	10.87	114.66	103.25
1	C	61	LYS	CA-CB-CG	10.84	135.77	114.10
1	A	3	GLU	CA-C-N	10.76	141.34	121.97
1	A	3	GLU	C-N-CA	10.76	141.34	121.97
1	A	56	LYS	CA-C-N	10.73	141.29	121.97
1	A	56	LYS	C-N-CA	10.73	141.29	121.97
1	B	217	ASP	CA-CB-CG	10.69	123.29	112.60
1	C	478	GLN	CB-CG-CD	-10.64	94.51	112.60
1	C	373	VAL	CA-C-O	10.49	134.13	121.75
1	A	481	ARG	CD-NE-CZ	10.47	139.06	124.40
1	C	228	ASP	CA-CB-CG	10.37	122.97	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	200	ARG	CD-NE-CZ	10.34	138.87	124.40
1	A	281	LEU	CA-C-O	10.20	132.65	120.92
1	B	492	PRO	N-CA-CB	10.15	113.91	103.25
1	C	17	SER	CA-C-O	10.12	132.26	120.92
1	B	252	VAL	CA-C-O	-10.12	110.89	121.41
1	A	392	ASN	CA-CB-CG	10.08	122.68	112.60
1	B	161	GLY	N-CA-C	10.06	127.05	115.08
1	C	28	ASN	CA-CB-CG	10.01	122.61	112.60
1	D	242	ARG	NE-CZ-NH2	-9.97	110.23	119.20
1	B	251	GLY	N-CA-C	9.95	136.75	113.18
1	C	344	GLY	CA-C-O	-9.94	110.81	121.05
1	A	193	ASP	CA-CB-CG	9.94	122.54	112.60
1	C	211	LEU	CA-C-O	9.94	132.00	121.07
1	C	270	ASP	CA-CB-CG	9.79	122.39	112.60
1	A	282	GLU	N-CA-C	9.79	122.45	110.41
1	C	274	ASN	OD1-CG-ND2	9.71	132.31	122.60
1	B	469	GLY	CA-C-O	9.67	130.85	120.40
1	D	25	GLY	CA-C-O	-9.66	115.94	122.22
1	A	242	ARG	NE-CZ-NH2	9.64	127.88	119.20
1	B	350	GLN	CB-CG-CD	9.63	128.97	112.60
1	A	16	ASP	CA-CB-CG	9.60	122.20	112.60
1	A	321	ARG	O-C-N	-9.54	112.17	122.09
1	D	356	ARG	NE-CZ-NH2	9.54	127.79	119.20
1	D	242	ARG	CD-NE-CZ	9.52	137.72	124.40
1	C	478	GLN	OE1-CD-NE2	9.51	132.11	122.60
1	D	546	GLY	CA-C-O	9.48	129.75	121.41
1	C	259	VAL	N-CA-CB	9.46	121.62	110.55
1	A	258	GLN	CA-C-O	-9.44	110.91	120.82
1	C	492	PRO	N-CA-CB	9.41	113.13	103.25
1	D	343	ASP	CA-CB-CG	9.39	121.99	112.60
1	D	16	ASP	CA-CB-CG	9.34	121.94	112.60
1	D	248	GLY	O-C-N	-9.27	116.11	123.80
1	D	492	PRO	CA-N-CD	-9.23	99.07	112.00
1	A	267	ARG	CA-C-O	-9.23	109.97	121.50
1	B	61	LYS	CA-CB-CG	9.22	132.55	114.10
1	B	252	VAL	CB-CA-C	-9.21	99.91	111.70
1	C	163	ASN	OD1-CG-ND2	-9.21	113.39	122.60
1	A	43	GLY	N-CA-C	-9.20	101.20	112.33
1	A	267	ARG	NE-CZ-NH1	-9.19	112.31	121.50
1	B	201	ASN	CA-CB-CG	9.18	121.78	112.60
1	A	69	ALA	CA-C-N	9.15	132.73	120.65
1	A	69	ALA	C-N-CA	9.15	132.73	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	242	ARG	NE-CZ-NH1	9.15	130.65	121.50
1	D	546	GLY	O-C-N	-9.12	113.90	122.93
1	A	19	HIS	O-C-N	-9.11	112.86	123.06
1	C	301	TYR	CA-CB-CG	9.09	130.25	113.90
1	B	475	LYS	O-C-N	9.07	133.65	123.40
1	A	393	ARG	CD-NE-CZ	9.07	137.09	124.40
1	C	569	LYS	CA-C-N	9.07	138.02	121.70
1	C	569	LYS	C-N-CA	9.07	138.02	121.70
1	D	526	ILE	N-CA-CB	9.06	120.88	110.82
1	A	38	CYS	CB-CA-C	-9.02	96.38	110.81
1	C	502	VAL	CA-C-O	-9.02	112.30	121.59
1	B	150	LYS	CB-CA-C	9.01	125.27	110.22
1	A	424	ILE	N-CA-CB	8.99	120.49	110.51
1	C	509	LEU	CA-C-O	-8.97	111.32	121.19
1	A	242	ARG	CD-NE-CZ	8.97	136.95	124.40
1	C	3	GLU	CA-C-N	8.96	138.11	121.97
1	C	3	GLU	C-N-CA	8.96	138.11	121.97
1	A	329	LEU	CA-C-O	-8.91	108.50	119.28
1	B	533	GLY	O-C-N	-8.90	114.44	122.90
1	B	259	VAL	N-CA-CB	8.90	123.92	110.58
1	B	19	HIS	CA-CB-CG	-8.84	104.96	113.80
1	A	321	ARG	NE-CZ-NH1	8.81	130.31	121.50
1	A	272	ARG	NE-CZ-NH2	-8.79	111.29	119.20
1	A	281	LEU	O-C-N	-8.79	112.97	123.16
1	B	283	ASP	CA-C-N	8.78	138.30	121.54
1	B	283	ASP	C-N-CA	8.78	138.30	121.54
1	C	141	ALA	CA-C-O	-8.74	111.64	120.82
1	D	279	ARG	NE-CZ-NH2	8.71	127.04	119.20
1	A	97	GLY	N-CA-C	8.70	123.38	111.54
1	D	356	ARG	CD-NE-CZ	8.69	136.56	124.40
1	A	526	ILE	CB-CA-C	8.65	121.42	110.96
1	A	570	ASP	CA-CB-CG	8.63	121.23	112.60
1	A	200	ARG	NE-CZ-NH1	8.62	130.12	121.50
1	D	185	GLU	CB-CG-CD	8.60	127.22	112.60
1	A	380	ARG	NE-CZ-NH1	-8.60	112.91	121.50
1	D	223	THR	O-C-N	-8.59	113.22	122.07
1	D	395	MET	CA-CB-CG	8.58	131.25	114.10
1	D	295	GLY	N-CA-C	-8.54	102.11	111.93
1	A	228	ASP	CA-CB-CG	8.52	121.12	112.60
1	A	27	THR	N-CA-C	-8.51	103.48	114.04
1	B	276	ARG	NE-CZ-NH2	-8.51	111.54	119.20
1	B	401	ARG	NE-CZ-NH2	-8.46	111.58	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	476	ASP	CA-CB-CG	8.46	121.06	112.60
1	A	357	ASP	CA-CB-CG	-8.46	104.14	112.60
1	C	558	ARG	CG-CD-NE	8.45	130.59	112.00
1	D	281	LEU	CA-C-O	8.44	130.17	120.80
1	B	252	VAL	O-C-N	8.44	131.07	121.96
1	C	234	ARG	NE-CZ-NH1	8.42	129.92	121.50
1	A	263	ASN	CA-C-O	-8.41	111.63	120.55
1	A	328	LYS	CB-CA-C	-8.41	96.39	110.68
1	C	223	THR	CA-C-O	8.41	129.46	120.55
1	A	29	ASP	CA-CB-CG	-8.40	104.20	112.60
1	C	530	TYR	O-C-N	-8.39	112.24	123.15
1	A	434	TYR	N-CA-C	-8.38	101.67	112.23
1	B	328	LYS	CA-CB-CG	8.36	130.81	114.10
1	C	503	HIS	N-CA-CB	-8.35	97.99	111.18
1	C	356	ARG	NE-CZ-NH1	-8.33	113.17	121.50
1	A	105	VAL	CA-C-O	8.33	125.05	119.38
1	D	56	LYS	N-CA-C	8.33	121.82	109.24
1	A	442	GLU	CA-CB-CG	8.33	130.75	114.10
1	C	543	ASN	CB-CG-ND2	-8.30	103.94	116.40
1	A	81	VAL	CA-C-O	-8.30	111.37	120.67
1	B	129	VAL	CA-C-O	-8.30	111.69	120.48
1	B	314	GLY	N-CA-C	8.29	124.85	112.41
1	A	479	PHE	CA-CB-CG	-8.27	105.53	113.80
1	B	479	PHE	CA-CB-CG	-8.26	105.54	113.80
1	C	540	HIS	CA-CB-CG	-8.26	105.54	113.80
1	C	234	ARG	NE-CZ-NH2	-8.22	111.80	119.20
1	C	523	GLY	CA-C-O	8.22	128.09	118.97
1	B	567	PHE	CA-C-O	-8.21	112.04	121.07
1	B	540	HIS	CA-CB-CG	-8.21	105.59	113.80
1	D	543	ASN	OD1-CG-ND2	8.21	130.81	122.60
1	C	204	ASP	CA-C-O	8.21	124.62	119.29
1	D	396	ASN	CB-CA-C	8.20	123.39	109.53
1	A	19	HIS	CA-C-O	8.18	131.18	121.36
1	B	422	ASP	CA-CB-CG	8.15	120.75	112.60
1	A	102	ARG	NE-CZ-NH1	-8.15	113.35	121.50
1	B	425	ARG	CB-CG-CD	8.14	130.02	111.30
1	B	157	GLU	CA-C-O	-8.13	111.92	120.87
1	C	492	PRO	CA-N-CD	-8.13	100.62	112.00
1	A	560	ALA	CA-C-O	-8.10	111.88	120.63
1	D	161	GLY	N-CA-C	8.09	126.06	115.47
1	C	161	GLY	O-C-N	-8.07	112.53	122.46
1	A	364	HIS	CA-CB-CG	8.07	121.87	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	318	ASN	CA-CB-CG	8.06	120.66	112.60
1	D	267	ARG	NE-CZ-NH1	-8.04	113.46	121.50
1	A	254	ALA	CA-C-O	-8.03	112.04	120.55
1	C	133	SER	CA-C-N	8.03	131.31	121.83
1	C	133	SER	C-N-CA	8.03	131.31	121.83
1	C	107	VAL	CA-C-N	8.01	132.49	120.31
1	C	107	VAL	C-N-CA	8.01	132.49	120.31
1	A	4	VAL	CA-C-O	-8.01	110.77	120.78
1	B	502	VAL	CA-C-O	-8.00	112.67	121.23
1	B	543	ASN	CA-CB-CG	-8.00	104.60	112.60
1	C	252	VAL	N-CA-CB	8.00	119.91	110.55
1	A	169	GLY	CA-C-O	-8.00	112.96	120.80
1	C	207	LEU	CA-C-O	-8.00	112.43	120.82
1	D	263	ASN	CA-CB-CG	-7.99	104.61	112.60
1	A	319	ASN	OD1-CG-ND2	-7.98	114.62	122.60
1	C	4	VAL	CA-C-N	7.98	131.31	120.54
1	C	4	VAL	C-N-CA	7.98	131.31	120.54
1	A	468	ASN	OD1-CG-ND2	-7.97	114.63	122.60
1	D	318	ASN	CA-CB-CG	7.96	120.56	112.60
1	C	4	VAL	N-CA-C	7.92	125.82	109.34
1	C	250	ALA	N-CA-C	7.92	127.68	110.80
1	C	525	PRO	CA-C-O	-7.91	112.77	121.23
1	C	121	GLY	CA-C-O	7.88	127.67	122.23
1	D	85	ASP	CA-CB-CG	-7.87	104.73	112.60
1	B	70	CYS	O-C-N	7.87	130.46	122.12
1	C	280	ILE	CA-C-O	-7.87	110.58	121.51
1	D	328	LYS	CA-C-O	7.86	130.21	121.02
1	C	293	VAL	CB-CA-C	-7.85	100.19	111.34
1	A	273	LEU	O-C-N	-7.80	113.90	122.79
1	A	148	GLY	CA-C-N	-7.79	108.46	121.39
1	A	148	GLY	C-N-CA	-7.79	108.46	121.39
1	A	219	ILE	CA-C-O	7.79	130.23	120.96
1	D	4	VAL	N-CA-CB	7.77	125.31	111.63
1	C	71	THR	CA-C-O	-7.76	110.45	119.61
1	D	522	THR	N-CA-C	7.76	122.01	112.23
1	B	283	ASP	O-C-N	-7.74	116.38	122.03
1	D	220	ASP	CA-CB-CG	7.73	120.33	112.60
1	B	526	ILE	N-CA-CB	7.72	120.26	110.99
1	D	350	GLN	CB-CG-CD	7.72	125.72	112.60
1	C	242	ARG	NE-CZ-NH1	-7.69	113.81	121.50
1	A	523	GLY	CA-C-O	7.68	127.67	119.07
1	A	172	ASN	CA-CB-CG	7.68	120.28	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	41	CYS	CA-C-O	-7.68	110.04	119.18
1	C	270	ASP	CA-C-O	7.67	129.13	120.84
1	C	218	SER	CB-CA-C	7.67	125.40	110.67
1	B	179	GLN	CA-C-O	7.65	128.79	119.38
1	A	162	GLY	O-C-N	-7.65	112.75	122.70
1	A	150	LYS	N-CA-C	-7.64	97.61	109.76
1	D	81	VAL	CB-CA-C	-7.64	98.74	110.50
1	C	30	ASN	OD1-CG-ND2	-7.64	114.96	122.60
1	A	231	ASP	CA-C-N	-7.63	113.14	123.14
1	A	231	ASP	C-N-CA	-7.63	113.14	123.14
1	D	362	GLN	OE1-CD-NE2	-7.62	114.98	122.60
1	D	74	HIS	CA-CB-CG	7.61	121.41	113.80
1	A	245	ARG	CA-C-O	7.61	126.67	120.13
1	D	217	ASP	CA-C-O	-7.61	112.49	120.55
1	C	523	GLY	N-CA-C	-7.60	104.05	115.00
1	A	274	ASN	OD1-CG-ND2	7.60	130.20	122.60
1	C	514	LYS	CA-C-O	7.59	128.23	119.35
1	A	522	THR	N-CA-C	7.59	122.60	113.12
1	D	401	ARG	NE-CZ-NH2	-7.57	112.39	119.20
1	A	28	ASN	O-C-N	-7.56	114.18	123.33
1	C	420	PHE	CA-CB-CG	7.54	121.34	113.80
1	C	401	ARG	CA-CB-CG	7.53	129.17	114.10
1	B	136	ALA	CA-C-N	7.53	128.30	119.94
1	B	136	ALA	C-N-CA	7.53	128.30	119.94
1	C	503	HIS	CA-CB-CG	7.50	121.30	113.80
1	D	151	VAL	N-CA-C	7.50	118.60	108.11
1	D	259	VAL	N-CA-CB	7.49	118.83	110.51
1	D	197	LYS	CA-C-O	-7.48	112.49	120.42
1	A	470	PHE	CA-CB-CG	7.46	121.26	113.80
1	C	230	THR	CA-C-O	-7.46	110.25	119.28
1	C	99	LYS	CA-C-O	-7.46	112.47	121.28
1	A	493	PHE	CA-CB-CG	-7.46	106.34	113.80
1	A	491	ALA	O-C-N	7.45	127.80	121.31
1	A	271	ILE	O-C-N	-7.44	114.49	122.83
1	A	272	ARG	NH1-CZ-NH2	7.44	128.97	119.30
1	B	145	ARG	N-CA-C	-7.44	103.25	111.36
1	D	230	THR	CA-C-O	-7.44	110.47	119.32
1	C	86	ALA	N-CA-C	-7.43	104.22	113.28
1	A	63	HIS	CA-CB-CG	-7.42	106.38	113.80
1	A	275	SER	N-CA-CB	-7.40	98.95	110.65
1	A	562	ALA	CA-C-O	7.40	128.40	120.55
1	B	560	ALA	CA-C-N	7.40	128.32	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	560	ALA	C-N-CA	7.40	128.32	120.03
1	C	19	HIS	CA-CB-CG	-7.39	106.41	113.80
1	B	85	ASP	CA-C-O	7.38	128.44	120.10
1	C	41	CYS	CA-C-N	-7.36	110.80	122.29
1	C	41	CYS	C-N-CA	-7.36	110.80	122.29
1	A	272	ARG	CA-C-O	7.35	128.32	120.46
1	D	359	GLU	CA-C-O	-7.34	110.61	119.49
1	C	246	PRO	CB-CA-C	7.33	120.56	110.95
1	B	69	ALA	CA-C-O	7.33	130.37	121.87
1	B	11	GLU	CA-CB-CG	7.32	128.73	114.10
1	B	94	MET	CA-C-O	7.32	125.09	119.46
1	A	231	ASP	CA-C-O	-7.30	112.54	120.36
1	B	478	GLN	OE1-CD-NE2	7.28	129.88	122.60
1	A	214	ASN	CB-CG-ND2	7.28	127.31	116.40
1	C	377	GLU	CB-CG-CD	7.26	124.95	112.60
1	D	25	GLY	N-CA-C	-7.26	105.06	111.95
1	B	38	CYS	CA-C-O	7.25	128.61	121.00
1	D	223	THR	CA-C-O	7.25	128.43	120.82
1	D	235	MET	N-CA-C	-7.24	96.75	109.06
1	B	294	LYS	CA-CB-CG	7.24	128.58	114.10
1	B	492	PRO	CA-N-CD	-7.24	101.86	112.00
1	D	400	THR	CA-C-N	7.24	135.36	121.54
1	D	400	THR	C-N-CA	7.24	135.36	121.54
1	A	26	VAL	CA-C-O	-7.24	114.77	121.72
1	C	449	LEU	N-CA-C	-7.24	102.39	112.45
1	A	217	ASP	N-CA-C	-7.23	103.40	111.28
1	B	356	ARG	NE-CZ-NH1	-7.23	114.27	121.50
1	A	519	SER	N-CA-C	7.23	121.18	110.48
1	B	534	GLU	O-C-N	-7.22	112.82	122.43
1	D	28	ASN	CA-C-O	-7.21	113.56	121.28
1	B	104	PHE	CA-C-O	7.21	129.10	120.81
1	C	5	LEU	CA-CB-CG	7.19	141.46	116.30
1	D	201	ASN	N-CA-C	7.19	121.63	112.86
1	A	314	GLY	CA-C-O	-7.18	114.36	122.33
1	B	339	GLY	O-C-N	-7.17	115.15	121.97
1	C	131	ILE	CB-CA-C	-7.17	103.48	111.23
1	A	345	LEU	N-CA-C	-7.17	102.87	111.69
1	A	110	ASP	CA-CB-CG	7.16	119.76	112.60
1	A	362	GLN	CA-C-O	-7.16	113.14	121.16
1	C	496	LEU	N-CA-C	7.16	120.19	108.52
1	D	200	ARG	CA-C-N	7.15	134.28	123.05
1	D	200	ARG	C-N-CA	7.15	134.28	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	492	PRO	N-CD-CG	7.14	113.91	103.20
1	C	4	VAL	N-CA-CB	-7.13	99.47	111.23
1	A	65	ILE	CA-C-O	-7.12	113.59	121.92
1	A	533	GLY	O-C-N	-7.12	115.74	122.86
1	C	211	LEU	CA-C-N	7.12	129.69	120.44
1	C	211	LEU	C-N-CA	7.12	129.69	120.44
1	A	88	HIS	CA-C-O	-7.12	111.99	121.46
1	C	373	VAL	O-C-N	-7.11	115.36	122.97
1	A	35	ASN	OD1-CG-ND2	7.09	129.69	122.60
1	C	165	LYS	CA-C-O	-7.08	111.25	119.61
1	A	56	LYS	CA-C-O	7.07	130.16	121.89
1	D	410	GLN	CA-CB-CG	7.06	128.21	114.10
1	D	65	ILE	CA-C-O	-7.04	116.12	121.68
1	A	3	GLU	N-CA-C	7.03	122.40	107.70
1	A	330	LYS	CA-C-O	-7.01	113.32	120.96
1	A	374	MET	CA-C-O	-6.99	113.33	121.16
1	D	357	ASP	CA-CB-CG	-6.99	105.61	112.60
1	A	3	GLU	CA-C-O	6.99	130.24	120.52
1	C	336	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	D	282	GLU	N-CA-C	6.98	120.81	110.48
1	C	285	SER	CA-C-N	6.96	135.06	121.41
1	C	285	SER	C-N-CA	6.96	135.06	121.41
1	C	125	THR	CA-CB-OG1	-6.96	99.16	109.60
1	D	229	MET	CA-C-O	-6.96	113.13	121.34
1	B	11	GLU	CA-C-N	6.95	132.57	121.18
1	B	11	GLU	C-N-CA	6.95	132.57	121.18
1	C	69	ALA	N-CA-C	6.94	119.53	110.43
1	D	68	ILE	CB-CA-C	6.94	122.67	111.29
1	D	10	GLY	CA-C-N	6.91	134.75	121.54
1	D	10	GLY	C-N-CA	6.91	134.75	121.54
1	B	265	VAL	O-C-N	-6.91	115.17	121.87
1	B	262	ASP	CA-CB-CG	6.89	119.49	112.60
1	C	336	ASN	CA-CB-CG	6.88	119.48	112.60
1	C	550	ILE	CA-C-O	-6.88	113.56	120.85
1	A	282	GLU	CA-C-O	-6.88	114.15	121.99
1	B	453	ILE	CA-C-N	6.87	134.67	121.54
1	B	453	ILE	C-N-CA	6.87	134.67	121.54
1	C	68	ILE	CA-CB-CG2	6.87	122.17	110.50
1	D	237	GLY	CA-C-O	6.87	127.21	119.59
1	B	74	HIS	O-C-N	6.87	131.22	123.05
1	B	157	GLU	O-C-N	6.85	128.86	121.60
1	B	271	ILE	N-CA-CB	-6.85	103.26	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	115	ASP	CA-C-O	-6.85	113.29	120.55
1	C	123	LYS	N-CA-C	6.83	119.56	111.71
1	D	261	TRP	CA-C-O	6.83	127.82	120.24
1	D	549	ALA	CA-C-O	6.83	127.82	120.24
1	A	318	ASN	CA-CB-CG	6.82	119.42	112.60
1	A	440	VAL	CB-CA-C	-6.81	101.65	110.98
1	D	563	SER	CA-CB-OG	6.81	124.72	111.10
1	B	204	ASP	CA-C-O	6.81	124.36	119.32
1	D	510	VAL	CA-C-O	-6.81	113.02	120.71
1	D	54	LYS	CA-C-O	6.80	127.27	120.88
1	D	366	THR	N-CA-C	6.79	120.39	107.75
1	B	267	ARG	CA-C-N	-6.79	108.10	121.41
1	B	267	ARG	C-N-CA	-6.79	108.10	121.41
1	C	46	LYS	CA-C-O	-6.79	113.69	120.82
1	D	231	ASP	CB-CA-C	6.78	120.92	109.80
1	A	366	THR	CA-C-O	6.77	133.21	121.09
1	D	516	GLU	N-CA-CB	-6.77	99.45	109.95
1	A	359	GLU	CA-CB-CG	6.76	127.63	114.10
1	A	556	TYR	CA-C-O	-6.76	113.72	120.82
1	C	422	ASP	CA-CB-CG	-6.74	105.86	112.60
1	A	185	GLU	CB-CA-C	6.74	121.47	110.22
1	C	220	ASP	CA-C-N	6.73	129.85	120.29
1	C	220	ASP	C-N-CA	6.73	129.85	120.29
1	C	426	LYS	CA-CB-CG	6.73	127.56	114.10
1	C	240	VAL	CA-C-O	6.73	128.10	120.90
1	B	467	TYR	CA-C-O	6.72	127.67	120.55
1	C	563	SER	CA-C-N	6.72	130.90	120.82
1	C	563	SER	C-N-CA	6.72	130.90	120.82
1	A	552	ASP	CA-CB-CG	6.72	119.32	112.60
1	B	77	HIS	CA-CB-CG	-6.72	107.08	113.80
1	B	269	THR	CA-C-O	-6.71	113.27	120.92
1	B	491	ALA	CA-C-N	6.71	128.23	119.84
1	B	491	ALA	C-N-CA	6.71	128.23	119.84
1	C	356	ARG	NH1-CZ-NH2	6.71	128.02	119.30
1	B	308	VAL	CA-C-O	-6.69	113.51	120.27
1	C	111	LYS	CA-CB-CG	6.69	127.47	114.10
1	C	37	GLN	OE1-CD-NE2	6.68	129.28	122.60
1	D	210	VAL	N-CA-C	-6.68	103.82	110.30
1	B	359	GLU	CB-CG-CD	6.68	123.95	112.60
1	A	534	GLU	O-C-N	-6.67	113.72	122.59
1	A	184	ILE	CA-C-N	-6.67	113.30	122.30
1	A	184	ILE	C-N-CA	-6.67	113.30	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	104	PHE	CA-CB-CG	6.67	120.47	113.80
1	A	159	ILE	CA-C-N	6.67	128.18	119.84
1	A	159	ILE	C-N-CA	6.67	128.18	119.84
1	C	247	THR	N-CA-CB	6.67	119.88	109.94
1	C	72	SER	CA-CB-OG	-6.66	97.78	111.10
1	A	96	PHE	CA-C-N	6.66	127.10	120.31
1	A	96	PHE	C-N-CA	6.66	127.10	120.31
1	A	267	ARG	O-C-N	-6.66	113.31	121.83
1	C	491	ALA	CA-C-N	6.65	128.15	119.84
1	C	491	ALA	C-N-CA	6.65	128.15	119.84
1	A	233	GLY	O-C-N	-6.64	118.83	123.95
1	A	100	TRP	CA-C-O	-6.64	112.88	120.58
1	C	524	LYS	CB-CA-C	6.62	119.04	108.91
1	B	218	SER	N-CA-C	-6.62	103.99	111.07
1	C	291	VAL	N-CA-C	6.62	119.64	108.86
1	B	249	GLY	N-CA-C	-6.61	97.51	113.18
1	B	309	VAL	CA-C-O	-6.60	113.51	120.57
1	D	262	ASP	N-CA-C	-6.60	104.01	111.14
1	D	525	PRO	CA-C-O	-6.60	114.13	121.32
1	D	23	LYS	N-CA-C	-6.59	103.72	111.03
1	A	400	THR	CA-C-N	6.58	130.32	120.31
1	A	400	THR	C-N-CA	6.58	130.32	120.31
1	C	252	VAL	CA-C-O	-6.58	114.19	121.17
1	D	135	GLY	CA-C-O	-6.58	113.68	120.66
1	C	55	ASP	N-CA-C	6.58	119.29	111.33
1	D	426	LYS	CA-CB-CG	6.58	127.25	114.10
1	D	250	ALA	CA-C-O	6.57	129.91	120.51
1	D	375	ILE	CA-C-O	-6.57	114.20	121.23
1	B	208	VAL	N-CA-C	-6.57	103.84	111.00
1	A	567	PHE	CA-C-O	-6.57	113.85	121.07
1	B	76	GLY	CA-C-N	6.57	133.30	122.73
1	B	76	GLY	C-N-CA	6.57	133.30	122.73
1	D	392	ASN	CA-CB-CG	6.56	119.16	112.60
1	A	31	LEU	N-CA-CB	-6.56	102.23	112.13
1	D	496	LEU	N-CA-CB	-6.55	100.89	110.84
1	C	31	LEU	N-CA-CB	-6.54	99.43	110.49
1	B	189	GLN	CA-C-O	-6.54	113.96	120.70
1	C	341	THR	CA-C-O	-6.54	111.54	119.32
1	C	276	ARG	CD-NE-CZ	-6.54	115.25	124.40
1	D	543	ASN	CA-CB-CG	-6.53	106.07	112.60
1	D	281	LEU	O-C-N	-6.53	115.55	123.19
1	C	161	GLY	N-CA-C	6.53	122.85	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	37	GLN	OE1-CD-NE2	6.53	129.12	122.60
1	B	209	LYS	N-CA-CB	6.53	119.47	110.01
1	B	570	ASP	N-CA-CB	6.53	121.59	110.50
1	B	421	ASP	N-CA-CB	-6.52	100.98	110.70
1	C	3	GLU	O-C-N	-6.52	112.57	123.00
1	C	401	ARG	NE-CZ-NH2	-6.52	113.33	119.20
1	D	241	ASN	CB-CG-ND2	-6.52	106.62	116.40
1	B	492	PRO	N-CD-CG	6.52	112.98	103.20
1	D	448	GLU	CA-CB-CG	6.51	127.13	114.10
1	C	47	GLU	O-C-N	-6.50	115.33	122.09
1	B	265	VAL	CA-C-N	6.50	128.99	120.28
1	B	265	VAL	C-N-CA	6.50	128.99	120.28
1	A	460	LEU	CA-C-O	6.50	127.64	120.82
1	B	24	GLY	CA-C-O	-6.49	115.88	122.56
1	B	426	LYS	CG-CD-CE	6.49	126.23	111.30
1	D	491	ALA	CA-C-N	6.49	127.95	119.84
1	D	491	ALA	C-N-CA	6.49	127.95	119.84
1	D	248	GLY	CA-C-O	6.49	126.16	121.04
1	B	539	VAL	CA-C-O	-6.47	113.78	120.71
1	D	197	LYS	O-C-N	6.47	129.52	122.15
1	A	154	LEU	O-C-N	-6.46	115.00	123.21
1	D	75	LYS	CA-C-O	-6.46	113.66	121.28
1	D	157	GLU	CA-C-O	-6.45	113.93	120.96
1	C	103	LYS	N-CA-C	-6.44	100.95	110.48
1	B	93	ASP	CA-C-O	6.43	128.78	121.58
1	D	63	HIS	CG-CD2-NE2	6.43	113.63	107.20
1	A	282	GLU	N-CA-CB	-6.43	101.58	110.38
1	A	366	THR	O-C-N	-6.42	114.47	122.82
1	A	422	ASP	CA-C-O	-6.42	112.21	119.79
1	B	328	LYS	N-CA-C	-6.42	104.20	111.07
1	A	267	ARG	NE-CZ-NH2	6.42	124.97	119.20
1	B	401	ARG	NE-CZ-NH1	6.42	127.92	121.50
1	C	350	GLN	CB-CG-CD	6.42	123.51	112.60
1	C	98	GLY	N-CA-C	-6.41	105.10	112.79
1	B	401	ARG	CD-NE-CZ	6.41	133.37	124.40
1	A	489	VAL	N-CA-CB	-6.41	100.66	111.23
1	B	68	ILE	CB-CG1-CD1	-6.39	100.39	113.80
1	A	64	LEU	CA-C-O	-6.38	114.60	121.56
1	D	36	GLY	O-C-N	-6.37	114.42	122.70
1	D	289	THR	CA-C-O	6.37	126.99	119.67
1	A	218	SER	CA-CB-OG	-6.36	98.39	111.10
1	D	558	ARG	CG-CD-NE	6.35	125.97	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	551	SER	CB-CA-C	-6.35	100.91	110.88
1	A	212	ALA	CA-C-N	6.34	129.41	120.28
1	A	212	ALA	C-N-CA	6.34	129.41	120.28
1	A	259	VAL	N-CA-CB	6.34	119.16	110.54
1	D	356	ARG	CA-C-O	-6.34	114.48	121.33
1	B	491	ALA	N-CA-C	6.34	118.60	109.48
1	C	252	VAL	CB-CA-C	-6.34	103.86	111.97
1	C	133	SER	O-C-N	-6.33	114.10	122.20
1	C	223	THR	O-C-N	-6.33	115.41	122.12
1	A	548	ASN	OD1-CG-ND2	-6.32	116.28	122.60
1	C	202	ILE	N-CA-C	-6.32	106.54	113.43
1	B	219	ILE	O-C-N	-6.32	115.70	121.89
1	C	89	SER	CA-CB-OG	-6.32	98.47	111.10
1	A	254	ALA	O-C-N	6.31	128.81	122.12
1	D	159	ILE	CA-C-O	6.31	128.40	119.95
1	A	231	ASP	CA-CB-CG	-6.31	106.29	112.60
1	D	282	GLU	N-CA-CB	-6.30	100.71	110.29
1	C	234	ARG	CA-C-O	6.30	127.39	120.71
1	C	17	SER	CA-C-N	6.30	132.19	122.42
1	C	17	SER	C-N-CA	6.30	132.19	122.42
1	A	4	VAL	N-CA-CB	6.30	121.62	111.23
1	A	41	CYS	N-CA-C	6.29	120.16	112.23
1	B	163	ASN	N-CA-C	-6.29	105.08	112.89
1	B	566	LYS	N-CA-CB	6.29	119.37	110.12
1	D	270	ASP	CA-C-O	6.28	127.29	120.58
1	D	372	GLY	N-CA-C	-6.28	106.58	115.43
1	A	118	ILE	CA-C-O	6.27	127.03	120.25
1	B	367	TYR	CA-C-O	6.27	127.13	120.36
1	C	241	ASN	OD1-CG-ND2	6.27	128.87	122.60
1	C	197	LYS	N-CA-CB	6.27	119.16	110.07
1	C	258	GLN	CA-C-N	-6.26	112.67	120.56
1	C	258	GLN	C-N-CA	-6.26	112.67	120.56
1	D	61	LYS	N-CA-CB	6.26	120.66	110.90
1	C	17	SER	O-C-N	-6.25	114.92	122.11
1	D	563	SER	N-CA-C	-6.25	105.47	113.23
1	A	212	ALA	O-C-N	-6.25	115.34	122.09
1	A	393	ARG	CA-C-O	-6.25	114.16	121.16
1	B	22	ASP	CA-CB-CG	6.25	118.85	112.60
1	D	175	GLU	N-CA-C	6.25	120.17	111.74
1	D	474	GLY	N-CA-C	-6.24	106.80	114.92
1	C	536	THR	CA-CB-OG1	-6.24	100.24	109.60
1	C	567	PHE	O-C-N	-6.23	114.08	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	260	LEU	O-C-N	-6.23	114.29	122.39
1	D	95	PRO	CA-C-N	6.22	130.97	122.07
1	D	95	PRO	C-N-CA	6.22	130.97	122.07
1	B	232	VAL	CA-C-O	-6.22	113.92	120.39
1	B	126	THR	CA-C-O	-6.22	113.98	121.32
1	A	536	THR	CA-CB-OG1	-6.22	100.28	109.60
1	C	19	HIS	CA-C-O	-6.21	114.48	121.81
1	C	150	LYS	CB-CA-C	6.20	120.45	109.72
1	A	341	THR	CA-C-O	-6.20	111.94	119.32
1	C	217	ASP	CA-C-O	6.20	127.10	119.97
1	A	149	ALA	CA-C-O	6.20	128.60	121.47
1	A	169	GLY	N-CA-C	6.20	120.39	112.83
1	A	340	ALA	CA-C-O	-6.20	114.90	122.64
1	C	54	LYS	CA-C-N	6.19	128.86	120.38
1	C	54	LYS	C-N-CA	6.19	128.86	120.38
1	A	426	LYS	O-C-N	-6.19	114.20	122.43
1	B	481	ARG	CA-C-N	6.19	125.75	119.19
1	B	481	ARG	C-N-CA	6.19	125.75	119.19
1	B	315	PHE	CA-C-N	6.19	129.41	120.38
1	B	315	PHE	C-N-CA	6.19	129.41	120.38
1	A	487	GLU	O-C-N	-6.19	114.29	122.33
1	C	352	GLY	N-CA-C	6.18	123.85	115.32
1	C	364	HIS	CA-CB-CG	-6.18	107.62	113.80
1	A	356	ARG	NE-CZ-NH2	6.18	124.76	119.20
1	D	57	VAL	CB-CA-C	-6.18	103.85	111.08
1	A	107	VAL	CA-C-N	6.17	131.93	121.14
1	A	107	VAL	C-N-CA	6.17	131.93	121.14
1	B	258	GLN	CA-C-N	-6.16	111.68	120.42
1	B	258	GLN	C-N-CA	-6.16	111.68	120.42
1	A	527	THR	N-CA-CB	6.16	119.11	109.69
1	B	134	GLY	O-C-N	-6.16	117.52	122.81
1	C	539	VAL	CA-C-O	-6.16	114.22	121.05
1	C	375	ILE	N-CA-CB	6.14	117.23	110.53
1	B	401	ARG	CA-CB-CG	6.14	126.38	114.10
1	B	215	SER	O-C-N	-6.14	114.42	122.59
1	A	520	GLU	N-CA-C	-6.13	104.15	111.69
1	A	133	SER	N-CA-C	6.12	119.49	112.57
1	C	200	ARG	O-C-N	-6.12	114.21	122.41
1	D	241	ASN	OD1-CG-ND2	6.12	128.72	122.60
1	B	537	GLY	O-C-N	-6.11	119.24	123.95
1	C	401	ARG	NE-CZ-NH1	6.11	127.61	121.50
1	C	235	MET	N-CA-C	-6.10	99.86	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	252	VAL	CB-CA-C	-6.10	101.29	111.29
1	D	239	SER	CA-C-O	6.10	125.23	118.52
1	D	429	LYS	CA-C-N	6.10	128.77	120.54
1	D	429	LYS	C-N-CA	6.10	128.77	120.54
1	C	512	ASP	N-CA-C	-6.10	100.91	109.69
1	A	214	ASN	OD1-CG-ND2	-6.09	116.51	122.60
1	D	324	LYS	O-C-N	-6.09	115.75	122.09
1	B	262	ASP	N-CA-C	-6.09	104.64	111.28
1	B	283	ASP	N-CA-CB	-6.09	105.92	111.59
1	D	251	GLY	N-CA-C	6.09	127.61	113.18
1	A	336	ASN	N-CA-C	6.09	119.53	110.52
1	B	40	SER	CA-C-O	-6.09	114.43	120.82
1	D	217	ASP	O-C-N	6.08	128.57	122.12
1	B	79	LYS	CA-C-O	6.08	128.00	121.55
1	A	107	VAL	CB-CA-C	-6.08	103.17	112.05
1	A	508	GLY	CA-C-N	6.07	129.75	120.82
1	A	508	GLY	C-N-CA	6.07	129.75	120.82
1	C	349	LEU	CB-CA-C	-6.07	100.36	110.68
1	A	143	SER	O-C-N	-6.07	114.52	122.59
1	D	236	GLY	N-CA-C	-6.07	105.65	112.33
1	A	453	ILE	CB-CA-C	-6.07	104.09	112.04
1	B	10	GLY	N-CA-C	-6.06	105.25	113.37
1	D	430	ALA	CA-C-O	6.06	127.38	120.90
1	A	563	SER	O-C-N	-6.05	115.55	122.09
1	D	185	GLU	O-C-N	-6.05	115.57	122.84
1	A	203	ASN	CA-CB-CG	6.05	118.65	112.60
1	B	263	ASN	CA-CB-CG	-6.05	106.55	112.60
1	C	567	PHE	CA-C-O	6.05	126.82	119.38
1	B	306	ASP	CA-CB-CG	-6.04	106.56	112.60
1	A	213	ASN	N-CA-C	6.04	118.66	111.71
1	A	503	HIS	N-CA-C	6.04	123.66	110.80
1	B	372	GLY	CA-C-O	6.03	125.72	119.02
1	A	490	VAL	CA-C-O	6.03	128.11	120.75
1	B	568	ALA	CA-C-O	-6.03	113.45	120.20
1	C	194	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	219	ILE	O-C-N	-6.03	114.06	121.90
1	D	357	ASP	N-CA-C	6.03	123.64	110.80
1	C	510	VAL	CA-C-O	6.03	127.52	120.71
1	D	63	HIS	CA-CB-CG	6.03	119.83	113.80
1	D	152	ILE	N-CA-CB	6.02	119.72	111.41
1	A	161	GLY	N-CA-C	6.01	123.96	115.30
1	A	156	LYS	CA-C-O	6.01	126.31	119.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	407	ALA	CA-C-O	-6.01	114.47	120.90
1	B	560	ALA	CA-C-O	6.01	128.06	121.02
1	B	35	ASN	CA-CB-CG	6.01	118.61	112.60
1	D	535	VAL	CA-C-O	6.00	127.30	120.03
1	D	185	GLU	N-CA-CB	-6.00	99.40	110.56
1	C	474	GLY	N-CA-C	-5.99	105.25	115.08
1	C	39	VAL	CB-CA-C	5.99	120.22	112.14
1	A	275	SER	CA-C-N	-5.98	114.74	123.00
1	A	275	SER	C-N-CA	-5.98	114.74	123.00
1	B	520	GLU	CA-CB-CG	5.98	126.06	114.10
1	A	440	VAL	CA-C-O	-5.98	114.08	120.59
1	D	252	VAL	N-CA-CB	5.98	121.09	111.23
1	A	480	GLU	N-CA-CB	-5.97	101.81	110.47
1	A	563	SER	CB-CA-C	5.97	120.33	110.90
1	B	4	VAL	N-CA-C	-5.97	100.47	108.35
1	B	12	MET	CB-CA-C	-5.97	99.73	110.35
1	A	270	ASP	CA-CB-CG	5.96	118.56	112.60
1	B	468	ASN	CB-CG-OD1	-5.96	108.88	120.80
1	C	216	SER	CA-C-O	-5.96	114.23	120.55
1	B	172	ASN	OD1-CG-ND2	5.96	128.56	122.60
1	C	279	ARG	CA-C-N	-5.96	111.64	122.43
1	C	279	ARG	C-N-CA	-5.96	111.64	122.43
1	C	88	HIS	CA-C-O	-5.96	114.28	120.89
1	C	439	ILE	CB-CA-C	-5.96	103.82	111.20
1	D	361	ILE	O-C-N	-5.95	116.83	123.26
1	A	512	ASP	CA-C-O	-5.95	114.59	121.49
1	C	550	ILE	CA-C-N	5.95	128.17	120.44
1	C	550	ILE	C-N-CA	5.95	128.17	120.44
1	A	163	ASN	O-C-N	-5.94	114.96	122.27
1	A	312	ALA	N-CA-C	5.94	120.38	113.20
1	A	115	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	388	ASN	CB-CG-ND2	5.93	125.30	116.40
1	B	307	ALA	O-C-N	-5.92	115.49	123.19
1	B	516	GLU	CA-C-O	-5.91	113.95	120.69
1	A	547	GLY	N-CA-C	-5.91	107.26	113.58
1	B	215	SER	CA-C-O	5.90	128.95	120.51
1	C	98	GLY	CA-C-O	-5.90	115.67	121.93
1	B	12	MET	N-CA-C	5.90	122.51	113.19
1	C	83	TYR	CA-C-N	5.90	128.99	120.38
1	C	83	TYR	C-N-CA	5.90	128.99	120.38
1	B	315	PHE	CA-CB-CG	5.90	119.70	113.80
1	D	283	ASP	O-C-N	-5.90	114.74	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	519	SER	O-C-N	-5.90	116.30	122.96
1	D	468	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	A	350	GLN	CB-CG-CD	5.89	122.62	112.60
1	C	222	LEU	CA-C-O	5.89	126.67	120.42
1	D	157	GLU	N-CA-CB	-5.89	102.90	109.74
1	C	273	LEU	O-C-N	-5.88	114.41	122.23
1	B	476	ASP	CA-CB-CG	5.88	118.48	112.60
1	D	159	ILE	O-C-N	-5.88	114.40	121.10
1	C	377	GLU	CA-C-O	5.88	126.72	119.79
1	C	326	ASP	CA-CB-CG	5.87	118.47	112.60
1	C	80	SER	CA-C-O	-5.87	114.89	121.81
1	B	536	THR	CA-CB-OG1	-5.86	100.80	109.60
1	A	20	VAL	CB-CA-C	-5.86	104.36	112.04
1	C	16	ASP	CA-C-N	5.86	129.61	120.82
1	C	16	ASP	C-N-CA	5.86	129.61	120.82
1	C	505	THR	O-C-N	-5.86	114.20	122.87
1	A	331	GLY	N-CA-C	5.86	123.44	115.30
1	A	123	LYS	CA-C-O	-5.85	112.42	119.27
1	B	356	ARG	CA-C-N	5.85	132.72	121.54
1	B	356	ARG	C-N-CA	5.85	132.72	121.54
1	C	328	LYS	O-C-N	-5.85	114.81	122.59
1	A	245	ARG	NE-CZ-NH2	-5.85	113.94	119.20
1	C	282	GLU	N-CA-C	5.85	118.77	109.65
1	B	513	THR	CA-CB-OG1	-5.85	100.83	109.60
1	B	161	GLY	CA-C-N	5.84	131.47	120.07
1	B	161	GLY	C-N-CA	5.84	131.47	120.07
1	D	424	ILE	N-CA-C	5.84	116.03	110.42
1	A	327	PRO	CA-C-N	5.84	128.38	120.38
1	A	327	PRO	C-N-CA	5.84	128.38	120.38
1	A	28	ASN	CA-C-O	5.84	127.60	120.60
1	A	423	SER	CA-C-O	-5.84	114.69	120.70
1	D	242	ARG	CA-C-N	-5.84	114.66	122.42
1	D	242	ARG	C-N-CA	-5.84	114.66	122.42
1	A	517	VAL	N-CA-CB	5.83	117.65	111.00
1	A	273	LEU	CA-C-N	5.83	130.66	122.08
1	A	273	LEU	C-N-CA	5.83	130.66	122.08
1	B	548	ASN	CA-C-O	-5.83	112.77	119.60
1	B	403	LYS	CA-CB-CG	5.83	125.76	114.10
1	B	521	LYS	CA-C-O	-5.83	113.51	120.10
1	C	67	GLU	CA-C-O	-5.83	114.04	120.69
1	C	152	ILE	CB-CG1-CD1	5.83	126.04	113.80
1	A	276	ARG	CA-CB-CG	5.83	125.75	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	108	ASP	CA-C-N	5.82	129.03	120.82
1	C	108	ASP	C-N-CA	5.82	129.03	120.82
1	D	354	ALA	CA-C-O	5.82	127.26	120.80
1	A	244	HIS	CA-CB-CG	-5.81	107.99	113.80
1	D	321	ARG	CD-NE-CZ	-5.81	116.26	124.40
1	B	224	SER	O-C-N	-5.81	114.86	122.59
1	C	525	PRO	CB-CA-C	-5.81	104.33	111.64
1	A	285	SER	N-CA-CB	5.80	117.61	110.53
1	B	181	LYS	CA-C-O	-5.80	112.94	119.79
1	C	539	VAL	CB-CA-C	-5.80	104.42	112.02
1	B	16	ASP	N-CA-CB	5.80	120.18	110.32
1	D	327	PRO	CA-C-O	-5.80	110.05	120.60
1	A	242	ARG	CA-CB-CG	5.79	125.69	114.10
1	D	202	ILE	CA-C-O	5.79	126.20	119.89
1	A	415	SER	CA-C-O	-5.79	114.74	121.10
1	C	553	ILE	CA-C-O	-5.79	115.25	121.27
1	D	35	ASN	CA-C-O	-5.79	114.36	120.55
1	D	3	GLU	N-CA-C	5.78	118.33	110.06
1	B	470	PHE	N-CA-CB	5.78	118.61	110.12
1	D	212	ALA	CA-C-O	5.78	126.65	120.70
1	A	28	ASN	CA-CB-CG	5.77	118.37	112.60
1	A	455	VAL	N-CA-CB	5.77	119.29	111.21
1	B	150	LYS	O-C-N	-5.77	116.50	123.13
1	B	197	LYS	CA-C-O	-5.76	114.77	120.82
1	D	214	ASN	CA-CB-CG	5.76	118.36	112.60
1	D	411	GLN	CA-CB-CG	5.76	125.62	114.10
1	B	566	LYS	N-CA-C	-5.75	105.01	111.28
1	B	246	PRO	O-C-N	-5.75	116.20	123.10
1	A	165	LYS	CA-C-O	-5.75	111.86	119.10
1	A	345	LEU	CB-CA-C	5.75	121.21	110.70
1	A	194	ASP	CA-CB-CG	5.74	118.34	112.60
1	D	283	ASP	CA-C-N	5.74	132.51	121.54
1	D	283	ASP	C-N-CA	5.74	132.51	121.54
1	D	543	ASN	N-CA-C	5.74	117.74	108.32
1	A	241	ASN	CA-CB-CG	-5.74	106.86	112.60
1	D	106	PRO	CA-C-O	-5.74	114.77	121.95
1	A	291	VAL	N-CA-CB	-5.74	101.76	111.23
1	B	42	HIS	CA-CB-CG	-5.74	108.06	113.80
1	A	355	THR	O-C-N	-5.73	115.70	123.15
1	C	151	VAL	N-CA-C	5.73	116.73	108.48
1	A	181	LYS	CA-C-O	-5.72	114.45	120.63
1	B	79	LYS	O-C-N	-5.72	115.77	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	480	GLU	N-CA-C	5.72	119.96	113.15
1	A	536	THR	CA-CB-CG2	5.72	120.22	110.50
1	A	70	CYS	CA-C-O	5.72	127.00	121.00
1	D	423	SER	CA-C-N	5.72	127.76	120.56
1	D	423	SER	C-N-CA	5.72	127.76	120.56
1	A	490	VAL	O-C-N	-5.72	115.68	122.77
1	D	104	PHE	N-CA-CB	5.72	118.81	109.95
1	D	483	ASP	CA-CB-CG	5.72	118.32	112.60
1	C	33	HIS	CA-CB-CG	-5.71	108.09	113.80
1	D	38	CYS	N-CA-C	-5.71	104.97	111.14
1	D	210	VAL	CB-CA-C	5.71	118.95	111.81
1	A	504	HIS	ND1-CE1-NE2	-5.71	102.69	108.40
1	B	396	ASN	CA-CB-CG	5.71	118.31	112.60
1	D	328	LYS	O-C-N	-5.71	115.29	122.20
1	B	192	ILE	CB-CA-C	-5.70	104.68	111.81
1	C	568	ALA	CA-C-O	-5.70	112.24	119.31
1	D	328	LYS	CB-CA-C	-5.70	101.38	110.84
1	C	45	LEU	CA-C-O	-5.70	114.51	120.55
1	D	42	HIS	CA-CB-CG	5.69	119.49	113.80
1	A	318	ASN	N-CA-CB	-5.69	102.07	110.49
1	A	520	GLU	CA-CB-CG	5.69	125.48	114.10
1	C	271	ILE	CA-C-O	5.69	126.80	120.59
1	A	67	GLU	CA-C-N	-5.69	115.13	123.10
1	A	67	GLU	C-N-CA	-5.69	115.13	123.10
1	B	494	TYR	N-CA-C	5.69	118.84	109.85
1	A	80	SER	CA-CB-OG	5.69	122.48	111.10
1	A	264	ALA	N-CA-CB	5.69	118.26	110.01
1	A	285	SER	CA-C-N	5.68	132.55	121.41
1	A	285	SER	C-N-CA	5.68	132.55	121.41
1	C	58	SER	CB-CA-C	-5.68	100.36	108.88
1	C	186	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	560	ALA	CA-C-N	5.67	126.11	119.94
1	A	560	ALA	C-N-CA	5.67	126.11	119.94
1	C	67	GLU	CA-C-N	-5.67	115.39	123.10
1	C	67	GLU	C-N-CA	-5.67	115.39	123.10
1	C	247	THR	CB-CA-C	-5.67	101.75	110.81
1	A	321	ARG	NE-CZ-NH2	-5.67	114.10	119.20
1	C	283	ASP	CA-CB-CG	5.66	118.26	112.60
1	D	194	ASP	CA-C-O	-5.66	114.84	120.90
1	A	217	ASP	CB-CA-C	-5.66	101.39	110.79
1	B	477	ALA	O-C-N	5.66	128.60	122.15
1	D	88	HIS	CA-CB-CG	5.66	119.46	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	90	PHE	CA-CB-CG	5.66	119.46	113.80
1	C	68	ILE	CB-CA-C	5.66	118.17	111.32
1	B	72	SER	CA-C-O	5.65	126.39	119.05
1	C	534	GLU	CA-CB-CG	5.64	125.38	114.10
1	A	398	ILE	CA-C-O	5.64	127.83	120.78
1	B	129	VAL	CB-CA-C	-5.64	102.43	110.83
1	D	181	LYS	CA-C-O	5.64	126.53	120.55
1	A	328	LYS	CA-CB-CG	5.63	125.37	114.10
1	B	64	LEU	CA-C-N	5.63	130.17	122.34
1	B	64	LEU	C-N-CA	5.63	130.17	122.34
1	D	337	HIS	CA-C-N	5.63	125.10	119.24
1	D	337	HIS	C-N-CA	5.63	125.10	119.24
1	C	292	LEU	CB-CA-C	-5.63	102.28	111.68
1	D	314	GLY	N-CA-C	5.63	120.65	112.60
1	A	127	ASP	CA-CB-CG	-5.63	106.97	112.60
1	A	559	ILE	CA-C-O	-5.63	115.21	121.17
1	D	78	GLU	CB-CA-C	5.62	120.82	109.68
1	A	395	MET	CB-CA-C	-5.62	100.15	111.17
1	A	541	GLY	CA-C-O	-5.62	113.53	121.40
1	D	71	THR	O-C-N	-5.62	115.65	122.22
1	B	74	HIS	CA-C-O	-5.62	114.70	120.54
1	C	201	ASN	CA-C-N	-5.62	115.08	122.16
1	C	201	ASN	C-N-CA	-5.62	115.08	122.16
1	D	63	HIS	ND1-CG-CD2	-5.62	100.48	106.10
1	A	567	PHE	O-C-N	5.61	128.09	122.08
1	A	436	HIS	CA-C-O	-5.61	112.48	119.38
1	C	202	ILE	CA-CB-CG1	5.61	119.94	110.40
1	C	425	ARG	N-CA-CB	5.61	118.47	110.16
1	B	237	GLY	CA-C-O	5.61	125.42	119.03
1	B	313	GLY	CA-C-O	-5.61	115.45	122.74
1	A	548	ASN	CB-CG-ND2	5.60	124.80	116.40
1	C	129	VAL	CA-CB-CG1	5.59	119.90	110.40
1	A	485	PRO	N-CA-C	5.59	120.89	113.40
1	B	296	GLU	CA-CB-CG	-5.59	102.92	114.10
1	B	421	ASP	N-CA-C	5.59	118.36	110.14
1	B	502	VAL	N-CA-C	-5.58	102.38	109.58
1	B	206	GLU	CA-C-O	-5.58	114.63	120.55
1	C	278	VAL	CB-CA-C	-5.58	102.14	111.29
1	B	420	PHE	CA-C-N	5.57	133.03	123.05
1	B	420	PHE	C-N-CA	5.57	133.03	123.05
1	D	81	VAL	N-CA-C	5.57	116.76	108.46
1	A	443	GLY	N-CA-C	-5.57	101.44	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	556	TYR	CA-CB-CG	-5.57	103.87	113.90
1	B	329	LEU	N-CA-C	5.57	121.05	113.37
1	B	534	GLU	CA-C-O	5.57	126.11	119.10
1	C	566	LYS	O-C-N	-5.57	116.30	122.09
1	C	185	GLU	CA-C-O	5.56	127.58	120.57
1	D	369	PRO	CA-C-N	5.56	128.28	120.28
1	D	369	PRO	C-N-CA	5.56	128.28	120.28
1	A	339	GLY	O-C-N	5.55	130.56	122.18
1	B	291	VAL	CA-C-O	5.54	126.90	121.19
1	D	194	ASP	CA-CB-CG	5.54	118.14	112.60
1	D	233	GLY	CA-C-O	-5.54	116.05	121.93
1	C	486	ARG	CA-C-N	5.54	129.47	120.60
1	C	486	ARG	C-N-CA	5.54	129.47	120.60
1	C	142	VAL	N-CA-CB	5.54	117.03	110.55
1	B	216	SER	CA-C-N	5.54	127.97	120.38
1	B	216	SER	C-N-CA	5.54	127.97	120.38
1	B	259	VAL	CA-C-O	-5.53	114.98	120.85
1	B	312	ALA	CA-C-O	-5.53	112.60	120.51
1	D	10	GLY	CA-C-O	5.52	126.97	121.00
1	B	311	ALA	N-CA-C	-5.52	105.23	112.41
1	B	364	HIS	O-C-N	5.52	127.47	121.23
1	B	477	ALA	N-CA-CB	-5.52	101.99	110.16
1	A	470	PHE	N-CA-C	-5.52	105.27	111.28
1	C	449	LEU	CA-C-O	5.51	126.73	120.00
1	C	388	ASN	CA-CB-CG	5.51	118.11	112.60
1	C	510	VAL	O-C-N	-5.51	116.67	122.95
1	B	478	GLN	N-CA-CB	-5.50	101.19	110.49
1	C	150	LYS	N-CA-C	-5.50	100.21	109.07
1	A	156	LYS	CA-CB-CG	5.50	125.10	114.10
1	B	271	ILE	O-C-N	-5.50	116.68	122.95
1	C	148	GLY	CA-C-O	-5.50	112.22	119.25
1	B	425	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	B	417	TYR	CB-CA-C	-5.49	101.36	110.14
1	C	525	PRO	O-C-N	5.49	129.32	123.01
1	B	77	HIS	N-CA-C	5.49	118.98	112.72
1	A	522	THR	CA-C-O	-5.49	113.14	119.78
1	B	200	ARG	NE-CZ-NH1	-5.49	116.02	121.50
1	C	218	SER	N-CA-C	-5.48	105.46	111.82
1	D	93	ASP	CA-CB-CG	5.48	118.08	112.60
1	C	198	GLY	CA-C-O	-5.48	115.43	120.80
1	A	514	LYS	CG-CD-CE	5.47	123.89	111.30
1	B	245	ARG	CA-CB-CG	5.47	125.05	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	396	ASN	N-CA-C	-5.47	101.55	110.20
1	A	29	ASP	O-C-N	-5.47	115.96	122.20
1	D	235	MET	CA-C-O	-5.47	114.04	120.60
1	C	561	GLY	N-CA-C	-5.47	105.77	112.77
1	A	411	GLN	CA-C-O	-5.46	115.23	121.68
1	A	332	PHE	CA-CB-CG	5.46	119.26	113.80
1	A	141	ALA	N-CA-C	-5.46	105.41	111.36
1	A	426	LYS	CA-CB-CG	5.45	125.00	114.10
1	D	519	SER	N-CA-C	5.45	118.55	110.48
1	A	67	GLU	CA-C-O	-5.45	114.44	120.60
1	B	254	ALA	CA-C-O	5.45	126.72	121.00
1	B	372	GLY	N-CA-C	-5.45	108.11	115.36
1	C	8	PHE	CA-C-O	-5.45	114.75	120.63
1	C	212	ALA	CA-C-O	-5.44	115.11	120.82
1	A	431	ILE	CA-C-N	5.44	129.39	120.63
1	A	431	ILE	C-N-CA	5.44	129.39	120.63
1	A	459	GLU	CB-CA-C	5.44	119.93	110.79
1	A	228	ASP	CB-CA-C	-5.44	102.79	111.17
1	B	262	ASP	N-CA-CB	5.44	118.11	110.12
1	B	93	ASP	CB-CA-C	5.43	120.81	111.68
1	A	333	LYS	CB-CA-C	5.43	118.76	109.80
1	A	481	ARG	CA-C-O	5.43	127.60	120.16
1	B	530	TYR	CA-C-O	-5.43	114.98	121.11
1	C	438	ASN	N-CA-C	5.42	119.18	112.24
1	A	385	ILE	CA-C-O	-5.42	115.35	121.75
1	A	490	VAL	CA-C-N	5.42	130.73	121.35
1	A	490	VAL	C-N-CA	5.42	130.73	121.35
1	C	102	ARG	NE-CZ-NH2	-5.42	114.32	119.20
1	C	335	THR	N-CA-C	-5.42	106.34	113.17
1	B	26	VAL	CA-C-O	-5.42	115.86	121.93
1	B	276	ARG	NH1-CZ-NH2	5.42	126.34	119.30
1	D	165	LYS	CA-C-O	-5.42	112.77	120.51
1	B	38	CYS	O-C-N	-5.41	116.40	122.03
1	C	279	ARG	CB-CG-CD	5.41	123.74	111.30
1	C	499	ALA	CA-C-N	5.41	125.41	119.89
1	C	499	ALA	C-N-CA	5.41	125.41	119.89
1	A	309	VAL	CB-CA-C	-5.41	103.49	110.84
1	D	382	ASN	N-CA-CB	-5.40	101.42	110.39
1	D	468	ASN	CB-CG-OD1	5.40	131.60	120.80
1	B	535	VAL	N-CA-C	-5.40	104.20	111.44
1	A	558	ARG	NE-CZ-NH1	-5.40	116.10	121.50
1	A	334	ALA	CA-C-O	5.39	128.08	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	217	ASP	CA-C-N	5.39	127.44	120.44
1	B	217	ASP	C-N-CA	5.39	127.44	120.44
1	C	357	ASP	N-CA-CB	-5.39	104.06	112.41
1	B	129	VAL	O-C-N	5.38	128.83	123.18
1	A	169	GLY	O-C-N	5.38	127.39	122.17
1	B	127	ASP	N-CA-C	-5.38	104.37	111.96
1	B	525	PRO	CA-C-O	-5.38	115.22	121.95
1	B	548	ASN	N-CA-C	-5.38	105.85	112.90
1	D	492	PRO	N-CD-CG	5.38	111.27	103.20
1	C	102	ARG	NE-CZ-NH1	5.38	126.88	121.50
1	B	503	HIS	N-CA-C	5.38	120.33	113.18
1	B	3	GLU	CA-C-N	5.37	130.69	122.25
1	B	3	GLU	C-N-CA	5.37	130.69	122.25
1	A	529	LEU	CA-C-O	-5.37	114.41	120.32
1	B	332	PHE	CA-CB-CG	5.37	119.17	113.80
1	C	377	GLU	N-CA-C	-5.37	105.47	112.23
1	B	245	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	D	220	ASP	CA-C-N	5.36	127.41	120.44
1	D	220	ASP	C-N-CA	5.36	127.41	120.44
1	D	342	GLY	CA-C-N	5.36	127.78	120.54
1	D	342	GLY	C-N-CA	5.36	127.78	120.54
1	D	11	GLU	CB-CG-CD	5.36	121.71	112.60
1	C	64	LEU	CA-C-N	5.36	128.00	122.27
1	C	64	LEU	C-N-CA	5.36	128.00	122.27
1	C	366	THR	O-C-N	-5.36	115.46	122.43
1	B	145	ARG	CB-CA-C	5.36	119.96	110.85
1	D	73	CYS	CB-CA-C	-5.36	99.76	110.42
1	A	9	HIS	CA-C-O	5.35	125.97	119.49
1	A	470	PHE	CA-C-O	-5.35	114.88	120.55
1	B	193	ASP	CA-CB-CG	-5.35	107.25	112.60
1	B	291	VAL	N-CA-CB	-5.35	101.46	111.62
1	C	84	CYS	O-C-N	-5.35	116.11	122.20
1	C	526	ILE	N-CA-CB	5.35	116.36	110.53
1	D	30	ASN	CA-CB-CG	-5.35	107.25	112.60
1	A	557	GLY	CA-C-O	-5.34	115.55	121.05
1	B	328	LYS	N-CA-CB	5.34	117.76	110.01
1	C	58	SER	CA-C-O	-5.34	113.63	120.04
1	D	123	LYS	CA-C-O	-5.34	114.06	120.10
1	D	332	PHE	CA-CB-CG	5.34	119.14	113.80
1	B	429	LYS	CA-CB-CG	5.34	124.78	114.10
1	A	349	LEU	N-CA-C	-5.34	105.54	111.36
1	C	26	VAL	CA-C-O	-5.34	114.63	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	12	MET	CA-CB-CG	5.34	124.78	114.10
1	D	131	ILE	CA-C-O	-5.34	114.55	120.74
1	C	193	ASP	CB-CA-C	5.34	119.33	110.90
1	A	350	GLN	N-CA-C	-5.33	106.47	112.87
1	C	222	LEU	N-CA-C	-5.33	105.55	111.36
1	A	509	LEU	CA-C-O	-5.33	115.69	121.44
1	D	245	ARG	N-CA-C	5.33	113.02	108.22
1	D	86	ALA	CA-C-O	-5.33	114.88	120.63
1	A	358	LEU	CA-C-O	-5.32	112.83	119.38
1	A	459	GLU	N-CA-CB	-5.32	102.26	110.13
1	A	271	ILE	N-CA-C	5.32	116.41	108.54
1	D	150	LYS	CB-CA-C	5.32	118.52	109.80
1	D	316	ALA	CA-C-O	-5.32	112.84	119.38
1	A	42	HIS	CA-C-O	-5.31	113.00	119.32
1	A	157	GLU	N-CA-CB	-5.31	103.49	109.49
1	A	272	ARG	O-C-N	-5.31	116.44	123.13
1	B	159	ILE	CA-C-N	5.31	126.48	119.84
1	B	159	ILE	C-N-CA	5.31	126.48	119.84
1	B	255	HIS	CA-C-O	-5.31	115.22	120.90
1	C	92	PHE	CA-C-O	-5.31	115.31	121.15
1	A	230	THR	O-C-N	-5.31	115.04	122.37
1	B	92	PHE	O-C-N	-5.31	116.41	122.89
1	C	558	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	A	318	ASN	OD1-CG-ND2	5.31	127.91	122.60
1	C	47	GLU	CB-CG-CD	5.31	121.62	112.60
1	C	12	MET	CA-CB-CG	5.30	124.71	114.10
1	A	43	GLY	CA-C-O	-5.30	118.33	122.52
1	D	362	GLN	CG-CD-NE2	5.30	124.35	116.40
1	C	493	PHE	CA-CB-CG	-5.30	108.50	113.80
1	D	252	VAL	CB-CA-C	-5.30	102.60	111.29
1	D	11	GLU	CA-C-N	5.30	131.66	121.54
1	D	11	GLU	C-N-CA	5.30	131.66	121.54
1	A	492	PRO	N-CA-CB	5.30	108.81	103.25
1	B	209	LYS	CB-CA-C	-5.30	102.56	110.88
1	A	526	ILE	CA-C-O	5.29	126.84	120.65
1	B	134	GLY	CA-C-N	5.29	125.97	119.99
1	B	134	GLY	C-N-CA	5.29	125.97	119.99
1	C	108	ASP	CA-C-O	5.29	126.06	119.97
1	C	272	ARG	O-C-N	5.29	129.41	123.27
1	A	303	ILE	CA-C-O	-5.29	114.84	120.39
1	B	495	ALA	N-CA-C	5.29	118.07	109.24
1	A	469	GLY	O-C-N	5.29	127.27	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	146	ASP	O-C-N	-5.29	115.56	122.59
1	B	253	GLY	CA-C-N	5.29	127.63	120.65
1	B	253	GLY	C-N-CA	5.29	127.63	120.65
1	B	360	TYR	CA-C-O	5.28	126.01	120.36
1	C	272	ARG	CA-C-O	-5.28	114.65	120.30
1	D	216	SER	CA-C-N	5.28	127.36	120.28
1	D	216	SER	C-N-CA	5.28	127.36	120.28
1	B	68	ILE	CB-CA-C	5.28	117.86	110.99
1	C	157	GLU	CA-C-N	5.28	124.97	119.64
1	C	157	GLU	C-N-CA	5.28	124.97	119.64
1	A	338	PRO	O-C-N	-5.27	115.42	122.22
1	C	483	ASP	CA-CB-CG	5.27	117.87	112.60
1	B	522	THR	CA-C-O	-5.27	112.54	118.55
1	B	64	LEU	CA-C-O	-5.27	115.39	121.19
1	B	481	ARG	NE-CZ-NH2	-5.27	114.46	119.20
1	C	373	VAL	CA-C-N	5.27	128.83	121.24
1	C	373	VAL	C-N-CA	5.27	128.83	121.24
1	D	279	ARG	CD-NE-CZ	-5.27	117.03	124.40
1	C	528	GLY	CA-C-O	-5.27	113.79	119.27
1	A	218	SER	CB-CA-C	5.26	120.91	110.17
1	D	438	ASN	N-CA-CB	-5.25	104.31	112.30
1	A	499	ALA	CA-C-N	5.25	125.19	119.78
1	A	499	ALA	C-N-CA	5.25	125.19	119.78
1	A	314	GLY	O-C-N	5.25	128.42	122.86
1	B	339	GLY	CA-C-O	5.25	123.81	119.04
1	C	238	ALA	N-CA-CB	5.25	119.18	110.52
1	A	252	VAL	CA-CB-CG1	5.24	119.31	110.40
1	A	381	GLY	CA-C-O	5.24	126.15	120.75
1	C	434	TYR	CA-C-N	5.24	129.31	120.29
1	C	434	TYR	C-N-CA	5.24	129.31	120.29
1	D	343	ASP	CA-C-O	5.24	126.51	120.90
1	A	484	LEU	O-C-N	5.24	126.13	121.36
1	A	563	SER	N-CA-CB	-5.24	102.47	110.07
1	B	503	HIS	CA-CB-CG	5.24	119.04	113.80
1	B	47	GLU	O-C-N	-5.24	116.64	122.09
1	B	305	ALA	CA-C-O	-5.23	115.68	121.33
1	D	356	ARG	NE-CZ-NH1	-5.23	116.27	121.50
1	A	107	VAL	N-CA-CB	5.23	118.75	110.54
1	A	200	ARG	CG-CD-NE	5.23	123.51	112.00
1	B	78	GLU	CA-C-O	-5.23	115.63	121.23
1	B	372	GLY	O-C-N	-5.23	115.75	122.39
1	A	167	ALA	CA-C-O	-5.23	113.04	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	367	TYR	CA-C-O	-5.23	115.05	120.70
1	D	19	HIS	CA-CB-CG	-5.23	108.57	113.80
1	D	279	ARG	NE-CZ-NH1	-5.23	116.27	121.50
1	A	71	THR	CA-CB-OG1	-5.23	101.76	109.60
1	A	79	LYS	CB-CG-CD	5.22	123.31	111.30
1	A	506	MET	N-CA-C	5.22	117.72	111.71
1	D	50	ALA	N-CA-C	-5.22	105.67	111.36
1	D	231	ASP	N-CA-C	-5.22	100.79	109.46
1	D	496	LEU	N-CA-C	5.22	117.31	108.02
1	D	68	ILE	CB-CG1-CD1	-5.22	102.84	113.80
1	A	395	MET	N-CA-C	5.21	116.21	108.60
1	A	491	ALA	CA-C-N	5.21	126.35	119.84
1	A	491	ALA	C-N-CA	5.21	126.35	119.84
1	C	401	ARG	CA-C-N	5.21	131.49	121.54
1	C	401	ARG	C-N-CA	5.21	131.49	121.54
1	B	83	TYR	CA-C-N	5.20	127.98	120.38
1	B	83	TYR	C-N-CA	5.20	127.98	120.38
1	A	29	ASP	N-CA-CB	-5.20	101.92	110.14
1	A	293	VAL	CA-C-N	-5.20	115.28	123.13
1	A	293	VAL	C-N-CA	-5.20	115.28	123.13
1	B	241	ASN	CB-CG-ND2	-5.20	108.61	116.40
1	D	134	GLY	CA-C-O	-5.20	117.08	122.28
1	D	350	GLN	CA-CB-CG	5.20	124.49	114.10
1	B	517	VAL	O-C-N	-5.19	117.04	122.81
1	B	242	ARG	CD-NE-CZ	5.19	131.67	124.40
1	A	160	PRO	N-CA-C	5.19	123.16	112.47
1	B	283	ASP	N-CA-C	5.19	115.97	108.34
1	C	152	ILE	N-CA-CB	5.19	118.39	111.64
1	A	242	ARG	NE-CZ-NH1	-5.19	116.31	121.50
1	C	341	THR	N-CA-C	5.19	120.25	113.30
1	A	387	VAL	CA-C-O	-5.19	115.06	120.76
1	A	467	TYR	CA-C-O	-5.19	114.24	120.10
1	C	143	SER	O-C-N	-5.19	116.70	122.09
1	C	67	GLU	N-CA-C	-5.18	101.52	109.76
1	C	18	CYS	N-CA-CB	-5.18	101.00	110.27
1	C	532	ALA	O-C-N	5.18	128.59	123.46
1	D	63	HIS	N-CA-C	-5.18	106.65	113.17
1	B	151	VAL	N-CA-C	5.17	116.42	108.71
1	A	309	VAL	N-CA-CB	5.17	117.20	110.99
1	C	543	ASN	CA-C-O	-5.17	113.83	120.14
1	C	549	ALA	O-C-N	5.17	127.67	122.09
1	B	304	LYS	CA-C-O	-5.17	114.80	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	557	GLY	N-CA-C	-5.17	106.39	112.64
1	D	233	GLY	O-C-N	5.17	127.86	122.79
1	B	86	ALA	N-CA-C	-5.17	104.91	111.11
1	C	393	ARG	NE-CZ-NH1	-5.17	116.33	121.50
1	A	46	LYS	N-CA-CB	5.16	117.67	109.82
1	A	95	PRO	N-CA-C	-5.16	103.08	111.03
1	B	255	HIS	N-CA-CB	5.16	117.64	109.94
1	C	275	SER	CA-C-O	-5.16	114.06	120.57
1	A	215	SER	CA-C-O	5.16	125.89	120.42
1	C	276	ARG	N-CA-C	5.16	116.72	108.41
1	C	3	GLU	CB-CA-C	5.16	119.90	110.10
1	D	476	ASP	CA-CB-CG	5.15	117.75	112.60
1	B	5	LEU	CA-C-O	-5.15	115.06	120.63
1	A	445	THR	CA-C-O	-5.15	115.94	121.45
1	A	492	PRO	CA-N-CD	-5.15	104.80	112.00
1	B	67	GLU	CA-C-N	-5.15	116.23	123.13
1	B	67	GLU	C-N-CA	-5.15	116.23	123.13
1	B	68	ILE	CA-CB-CG2	5.14	119.25	110.50
1	C	200	ARG	CA-C-N	5.14	131.37	121.54
1	C	200	ARG	C-N-CA	5.14	131.37	121.54
1	B	39	VAL	CA-C-O	-5.14	115.60	120.95
1	C	130	ILE	N-CA-C	5.14	115.26	107.80
1	B	420	PHE	CA-C-O	5.14	127.27	121.51
1	B	464	VAL	N-CA-C	5.14	115.91	110.72
1	B	279	ARG	NE-CZ-NH2	5.14	123.82	119.20
1	C	283	ASP	CA-C-N	5.13	131.34	121.54
1	C	283	ASP	C-N-CA	5.13	131.34	121.54
1	C	467	TYR	CA-C-N	5.13	127.16	120.28
1	C	467	TYR	C-N-CA	5.13	127.16	120.28
1	D	61	LYS	CA-CB-CG	5.13	124.36	114.10
1	D	318	ASN	N-CA-CB	-5.13	103.64	110.57
1	A	3	GLU	O-C-N	-5.13	115.19	122.99
1	A	128	VAL	O-C-N	-5.13	117.80	123.18
1	B	219	ILE	CA-C-O	5.13	126.39	121.05
1	D	435	VAL	CA-C-O	-5.13	115.08	120.57
1	A	68	ILE	O-C-N	-5.13	115.44	122.62
1	C	130	ILE	CA-C-O	-5.13	115.04	120.53
1	C	259	VAL	CG1-CB-CG2	5.13	122.08	110.80
1	D	8	PHE	O-C-N	-5.13	116.22	122.22
1	D	318	ASN	CA-C-O	-5.13	116.47	122.37
1	C	176	THR	N-CA-C	5.12	117.67	110.14
1	A	259	VAL	CG1-CB-CG2	5.12	122.07	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	277	VAL	CB-CA-C	5.12	117.07	111.08
1	A	508	GLY	O-C-N	-5.12	118.89	123.96
1	D	27	THR	CA-CB-OG1	5.12	117.28	109.60
1	A	274	ASN	CB-CA-C	-5.12	103.63	111.66
1	C	218	SER	N-CA-CB	-5.12	102.35	110.28
1	D	548	ASN	CA-C-O	-5.12	112.56	119.11
1	A	272	ARG	N-CA-C	5.11	117.04	107.99
1	C	429	LYS	O-C-N	-5.11	116.77	122.09
1	B	564	ALA	CA-C-O	-5.11	114.09	119.97
1	C	306	ASP	CA-C-O	-5.11	114.57	120.24
1	C	46	LYS	N-CA-CB	5.11	117.42	110.01
1	C	249	GLY	CA-C-N	5.10	131.29	121.54
1	C	249	GLY	C-N-CA	5.10	131.29	121.54
1	D	267	ARG	CA-C-O	-5.10	113.21	120.51
1	D	184	ILE	N-CA-CB	5.10	116.09	110.53
1	A	382	ASN	OD1-CG-ND2	-5.10	117.50	122.60
1	C	14	GLY	N-CA-C	5.10	125.26	113.18
1	C	321	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	C	380	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	C	313	GLY	O-C-N	-5.10	117.80	123.05
1	A	359	GLU	CB-CG-CD	5.09	121.26	112.60
1	B	88	HIS	CA-CB-CG	5.09	118.89	113.80
1	C	129	VAL	CA-C-N	-5.09	116.50	123.12
1	C	129	VAL	C-N-CA	-5.09	116.50	123.12
1	B	256	VAL	CA-C-O	-5.09	115.46	120.85
1	A	545	LEU	CA-C-O	-5.09	115.25	121.05
1	A	323	SER	N-CA-C	5.08	118.74	112.54
1	B	280	ILE	CA-C-O	-5.08	115.09	120.48
1	D	330	LYS	N-CA-C	-5.08	102.53	110.10
1	A	333	LYS	CB-CG-CD	5.08	122.99	111.30
1	B	401	ARG	N-CA-CB	5.08	119.08	110.49
1	C	495	ALA	N-CA-C	5.08	116.86	108.13
1	D	269	THR	N-CA-C	5.08	117.83	110.42
1	C	43	GLY	N-CA-C	-5.07	106.61	112.29
1	D	429	LYS	O-C-N	-5.07	116.42	122.20
1	A	338	PRO	N-CA-C	5.07	120.50	113.65
1	B	269	THR	CA-CB-OG1	-5.07	102.00	109.60
1	A	73	CYS	O-C-N	5.07	129.33	122.59
1	D	536	THR	CA-C-O	5.07	127.70	121.72
1	C	5	LEU	O-C-N	-5.06	116.82	122.09
1	A	128	VAL	CA-C-N	5.06	129.31	122.93
1	A	128	VAL	C-N-CA	5.06	129.31	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	301	TYR	CA-CB-CG	5.06	123.01	113.90
1	A	188	LYS	N-CA-CB	5.06	118.01	110.22
1	B	479	PHE	CA-C-O	-5.06	115.30	121.88
1	A	271	ILE	N-CA-CB	-5.05	105.29	110.95
1	D	302	VAL	CA-C-N	-5.05	116.55	123.12
1	D	302	VAL	C-N-CA	-5.05	116.55	123.12
1	B	95	PRO	CA-C-N	5.05	129.53	122.36
1	B	95	PRO	C-N-CA	5.05	129.53	122.36
1	A	285	SER	N-CA-C	-5.05	102.04	109.62
1	B	379	VAL	N-CA-C	-5.05	105.57	110.42
1	C	180	ALA	O-C-N	-5.05	115.87	122.59
1	A	267	ARG	CA-CB-CG	-5.05	104.00	114.10
1	C	75	LYS	CA-C-O	5.05	127.27	121.47
1	C	17	SER	N-CA-CB	-5.04	101.56	109.78
1	C	537	GLY	O-C-N	-5.04	119.21	123.60
1	B	22	ASP	N-CA-CB	5.04	118.88	110.41
1	C	73	CYS	O-C-N	5.04	129.29	122.59
1	C	213	ASN	OD1-CG-ND2	5.04	127.64	122.60
1	C	268	GLY	CA-C-N	-5.03	113.04	120.94
1	C	268	GLY	C-N-CA	-5.03	113.04	120.94
1	A	429	LYS	CA-C-O	-5.03	113.40	119.49
1	B	36	GLY	CA-C-O	5.03	125.99	120.66
1	D	240	VAL	CB-CA-C	-5.03	101.80	110.65
1	A	30	ASN	CA-C-O	-5.03	113.20	119.38
1	B	8	PHE	O-C-N	-5.03	116.66	122.09
1	D	357	ASP	N-CA-CB	-5.03	101.99	110.49
1	A	51	ALA	N-CA-CB	-5.03	103.04	110.53
1	A	308	VAL	CA-C-O	-5.03	115.19	120.27
1	B	540	HIS	N-CA-C	5.02	119.09	112.92
1	C	93	ASP	CB-CA-C	5.02	119.74	111.31
1	D	322	VAL	N-CA-C	5.02	115.74	110.62
1	C	345	LEU	CB-CA-C	-5.02	102.78	110.81
1	D	38	CYS	CA-C-O	5.02	125.87	120.70
1	D	267	ARG	CA-C-N	-5.02	111.58	121.41
1	D	267	ARG	C-N-CA	-5.02	111.58	121.41
1	C	427	SER	N-CA-C	5.01	117.40	111.33
1	D	136	ALA	CA-C-N	5.01	125.55	119.98
1	D	136	ALA	C-N-CA	5.01	125.55	119.98
1	A	334	ALA	O-C-N	-5.01	116.63	123.10
1	C	380	ARG	NH1-CZ-NH2	-5.01	112.79	119.30
1	D	526	ILE	CA-C-O	5.01	127.01	120.95
1	A	520	GLU	CB-CA-C	5.01	119.87	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	257	ALA	CA-C-N	5.01	126.95	120.44
1	C	257	ALA	C-N-CA	5.01	126.95	120.44
1	A	144	ALA	CB-CA-C	-5.00	103.02	110.88
1	B	231	ASP	N-CA-C	-5.00	101.80	109.76
1	C	78	GLU	N-CA-CB	-5.00	103.30	111.66
1	A	490	VAL	N-CA-C	5.00	115.54	107.73
1	A	9	HIS	O-C-N	-5.00	115.89	122.39
1	A	476	ASP	CA-CB-CG	5.00	117.60	112.60
1	C	231	ASP	CA-C-N	-5.00	116.99	123.19
1	C	231	ASP	C-N-CA	-5.00	116.99	123.19

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	ASP	Mainchain
1	A	491	ALA	Peptide,Mainchain
1	B	491	ALA	Peptide,Mainchain
1	C	477	ALA	Mainchain
1	C	491	ALA	Peptide,Mainchain
1	D	491	ALA	Peptide,Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4124	0	4013	191	1
1	B	4093	0	3976	185	0
1	C	4099	0	3977	203	2
1	D	4113	0	3988	224	1
2	A	172	0	121	15	0
2	B	172	0	121	13	0
2	C	172	0	120	13	0
2	D	172	0	121	21	0
3	A	53	0	31	9	0
3	B	53	0	31	8	0
3	C	53	0	31	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	53	0	30	9	0
4	B	5	0	0	1	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	48	0	0	2	0
5	B	29	0	0	3	0
5	C	30	0	0	2	0
5	D	19	0	0	2	0
All	All	17470	0	16560	831	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (831) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:CYS:SG	2:D:603:HEC:HAC	1.21	1.71
3:B:700:FAD:C2'	3:B:700:FAD:C1'	1.77	1.62
3:D:900:FAD:C2'	3:D:900:FAD:C1'	1.78	1.59
3:A:600:FAD:C1'	3:A:600:FAD:C2'	1.78	1.57
3:C:800:FAD:C2'	3:C:800:FAD:C1'	1.78	1.56
1:A:41:CYS:SG	2:A:604:HEC:HAC	1.46	1.55
1:B:73:CYS:SG	2:B:602:HEC:HAC	1.48	1.51
1:D:70:CYS:SG	2:D:602:HEC:CAB	2.04	1.46
1:C:87:CYS:SG	2:C:601:HEC:CAC	2.01	1.46
1:B:87:CYS:SG	2:B:601:HEC:CAC	2.03	1.45
1:D:41:CYS:SG	2:D:604:HEC:CAC	2.03	1.44
1:D:73:CYS:SG	2:D:602:HEC:CAC	2.05	1.43
1:A:41:CYS:SG	2:A:604:HEC:CAC	2.07	1.42
1:D:18:CYS:SG	2:D:603:HEC:CAC	2.12	1.34
1:B:73:CYS:SG	2:B:602:HEC:CAC	2.15	1.33
1:D:506:MET:HE3	1:D:543:ASN:HA	1.29	1.14
1:C:379:VAL:HG11	1:C:418:LEU:HD13	1.45	0.97
1:A:288:VAL:HG23	1:A:526:ILE:HD11	1.46	0.95
1:D:64:LEU:HD13	1:D:159:ILE:HD12	1.53	0.91
1:C:35:ASN:HD21	1:C:71:THR:H	1.16	0.91
1:A:66:GLY:H	1:A:258:GLN:HE22	1.07	0.91
1:A:319:ASN:HD21	1:A:331:GLY:H	1.09	0.91
1:A:452:GLN:HE21	1:A:452:GLN:HA	1.35	0.91
1:A:393:ARG:HH11	1:A:478:GLN:NE2	1.67	0.91
1:B:166:LEU:HD21	2:B:601:HEC:HBC2	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ASN:HD21	1:A:71:THR:H	1.18	0.89
1:B:66:GLY:H	1:B:258:GLN:HE22	1.19	0.89
1:C:319:ASN:HD21	1:C:331:GLY:H	0.94	0.88
1:D:316:ALA:HB1	1:D:502:VAL:HG12	1.55	0.88
1:B:455:VAL:HG21	1:B:460:LEU:HD12	1.53	0.87
1:D:447:GLU:HB3	1:D:457:ALA:HB1	1.57	0.87
1:C:9:HIS:HA	1:C:12:MET:HE3	1.57	0.86
1:C:319:ASN:ND2	1:C:331:GLY:H	1.75	0.82
1:D:31:LEU:HD21	2:D:603:HEC:HAD1	1.62	0.82
1:C:421:ASP:HB2	1:C:488:LEU:HD12	1.61	0.81
1:B:125:THR:HG22	1:B:304:LYS:HB3	1.63	0.81
1:D:526:ILE:HG12	1:D:529:LEU:HB2	1.63	0.81
1:D:424:ILE:HD13	1:D:486:ARG:HD2	1.62	0.80
1:A:66:GLY:H	1:A:258:GLN:NE2	1.79	0.80
1:C:392:ASN:HA	1:C:463:THR:HG21	1.64	0.80
1:D:362:GLN:HB2	1:D:506:MET:HE1	1.63	0.80
1:C:186:ASP:HB2	1:C:240:VAL:HG11	1.64	0.79
1:B:409:LEU:HD23	1:B:414:GLU:HB3	1.64	0.78
1:C:280:ILE:HD12	1:C:347:VAL:HG13	1.64	0.77
1:C:181:LYS:H	1:C:181:LYS:HD3	1.48	0.77
1:D:471:VAL:HG22	1:D:484:LEU:HB3	1.63	0.77
1:C:175:GLU:OE2	1:C:188:LYS:HG3	1.84	0.76
1:D:52:ALA:CA	1:D:53:PRO:N	2.48	0.76
1:B:533:GLY:HA2	1:B:553:ILE:HG22	1.65	0.76
1:C:233:GLY:HA3	1:C:245:ARG:NH2	2.01	0.76
1:D:506:MET:CE	1:D:543:ASN:HA	2.13	0.75
1:C:416:ALA:HB3	1:C:498:ILE:HD11	1.69	0.75
1:B:366:THR:HG22	1:B:498:ILE:HD12	1.68	0.75
1:C:319:ASN:HD21	1:C:331:GLY:N	1.79	0.74
1:C:421:ASP:HB3	1:C:424:ILE:HG12	1.68	0.74
1:A:322:VAL:HG13	1:A:361:ILE:HD13	1.69	0.74
1:A:62:SER:HB3	2:A:601:HEC:HBB3	1.70	0.73
1:C:446:ILE:HD13	1:C:464:VAL:HG11	1.71	0.73
1:A:145:ARG:HH11	1:A:268:GLY:H	1.36	0.72
1:B:68:ILE:HD11	2:B:602:HEC:CMC	2.19	0.72
1:B:175:GLU:OE2	1:B:188:LYS:HG3	1.90	0.72
1:A:135:GLY:HA3	1:A:553:ILE:HD12	1.72	0.72
1:A:177:LYS:HB2	1:A:178:PRO:HD3	1.71	0.72
1:D:453:ILE:O	1:D:454:ASP:HB2	1.89	0.72
1:D:66:GLY:H	1:D:258:GLN:HE22	1.36	0.71
1:B:319:ASN:HD21	1:B:331:GLY:H	1.36	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:VAL:HG21	1:A:225:MET:HE1	1.72	0.71
1:C:452:GLN:HE21	1:C:452:GLN:HA	1.55	0.71
1:C:409:LEU:HD22	1:C:414:GLU:HB3	1.73	0.71
3:D:900:FAD:C2'	3:D:900:FAD:N10	2.52	0.71
1:A:366:THR:HG22	1:A:498:ILE:HD13	1.72	0.70
1:D:366:THR:HG21	1:D:380:ARG:HE	1.56	0.70
1:D:453:ILE:HG22	1:D:455:VAL:HG13	1.73	0.70
1:C:194:ASP:OD2	1:C:242:ARG:NH2	2.24	0.70
1:D:68:ILE:HD11	2:D:602:HEC:HMC1	1.73	0.70
1:A:393:ARG:NH1	1:A:478:GLN:NE2	2.39	0.70
1:D:35:ASN:HD21	1:D:71:THR:H	1.38	0.70
1:D:225:MET:HE3	1:D:263:ASN:CB	2.22	0.69
1:C:181:LYS:H	1:C:181:LYS:CD	2.00	0.69
1:D:393:ARG:HD3	1:D:478:GLN:HE22	1.56	0.69
1:B:28:ASN:C	1:B:28:ASN:HD22	2.00	0.69
1:B:392:ASN:HA	1:B:463:THR:HG21	1.75	0.68
1:B:455:VAL:CG2	1:B:460:LEU:HD12	2.23	0.68
1:B:550:ILE:HG12	3:B:700:FAD:C2	2.23	0.68
1:A:319:ASN:ND2	1:A:331:GLY:H	1.89	0.68
1:D:455:VAL:HB	1:D:456:PRO:HD2	1.75	0.68
1:A:68:ILE:HD11	2:A:602:HEC:HMC1	1.76	0.68
1:A:117:ALA:HA	1:A:120:ALA:HB3	1.76	0.68
1:B:68:ILE:HD11	2:B:602:HEC:HMC3	1.74	0.68
1:A:186:ASP:HB2	1:A:240:VAL:HG11	1.74	0.68
1:D:52:ALA:O	1:D:53:PRO:N	2.27	0.68
1:B:460:LEU:O	1:B:464:VAL:HG23	1.94	0.67
1:B:549:ALA:HB3	3:B:700:FAD:N1	2.10	0.67
1:C:35:ASN:ND2	1:C:71:THR:H	1.92	0.67
1:B:58:SER:H	1:B:61:LYS:CE	2.06	0.67
1:C:326:ASP:OD2	1:C:328:LYS:HB2	1.94	0.67
1:D:310:ILE:HD11	1:D:529:LEU:HD21	1.76	0.67
1:C:516:GLU:HG2	5:C:843:HOH:O	1.94	0.67
1:C:129:VAL:HB	1:C:308:VAL:HG22	1.77	0.67
3:A:600:FAD:C1'	3:A:600:FAD:C3'	2.71	0.66
1:B:526:ILE:HG12	1:B:529:LEU:HB2	1.78	0.66
1:D:64:LEU:HD13	1:D:159:ILE:CD1	2.23	0.66
1:C:549:ALA:HB3	3:C:800:FAD:N1	2.11	0.66
1:B:58:SER:H	1:B:61:LYS:HE2	1.60	0.66
1:A:393:ARG:HH11	1:A:478:GLN:HE21	1.42	0.66
1:C:163:ASN:HD21	1:C:336:ASN:ND2	1.93	0.66
1:D:72:SER:HB2	1:D:158:PRO:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:VAL:HG21	1:A:297:TYR:HB3	1.78	0.66
1:D:68:ILE:HD11	2:D:602:HEC:CMC	2.26	0.65
1:A:393:ARG:NH1	1:A:478:GLN:HE21	1.95	0.65
1:B:280:ILE:HG13	1:B:347:VAL:HG13	1.79	0.65
1:D:283:ASP:CG	1:D:284:ALA:H	2.03	0.65
1:A:319:ASN:HD21	1:A:331:GLY:N	1.91	0.65
1:B:446:ILE:HG23	1:B:460:LEU:HD22	1.78	0.65
1:A:41:CYS:SG	2:A:604:HEC:C3C	2.84	0.65
1:B:321:ARG:NH2	1:B:346:ASP:OD1	2.20	0.65
1:A:468:ASN:ND2	1:A:487:GLU:O	2.30	0.65
1:D:514:LYS:O	1:D:515:ALA:HB3	1.97	0.65
1:D:225:MET:HE1	1:D:260:LEU:HD23	1.77	0.65
1:B:319:ASN:ND2	1:B:331:GLY:H	1.94	0.64
1:D:288:VAL:HG22	1:D:526:ILE:HD11	1.79	0.64
1:D:460:LEU:O	1:D:464:VAL:HG23	1.96	0.64
1:D:506:MET:HE3	1:D:543:ASN:CA	2.19	0.64
1:A:75:LYS:H	1:A:80:SER:HB3	1.62	0.64
1:D:45:LEU:HD23	2:D:602:HEC:HBB2	1.78	0.64
2:A:601:HEC:HHA	2:A:601:HEC:HBA1	1.79	0.64
1:B:389:ARG:NH2	1:B:413:GLY:HA3	2.13	0.64
1:A:68:ILE:HD11	2:A:602:HEC:CMC	2.27	0.64
1:D:135:GLY:HA3	1:D:553:ILE:HD12	1.80	0.64
1:D:393:ARG:NH1	1:D:467:TYR:HD2	1.94	0.64
1:D:117:ALA:HA	1:D:120:ALA:HB3	1.80	0.64
1:B:471:VAL:HG11	1:B:487:GLU:HA	1.80	0.64
1:C:94:MET:HE2	2:C:602:HEC:HMD2	1.80	0.64
1:C:530:TYR:CE2	1:C:563:SER:HB3	2.32	0.64
1:A:83:TYR:CE1	1:A:159:ILE:HD11	2.34	0.63
1:A:445:THR:OG1	1:A:448:GLU:HB2	1.98	0.63
1:A:26:VAL:HG21	1:A:297:TYR:CB	2.28	0.63
3:C:800:FAD:C1'	3:C:800:FAD:C3'	2.74	0.63
1:C:231:ASP:HB3	1:C:245:ARG:HG3	1.78	0.63
1:D:145:ARG:HH11	1:D:268:GLY:H	1.44	0.63
1:D:154:LEU:HD13	1:D:277:VAL:CG2	2.28	0.63
1:B:362:GLN:NE2	1:B:544:ARG:HH21	1.97	0.63
1:A:514:LYS:HE3	1:A:516:GLU:CD	2.24	0.63
1:A:127:ASP:HB2	1:A:150:LYS:O	1.96	0.63
1:B:173:ALA:HA	1:B:215:SER:HB2	1.81	0.63
1:B:228:ASP:HB3	1:B:247:THR:OG1	1.98	0.63
1:B:449:LEU:HD22	1:B:495:ALA:HB2	1.81	0.63
1:A:514:LYS:HE3	1:A:516:GLU:OE1	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:600:FAD:C2'	3:A:600:FAD:N10	2.58	0.63
1:A:387:VAL:O	1:A:416:ALA:HB1	1.98	0.62
1:B:35:ASN:HD21	1:B:71:THR:H	1.46	0.62
1:B:509:LEU:H	1:B:536:THR:HA	1.64	0.62
1:A:106:PRO:HG2	1:A:109:ALA:HB2	1.81	0.62
3:B:700:FAD:C2'	3:B:700:FAD:N10	2.58	0.62
1:C:431:ILE:O	1:C:435:VAL:HG23	1.99	0.62
1:A:392:ASN:HA	1:A:463:THR:HG21	1.79	0.62
1:B:71:THR:HA	1:B:74:HIS:O	1.99	0.62
1:D:20:VAL:HG22	1:D:33:HIS:CG	2.34	0.62
1:B:337:HIS:HB2	1:B:338:PRO:HD2	1.82	0.62
1:A:246:PRO:HD2	1:A:250:ALA:O	2.00	0.62
1:D:52:ALA:CA	1:D:52:ALA:O	2.47	0.62
1:B:450:ALA:HA	1:B:455:VAL:HG22	1.81	0.62
1:C:388:ASN:ND2	1:C:390:GLU:HB2	2.15	0.62
1:D:553:ILE:HG13	1:D:554:VAL:N	2.13	0.62
1:C:87:CYS:SG	2:C:601:HEC:C3C	2.87	0.61
1:D:52:ALA:CA	1:D:53:PRO:CD	2.79	0.61
1:C:409:LEU:HA	1:C:414:GLU:HB3	1.82	0.61
1:B:73:CYS:CB	2:B:602:HEC:HAC	2.31	0.61
1:B:325:TYR:O	2:D:604:HEC:HMD3	2.00	0.61
1:B:154:LEU:HD22	1:B:293:VAL:HG11	1.82	0.61
1:C:445:THR:OG1	1:C:448:GLU:HB2	2.01	0.61
1:D:431:ILE:HA	1:D:434:TYR:CD2	2.36	0.61
1:A:453:ILE:O	1:A:454:ASP:HB2	2.00	0.61
1:B:435:VAL:HG22	1:B:440:VAL:HG21	1.82	0.60
1:C:374:MET:HE1	3:C:800:FAD:H6	1.81	0.60
1:D:405:SER:O	1:D:409:LEU:HD12	2.01	0.60
1:B:259:VAL:O	1:B:263:ASN:ND2	2.35	0.60
3:C:800:FAD:C1'	3:C:800:FAD:O2'	2.47	0.60
1:A:283:ASP:OD2	1:A:284:ALA:N	2.34	0.60
1:B:332:PHE:HZ	1:B:409:LEU:HD11	1.66	0.60
1:C:155:GLU:OE1	3:C:800:FAD:H1B	2.01	0.60
1:C:231:ASP:OD2	1:C:245:ARG:HD2	2.00	0.60
1:D:228:ASP:O	1:D:229:MET:HE2	2.02	0.60
1:A:35:ASN:ND2	1:A:70:CYS:HB2	2.15	0.60
1:A:142:VAL:HG21	1:A:225:MET:CE	2.30	0.60
1:A:153:LEU:HD22	1:A:271:ILE:HG23	1.84	0.60
3:D:900:FAD:C1'	3:D:900:FAD:O2'	2.47	0.60
1:C:409:LEU:HD21	1:C:500:PRO:HG3	1.84	0.59
1:C:558:ARG:HH11	1:C:558:ARG:HG2	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:PHE:CE1	1:D:395:MET:HE3	2.36	0.59
1:B:467:TYR:HA	1:B:470:PHE:CD2	2.36	0.59
1:C:389:ARG:HD2	1:C:412:LYS:CB	2.31	0.59
1:C:467:TYR:HA	1:C:470:PHE:CD2	2.37	0.59
1:D:73:CYS:SG	2:D:602:HEC:C3C	2.89	0.59
1:C:131:ILE:HG12	1:C:277:VAL:HG21	1.83	0.59
1:C:388:ASN:HB3	1:C:411:GLN:HE21	1.67	0.59
1:C:514:LYS:O	1:C:515:ALA:HB3	2.03	0.59
1:C:68:ILE:HG13	1:C:68:ILE:O	2.02	0.59
1:A:294:LYS:HB2	1:A:300:TYR:CE2	2.38	0.59
1:B:527:THR:HG22	1:B:567:PHE:CZ	2.37	0.59
1:D:234:ARG:HB2	1:D:241:ASN:OD1	2.02	0.59
1:C:166:LEU:HD13	2:C:601:HEC:HMD1	1.84	0.59
1:D:49:ALA:HB1	1:D:61:LYS:HB3	1.84	0.59
1:D:218:SER:HB3	1:D:554:VAL:HG12	1.85	0.59
1:B:68:ILE:HG13	1:B:68:ILE:O	2.03	0.58
1:B:375:ILE:HG21	1:B:418:LEU:HD11	1.84	0.58
1:B:421:ASP:HB3	1:B:424:ILE:HG12	1.85	0.58
1:B:375:ILE:HG12	1:B:496:LEU:HD22	1.85	0.58
1:D:78:GLU:O	1:D:79:LYS:C	2.45	0.58
1:A:145:ARG:NH1	1:A:268:GLY:H	1.99	0.58
1:A:163:ASN:HD21	1:A:336:ASN:ND2	2.01	0.58
3:B:700:FAD:C1'	3:B:700:FAD:C3'	2.76	0.58
1:A:170:GLY:HA2	1:A:252:VAL:HG21	1.85	0.58
1:C:87:CYS:O	1:C:372:GLY:HA3	2.03	0.58
1:B:375:ILE:HG21	1:B:418:LEU:CD1	2.33	0.58
1:D:470:PHE:CG	1:D:476:ASP:HA	2.39	0.58
1:C:375:ILE:HG13	1:C:496:LEU:HD22	1.86	0.58
1:D:35:ASN:ND2	1:D:70:CYS:H	2.01	0.58
1:A:171:MET:HE3	1:A:551:SER:HA	1.85	0.58
1:C:558:ARG:HH11	1:C:558:ARG:CG	2.15	0.58
1:D:159:ILE:HG13	5:D:930:HOH:O	2.04	0.58
1:D:235:MET:HE3	1:D:547:GLY:N	2.19	0.58
1:D:453:ILE:HD11	1:D:495:ALA:CB	2.34	0.57
3:D:900:FAD:C1'	3:D:900:FAD:C3'	2.74	0.57
1:C:343:ASP:HB3	3:C:800:FAD:H61A	1.69	0.57
1:D:28:ASN:C	1:D:28:ASN:HD22	2.12	0.57
1:A:452:GLN:HA	1:A:452:GLN:NE2	2.11	0.57
1:B:196:MET:CE	1:B:203:ASN:HB2	2.33	0.57
1:C:294:LYS:O	1:C:294:LYS:HG3	2.04	0.57
1:B:66:GLY:H	1:B:258:GLN:NE2	1.97	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:ASP:OD2	1:D:328:LYS:HG3	2.04	0.57
1:C:118:ILE:CD1	1:C:279:ARG:NH1	2.67	0.57
3:C:800:FAD:C2'	3:C:800:FAD:N10	2.63	0.57
1:D:83:TYR:CE1	1:D:159:ILE:HD13	2.39	0.57
1:C:429:LYS:O	1:C:430:ALA:C	2.47	0.57
1:A:470:PHE:CG	1:A:476:ASP:HA	2.40	0.57
1:A:517:VAL:HG21	1:A:529:LEU:HD22	1.87	0.57
1:B:455:VAL:HB	1:B:456:PRO:HD2	1.87	0.57
1:A:293:VAL:HG21	1:A:303:ILE:HD12	1.86	0.56
1:A:71:THR:HA	1:A:74:HIS:O	2.05	0.56
1:B:228:ASP:OD1	1:B:247:THR:HG21	2.06	0.56
1:D:470:PHE:HA	1:D:475:LYS:O	2.05	0.56
1:B:114:GLN:HE21	1:B:279:ARG:HH21	1.54	0.56
1:D:516:GLU:HG2	1:D:525:PRO:HB3	1.87	0.56
1:D:192:ILE:HG23	1:D:208:VAL:HG12	1.88	0.56
1:B:283:ASP:CG	1:B:284:ALA:H	2.13	0.56
1:C:409:LEU:CD2	1:C:414:GLU:HB3	2.36	0.56
1:C:235:MET:HE2	1:C:243:SER:OG	2.05	0.56
1:C:388:ASN:HD22	1:C:390:GLU:H	1.53	0.56
1:A:28:ASN:HD21	1:A:32:THR:H	1.53	0.56
1:A:68:ILE:C	1:A:68:ILE:HD12	2.30	0.56
1:A:388:ASN:HD21	1:A:392:ASN:HB2	1.71	0.56
1:B:230:THR:OG1	1:B:247:THR:HG23	2.06	0.56
1:C:453:ILE:CG2	1:C:455:VAL:HG13	2.36	0.56
1:D:319:ASN:ND2	1:D:331:GLY:H	2.04	0.56
1:A:470:PHE:HB3	1:A:476:ASP:HA	1.87	0.55
1:B:102:ARG:NH2	1:B:157:GLU:OE1	2.39	0.55
1:B:403:LYS:O	1:B:406:ALA:HB3	2.06	0.55
1:C:421:ASP:HB3	1:C:424:ILE:CG1	2.36	0.55
1:D:41:CYS:SG	2:D:604:HEC:C3C	2.92	0.55
1:D:393:ARG:HD3	1:D:478:GLN:NE2	2.20	0.55
1:B:234:ARG:HB2	1:B:241:ASN:OD1	2.07	0.55
1:D:403:LYS:O	1:D:406:ALA:HB3	2.07	0.55
1:B:122:VAL:HG22	1:B:302:VAL:HG11	1.89	0.55
1:C:380:ARG:HA	1:C:384:ALA:HB3	1.88	0.55
1:C:420:PHE:CE2	1:C:431:ILE:HG21	2.42	0.55
1:D:384:ALA:HB2	1:D:420:PHE:HB3	1.89	0.55
1:B:366:THR:HA	1:B:498:ILE:HB	1.89	0.55
1:C:376:THR:HG23	1:C:379:VAL:H	1.71	0.55
1:A:135:GLY:O	1:A:136:ALA:C	2.49	0.55
1:D:70:CYS:SG	2:D:602:HEC:C3B	2.93	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:VAL:HG12	1:C:241:ASN:N	2.21	0.55
1:C:281:LEU:N	1:C:290:GLY:O	2.26	0.55
1:D:52:ALA:CA	1:D:53:PRO:HD3	2.37	0.55
1:C:376:THR:HG22	1:C:379:VAL:HG23	1.89	0.54
1:C:452:GLN:HA	1:C:452:GLN:NE2	2.21	0.54
1:C:471:VAL:CG1	1:C:487:GLU:HG3	2.37	0.54
1:D:19:HIS:ND1	1:D:34:GLU:OE2	2.40	0.54
1:A:461:ALA:O	1:A:465:THR:HG23	2.07	0.54
1:D:468:ASN:OD1	1:D:487:GLU:HB3	2.06	0.54
1:C:28:ASN:C	1:C:28:ASN:HD22	2.16	0.54
1:C:453:ILE:O	1:C:454:ASP:HB2	2.07	0.54
1:D:225:MET:CE	1:D:260:LEU:HD23	2.38	0.54
1:A:367:TYR:HB3	1:A:499:ALA:O	2.07	0.54
1:C:375:ILE:HG21	1:C:418:LEU:CD1	2.37	0.54
1:A:393:ARG:HH11	1:A:478:GLN:HE22	1.53	0.54
1:B:540:HIS:ND1	1:B:544:ARG:HG3	2.23	0.54
1:D:175:GLU:OE2	1:D:188:LYS:HG3	2.07	0.54
1:D:198:GLY:HA3	1:D:545:LEU:HD21	1.89	0.54
1:B:80:SER:HB3	1:B:94:MET:HE3	1.90	0.54
1:D:421:ASP:OD2	1:D:424:ILE:HG12	2.08	0.54
1:A:79:LYS:HG2	1:A:96:PHE:O	2.08	0.54
1:D:322:VAL:HG22	1:D:361:ILE:HD13	1.89	0.54
1:A:343:ASP:HB2	5:A:609:HOH:O	2.08	0.54
1:A:459:GLU:O	1:A:463:THR:HG23	2.07	0.54
1:A:172:ASN:OD1	1:A:548:ASN:ND2	2.41	0.53
1:A:231:ASP:HB3	1:A:245:ARG:HG2	1.89	0.53
1:B:393:ARG:HD3	1:B:478:GLN:NE2	2.23	0.53
1:C:385:ILE:HG12	1:C:488:LEU:HD21	1.89	0.53
1:A:367:TYR:O	1:A:369:PRO:HD3	2.08	0.53
1:A:504:HIS:CD2	1:A:544:ARG:HE	2.27	0.53
3:A:600:FAD:C1'	3:A:600:FAD:O2'	2.51	0.53
1:B:319:ASN:HD21	1:B:330:LYS:HA	1.74	0.53
1:D:145:ARG:HG2	1:D:151:VAL:CG2	2.39	0.53
1:D:145:ARG:NH1	1:D:268:GLY:H	2.06	0.53
1:B:527:THR:HG22	1:B:567:PHE:HZ	1.72	0.53
1:A:394:PHE:CE1	1:A:395:MET:HE3	2.44	0.53
1:C:8:PHE:HE2	2:C:604:HEC:HHA	1.74	0.53
1:C:187:LYS:HB2	1:C:190:ILE:CD1	2.38	0.53
1:C:420:PHE:CE2	1:C:431:ILE:HD13	2.43	0.53
1:C:453:ILE:HG21	1:C:455:VAL:HG13	1.90	0.53
1:C:461:ALA:O	1:C:465:THR:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ARG:HD3	1:A:249:GLY:HA2	1.90	0.53
1:A:422:ASP:OD1	1:A:494:TYR:OH	2.22	0.53
1:B:58:SER:HB3	1:B:61:LYS:HE3	1.91	0.53
1:B:446:ILE:CD1	1:B:464:VAL:HG11	2.38	0.53
1:A:317:LYS:HB3	1:A:340:ALA:O	2.09	0.53
1:C:187:LYS:HB2	1:C:190:ILE:HD12	1.90	0.53
1:A:550:ILE:HA	1:A:553:ILE:HG12	1.90	0.53
1:B:393:ARG:HD3	1:B:478:GLN:HE22	1.73	0.53
1:B:455:VAL:HB	1:B:456:PRO:CD	2.39	0.53
1:C:172:ASN:O	1:C:551:SER:OG	2.26	0.53
1:D:389:ARG:HG3	1:D:389:ARG:HH11	1.73	0.53
1:A:167:ALA:HA	3:A:600:FAD:N5	2.24	0.52
1:A:176:THR:HB	1:A:178:PRO:HD2	1.89	0.52
1:D:179:GLN:NE2	1:D:242:ARG:HB3	2.23	0.52
1:A:206:GLU:HA	1:A:209:LYS:HD2	1.90	0.52
1:B:450:ALA:HA	1:B:455:VAL:CG2	2.40	0.52
1:B:544:ARG:HD2	1:B:549:ALA:HB2	1.91	0.52
1:C:173:ALA:HA	1:C:215:SER:HB2	1.91	0.52
1:C:315:PHE:CD1	1:C:321:ARG:HG2	2.45	0.52
1:A:458:ALA:O	1:A:462:LYS:HB2	2.09	0.52
1:B:376:THR:HG22	1:B:434:TYR:OH	2.10	0.52
1:B:288:VAL:CG2	1:B:526:ILE:HD11	2.39	0.52
1:A:35:ASN:HD22	1:A:70:CYS:HB2	1.75	0.52
1:D:377:GLU:OE1	1:D:401:ARG:HD3	2.10	0.52
1:D:463:THR:O	1:D:464:VAL:C	2.52	0.52
1:D:467:TYR:O	1:D:470:PHE:HB2	2.09	0.52
1:B:428:LEU:O	1:B:429:LYS:C	2.53	0.52
1:D:446:ILE:HD13	1:D:464:VAL:HG11	1.92	0.52
1:C:225:MET:HE3	1:C:260:LEU:HD23	1.92	0.52
1:D:233:GLY:HA3	1:D:245:ARG:NH2	2.24	0.52
1:D:376:THR:OG1	1:D:377:GLU:N	2.41	0.51
1:A:550:ILE:O	1:A:554:VAL:HG23	2.09	0.51
1:D:225:MET:HE3	1:D:263:ASN:HB2	1.91	0.51
1:D:68:ILE:HD12	1:D:68:ILE:C	2.34	0.51
1:D:192:ILE:HD13	1:D:209:LYS:HG2	1.92	0.51
1:C:146:ASP:CG	1:C:267:ARG:HH11	2.18	0.51
1:C:450:ALA:HA	1:C:455:VAL:CG2	2.40	0.51
3:B:700:FAD:C1'	3:B:700:FAD:O2'	2.52	0.51
1:A:142:VAL:O	1:A:143:SER:C	2.54	0.51
1:B:28:ASN:C	1:B:28:ASN:ND2	2.69	0.51
1:B:44:ASP:OD2	1:B:44:ASP:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:LYS:HB2	1:B:190:ILE:HD12	1.91	0.51
1:C:387:VAL:HG12	1:C:388:ASN:O	2.10	0.51
1:C:394:PHE:O	1:C:395:MET:HB3	2.09	0.51
1:D:441:LYS:O	1:D:494:TYR:HA	2.11	0.51
1:D:498:ILE:HD12	1:D:498:ILE:O	2.10	0.51
1:A:526:ILE:HG12	1:A:529:LEU:HB2	1.93	0.51
1:B:175:GLU:HG2	1:B:186:ASP:O	2.10	0.51
1:B:362:GLN:NE2	1:B:544:ARG:NH2	2.58	0.51
1:B:446:ILE:HD11	1:B:464:VAL:HG11	1.92	0.51
1:C:37:GLN:O	1:C:40:SER:HB2	2.11	0.51
1:D:62:SER:HB3	2:D:601:HEC:HBB3	1.93	0.51
1:D:80:SER:O	1:D:97:GLY:HA2	2.11	0.51
1:B:362:GLN:HE22	1:B:544:ARG:NH2	2.09	0.51
1:C:450:ALA:HA	1:C:455:VAL:HG22	1.93	0.51
1:C:455:VAL:HB	1:C:456:PRO:HD2	1.91	0.51
1:D:368:SER:HB2	1:D:375:ILE:HD13	1.92	0.51
1:D:428:LEU:HB3	1:D:431:ILE:HG13	1.91	0.51
1:A:366:THR:HA	1:A:498:ILE:HB	1.92	0.51
1:A:322:VAL:HG13	1:A:361:ILE:HG21	1.93	0.50
1:C:270:ASP:OD1	1:C:272:ARG:NH2	2.43	0.50
1:D:453:ILE:CG2	1:D:455:VAL:HG13	2.41	0.50
1:A:35:ASN:ND2	1:A:71:THR:H	1.99	0.50
1:A:166:LEU:HD11	2:A:601:HEC:HBC2	1.93	0.50
1:B:48:LEU:HD11	2:B:602:HEC:HMB2	1.93	0.50
1:B:394:PHE:O	1:B:395:MET:HB3	2.11	0.50
1:B:540:HIS:CG	1:B:544:ARG:HG3	2.47	0.50
1:D:155:GLU:HB3	1:D:273:LEU:CD2	2.42	0.50
1:D:280:ILE:HG23	1:D:288:VAL:HG13	1.93	0.50
1:D:4:VAL:O	1:D:5:LEU:C	2.52	0.50
1:A:80:SER:O	1:A:97:GLY:HA2	2.11	0.50
1:B:441:LYS:HB2	1:B:495:ALA:HB3	1.93	0.50
1:C:556:TYR:O	1:C:557:GLY:C	2.54	0.50
1:D:251:GLY:O	1:D:252:VAL:C	2.54	0.50
1:A:181:LYS:HE3	1:A:181:LYS:H	1.77	0.50
1:A:236:GLY:N	1:A:377:GLU:OE2	2.27	0.50
1:B:153:LEU:HD22	1:B:271:ILE:HG23	1.93	0.50
1:A:388:ASN:ND2	1:A:392:ASN:H	2.09	0.50
1:B:388:ASN:OD1	1:B:411:GLN:NE2	2.44	0.50
1:C:277:VAL:HG13	1:C:291:VAL:CG2	2.42	0.50
1:D:453:ILE:HD11	1:D:495:ALA:HB3	1.94	0.50
1:B:68:ILE:HD12	1:B:68:ILE:C	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:THR:HG22	1:B:367:TYR:CD2	2.46	0.50
1:C:526:ILE:HG12	1:C:529:LEU:HB2	1.92	0.50
1:D:383:GLY:HA3	1:D:424:ILE:HD12	1.94	0.50
1:C:153:LEU:HD23	1:C:153:LEU:C	2.36	0.50
1:C:376:THR:CG2	1:C:378:ALA:HB3	2.41	0.50
1:D:385:ILE:HD13	1:D:488:LEU:HD13	1.94	0.50
1:A:446:ILE:HD11	1:A:493:PHE:CZ	2.47	0.49
1:B:394:PHE:HD1	1:B:407:ALA:HB1	1.76	0.49
1:C:399:THR:CG2	1:C:404:ALA:HB2	2.43	0.49
1:D:31:LEU:HD21	2:D:603:HEC:CAD	2.39	0.49
1:D:380:ARG:HH11	1:D:380:ARG:HB2	1.77	0.49
1:A:187:LYS:HB2	1:A:190:ILE:HG13	1.94	0.49
1:B:194:ASP:OD2	1:B:242:ARG:NH2	2.45	0.49
2:C:604:HEC:HBC2	2:C:604:HEC:HHD	1.94	0.49
1:A:246:PRO:HG3	1:A:255:HIS:CD2	2.47	0.49
1:D:468:ASN:OD1	1:D:487:GLU:OE1	2.30	0.49
1:A:234:ARG:HG3	1:A:235:MET:N	2.27	0.49
1:B:228:ASP:O	1:B:246:PRO:HA	2.12	0.49
1:C:203:ASN:O	1:C:205:PRO:HD3	2.12	0.49
1:C:386:VAL:HG22	1:C:418:LEU:HD23	1.95	0.49
1:A:171:MET:HB2	1:A:550:ILE:HB	1.93	0.49
1:A:177:LYS:HE3	1:A:220:ASP:OD2	2.11	0.49
1:B:196:MET:HE1	1:B:203:ASN:HB2	1.94	0.49
1:D:207:LEU:O	1:D:211:LEU:HB2	2.13	0.49
1:A:39:VAL:HG13	1:A:44:ASP:HB3	1.95	0.49
1:A:566:LYS:O	1:A:567:PHE:C	2.55	0.49
1:B:263:ASN:O	1:B:267:ARG:HG2	2.13	0.49
1:B:368:SER:OG	1:B:371:GLY:N	2.38	0.49
1:A:368:SER:HB2	1:A:375:ILE:HD13	1.93	0.49
1:B:5:LEU:HD22	1:B:9:HIS:CE1	2.48	0.49
2:B:603:HEC:HBA2	2:B:603:HEC:HHA	1.95	0.49
3:C:800:FAD:O2'	3:C:800:FAD:C9A	2.61	0.49
1:D:349:LEU:HD21	1:D:355:THR:CG2	2.43	0.49
1:D:549:ALA:HB3	3:D:900:FAD:N1	2.27	0.49
1:A:154:LEU:HD23	1:A:272:ARG:HB2	1.95	0.48
1:A:506:MET:HE3	1:A:542:ALA:C	2.38	0.48
1:C:346:ASP:O	1:C:350:GLN:HG2	2.12	0.48
1:A:127:ASP:O	1:A:305:ALA:HB1	2.13	0.48
1:B:5:LEU:HD23	1:B:96:PHE:CE1	2.49	0.48
1:B:389:ARG:HH21	1:B:413:GLY:HA3	1.79	0.48
1:B:453:ILE:HD11	1:B:495:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:VAL:CG2	1:A:303:ILE:HD12	2.43	0.48
1:C:240:VAL:CG1	1:C:241:ASN:N	2.76	0.48
1:C:367:TYR:HB3	1:C:499:ALA:O	2.14	0.48
1:D:73:CYS:SG	2:D:602:HEC:CBC	2.89	0.48
1:D:128:VAL:HG22	1:D:307:ALA:HB3	1.94	0.48
1:D:459:GLU:OE1	1:D:459:GLU:HA	2.13	0.48
1:A:52:ALA:HB1	1:A:53:PRO:HD2	1.94	0.48
1:A:175:GLU:OE2	1:A:188:LYS:HG3	2.13	0.48
1:A:360:TYR:CD2	1:A:542:ALA:HB1	2.49	0.48
1:B:505:THR:HB	5:B:732:HOH:O	2.13	0.48
1:C:291:VAL:HG12	1:C:303:ILE:HB	1.95	0.48
1:C:394:PHE:CE1	1:C:395:MET:HE3	2.48	0.48
1:A:109:ALA:O	1:A:110:ASP:CB	2.61	0.48
1:A:326:ASP:OD2	1:A:328:LYS:HG3	2.14	0.48
1:B:320:GLU:O	1:B:324:LYS:HG3	2.13	0.48
1:B:533:GLY:CA	1:B:553:ILE:HG22	2.38	0.48
1:C:512:ASP:OD1	1:C:512:ASP:C	2.56	0.48
1:D:205:PRO:O	1:D:209:LYS:HG3	2.13	0.48
1:D:249:GLY:O	1:D:250:ALA:CB	2.62	0.48
1:D:267:ARG:HG3	1:D:267:ARG:HH21	1.78	0.48
1:B:337:HIS:CE1	1:B:339:GLY:H	2.32	0.48
1:C:459:GLU:HA	1:C:459:GLU:OE1	2.14	0.48
1:D:102:ARG:NH2	1:D:157:GLU:OE1	2.47	0.48
1:D:196:MET:CE	1:D:203:ASN:HB2	2.44	0.48
1:B:468:ASN:O	1:B:471:VAL:HB	2.14	0.48
1:C:533:GLY:HA2	1:C:553:ILE:HG22	1.96	0.48
1:D:114:GLN:O	1:D:118:ILE:HG13	2.13	0.48
1:A:72:SER:HB2	1:A:158:PRO:HB2	1.95	0.48
1:A:394:PHE:HE1	1:A:395:MET:HE3	1.79	0.48
2:A:601:HEC:HBA1	2:A:601:HEC:CHA	2.44	0.48
1:C:421:ASP:HB3	1:C:424:ILE:CD1	2.44	0.48
1:D:82:ALA:O	1:D:83:TYR:C	2.54	0.48
1:A:310:ILE:CD1	1:A:529:LEU:HD21	2.43	0.47
1:B:115:ASP:HA	1:B:118:ILE:HD12	1.96	0.47
1:C:376:THR:HG21	1:C:428:LEU:HD21	1.95	0.47
1:D:418:LEU:O	1:D:495:ALA:HA	2.14	0.47
1:D:421:ASP:HB2	1:D:490:VAL:O	2.13	0.47
1:A:283:ASP:CG	1:A:284:ALA:N	2.72	0.47
3:B:700:FAD:H9	3:B:700:FAD:H1'1	1.60	0.47
1:B:429:LYS:O	1:B:432:GLU:HB2	2.14	0.47
1:C:375:ILE:HG21	1:C:418:LEU:HD11	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:GLY:O	1:C:414:GLU:C	2.56	0.47
1:C:446:ILE:CD1	1:C:464:VAL:HG11	2.43	0.47
1:B:433:GLY:CA	2:B:601:HEC:HBA2	2.44	0.47
1:C:10:GLY:HA2	1:C:14:GLY:HA2	1.95	0.47
1:C:225:MET:HG2	1:C:263:ASN:CG	2.39	0.47
1:A:56:LYS:HB3	1:A:57:VAL:HG23	1.96	0.47
1:A:167:ALA:HA	3:A:600:FAD:C6	2.43	0.47
1:C:249:GLY:O	1:C:250:ALA:HB3	2.15	0.47
1:C:87:CYS:SG	2:C:601:HEC:CBC	2.90	0.47
1:D:156:LYS:HD3	3:D:900:FAD:C4A	2.44	0.47
1:D:249:GLY:O	1:D:250:ALA:HB3	2.15	0.47
1:D:293:VAL:O	1:D:300:TYR:HA	2.15	0.47
1:D:506:MET:HG3	1:D:540:HIS:HB2	1.96	0.47
1:D:510:VAL:HG12	1:D:518:LYS:HG3	1.96	0.47
1:A:174:ALA:O	1:A:175:GLU:HB2	2.15	0.47
1:C:68:ILE:HA	5:C:824:HOH:O	2.15	0.47
1:C:154:LEU:HD22	1:C:293:VAL:HG11	1.96	0.47
1:C:180:ALA:O	1:C:181:LYS:C	2.58	0.47
1:C:192:ILE:HD13	1:C:209:LYS:HG2	1.96	0.47
1:D:28:ASN:ND2	1:D:31:LEU:H	2.11	0.47
1:D:319:ASN:HD21	1:D:331:GLY:H	1.61	0.47
1:A:133:SER:HB3	1:A:155:GLU:HB2	1.96	0.47
1:C:59:PRO:HG3	2:C:602:HEC:CMD	2.45	0.47
1:C:358:LEU:HA	1:C:507:GLY:HA3	1.96	0.47
1:C:549:ALA:CB	3:C:800:FAD:H1'2	2.45	0.47
1:D:145:ARG:HG2	1:D:151:VAL:HG21	1.95	0.47
1:D:173:ALA:HA	1:D:215:SER:HB2	1.96	0.47
1:A:5:LEU:HD23	1:A:96:PHE:CE1	2.50	0.47
1:B:279:ARG:HB3	1:B:292:LEU:HB3	1.97	0.47
1:B:431:ILE:HG22	1:B:431:ILE:O	2.15	0.47
1:C:245:ARG:HA	1:C:252:VAL:HG13	1.97	0.47
1:C:421:ASP:OD1	1:C:490:VAL:O	2.33	0.47
1:D:210:VAL:O	1:D:211:LEU:C	2.57	0.47
1:B:20:VAL:HG22	1:B:33:HIS:CD2	2.50	0.47
1:B:534:GLU:OE2	3:B:700:FAD:O3'	2.30	0.47
1:C:395:MET:HG2	1:C:396:ASN:N	2.28	0.47
1:C:498:ILE:HD12	1:C:498:ILE:O	2.15	0.47
1:D:364:HIS:O	1:D:500:PRO:HA	2.15	0.47
1:A:170:GLY:HA2	1:A:252:VAL:CG2	2.45	0.46
1:B:35:ASN:ND2	1:B:70:CYS:H	2.14	0.46
1:B:356:ARG:NH1	1:B:357:ASP:OD2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ILE:HG22	1:B:361:ILE:O	2.15	0.46
1:A:198:GLY:O	1:A:543:ASN:HB3	2.15	0.46
1:A:356:ARG:NE	1:A:357:ASP:OD2	2.43	0.46
1:B:231:ASP:HB3	1:B:245:ARG:HG3	1.97	0.46
1:B:240:VAL:HG13	1:B:241:ASN:N	2.29	0.46
1:C:422:ASP:OD1	1:C:492:PRO:HD2	2.15	0.46
1:D:26:VAL:HG21	1:D:297:TYR:HB3	1.97	0.46
1:C:421:ASP:OD1	1:C:422:ASP:N	2.47	0.46
1:D:424:ILE:HD11	1:D:486:ARG:HB2	1.97	0.46
1:A:235:MET:SD	1:A:377:GLU:HB3	2.56	0.46
1:A:504:HIS:CG	1:A:544:ARG:HE	2.33	0.46
1:B:32:THR:O	1:B:33:HIS:C	2.58	0.46
1:B:158:PRO:O	1:B:273:LEU:HD13	2.16	0.46
1:B:402:ASP:OD1	1:B:403:LYS:N	2.44	0.46
1:C:26:VAL:HG21	1:C:297:TYR:HB3	1.96	0.46
1:D:28:ASN:C	1:D:28:ASN:ND2	2.74	0.46
1:D:52:ALA:O	1:D:52:ALA:HB3	2.16	0.46
1:D:367:TYR:O	1:D:369:PRO:HD3	2.15	0.46
1:D:498:ILE:HD12	1:D:498:ILE:C	2.40	0.46
3:D:900:FAD:H1'1	5:D:922:HOH:O	2.14	0.46
1:A:517:VAL:CG2	1:A:529:LEU:HD22	2.45	0.46
1:A:177:LYS:HG3	5:A:650:HOH:O	2.15	0.46
1:C:74:HIS:HB3	2:C:604:HEC:HMB2	1.97	0.46
1:C:393:ARG:NH1	1:C:467:TYR:HD2	2.14	0.46
1:A:246:PRO:O	1:A:247:THR:C	2.56	0.46
3:A:600:FAD:C1'	3:A:600:FAD:O3'	2.64	0.46
1:B:222:LEU:HD13	1:B:256:VAL:HG22	1.97	0.46
1:B:424:ILE:O	1:B:425:ARG:C	2.58	0.46
1:B:481:ARG:HA	1:B:482:PRO:HD3	1.79	0.46
1:C:164:THR:O	1:C:253:GLY:HA3	2.15	0.46
1:C:409:LEU:HD21	1:C:500:PRO:CG	2.46	0.46
1:C:420:PHE:HE2	1:C:431:ILE:HG21	1.80	0.46
1:C:505:THR:O	1:C:506:MET:C	2.57	0.46
1:A:118:ILE:HD13	1:A:281:LEU:CD2	2.46	0.46
1:A:375:ILE:HG12	1:A:496:LEU:HD22	1.98	0.46
1:B:8:PHE:HE2	2:B:604:HEC:HHA	1.81	0.46
1:D:376:THR:HG22	1:D:434:TYR:OH	2.15	0.46
1:A:282:GLU:O	1:A:283:ASP:HB3	2.15	0.46
1:C:177:LYS:O	1:C:181:LYS:HG2	2.15	0.46
1:C:184:ILE:HD13	1:C:241:ASN:CB	2.46	0.46
1:C:422:ASP:HB2	1:C:492:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:477:ALA:O	1:D:478:GLN:C	2.59	0.46
1:A:266:LYS:O	1:A:266:LYS:HG2	2.15	0.46
1:A:368:SER:HB2	1:A:375:ILE:CD1	2.46	0.46
1:C:163:ASN:ND2	1:C:336:ASN:ND2	2.62	0.46
1:C:506:MET:HE3	1:C:542:ALA:O	2.16	0.46
1:D:5:LEU:HD23	1:D:96:PHE:CD1	2.50	0.46
1:D:291:VAL:HG12	1:D:303:ILE:HB	1.97	0.46
1:A:48:LEU:HD13	1:A:60:HIS:CE1	2.51	0.45
1:A:170:GLY:CA	1:A:252:VAL:HG21	2.45	0.45
1:A:222:LEU:O	1:A:223:THR:C	2.59	0.45
1:A:346:ASP:O	1:A:347:VAL:C	2.59	0.45
1:A:422:ASP:O	1:A:426:LYS:HG3	2.15	0.45
1:C:393:ARG:O	1:C:394:PHE:HB3	2.16	0.45
1:C:471:VAL:HG11	1:C:487:GLU:HG3	1.96	0.45
1:D:394:PHE:HE1	1:D:395:MET:HE3	1.79	0.45
1:A:186:ASP:CB	1:A:240:VAL:HG11	2.43	0.45
1:B:145:ARG:HH11	1:B:268:GLY:H	1.64	0.45
1:B:366:THR:HG21	1:B:380:ARG:HE	1.81	0.45
1:C:68:ILE:HD11	2:C:602:HEC:HMC2	1.97	0.45
1:C:407:ALA:O	1:C:411:GLN:HG2	2.16	0.45
1:B:512:ASP:OD2	1:B:516:GLU:OE2	2.34	0.45
1:C:330:LYS:HB2	1:C:330:LYS:NZ	2.31	0.45
1:D:195:THR:HG22	1:D:203:ASN:ND2	2.31	0.45
1:D:240:VAL:O	1:D:242:ARG:HG2	2.16	0.45
1:D:471:VAL:HG11	1:D:487:GLU:HG2	1.97	0.45
1:C:109:ALA:O	1:C:110:ASP:CB	2.63	0.45
1:C:402:ASP:OD1	1:C:402:ASP:N	2.44	0.45
1:C:429:LYS:O	1:C:431:ILE:N	2.50	0.45
1:B:135:GLY:HA3	1:B:553:ILE:HD12	1.99	0.45
1:C:512:ASP:OD1	1:C:514:LYS:N	2.39	0.45
1:D:378:ALA:O	1:D:382:ASN:HB2	2.17	0.45
1:D:514:LYS:O	1:D:515:ALA:CB	2.64	0.45
1:A:94:MET:HE2	2:A:602:HEC:HMD2	1.97	0.45
1:A:145:ARG:HG2	1:A:151:VAL:CG2	2.46	0.45
1:A:544:ARG:HD2	1:A:549:ALA:HB2	1.97	0.45
1:B:326:ASP:OD2	1:B:328:LYS:HG3	2.16	0.45
1:C:28:ASN:HD21	1:C:32:THR:H	1.65	0.45
1:D:118:ILE:HD12	1:D:279:ARG:NH1	2.31	0.45
1:B:267:ARG:HG2	1:B:267:ARG:H	1.63	0.45
1:B:510:VAL:HA	5:B:734:HOH:O	2.16	0.45
1:D:232:VAL:HA	1:D:243:SER:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:601:HEC:CBD	2:D:601:HEC:HHA	2.47	0.45
1:B:26:VAL:HG21	1:B:297:TYR:HB2	1.98	0.45
1:B:276:ARG:NH2	1:B:343:ASP:OD1	2.38	0.45
1:B:396:ASN:OD1	1:B:481:ARG:HA	2.16	0.45
1:C:26:VAL:HG21	1:C:297:TYR:CB	2.46	0.45
1:D:326:ASP:OD2	1:D:326:ASP:C	2.58	0.45
1:A:90:PHE:O	1:A:91:GLY:C	2.59	0.45
1:A:480:GLU:CD	1:A:480:GLU:H	2.25	0.45
1:B:410:GLN:HE21	1:B:410:GLN:HB2	1.38	0.45
1:D:268:GLY:O	1:D:269:THR:C	2.59	0.45
1:B:395:MET:HE2	1:B:404:ALA:HB1	1.98	0.44
1:C:418:LEU:O	1:C:495:ALA:HA	2.17	0.44
1:A:146:ASP:O	1:A:147:ALA:HB2	2.17	0.44
1:A:366:THR:HG21	1:A:380:ARG:HE	1.82	0.44
1:A:379:VAL:HG12	1:A:384:ALA:HB2	1.98	0.44
1:A:413:GLY:O	1:A:414:GLU:C	2.60	0.44
1:A:453:ILE:O	1:A:454:ASP:CB	2.66	0.44
1:C:424:ILE:HD13	1:C:424:ILE:N	2.32	0.44
1:C:459:GLU:O	1:C:460:LEU:C	2.60	0.44
1:D:87:CYS:O	1:D:372:GLY:HA3	2.16	0.44
1:D:371:GLY:CA	1:D:439:ILE:HG21	2.46	0.44
1:A:417:TYR:CZ	1:A:453:ILE:HG23	2.52	0.44
1:B:263:ASN:O	1:B:264:ALA:C	2.59	0.44
1:B:282:GLU:HA	1:B:287:LYS:O	2.17	0.44
1:D:192:ILE:O	1:D:193:ASP:C	2.61	0.44
1:D:288:VAL:CG2	1:D:526:ILE:HD11	2.45	0.44
1:D:336:ASN:HD22	1:D:340:ALA:CB	2.30	0.44
1:D:375:ILE:HG21	1:D:418:LEU:HD11	1.99	0.44
1:C:199:GLY:O	1:C:202:ILE:HG23	2.18	0.44
1:C:200:ARG:O	1:C:202:ILE:HG22	2.18	0.44
1:D:326:ASP:OD1	1:D:328:LYS:HD2	2.17	0.44
1:B:85:ASP:O	1:B:86:ALA:C	2.56	0.44
1:B:449:LEU:HD22	1:B:495:ALA:CB	2.46	0.44
1:A:62:SER:CB	2:A:601:HEC:HBB3	2.44	0.44
1:A:167:ALA:HA	3:A:600:FAD:C5X	2.48	0.44
1:C:7:ASP:O	1:C:8:PHE:C	2.58	0.44
1:D:52:ALA:O	1:D:52:ALA:CB	2.66	0.44
1:D:431:ILE:HA	1:D:434:TYR:HD2	1.83	0.44
1:A:12:MET:HE1	2:A:604:HEC:CAD	2.47	0.44
1:A:46:LYS:O	1:A:49:ALA:HB3	2.18	0.44
1:A:280:ILE:HA	1:A:291:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ARG:HH21	1:A:435:VAL:HG21	1.83	0.44
1:B:422:ASP:OD1	1:B:494:TYR:OH	2.36	0.44
1:C:321:ARG:NH2	1:C:342:GLY:HA3	2.32	0.44
1:C:511:ILE:HA	1:C:516:GLU:O	2.17	0.44
1:D:66:GLY:H	1:D:258:GLN:NE2	2.10	0.44
1:D:187:LYS:HB2	1:D:190:ILE:HG13	1.99	0.44
1:D:470:PHE:CD1	1:D:476:ASP:HA	2.52	0.44
1:A:177:LYS:O	1:A:181:LYS:HE3	2.18	0.44
1:B:394:PHE:CD1	1:B:407:ALA:HB1	2.52	0.44
1:C:35:ASN:ND2	1:C:69:ALA:HB1	2.33	0.44
1:C:428:LEU:HD23	1:C:431:ILE:HG13	1.99	0.44
1:D:225:MET:HE3	1:D:263:ASN:HB3	1.99	0.44
1:A:82:ALA:O	1:A:85:ASP:HB2	2.18	0.43
1:A:294:LYS:HB2	1:A:300:TYR:CD2	2.53	0.43
1:A:410:GLN:HE21	1:A:410:GLN:HB2	1.38	0.43
1:B:283:ASP:OD2	1:B:284:ALA:N	2.51	0.43
1:D:280:ILE:HD12	1:D:347:VAL:HG13	2.00	0.43
1:A:141:ALA:O	1:A:142:VAL:O	2.36	0.43
1:A:478:GLN:HB3	1:A:479:PHE:CD1	2.53	0.43
1:B:467:TYR:O	1:B:471:VAL:HG23	2.18	0.43
1:B:26:VAL:HG21	1:B:297:TYR:CB	2.49	0.43
1:B:516:GLU:HG2	5:B:741:HOH:O	2.18	0.43
1:B:87:CYS:O	1:B:372:GLY:HA3	2.19	0.43
1:B:514:LYS:O	1:B:515:ALA:HB3	2.18	0.43
1:B:557:GLY:O	1:B:558:ARG:C	2.59	0.43
1:C:28:ASN:C	1:C:28:ASN:ND2	2.76	0.43
1:C:366:THR:HG23	1:C:380:ARG:HH21	1.83	0.43
1:D:471:VAL:CG1	1:D:487:GLU:HG2	2.48	0.43
1:A:130:ILE:O	1:A:153:LEU:HA	2.18	0.43
1:B:246:PRO:HD3	1:B:252:VAL:HG13	2.00	0.43
1:B:448:GLU:HA	1:B:451:LYS:HD2	2.00	0.43
1:C:514:LYS:O	1:C:515:ALA:CB	2.66	0.43
1:A:145:ARG:HG2	1:A:151:VAL:HG21	2.00	0.43
1:A:206:GLU:OE2	1:A:209:LYS:NZ	2.48	0.43
1:D:155:GLU:HB3	1:D:273:LEU:HD22	1.99	0.43
1:D:196:MET:HE1	1:D:203:ASN:HB2	1.99	0.43
1:D:383:GLY:HA3	1:D:424:ILE:CD1	2.49	0.43
1:A:225:MET:HG2	1:A:263:ASN:OD1	2.18	0.43
1:A:470:PHE:CB	1:A:476:ASP:HA	2.49	0.43
1:B:33:HIS:O	1:B:34:GLU:C	2.60	0.43
1:C:163:ASN:HD21	1:C:336:ASN:CG	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:GLU:CD	1:C:188:LYS:HG3	2.44	0.43
1:C:397:GLU:HB2	1:C:481:ARG:NH1	2.34	0.43
1:D:44:ASP:H	1:D:47:GLU:HB2	1.83	0.43
1:D:179:GLN:HE22	1:D:242:ARG:HB3	1.84	0.43
1:D:400:THR:O	1:D:403:LYS:N	2.47	0.43
1:A:132:GLY:CA	3:A:600:FAD:H4B	2.49	0.43
1:B:171:MET:O	1:B:244:HIS:HB2	2.19	0.43
1:B:195:THR:HG21	1:B:208:VAL:HG13	2.01	0.43
1:B:317:LYS:HG3	1:B:317:LYS:O	2.19	0.43
1:B:349:LEU:HD21	1:B:355:THR:HG23	2.01	0.43
1:B:433:GLY:HA2	2:B:601:HEC:HBA2	2.01	0.43
1:C:127:ASP:HB2	1:C:150:LYS:O	2.19	0.43
1:D:53:PRO:O	1:D:54:LYS:C	2.61	0.43
1:D:198:GLY:O	1:D:543:ASN:HB3	2.18	0.43
1:D:422:ASP:HB3	1:D:490:VAL:HG12	2.00	0.43
1:B:234:ARG:HB2	1:B:234:ARG:HE	1.74	0.43
1:B:435:VAL:CG2	1:B:440:VAL:HG21	2.49	0.43
1:D:172:ASN:OD1	1:D:548:ASN:ND2	2.52	0.43
1:A:225:MET:HE2	1:A:263:ASN:HB2	2.00	0.42
1:B:240:VAL:HG22	1:B:241:ASN:H	1.84	0.42
1:B:278:VAL:HG23	1:B:292:LEU:HD12	2.01	0.42
1:C:170:GLY:HA2	1:C:252:VAL:HG21	2.01	0.42
1:D:65:ILE:HB	1:D:258:GLN:NE2	2.33	0.42
1:D:177:LYS:HB2	1:D:178:PRO:HD3	2.00	0.42
1:D:375:ILE:HG21	1:D:418:LEU:CD1	2.49	0.42
1:A:428:LEU:HB3	1:A:431:ILE:HD12	2.02	0.42
1:B:164:THR:O	1:B:253:GLY:HA3	2.19	0.42
1:D:204:ASP:O	1:D:208:VAL:HG23	2.19	0.42
1:D:266:LYS:C	1:D:267:ARG:O	2.61	0.42
1:D:488:LEU:HD23	1:D:488:LEU:O	2.19	0.42
1:B:127:ASP:HB2	1:B:150:LYS:H	1.84	0.42
1:B:456:PRO:HB2	1:B:459:GLU:HB2	2.00	0.42
1:D:42:HIS:CE1	2:D:604:HEC:ND	2.87	0.42
1:D:455:VAL:HB	1:D:456:PRO:CD	2.46	0.42
1:A:153:LEU:HD23	1:A:153:LEU:C	2.44	0.42
1:A:326:ASP:OD2	1:A:328:LYS:HB2	2.18	0.42
1:A:334:ALA:HA	1:A:502:VAL:O	2.19	0.42
1:A:453:ILE:CG2	1:A:455:VAL:HG13	2.49	0.42
1:C:145:ARG:NH1	1:C:267:ARG:O	2.52	0.42
1:C:184:ILE:HD13	1:C:241:ASN:HB3	2.02	0.42
1:C:367:TYR:O	1:C:369:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:PHE:O	1:C:395:MET:CB	2.67	0.42
1:D:376:THR:O	1:D:379:VAL:HG23	2.20	0.42
1:A:74:HIS:CE1	2:A:602:HEC:ND	2.87	0.42
1:B:394:PHE:CE1	1:B:395:MET:SD	3.13	0.42
1:D:119:ALA:O	1:D:121:GLY:N	2.38	0.42
1:D:192:ILE:HG23	1:D:208:VAL:CG1	2.49	0.42
1:A:65:ILE:H	1:A:65:ILE:HG13	1.71	0.42
1:A:272:ARG:O	1:A:275:SER:HB2	2.20	0.42
1:B:204:ASP:OD1	1:B:206:GLU:N	2.53	0.42
1:C:234:ARG:HE	1:C:234:ARG:HB2	1.43	0.42
1:D:68:ILE:HG13	1:D:68:ILE:O	2.20	0.42
1:D:450:ALA:HA	1:D:455:VAL:HG22	2.02	0.42
1:A:506:MET:HE3	1:A:542:ALA:O	2.20	0.42
1:B:171:MET:HG3	1:B:550:ILE:HG22	2.01	0.42
1:B:401:ARG:NH2	4:B:714:SO4:O1	2.38	0.42
1:B:409:LEU:HD23	1:B:409:LEU:HA	1.89	0.42
1:C:471:VAL:HG21	1:C:487:GLU:HA	2.01	0.42
1:D:136:ALA:HB2	1:D:553:ILE:HB	2.01	0.42
1:D:188:LYS:O	1:D:192:ILE:HG13	2.19	0.42
1:A:26:VAL:CG2	1:A:297:TYR:HB3	2.49	0.42
1:B:196:MET:HE3	1:B:196:MET:HA	2.02	0.42
1:B:396:ASN:O	1:B:397:GLU:C	2.62	0.42
1:C:154:LEU:HD13	1:C:293:VAL:HG22	2.01	0.42
1:C:279:ARG:HB3	1:C:292:LEU:HB2	2.01	0.42
1:C:374:MET:CE	3:C:800:FAD:H6	2.48	0.42
1:D:460:LEU:HD23	1:D:460:LEU:HA	1.91	0.42
1:A:181:LYS:HE3	1:A:181:LYS:N	2.34	0.42
1:B:445:THR:O	1:B:446:ILE:C	2.63	0.42
1:C:146:ASP:OD2	1:C:267:ARG:NH1	2.51	0.42
1:C:364:HIS:O	1:C:500:PRO:HA	2.20	0.42
1:C:484:LEU:HA	1:C:485:PRO:HD2	1.89	0.42
3:C:800:FAD:H8A	3:C:800:FAD:H2B	1.90	0.42
1:D:39:VAL:HA	1:D:43:GLY:O	2.20	0.42
3:D:900:FAD:N10	3:D:900:FAD:O2'	2.52	0.42
1:A:433:GLY:HA3	2:A:601:HEC:HBA2	2.02	0.42
1:C:60:HIS:CD2	2:C:602:HEC:NC	2.87	0.42
1:C:80:SER:O	1:C:97:GLY:HA2	2.20	0.42
1:C:233:GLY:HA3	1:C:245:ARG:HH22	1.78	0.42
1:D:181:LYS:HE2	1:D:181:LYS:HA	2.02	0.42
1:D:26:VAL:HG11	1:D:31:LEU:HD11	2.02	0.41
1:D:319:ASN:HD21	1:D:331:GLY:N	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:PRO:HB2	1:D:486:ARG:H	1.58	0.41
1:D:83:TYR:O	1:D:84:CYS:C	2.62	0.41
1:A:68:ILE:O	1:A:68:ILE:HG13	2.20	0.41
1:B:199:GLY:HA3	1:B:203:ASN:OD1	2.19	0.41
1:B:210:VAL:HG13	1:B:214:ASN:ND2	2.36	0.41
1:B:316:ALA:HB3	1:B:336:ASN:ND2	2.35	0.41
1:D:37:GLN:O	1:D:40:SER:HB2	2.21	0.41
1:D:376:THR:HG23	1:D:379:VAL:HG23	2.03	0.41
1:D:430:ALA:O	1:D:433:GLY:N	2.47	0.41
1:D:458:ALA:O	1:D:462:LYS:HB2	2.20	0.41
1:A:310:ILE:HD12	1:A:529:LEU:HD21	2.02	0.41
1:A:449:LEU:HD11	1:A:495:ALA:HB2	2.00	0.41
1:B:220:ASP:O	1:B:224:SER:HB3	2.20	0.41
1:D:37:GLN:HA	1:D:40:SER:HB2	2.03	0.41
1:D:105:VAL:HA	1:D:106:PRO:HD2	1.90	0.41
1:D:114:GLN:HG2	1:D:300:TYR:CE2	2.55	0.41
1:D:329:LEU:HD13	1:D:502:VAL:HG22	2.02	0.41
1:D:446:ILE:HG21	1:D:464:VAL:HG21	2.02	0.41
1:D:499:ALA:HA	1:D:500:PRO:HD3	1.96	0.41
3:D:900:FAD:H1'1	3:D:900:FAD:H9	1.82	0.41
1:A:26:VAL:HG21	1:A:297:TYR:HB2	2.01	0.41
1:A:433:GLY:O	1:A:437:LEU:HG	2.20	0.41
1:C:63:HIS:CD2	2:C:601:HEC:NA	2.89	0.41
1:C:409:LEU:CD2	1:C:500:PRO:HG3	2.50	0.41
1:A:409:LEU:HD23	1:A:409:LEU:HA	1.92	0.41
1:A:453:ILE:HG21	1:A:455:VAL:HG13	2.01	0.41
2:A:602:HEC:HBA2	1:C:360:TYR:OH	2.21	0.41
1:C:376:THR:HG23	1:C:378:ALA:HB3	2.03	0.41
1:C:376:THR:HG21	1:C:378:ALA:HB3	2.02	0.41
1:D:62:SER:CB	2:D:601:HEC:HBB3	2.51	0.41
1:B:79:LYS:NZ	1:B:97:GLY:O	2.46	0.41
1:C:471:VAL:HB	1:C:487:GLU:HG3	2.03	0.41
1:D:110:ASP:O	1:D:114:GLN:HG3	2.21	0.41
1:D:270:ASP:OD2	1:D:270:ASP:C	2.64	0.41
1:D:371:GLY:HA2	1:D:439:ILE:HG21	2.01	0.41
1:A:204:ASP:HB3	1:A:207:LEU:HD12	2.02	0.41
1:A:286:GLY:O	1:A:526:ILE:HD12	2.20	0.41
1:A:471:VAL:HG22	1:A:484:LEU:HB3	2.03	0.41
1:B:87:CYS:SG	2:B:601:HEC:CBC	2.94	0.41
1:B:186:ASP:OD2	1:B:242:ARG:HD3	2.21	0.41
1:B:499:ALA:HA	1:B:500:PRO:HD3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:ARG:HD2	1:C:432:GLU:OE1	2.21	0.41
1:D:153:LEU:C	1:D:153:LEU:HD23	2.46	0.41
1:D:428:LEU:HD23	1:D:431:ILE:HG13	2.03	0.41
1:A:44:ASP:O	1:A:45:LEU:C	2.64	0.41
1:C:483:ASP:OD2	1:C:485:PRO:HD3	2.21	0.41
1:D:75:LYS:HB2	1:D:78:GLU:O	2.21	0.41
1:D:166:LEU:HD21	2:D:601:HEC:HBC2	2.02	0.41
1:C:342:GLY:O	1:C:343:ASP:C	2.62	0.40
1:C:540:HIS:O	1:C:541:GLY:C	2.63	0.40
1:D:94:MET:HB2	2:D:602:HEC:HMD2	2.01	0.40
1:A:554:VAL:O	1:A:555:THR:C	2.64	0.40
1:C:15:CYS:HB3	1:C:22:ASP:HA	2.03	0.40
1:C:116:LYS:O	1:C:120:ALA:HB2	2.22	0.40
1:B:280:ILE:HG13	1:B:347:VAL:CG1	2.51	0.40
1:B:400:THR:O	1:B:401:ARG:C	2.64	0.40
1:C:8:PHE:HE2	2:C:604:HEC:CHA	2.34	0.40
1:C:109:ALA:O	1:C:110:ASP:HB2	2.21	0.40
1:C:409:LEU:HD22	1:C:414:GLU:CB	2.49	0.40
1:C:455:VAL:HB	1:C:456:PRO:CD	2.51	0.40
1:C:263:ASN:O	1:C:264:ALA:C	2.64	0.40
1:C:398:ILE:CD1	1:C:482:PRO:HD2	2.51	0.40
1:D:190:ILE:O	1:D:194:ASP:HB2	2.22	0.40
1:D:380:ARG:O	1:D:481:ARG:NH2	2.55	0.40
1:A:316:ALA:HB1	1:A:502:VAL:HG12	2.03	0.40
1:B:82:ALA:O	1:B:83:TYR:C	2.64	0.40
1:C:39:VAL:O	1:C:40:SER:C	2.65	0.40
1:C:332:PHE:HE1	1:C:500:PRO:HB2	1.87	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:THR:OG1	1:C:247:THR:OG1[4_555]	2.12	0.08
1:C:125:THR:OG1	1:D:247:THR:OG1[4_456]	2.15	0.05

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	568/572 (99%)	504 (89%)	51 (9%)	13 (2%)	5 19
1	B	562/572 (98%)	495 (88%)	52 (9%)	15 (3%)	4 16
1	C	566/572 (99%)	482 (85%)	64 (11%)	20 (4%)	3 12
1	D	566/572 (99%)	488 (86%)	61 (11%)	17 (3%)	3 14
All	All	2262/2288 (99%)	1969 (87%)	228 (10%)	65 (3%)	3 15

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	VAL
1	A	142	VAL
1	A	147	ALA
1	A	454	ASP
1	B	250	ALA
1	B	357	ASP
1	B	388	ASN
1	B	454	ASP
1	C	250	ALA
1	C	284	ALA
1	C	394	PHE
1	C	401	ARG
1	C	454	ASP
1	D	120	ALA
1	D	250	ALA
1	D	357	ASP
1	D	454	ASP
1	D	485	PRO
1	A	143	SER
1	A	283	ASP
1	A	513	THR
1	B	240	VAL

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Mol	Chain	Res	Type
1	B	247	THR
1	B	251	GLY
1	B	412	LYS
1	B	478	GLN
1	C	120	ALA
1	C	414	GLU
1	C	415	SER
1	C	451	LYS
1	C	485	PRO
1	D	267	ARG
1	D	401	ARG
1	D	478	GLN
1	A	110	ASP
1	A	120	ALA
1	A	343	ASP
1	B	148	GLY
1	B	201	ASN
1	B	489	VAL
1	C	180	ALA
1	C	343	ASP
1	C	410	GLN
1	D	11	GLU
1	D	17	SER
1	D	148	GLY
1	B	215	SER
1	B	284	ALA
1	C	56	LYS
1	C	201	ASN
1	C	492	PRO
1	D	329	LEU
1	A	55	ASP
1	C	430	ALA
1	D	464	VAL
1	B	13	GLY
1	C	412	LYS
1	D	13	GLY
1	D	283	ASP
1	A	4	VAL
1	A	162	GLY
1	D	369	PRO
1	C	286	GLY
1	C	398	ILE

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Mol	Chain	Res	Type
1	D	482	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	409/429 (95%)	343 (84%)	66 (16%)	2 8
1	B	406/429 (95%)	339 (84%)	67 (16%)	2 8
1	C	405/429 (94%)	328 (81%)	77 (19%)	1 5
1	D	407/429 (95%)	339 (83%)	68 (17%)	2 7
All	All	1627/1716 (95%)	1349 (83%)	278 (17%)	2 7

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	16	ASP
1	A	17	SER
1	A	20	VAL
1	A	28	ASN
1	A	31	LEU
1	A	32	THR
1	A	55	ASP
1	A	67	GLU
1	A	68	ILE
1	A	79	LYS
1	A	80	SER
1	A	102	ARG
1	A	105	VAL
1	A	150	LYS
1	A	156	LYS
1	A	181	LYS
1	A	192	ILE
1	A	211	LEU
1	A	239	SER

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Mol	Chain	Res	Type
1	A	245	ARG
1	A	252	VAL
1	A	259	VAL
1	A	273	LEU
1	A	282	GLU
1	A	283	ASP
1	A	291	VAL
1	A	292	LEU
1	A	296	GLU
1	A	328	LYS
1	A	330	LYS
1	A	345	LEU
1	A	350	GLN
1	A	359	GLU
1	A	375	ILE
1	A	385	ILE
1	A	387	VAL
1	A	388	ASN
1	A	390	GLU
1	A	395	MET
1	A	401	ARG
1	A	402	ASP
1	A	414	GLU
1	A	423	SER
1	A	426	LYS
1	A	432	GLU
1	A	442	GLU
1	A	444	LYS
1	A	446	ILE
1	A	448	GLU
1	A	449	LEU
1	A	452	GLN
1	A	459	GLU
1	A	460	LEU
1	A	463	THR
1	A	465	THR
1	A	480	GLU
1	A	487	GLU
1	A	488	LEU
1	A	489	VAL
1	A	496	LEU
1	A	518	LYS

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Mol	Chain	Res	Type
1	A	520	GLU
1	A	526	ILE
1	A	529	LEU
1	A	534	GLU
1	B	5	LEU
1	B	16	ASP
1	B	26	VAL
1	B	28	ASN
1	B	31	LEU
1	B	54	LYS
1	B	61	LYS
1	B	68	ILE
1	B	78	GLU
1	B	79	LYS
1	B	81	VAL
1	B	89	SER
1	B	93	ASP
1	B	102	ARG
1	B	105	VAL
1	B	165	LYS
1	B	184	ILE
1	B	201	ASN
1	B	206	GLU
1	B	211	LEU
1	B	219	ILE
1	B	224	SER
1	B	232	VAL
1	B	234	ARG
1	B	240	VAL
1	B	247	THR
1	B	252	VAL
1	B	259	VAL
1	B	267	ARG
1	B	282	GLU
1	B	287	LYS
1	B	291	VAL
1	B	294	LYS
1	B	322	VAL
1	B	345	LEU
1	B	347	VAL
1	B	350	GLN
1	B	374	MET

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Mol	Chain	Res	Type
1	B	375	ILE
1	B	376	THR
1	B	377	GLU
1	B	386	VAL
1	B	387	VAL
1	B	392	ASN
1	B	395	MET
1	B	405	SER
1	B	410	GLN
1	B	415	SER
1	B	423	SER
1	B	429	LYS
1	B	432	GLU
1	B	444	LYS
1	B	445	THR
1	B	447	GLU
1	B	452	GLN
1	B	460	LEU
1	B	463	THR
1	B	478	GLN
1	B	480	GLU
1	B	488	LEU
1	B	489	VAL
1	B	496	LEU
1	B	506	MET
1	B	518	LYS
1	B	522	THR
1	B	526	ILE
1	B	529	LEU
1	C	15	CYS
1	C	16	ASP
1	C	17	SER
1	C	21	SER
1	C	26	VAL
1	C	27	THR
1	C	28	ASN
1	C	31	LEU
1	C	40	SER
1	C	61	LYS
1	C	68	ILE
1	C	75	LYS
1	C	79	LYS

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Mol	Chain	Res	Type
1	C	102	ARG
1	C	106	PRO
1	C	124	GLU
1	C	129	VAL
1	C	143	SER
1	C	145	ARG
1	C	201	ASN
1	C	202	ILE
1	C	203	ASN
1	C	205	PRO
1	C	211	LEU
1	C	223	THR
1	C	224	SER
1	C	225	MET
1	C	234	ARG
1	C	242	ARG
1	C	243	SER
1	C	245	ARG
1	C	252	VAL
1	C	259	VAL
1	C	280	ILE
1	C	288	VAL
1	C	292	LEU
1	C	294	LYS
1	C	320	GLU
1	C	321	ARG
1	C	322	VAL
1	C	324	LYS
1	C	330	LYS
1	C	347	VAL
1	C	368	SER
1	C	373	VAL
1	C	374	MET
1	C	376	THR
1	C	387	VAL
1	C	388	ASN
1	C	395	MET
1	C	398	ILE
1	C	400	THR
1	C	402	ASP
1	C	409	LEU
1	C	410	GLN

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Mol	Chain	Res	Type
1	C	424	ILE
1	C	426	LYS
1	C	435	VAL
1	C	444	LYS
1	C	448	GLU
1	C	452	GLN
1	C	459	GLU
1	C	460	LEU
1	C	462	LYS
1	C	463	THR
1	C	465	THR
1	C	480	GLU
1	C	484	LEU
1	C	487	GLU
1	C	489	VAL
1	C	496	LEU
1	C	520	GLU
1	C	526	ILE
1	C	529	LEU
1	C	551	SER
1	C	558	ARG
1	C	570	ASP
1	D	5	LEU
1	D	11	GLU
1	D	17	SER
1	D	20	VAL
1	D	28	ASN
1	D	31	LEU
1	D	32	THR
1	D	40	SER
1	D	45	LEU
1	D	68	ILE
1	D	72	SER
1	D	75	LYS
1	D	78	GLU
1	D	81	VAL
1	D	89	SER
1	D	126	THR
1	D	130	ILE
1	D	145	ARG
1	D	159	ILE
1	D	175	GLU

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Mol	Chain	Res	Type
1	D	210	VAL
1	D	211	LEU
1	D	230	THR
1	D	235	MET
1	D	243	SER
1	D	247	THR
1	D	252	VAL
1	D	259	VAL
1	D	273	LEU
1	D	282	GLU
1	D	283	ASP
1	D	291	VAL
1	D	292	LEU
1	D	303	ILE
1	D	328	LYS
1	D	330	LYS
1	D	345	LEU
1	D	347	VAL
1	D	350	GLN
1	D	368	SER
1	D	376	THR
1	D	382	ASN
1	D	385	ILE
1	D	387	VAL
1	D	388	ASN
1	D	392	ASN
1	D	395	MET
1	D	396	ASN
1	D	401	ARG
1	D	415	SER
1	D	440	VAL
1	D	444	LYS
1	D	447	GLU
1	D	449	LEU
1	D	452	GLN
1	D	459	GLU
1	D	460	LEU
1	D	462	LYS
1	D	463	THR
1	D	473	SER
1	D	480	GLU
1	D	488	LEU

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Mol	Chain	Res	Type
1	D	496	LEU
1	D	526	ILE
1	D	529	LEU
1	D	555	THR
1	D	558	ARG
1	D	570	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	33	HIS
1	A	35	ASN
1	A	114	GLN
1	A	172	ASN
1	A	258	GLN
1	A	319	ASN
1	A	336	ASN
1	A	362	GLN
1	A	382	ASN
1	A	388	ASN
1	A	396	ASN
1	A	410	GLN
1	A	411	GLN
1	A	452	GLN
1	A	468	ASN
1	A	478	GLN
1	A	548	ASN
1	B	28	ASN
1	B	35	ASN
1	B	114	GLN
1	B	172	ASN
1	B	258	GLN
1	B	319	ASN
1	B	336	ASN
1	B	362	GLN
1	B	388	ASN
1	B	392	ASN
1	B	410	GLN
1	B	411	GLN
1	B	452	GLN
1	B	478	GLN

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Mol	Chain	Res	Type
1	B	548	ASN
1	C	28	ASN
1	C	35	ASN
1	C	37	GLN
1	C	114	GLN
1	C	172	ASN
1	C	213	ASN
1	C	214	ASN
1	C	319	ASN
1	C	336	ASN
1	C	350	GLN
1	C	362	GLN
1	C	364	HIS
1	C	388	ASN
1	C	411	GLN
1	C	452	GLN
1	C	548	ASN
1	D	28	ASN
1	D	35	ASN
1	D	37	GLN
1	D	114	GLN
1	D	172	ASN
1	D	258	GLN
1	D	319	ASN
1	D	336	ASN
1	D	350	GLN
1	D	382	ASN
1	D	411	GLN
1	D	452	GLN
1	D	468	ASN
1	D	478	GLN
1	D	548	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

23 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	B	714	-	4,4,4	0.58	0	6,6,6	0.45	0
3	FAD	A	600	-	58,58,58	2.90	11 (18%)	85,89,89	2.82	31 (36%)
2	HEC	C	604	1	50,50,50	1.44	6 (12%)	68,82,82	2.12	18 (26%)
2	HEC	C	602	1	50,50,50	1.39	9 (18%)	68,82,82	1.45	9 (13%)
4	SO4	C	814	-	4,4,4	0.65	0	6,6,6	0.65	0
2	HEC	B	603	1	50,50,50	1.41	5 (10%)	68,82,82	1.35	8 (11%)
2	HEC	D	602	1	50,50,50	1.39	9 (18%)	68,82,82	1.46	6 (8%)
3	FAD	C	800	-	58,58,58	2.92	10 (17%)	85,89,89	3.42	27 (31%)
2	HEC	D	601	1	50,50,50	1.50	6 (12%)	68,82,82	1.75	11 (16%)
2	HEC	D	604	1	50,50,50	1.30	5 (10%)	68,82,82	1.75	13 (19%)
2	HEC	A	603	1	50,50,50	1.39	7 (14%)	68,82,82	1.17	6 (8%)
2	HEC	A	602	1	50,50,50	1.45	10 (20%)	68,82,82	1.48	10 (14%)
2	HEC	A	601	1	50,50,50	1.44	7 (14%)	68,82,82	2.08	21 (30%)
2	HEC	A	604	1	50,50,50	1.38	8 (16%)	68,82,82	1.52	12 (17%)
2	HEC	B	602	1	50,50,50	1.39	3 (6%)	68,82,82	1.16	4 (5%)
2	HEC	C	603	1	50,50,50	1.36	5 (10%)	68,82,82	1.25	8 (11%)
2	HEC	C	601	1	50,50,50	1.28	6 (12%)	68,82,82	1.57	9 (13%)
2	HEC	D	603	1	50,50,50	1.40	6 (12%)	68,82,82	1.10	4 (5%)
2	HEC	B	601	1	50,50,50	1.39	7 (14%)	68,82,82	1.56	10 (14%)
2	HEC	B	604	1	50,50,50	1.29	5 (10%)	68,82,82	1.69	18 (26%)
3	FAD	D	900	-	58,58,58	2.87	10 (17%)	85,89,89	2.93	22 (25%)
3	FAD	B	700	-	58,58,58	2.89	9 (15%)	85,89,89	2.77	34 (40%)
4	SO4	D	914	-	4,4,4	0.57	0	6,6,6	0.68	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	A	600	-	2/2/9/9	14/34/50/50	0/6/6/6
2	HEC	C	604	1	1/1/3/7	8/14/54/54	-
2	HEC	C	602	1	1/1/3/7	8/14/54/54	-
2	HEC	B	603	1	1/1/3/7	2/14/54/54	-
2	HEC	D	602	1	1/1/3/7	7/14/54/54	-
3	FAD	C	800	-	3/3/9/9	15/34/50/50	0/5/6/6
2	HEC	D	601	1	1/1/3/7	9/14/54/54	-
2	HEC	D	604	1	1/1/3/7	4/14/54/54	-
2	HEC	A	603	1	1/1/3/7	5/14/54/54	-
2	HEC	A	602	1	1/1/3/7	8/14/54/54	-
2	HEC	A	601	1	1/1/3/7	9/14/54/54	-
2	HEC	A	604	1	1/1/3/7	4/14/54/54	-
2	HEC	B	602	1	1/1/3/7	7/14/54/54	-
2	HEC	C	603	1	1/1/3/7	7/14/54/54	-
2	HEC	C	601	1	1/1/3/7	7/14/54/54	-
2	HEC	D	603	1	-	3/14/54/54	-
2	HEC	B	601	1	1/1/3/7	8/14/54/54	-
2	HEC	B	604	1	1/1/3/7	4/14/54/54	-
3	FAD	D	900	-	2/2/9/9	16/34/50/50	0/6/6/6
3	FAD	B	700	-	2/2/9/9	13/34/50/50	0/6/6/6

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	800	FAD	C1'-C2'	18.79	1.78	1.52
3	D	900	FAD	C1'-C2'	18.35	1.78	1.52
3	A	600	FAD	C1'-C2'	18.22	1.78	1.52
3	B	700	FAD	C1'-C2'	17.72	1.77	1.52
3	A	600	FAD	C5B-C4B	6.83	1.72	1.51
3	D	900	FAD	C5B-C4B	6.73	1.71	1.51
3	B	700	FAD	C5B-C4B	6.61	1.71	1.51
3	C	800	FAD	P-O3P	-5.42	1.53	1.59
3	C	800	FAD	C5B-C4B	5.41	1.67	1.51
3	B	700	FAD	P-O3P	-5.39	1.53	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	900	FAD	P-O3P	-4.26	1.54	1.59
2	C	604	HEC	CBC-CAC	-4.20	1.33	1.51
2	D	601	HEC	CBB-CAB	-4.20	1.33	1.51
2	B	604	HEC	CBC-CAC	-4.10	1.34	1.51
2	B	603	HEC	CBC-CAC	-4.09	1.34	1.51
2	B	602	HEC	CBC-CAC	-4.00	1.34	1.51
2	D	604	HEC	CBC-CAC	-4.00	1.34	1.51
2	D	603	HEC	CBC-CAC	-3.90	1.34	1.51
2	C	603	HEC	CBC-CAC	-3.87	1.35	1.51
2	B	603	HEC	CBB-CAB	-3.87	1.35	1.51
2	C	601	HEC	CBC-CAC	-3.84	1.35	1.51
2	D	603	HEC	CBB-CAB	-3.79	1.35	1.51
2	A	601	HEC	CBC-CAC	-3.78	1.35	1.51
2	C	601	HEC	CBB-CAB	-3.78	1.35	1.51
2	D	601	HEC	CBC-CAC	-3.67	1.35	1.51
2	B	602	HEC	CBB-CAB	-3.66	1.36	1.51
2	B	601	HEC	CBB-CAB	-3.64	1.36	1.51
3	A	600	FAD	P-O3P	-3.62	1.55	1.59
2	A	603	HEC	CBB-CAB	-3.61	1.36	1.51
2	C	603	HEC	CBB-CAB	-3.54	1.36	1.51
2	A	603	HEC	CBC-CAC	-3.52	1.36	1.51
2	A	601	HEC	CBB-CAB	-3.49	1.36	1.51
2	A	602	HEC	CBC-CAC	-3.45	1.36	1.51
2	A	602	HEC	CBB-CAB	-3.42	1.37	1.51
3	A	600	FAD	C5'-C4'	-3.40	1.47	1.51
2	A	604	HEC	CBC-CAC	-3.35	1.37	1.51
2	D	602	HEC	CBC-CAC	-3.28	1.37	1.51
2	A	604	HEC	CBB-CAB	-3.27	1.37	1.51
2	D	602	HEC	CBB-CAB	-3.25	1.37	1.51
2	C	604	HEC	CBB-CAB	-3.24	1.37	1.51
2	B	601	HEC	CBC-CAC	-3.24	1.37	1.51
2	B	604	HEC	CBB-CAB	-3.19	1.38	1.51
2	C	602	HEC	CBC-CAC	-3.18	1.38	1.51
2	C	602	HEC	CBB-CAB	-3.14	1.38	1.51
2	D	604	HEC	CBB-CAB	-3.10	1.38	1.51
3	B	700	FAD	C6-C7	3.08	1.43	1.39
3	C	800	FAD	C8-C7	3.06	1.48	1.40
3	D	900	FAD	C5X-N5	-3.03	1.33	1.39
2	D	601	HEC	CAC-C3C	2.99	1.58	1.51
2	D	601	HEC	FE-NC	2.99	2.05	1.95
3	A	600	FAD	PA-O3P	2.98	1.62	1.59
2	B	602	HEC	CMB-C2B	2.97	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	604	HEC	CMD-C2D	2.91	1.56	1.50
3	B	700	FAD	C5X-N5	-2.87	1.34	1.39
2	A	602	HEC	CAC-C3C	2.85	1.58	1.51
3	C	800	FAD	C5'-C4'	-2.84	1.47	1.51
2	A	602	HEC	O1A-CGA	2.82	1.31	1.22
3	C	800	FAD	P-O1P	-2.79	1.41	1.50
2	B	601	HEC	CAB-C3B	2.78	1.58	1.51
2	A	604	HEC	CAB-C3B	2.76	1.58	1.51
2	C	604	HEC	CMC-C2C	2.76	1.56	1.50
3	B	700	FAD	PA-O3P	-2.72	1.56	1.59
2	C	602	HEC	FE-NA	2.70	2.04	1.95
2	A	601	HEC	C3B-C2B	-2.68	1.31	1.36
3	D	900	FAD	C5A-C4A	2.67	1.43	1.39
3	A	600	FAD	PA-O2A	-2.65	1.43	1.55
3	A	600	FAD	C6-C7	2.61	1.43	1.39
2	C	602	HEC	CAB-C3B	2.61	1.57	1.51
3	A	600	FAD	P-O2P	-2.61	1.43	1.55
2	C	604	HEC	FE-NB	2.60	2.02	1.94
2	D	603	HEC	FE-NA	2.60	2.03	1.95
2	B	601	HEC	CAC-C3C	2.59	1.57	1.51
2	A	604	HEC	FE-ND	2.59	2.02	1.94
2	A	602	HEC	CAB-C3B	2.58	1.57	1.51
2	A	603	HEC	FE-NB	2.57	2.02	1.94
3	B	700	FAD	C5A-C4A	2.53	1.43	1.39
2	A	603	HEC	CAB-C3B	2.52	1.57	1.51
2	D	602	HEC	FE-NA	2.50	2.03	1.95
3	C	800	FAD	C6-C7	2.50	1.43	1.39
3	D	900	FAD	P-O2P	-2.50	1.43	1.55
2	D	602	HEC	FE-NB	2.50	2.02	1.94
2	C	602	HEC	CMB-C2B	2.49	1.55	1.50
2	D	604	HEC	CAB-C3B	2.48	1.57	1.51
2	D	602	HEC	CMB-C2B	2.46	1.55	1.50
2	C	604	HEC	CAC-C3C	2.46	1.57	1.51
2	B	603	HEC	FE-NB	2.46	2.02	1.94
2	D	602	HEC	CAC-C3C	2.43	1.57	1.51
2	C	604	HEC	CAB-C3B	2.42	1.57	1.51
2	C	602	HEC	C3C-C2C	-2.41	1.32	1.38
2	D	603	HEC	CAB-C3B	2.41	1.57	1.51
3	B	700	FAD	C8-C7	2.39	1.46	1.40
3	A	600	FAD	P-O1P	-2.39	1.42	1.50
2	A	601	HEC	O2D-CGD	-2.36	1.23	1.30
2	B	601	HEC	FE-NB	2.36	2.02	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	FAD	O4'-C4'	-2.35	1.38	1.43
2	A	603	HEC	C3C-C2C	-2.35	1.32	1.38
2	B	604	HEC	CMB-C2B	2.35	1.55	1.50
2	A	603	HEC	CAC-C3C	2.33	1.57	1.51
2	B	603	HEC	CAB-C3B	2.31	1.57	1.51
2	A	602	HEC	FE-ND	2.31	2.02	1.94
2	D	601	HEC	CMC-C2C	2.30	1.55	1.50
2	D	604	HEC	CAC-C3C	2.30	1.57	1.51
2	A	601	HEC	CMC-C2C	2.28	1.55	1.50
2	B	604	HEC	CAC-C3C	2.28	1.56	1.51
3	D	900	FAD	C6-C7	2.27	1.42	1.39
3	C	800	FAD	C5X-N5	-2.27	1.35	1.39
2	C	603	HEC	C3C-C2C	-2.27	1.33	1.38
3	B	700	FAD	PA-O2A	-2.27	1.44	1.55
2	D	602	HEC	O1D-CGD	2.26	1.29	1.22
2	A	602	HEC	O1D-CGD	2.25	1.29	1.22
2	C	603	HEC	FE-NB	2.24	2.01	1.94
2	D	602	HEC	CMC-C2C	2.24	1.55	1.50
2	D	603	HEC	FE-NB	2.22	2.01	1.94
2	D	601	HEC	C2A-C3A	-2.21	1.32	1.36
2	C	603	HEC	CAB-C3B	2.21	1.56	1.51
2	B	601	HEC	C3C-C2C	-2.19	1.33	1.38
2	C	601	HEC	FE-NB	2.18	2.01	1.94
2	A	602	HEC	FE-NC	2.16	2.02	1.95
2	A	601	HEC	CAC-C3C	2.15	1.56	1.51
2	B	604	HEC	CAB-C3B	2.15	1.56	1.51
3	A	600	FAD	P-O5'	-2.15	1.51	1.59
2	C	602	HEC	CMA-C3A	2.15	1.55	1.50
3	C	800	FAD	O4B-C4B	-2.15	1.40	1.45
2	D	604	HEC	CMB-C2B	2.14	1.55	1.50
2	A	604	HEC	C3C-C2C	-2.14	1.33	1.38
2	A	604	HEC	CMB-C2B	2.13	1.55	1.50
2	A	602	HEC	C3C-C2C	-2.12	1.33	1.38
2	A	602	HEC	CMB-C2B	2.12	1.55	1.50
2	A	603	HEC	O1A-CGA	2.11	1.29	1.22
2	A	604	HEC	CMC-C2C	2.11	1.55	1.50
2	D	603	HEC	C3C-C2C	-2.11	1.33	1.38
2	C	602	HEC	CAC-C3C	2.11	1.56	1.51
2	C	601	HEC	CAC-C3C	2.10	1.56	1.51
2	B	601	HEC	CMA-C3A	2.10	1.55	1.50
2	C	601	HEC	CMB-C2B	2.09	1.55	1.50
3	D	900	FAD	C2'-C3'	-2.08	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	900	FAD	PA-O3P	-2.07	1.57	1.59
3	D	900	FAD	PA-O2A	-2.06	1.45	1.55
2	B	603	HEC	CAC-C3C	2.05	1.56	1.51
2	D	602	HEC	CAB-C3B	2.03	1.56	1.51
2	A	601	HEC	CBD-CAD	2.03	1.59	1.51
2	C	602	HEC	O1D-CGD	2.03	1.28	1.22
2	C	601	HEC	CAB-C3B	2.02	1.56	1.51
3	C	800	FAD	PA-O2A	-2.01	1.46	1.55

All (281) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	800	FAD	O4B-C4B-C5B	16.97	163.68	109.33
3	C	800	FAD	O5B-C5B-C4B	16.46	165.03	108.99
3	D	900	FAD	O5B-C5B-C4B	11.62	148.57	108.99
3	D	900	FAD	C5B-C4B-C3B	-11.44	74.02	115.21
3	A	600	FAD	C5B-C4B-C3B	-11.29	74.55	115.21
3	C	800	FAD	C5B-C4B-C3B	-11.26	74.68	115.21
3	B	700	FAD	C5B-C4B-C3B	-11.19	74.91	115.21
3	A	600	FAD	O5B-C5B-C4B	10.61	145.13	108.99
3	D	900	FAD	O4B-C4B-C5B	9.88	140.99	109.33
2	C	604	HEC	CBD-CAD-C3D	9.87	139.81	112.53
3	B	700	FAD	O5B-C5B-C4B	9.58	141.62	108.99
3	B	700	FAD	O4B-C4B-C5B	8.90	137.85	109.33
3	A	600	FAD	O4B-C1B-N9A	-8.71	91.36	108.09
2	D	601	HEC	O2D-CGD-O1D	7.13	141.68	123.33
3	A	600	FAD	O4B-C4B-C5B	6.89	131.40	109.33
2	D	604	HEC	O2D-CGD-O1D	6.38	139.75	123.33
3	D	900	FAD	O3'-C3'-C4'	6.27	123.17	108.93
2	A	602	HEC	CAA-CBA-CGA	6.11	129.87	113.67
2	B	603	HEC	CAA-CBA-CGA	5.83	129.12	113.67
3	B	700	FAD	N3A-C2A-N1A	5.80	137.35	128.58
2	A	601	HEC	CBD-CAD-C3D	-5.69	96.80	112.53
2	C	604	HEC	CHB-C4A-NA	5.61	130.57	124.45
3	D	900	FAD	N3A-C2A-N1A	5.58	137.03	128.58
3	B	700	FAD	C4-N3-C2	-5.54	115.80	125.64
3	C	800	FAD	N6A-C6A-N1A	5.52	130.66	118.38
3	D	900	FAD	C4-N3-C2	-5.46	115.94	125.64
3	D	900	FAD	C4'-C3'-C2'	5.37	122.50	113.57
3	D	900	FAD	C9A-C5X-N5	-5.35	116.77	122.45
2	C	604	HEC	CBA-CAA-C2A	5.35	127.32	112.53
2	A	601	HEC	O1D-CGD-CBD	-5.30	106.29	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	604	HEC	CAD-CBD-CGD	-5.19	99.91	113.67
3	C	800	FAD	O5'-C5'-C4'	5.18	123.19	109.36
2	D	602	HEC	CBC-CAC-C3C	5.12	126.31	112.42
2	B	601	HEC	CBD-CAD-C3D	4.97	126.27	112.53
2	C	602	HEC	CBA-CAA-C2A	4.96	126.25	112.53
2	A	601	HEC	C3D-C4D-ND	-4.89	105.63	110.35
2	A	601	HEC	O1A-CGA-CBA	-4.86	107.67	123.09
3	B	700	FAD	O4'-C4'-C5'	-4.81	99.39	109.99
3	B	700	FAD	C1'-N10-C9A	-4.78	111.34	120.63
3	A	600	FAD	C2A-N1A-C6A	4.65	126.38	118.73
3	C	800	FAD	O4-C4-C4X	-4.62	114.34	126.53
2	C	601	HEC	O2D-CGD-O1D	4.52	134.96	123.33
2	A	604	HEC	O2D-CGD-O1D	4.38	134.60	123.33
3	D	900	FAD	O4'-C4'-C5'	-4.35	100.39	109.99
3	C	800	FAD	O4B-C1B-N9A	-4.32	99.79	108.09
2	A	601	HEC	O2D-CGD-O1D	4.30	134.38	123.33
2	B	601	HEC	O2D-CGD-O1D	4.29	134.37	123.33
3	A	600	FAD	O4B-C1B-C2B	-4.28	97.45	106.62
3	A	600	FAD	N6A-C6A-N1A	4.28	127.91	118.38
2	C	601	HEC	CBD-CAD-C3D	4.27	124.35	112.53
2	D	601	HEC	CAA-CBA-CGA	-4.24	102.42	113.67
2	A	602	HEC	CBC-CAC-C3C	4.22	123.86	112.42
3	A	600	FAD	O2-C2-N1	-4.22	114.79	121.80
2	D	601	HEC	CAD-CBD-CGD	-4.18	102.57	113.67
3	C	800	FAD	O4-C4-N3	4.14	127.90	120.11
2	A	601	HEC	O2A-CGA-O1A	4.06	133.78	123.33
3	A	600	FAD	C4B-O4B-C1B	-4.05	100.52	109.47
2	B	604	HEC	CBD-CAD-C3D	3.97	123.52	112.53
2	C	602	HEC	CHA-C4D-ND	3.92	128.65	124.42
3	A	600	FAD	C4A-N9A-C8A	3.89	109.82	105.74
2	C	601	HEC	O2A-CGA-O1A	3.85	133.23	123.33
2	D	604	HEC	O1D-CGD-CBD	-3.79	111.06	123.09
2	B	601	HEC	CAD-CBD-CGD	-3.77	103.67	113.67
2	A	601	HEC	CBC-CAC-C3C	3.76	122.60	112.42
3	A	600	FAD	C4X-C10-N10	3.69	121.76	116.48
3	D	900	FAD	C7M-C7-C6	3.65	126.00	119.57
3	B	700	FAD	C5X-C9A-N10	-3.59	114.72	117.97
2	C	601	HEC	O1A-CGA-CBA	-3.58	111.73	123.09
2	D	604	HEC	CBA-CAA-C2A	3.56	122.37	112.53
3	B	700	FAD	C4A-C5A-N7A	-3.53	106.55	110.58
3	C	800	FAD	C4-N3-C2	-3.52	119.40	125.64
3	A	600	FAD	C4-C4X-N5	3.49	123.03	118.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	602	HEC	O1A-CGA-CBA	-3.39	112.33	123.09
2	D	601	HEC	O1A-CGA-CBA	-3.36	112.42	123.09
2	D	602	HEC	CAA-CBA-CGA	3.35	122.54	113.67
3	A	600	FAD	O2A-PA-O1A	3.33	127.95	112.44
2	D	604	HEC	C3D-C4D-ND	-3.33	107.14	110.35
3	A	600	FAD	C10-C4X-N5	-3.30	118.07	124.81
3	D	900	FAD	O2-C2-N3	-3.29	112.28	118.58
2	A	604	HEC	CMA-C3A-C4A	-3.28	118.96	124.73
2	C	604	HEC	CHC-C1C-NC	3.28	129.80	123.86
2	C	603	HEC	CHA-C4D-ND	3.27	127.94	124.42
3	A	600	FAD	C4'-C3'-C2'	-3.26	108.15	113.57
2	B	604	HEC	CAD-CBD-CGD	-3.23	105.10	113.67
2	B	602	HEC	CAA-CBA-CGA	3.23	122.23	113.67
3	D	900	FAD	O2'-C2'-C3'	3.23	116.80	109.25
3	B	700	FAD	O3'-C3'-C4'	3.22	116.26	108.93
3	A	600	FAD	O4'-C4'-C3'	-3.21	101.72	109.25
2	C	602	HEC	CAD-CBD-CGD	-3.21	105.15	113.67
2	B	603	HEC	CBB-CAB-C3B	3.20	121.10	112.42
3	C	800	FAD	O2-C2-N1	-3.18	116.52	121.80
2	C	601	HEC	CAD-CBD-CGD	-3.13	105.36	113.67
3	B	700	FAD	C4'-C3'-C2'	-3.12	108.37	113.57
2	A	604	HEC	CBA-CAA-C2A	3.11	121.13	112.53
3	C	800	FAD	C4A-N9A-C8A	3.11	109.00	105.74
2	D	603	HEC	CBC-CAC-C3C	3.11	120.85	112.42
2	A	602	HEC	CBA-CAA-C2A	3.08	121.06	112.53
2	B	604	HEC	O1A-CGA-CBA	-3.08	113.33	123.09
2	B	602	HEC	CBC-CAC-C3C	3.07	120.73	112.42
3	B	700	FAD	O4'-C4'-C3'	-3.04	102.14	109.25
2	D	601	HEC	O2D-CGD-CBD	-3.02	104.45	114.00
2	D	601	HEC	CBC-CAC-C3C	3.00	120.56	112.42
2	C	604	HEC	C1C-CHC-C4B	-3.00	119.19	126.25
2	C	603	HEC	CAD-C3D-C2D	3.00	133.48	127.87
2	B	602	HEC	CBA-CAA-C2A	2.99	120.79	112.53
2	D	601	HEC	O1D-CGD-CBD	-2.98	113.63	123.09
2	B	604	HEC	C3C-C4C-NC	-2.98	106.84	110.15
2	B	601	HEC	CBA-CAA-C2A	2.98	120.77	112.53
2	B	604	HEC	C2A-C1A-NA	-2.98	107.45	110.32
2	C	604	HEC	C4A-CHB-C1B	-2.97	119.72	126.02
2	C	604	HEC	C2A-C1A-NA	-2.96	107.47	110.32
2	A	601	HEC	C1D-ND-C4D	2.95	108.70	105.21
3	C	800	FAD	O2B-C2B-C3B	-2.95	102.36	111.82
2	C	603	HEC	CBC-CAC-C3C	2.95	120.41	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	602	HEC	CBB-CAB-C3B	2.94	120.39	112.42
2	D	602	HEC	O2D-CGD-O1D	2.94	130.89	123.33
2	D	604	HEC	C1D-ND-C4D	2.93	108.68	105.21
2	B	604	HEC	O2D-CGD-O1D	2.93	130.87	123.33
2	C	601	HEC	O1D-CGD-CBD	-2.93	113.80	123.09
3	B	700	FAD	C10-C4X-N5	-2.90	118.89	124.81
2	D	601	HEC	CAA-C2A-C1A	-2.90	118.96	124.85
2	A	603	HEC	O2A-CGA-O1A	2.89	130.75	123.33
2	A	601	HEC	CHB-C4A-NA	2.87	127.58	124.45
3	B	700	FAD	C4X-C10-N1	-2.86	117.58	124.59
3	D	900	FAD	C2A-N1A-C6A	-2.82	114.09	118.73
3	B	700	FAD	C2A-N3A-C4A	-2.82	104.95	111.83
2	B	603	HEC	CBC-CAC-C3C	2.81	120.05	112.42
3	C	800	FAD	O2A-PA-O3P	2.81	114.87	107.27
2	B	601	HEC	O1D-CGD-CBD	-2.80	114.20	123.09
2	A	601	HEC	C4D-C3D-C2D	2.80	110.97	106.89
2	C	603	HEC	CAA-CBA-CGA	2.80	121.09	113.67
3	D	900	FAD	C4A-C5A-N7A	-2.80	107.39	110.58
2	A	602	HEC	O2A-CGA-O1A	2.78	130.48	123.33
2	A	601	HEC	CAD-C3D-C4D	-2.76	119.89	124.70
3	A	600	FAD	O2A-PA-O3P	2.75	114.71	107.27
2	B	604	HEC	C3D-C4D-ND	-2.74	107.70	110.35
2	C	602	HEC	O2A-CGA-O1A	2.74	130.38	123.33
2	A	602	HEC	CAD-CBD-CGD	-2.74	106.40	113.67
2	C	602	HEC	C3D-C4D-ND	-2.73	107.72	110.35
2	A	601	HEC	CAD-CBD-CGD	-2.72	106.44	113.67
3	B	700	FAD	C9-C8-C7	2.71	123.66	119.69
2	A	602	HEC	O1A-CGA-CBA	-2.71	114.51	123.09
3	C	800	FAD	C2A-N3A-C4A	-2.70	105.25	111.83
3	C	800	FAD	C6-C5X-N5	-2.69	113.98	118.44
3	D	900	FAD	C5X-N5-C4X	2.68	122.42	118.09
3	B	700	FAD	C5'-C4'-C3'	2.67	117.26	112.22
2	A	604	HEC	CMA-C3A-C2A	2.67	133.36	126.15
2	A	603	HEC	O1A-CGA-CBA	-2.66	114.67	123.09
2	C	603	HEC	CAD-C3D-C4D	-2.65	120.08	124.70
2	B	601	HEC	O1A-CGA-CBA	-2.64	114.73	123.09
2	A	602	HEC	CHA-C1A-NA	-2.63	121.59	124.45
3	A	600	FAD	C4-N3-C2	-2.61	121.01	125.64
2	D	602	HEC	C3D-C4D-ND	-2.61	107.83	110.35
3	B	700	FAD	C10-N1-C2	2.60	122.49	116.85
3	C	800	FAD	N3A-C2A-N1A	2.60	132.52	128.58
2	B	603	HEC	CHB-C4A-NA	2.59	127.28	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	800	FAD	C5A-C6A-N6A	-2.58	116.90	123.29
2	B	601	HEC	CAD-C3D-C4D	-2.57	120.21	124.70
3	B	700	FAD	C5X-N5-C4X	2.57	122.25	118.09
3	B	700	FAD	O4B-C1B-N9A	-2.57	103.16	108.09
2	D	604	HEC	C3B-C4B-NB	-2.56	107.36	110.17
3	B	700	FAD	O3P-PA-O1A	2.56	118.41	110.70
2	D	602	HEC	C1D-ND-C4D	2.56	108.23	105.21
3	D	900	FAD	C4X-C4-N3	2.55	119.75	113.25
2	D	603	HEC	O1A-CGA-CBA	-2.55	115.00	123.09
2	D	601	HEC	CHD-C1D-ND	2.54	127.51	124.37
2	C	604	HEC	O2D-CGD-O1D	2.54	129.86	123.33
2	A	604	HEC	CMC-C2C-C1C	-2.53	121.57	125.42
3	D	900	FAD	N3-C2-N1	2.52	124.85	119.50
3	A	600	FAD	O5'-C5'-C4'	2.51	116.06	109.36
2	B	601	HEC	C3D-C4D-ND	-2.51	107.93	110.35
2	B	604	HEC	O1D-CGD-CBD	-2.50	115.15	123.09
3	A	600	FAD	O5B-PA-O1A	-2.50	99.02	108.94
2	C	604	HEC	O2A-CGA-O1A	2.50	129.76	123.33
2	B	604	HEC	CAA-C2A-C1A	-2.50	119.77	124.85
2	D	604	HEC	CHA-C1A-C2A	2.49	128.80	124.86
3	B	700	FAD	C9A-C5X-N5	-2.49	119.81	122.45
2	C	601	HEC	CBC-CAC-C3C	2.48	119.16	112.42
2	C	604	HEC	CHA-C4D-C3D	2.48	128.40	124.77
3	B	700	FAD	N3-C2-N1	2.48	124.76	119.50
3	A	600	FAD	C9A-C5X-N5	-2.46	119.84	122.45
3	C	800	FAD	C6-C5X-C9A	2.46	122.43	119.05
2	A	601	HEC	C4A-CHB-C1B	-2.46	120.80	126.02
3	A	600	FAD	C2A-N3A-C4A	-2.46	105.83	111.83
3	A	600	FAD	N9A-C8A-N7A	-2.45	110.46	113.94
2	A	601	HEC	CHC-C4B-C3B	2.45	129.74	125.23
3	B	700	FAD	C9A-C9-C8	-2.44	114.31	119.22
2	B	604	HEC	CMB-C2B-C1B	-2.44	121.22	125.03
3	B	700	FAD	C4X-C4-N3	2.43	119.43	113.25
2	B	604	HEC	C4B-NB-C1B	2.43	108.08	105.21
3	C	800	FAD	C5'-C4'-C3'	-2.42	107.65	112.22
2	A	602	HEC	CBD-CAD-C3D	2.42	119.22	112.53
2	A	603	HEC	CMA-C3A-C4A	-2.42	120.47	124.73
2	B	603	HEC	CMA-C3A-C4A	-2.40	120.50	124.73
2	A	603	HEC	CAC-C3C-C4C	-2.40	121.61	124.91
2	B	601	HEC	CHB-C4A-NA	-2.39	121.85	124.45
2	A	604	HEC	O1D-CGD-CBD	-2.38	115.53	123.09
2	D	604	HEC	C4C-CHD-C1D	-2.37	120.67	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	602	HEC	O1D-CGD-CBD	-2.36	115.60	123.09
3	A	600	FAD	C7M-C7-C6	2.35	123.72	119.57
2	A	604	HEC	C3D-C4D-ND	-2.35	108.08	110.35
2	C	602	HEC	C1A-CHA-C4D	-2.35	121.02	126.02
2	C	604	HEC	CAA-CBA-CGA	-2.35	107.44	113.67
2	A	601	HEC	C3B-C4B-NB	-2.35	107.60	110.17
3	B	700	FAD	O3B-C3B-C4B	2.34	117.81	111.08
3	C	800	FAD	C6A-C5A-C4A	2.34	120.38	117.18
3	A	600	FAD	C5'-C4'-C3'	-2.34	107.80	112.22
2	D	604	HEC	CHD-C1D-ND	2.33	127.25	124.37
2	D	604	HEC	CHA-C4D-C3D	2.30	128.13	124.77
2	B	604	HEC	C3B-C4B-NB	-2.29	107.67	110.17
2	A	601	HEC	CMC-C2C-C3C	2.28	130.46	125.62
2	D	601	HEC	CAA-C2A-C3A	2.28	132.14	127.87
2	C	603	HEC	CHA-C4D-C3D	-2.28	121.45	124.77
3	B	700	FAD	C9-C9A-C5X	2.28	124.05	120.03
2	B	602	HEC	O1A-CGA-CBA	-2.28	115.87	123.09
3	A	600	FAD	C7M-C7-C8	-2.27	116.12	120.76
2	C	602	HEC	CHA-C1A-NA	2.27	126.92	124.45
2	B	604	HEC	CAA-CBA-CGA	-2.26	107.67	113.67
2	A	604	HEC	CMC-C2C-C3C	2.24	130.37	125.62
3	A	600	FAD	C5A-C6A-N1A	-2.24	111.83	117.51
3	C	800	FAD	C5X-C9A-N10	-2.23	115.95	117.97
2	C	602	HEC	C1D-ND-C4D	2.23	107.84	105.21
2	A	601	HEC	CHA-C4D-ND	2.22	126.81	124.42
2	A	604	HEC	CBC-CAC-C3C	2.22	118.43	112.42
2	B	603	HEC	C3D-C4D-ND	-2.21	108.21	110.35
3	C	800	FAD	C2A-N1A-C6A	2.21	122.36	118.73
2	D	601	HEC	O2A-CGA-O1A	2.21	129.01	123.33
2	C	604	HEC	CMC-C2C-C3C	2.21	130.30	125.62
2	D	604	HEC	C4B-NB-C1B	2.20	107.82	105.21
2	C	602	HEC	O2A-CGA-CBA	-2.19	107.07	114.00
2	C	604	HEC	C3D-C4D-ND	-2.19	108.23	110.35
2	D	603	HEC	CAD-C3D-C4D	-2.19	120.89	124.70
2	A	603	HEC	CMA-C3A-C2A	2.18	132.06	126.15
3	D	900	FAD	C7M-C7-C8	-2.18	116.30	120.76
3	B	700	FAD	C5A-N7A-C8A	2.17	106.86	103.45
3	B	700	FAD	C8M-C8-C7	-2.17	116.33	120.76
3	B	700	FAD	C4-C4X-N5	2.16	121.19	118.21
2	B	601	HEC	C1D-ND-C4D	2.16	107.76	105.21
2	C	604	HEC	CHA-C1A-C2A	2.15	128.26	124.86
2	B	603	HEC	CMA-C3A-C2A	2.15	131.96	126.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	HEC	CMB-C2B-C1B	-2.14	121.68	125.03
2	A	604	HEC	CHC-C1C-NC	2.14	127.74	123.86
2	B	604	HEC	CAC-C3C-C4C	-2.14	121.97	124.91
2	B	604	HEC	CHC-C4B-C3B	2.14	129.16	125.23
2	C	601	HEC	CAA-C2A-C1A	-2.13	120.52	124.85
2	B	604	HEC	C2B-C1B-NB	-2.13	107.44	109.90
3	D	900	FAD	O2'-C2'-C1'	-2.13	101.46	110.20
2	A	604	HEC	CHB-C4A-NA	2.12	126.77	124.45
3	C	800	FAD	O2'-C2'-C1'	-2.12	101.49	110.20
3	D	900	FAD	O4B-C1B-C2B	-2.11	102.09	106.62
3	B	700	FAD	O5B-PA-O1A	-2.11	100.56	108.94
3	B	700	FAD	N10-C10-N1	2.11	124.71	118.51
2	C	601	HEC	C3B-C4B-NB	-2.10	107.86	110.17
3	A	600	FAD	C8M-C8-C9	2.10	123.27	119.57
2	A	601	HEC	C2A-C1A-NA	-2.10	108.30	110.32
2	C	604	HEC	CHC-C1C-C2C	-2.10	121.34	127.43
3	C	800	FAD	O2A-PA-O1A	2.10	122.20	112.44
2	A	604	HEC	CHA-C1A-C2A	2.09	128.17	124.86
2	A	601	HEC	CMC-C2C-C1C	-2.07	122.26	125.42
2	D	604	HEC	C2A-C1A-NA	-2.06	108.33	110.32
3	D	900	FAD	C6-C5X-N5	2.06	121.86	118.44
2	C	603	HEC	O1A-CGA-CBA	-2.05	116.59	123.09
3	C	800	FAD	O3B-C3B-C2B	-2.05	105.26	111.82
2	B	604	HEC	CHA-C1A-NA	2.04	126.67	124.45
3	A	600	FAD	C5A-C4A-N3A	2.04	129.52	126.72
2	A	603	HEC	CHC-C1C-NC	2.04	127.55	123.86
2	C	604	HEC	CMD-C2D-C1D	-2.03	121.86	125.03
3	C	800	FAD	C5A-C6A-N1A	-2.03	112.35	117.51
2	C	604	HEC	CHB-C4A-C3A	-2.03	121.26	125.49
3	A	600	FAD	C5A-N7A-C8A	2.03	106.64	103.45
3	D	900	FAD	C5A-N7A-C8A	2.03	106.64	103.45
3	B	700	FAD	C2B-C3B-C4B	2.03	106.53	102.61
3	A	600	FAD	C5A-C4A-N9A	-2.02	103.61	105.81
2	B	603	HEC	CBA-CAA-C2A	-2.02	106.95	112.53
2	C	603	HEC	CMC-C2C-C3C	2.02	129.91	125.62
2	A	601	HEC	CAA-CBA-CGA	-2.02	108.31	113.67
2	D	603	HEC	O1D-CGD-CBD	-2.02	116.69	123.09
2	B	604	HEC	CBA-CAA-C2A	2.02	118.11	112.53
2	C	604	HEC	CAA-C2A-C3A	-2.01	124.10	127.87
3	C	800	FAD	C9A-N10-C10	-2.01	117.69	120.75
3	B	700	FAD	O4-C4-N3	-2.01	116.34	120.11

All (24) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	HEC	NA
2	A	602	HEC	NA
2	A	603	HEC	NA
2	A	604	HEC	NA
2	B	601	HEC	NA
2	B	602	HEC	NA
2	B	603	HEC	NA
2	B	604	HEC	NA
2	C	601	HEC	NA
2	C	602	HEC	NA
2	C	603	HEC	NA
2	C	604	HEC	NA
2	D	601	HEC	NA
2	D	602	HEC	NA
2	D	604	HEC	NA
3	A	600	FAD	C3'
3	A	600	FAD	C4'
3	B	700	FAD	C3'
3	B	700	FAD	C4'
3	C	800	FAD	C3'
3	C	800	FAD	C4B
3	C	800	FAD	C4'
3	D	900	FAD	C3'
3	D	900	FAD	C4'

All (158) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	HEC	C3D-CAD-CBD-CGD
2	B	602	HEC	C2A-CAA-CBA-CGA
2	C	602	HEC	C2A-CAA-CBA-CGA
2	C	604	HEC	C2D-C3D-CAD-CBD
3	A	600	FAD	C5B-O5B-PA-O1A
3	A	600	FAD	C3B-C4B-C5B-O5B
3	A	600	FAD	C1'-C2'-C3'-O3'
3	A	600	FAD	C1'-C2'-C3'-C4'
3	A	600	FAD	C3'-C4'-C5'-O5'
3	A	600	FAD	O4'-C4'-C5'-O5'
3	B	700	FAD	C3B-C4B-C5B-O5B
3	B	700	FAD	C1'-C2'-C3'-O3'
3	B	700	FAD	C1'-C2'-C3'-C4'
3	B	700	FAD	O2'-C2'-C3'-O3'
3	B	700	FAD	O2'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
3	B	700	FAD	C3'-C4'-C5'-O5'
3	B	700	FAD	O4'-C4'-C5'-O5'
3	C	800	FAD	C1'-C2'-C3'-O3'
3	C	800	FAD	C1'-C2'-C3'-C4'
3	C	800	FAD	C3'-C4'-C5'-O5'
3	C	800	FAD	O4'-C4'-C5'-O5'
3	D	900	FAD	C1'-C2'-C3'-C4'
3	D	900	FAD	O2'-C2'-C3'-C4'
3	D	900	FAD	C3'-C4'-C5'-O5'
3	D	900	FAD	O4'-C4'-C5'-O5'
2	C	604	HEC	C1A-C2A-CAA-CBA
2	C	604	HEC	C4D-C3D-CAD-CBD
2	C	604	HEC	C2C-C3C-CAC-CBC
3	C	800	FAD	O2'-C2'-C3'-O3'
3	D	900	FAD	O3'-C3'-C4'-O4'
3	A	600	FAD	O2'-C2'-C3'-C4'
3	C	800	FAD	O2'-C2'-C3'-C4'
3	C	800	FAD	C3B-C4B-C5B-O5B
3	D	900	FAD	O4B-C4B-C5B-O5B
3	D	900	FAD	C3B-C4B-C5B-O5B
2	B	601	HEC	C3D-CAD-CBD-CGD
2	C	603	HEC	C3D-CAD-CBD-CGD
2	D	603	HEC	C3D-CAD-CBD-CGD
2	C	601	HEC	C4C-C3C-CAC-CBC
3	D	900	FAD	O2'-C2'-C3'-O3'
2	C	601	HEC	C2C-C3C-CAC-CBC
3	A	600	FAD	O4B-C4B-C5B-O5B
2	A	602	HEC	C2A-CAA-CBA-CGA
2	B	601	HEC	C2A-CAA-CBA-CGA
2	C	601	HEC	C3D-CAD-CBD-CGD
2	D	601	HEC	C3D-CAD-CBD-CGD
2	D	602	HEC	C2A-CAA-CBA-CGA
2	C	604	HEC	C3A-C2A-CAA-CBA
3	B	700	FAD	O4B-C4B-C5B-O5B
3	C	800	FAD	O4B-C4B-C5B-O5B
3	A	600	FAD	O2'-C2'-C3'-O3'
2	C	604	HEC	C4C-C3C-CAC-CBC
2	B	604	HEC	C4D-C3D-CAD-CBD
2	D	601	HEC	C4D-C3D-CAD-CBD
2	D	601	HEC	C2D-C3D-CAD-CBD
2	A	601	HEC	C1A-C2A-CAA-CBA
2	D	601	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
2	B	601	HEC	C2C-C3C-CAC-CBC
2	D	602	HEC	C4C-C3C-CAC-CBC
3	D	900	FAD	P-O3P-PA-O1A
2	A	601	HEC	C3A-C2A-CAA-CBA
2	A	604	HEC	C4C-C3C-CAC-CBC
3	D	900	FAD	O3'-C3'-C4'-C5'
2	B	604	HEC	C2D-C3D-CAD-CBD
2	A	603	HEC	C3D-CAD-CBD-CGD
3	A	600	FAD	PA-O3P-P-O5'
3	B	700	FAD	PA-O3P-P-O5'
3	C	800	FAD	PA-O3P-P-O5'
3	D	900	FAD	PA-O3P-P-O5'
3	C	800	FAD	C2B-C1B-N9A-C8A
2	D	601	HEC	C2C-C3C-CAC-CBC
3	D	900	FAD	C1'-C2'-C3'-O3'
2	C	602	HEC	C2B-C3B-CAB-CBB
3	A	600	FAD	P-O3P-PA-O2A
3	D	900	FAD	P-O3P-PA-O2A
2	D	602	HEC	C2C-C3C-CAC-CBC
2	A	602	HEC	C3A-C2A-CAA-CBA
3	A	600	FAD	C5B-O5B-PA-O2A
3	A	600	FAD	C5B-O5B-PA-O3P
3	D	900	FAD	C5B-O5B-PA-O2A
3	D	900	FAD	C5B-O5B-PA-O3P
2	A	601	HEC	C4C-C3C-CAC-CBC
2	B	601	HEC	C4C-C3C-CAC-CBC
2	B	602	HEC	C4B-C3B-CAB-CBB
3	B	700	FAD	PA-O3P-P-O1P
3	C	800	FAD	P-O3P-PA-O2A
2	D	604	HEC	C3D-CAD-CBD-CGD
2	B	602	HEC	C2B-C3B-CAB-CBB
2	D	601	HEC	CAA-CBA-CGA-O1A
2	D	603	HEC	CAD-CBD-CGD-O1D
2	C	602	HEC	CAA-CBA-CGA-O1A
2	D	604	HEC	CAD-CBD-CGD-O1D
2	D	604	HEC	CAD-CBD-CGD-O2D
2	D	602	HEC	CAA-CBA-CGA-O1A
2	D	603	HEC	CAD-CBD-CGD-O2D
2	C	602	HEC	CAD-CBD-CGD-O2D
2	A	602	HEC	C4C-C3C-CAC-CBC
2	A	602	HEC	C1A-C2A-CAA-CBA
2	C	602	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	A	602	HEC	CAD-CBD-CGD-O2D
2	C	602	HEC	CAA-CBA-CGA-O2A
2	A	604	HEC	C2C-C3C-CAC-CBC
2	B	601	HEC	CAD-CBD-CGD-O1D
2	C	602	HEC	CAD-CBD-CGD-O1D
2	B	603	HEC	CAD-CBD-CGD-O1D
2	C	601	HEC	CAD-CBD-CGD-O2D
2	C	603	HEC	CAA-CBA-CGA-O1A
2	A	602	HEC	CAD-CBD-CGD-O1D
2	A	603	HEC	CAD-CBD-CGD-O1D
2	C	603	HEC	CAD-CBD-CGD-O1D
2	D	601	HEC	CAD-CBD-CGD-O2D
2	D	602	HEC	CAD-CBD-CGD-O2D
2	A	602	HEC	CAA-CBA-CGA-O2A
2	C	603	HEC	CAA-CBA-CGA-O2A
2	D	601	HEC	CAA-CBA-CGA-O2A
2	B	601	HEC	CAD-CBD-CGD-O2D
2	B	602	HEC	CAA-CBA-CGA-O1A
3	B	700	FAD	P-O3P-PA-O2A
3	C	800	FAD	P-O3P-PA-O1A
3	C	800	FAD	PA-O3P-P-O1P
2	C	601	HEC	CAD-CBD-CGD-O1D
2	D	601	HEC	CAD-CBD-CGD-O1D
2	D	602	HEC	CAA-CBA-CGA-O2A
2	D	602	HEC	CAD-CBD-CGD-O1D
3	C	800	FAD	O4B-C1B-N9A-C8A
2	A	602	HEC	CAA-CBA-CGA-O1A
2	B	601	HEC	CAA-CBA-CGA-O2A
3	A	600	FAD	O3'-C3'-C4'-C5'
2	A	603	HEC	CAD-CBD-CGD-O2D
2	B	602	HEC	CAA-CBA-CGA-O2A
2	C	601	HEC	CAA-CBA-CGA-O2A
2	C	603	HEC	CAD-CBD-CGD-O2D
2	C	603	HEC	C4B-C3B-CAB-CBB
2	A	603	HEC	C2B-C3B-CAB-CBB
2	A	604	HEC	CAD-CBD-CGD-O1D
2	B	603	HEC	CAD-CBD-CGD-O2D
2	A	604	HEC	CAD-CBD-CGD-O2D
2	C	601	HEC	CAA-CBA-CGA-O1A
2	B	602	HEC	CAD-CBD-CGD-O2D
2	A	601	HEC	CAD-CBD-CGD-O2D
2	C	602	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
2	B	601	HEC	CAA-CBA-CGA-O1A
2	A	601	HEC	C2C-C3C-CAC-CBC
2	B	602	HEC	CAD-CBD-CGD-O1D
2	A	601	HEC	CAD-CBD-CGD-O1D
2	B	604	HEC	CAD-CBD-CGD-O1D
2	C	603	HEC	C2B-C3B-CAB-CBB
2	C	604	HEC	CAA-CBA-CGA-O2A
3	B	700	FAD	C2B-C1B-N9A-C8A
2	D	604	HEC	C4D-C3D-CAD-CBD
2	A	603	HEC	C4B-C3B-CAB-CBB
3	D	900	FAD	C2B-C1B-N9A-C8A
2	A	601	HEC	CAA-CBA-CGA-O2A
2	B	604	HEC	CAD-CBD-CGD-O2D
2	C	604	HEC	CAA-CBA-CGA-O1A
3	C	800	FAD	C2'-C3'-C4'-O4'
3	B	700	FAD	P-O3P-PA-O1A
2	A	601	HEC	CAA-CBA-CGA-O1A

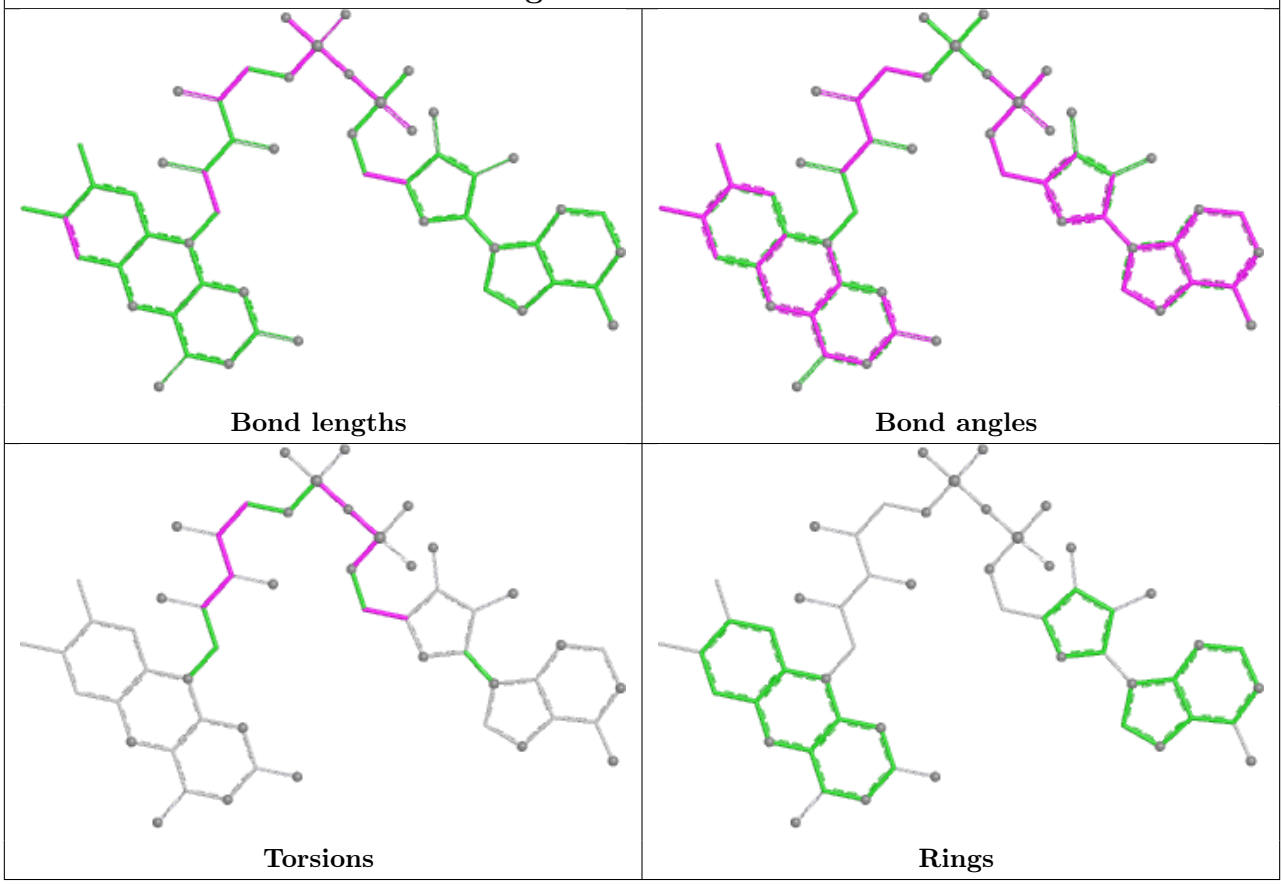
There are no ring outliers.

19 monomers are involved in 101 short contacts:

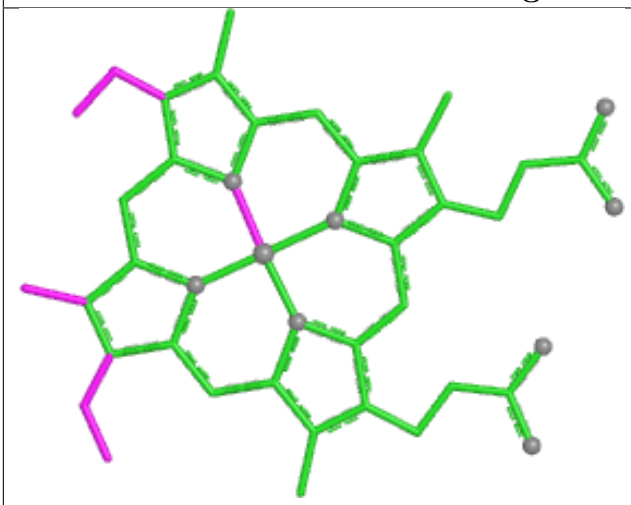
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	714	SO4	1	0
3	A	600	FAD	9	0
2	C	604	HEC	4	0
2	C	602	HEC	4	0
2	B	603	HEC	1	0
2	D	602	HEC	9	0
3	C	800	FAD	12	0
2	D	601	HEC	4	0
2	D	604	HEC	4	0
2	A	602	HEC	5	0
2	A	601	HEC	6	0
2	A	604	HEC	4	0
2	B	602	HEC	6	0
2	C	601	HEC	5	0
2	D	603	HEC	4	0
2	B	601	HEC	5	0
2	B	604	HEC	1	0
3	D	900	FAD	9	0
3	B	700	FAD	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

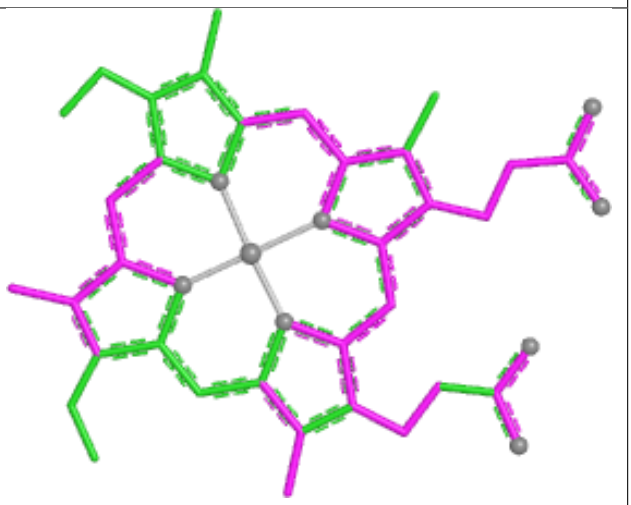
Ligand FAD A 600



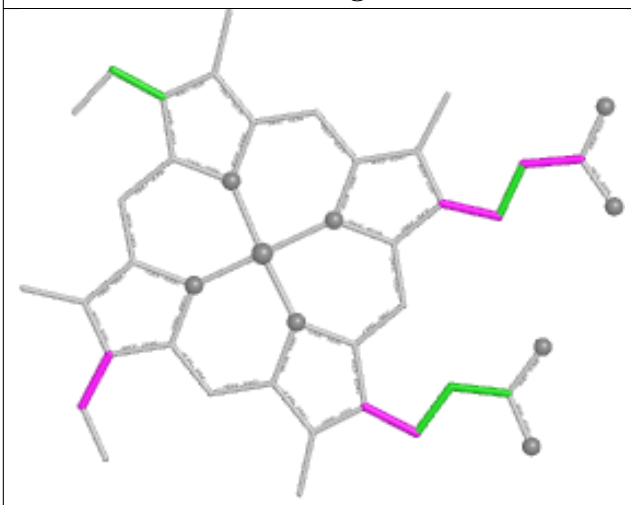
Ligand HEC C 604



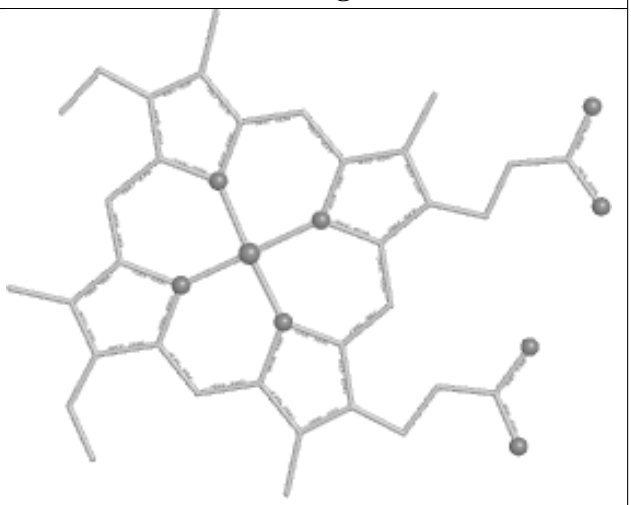
Bond lengths



Bond angles

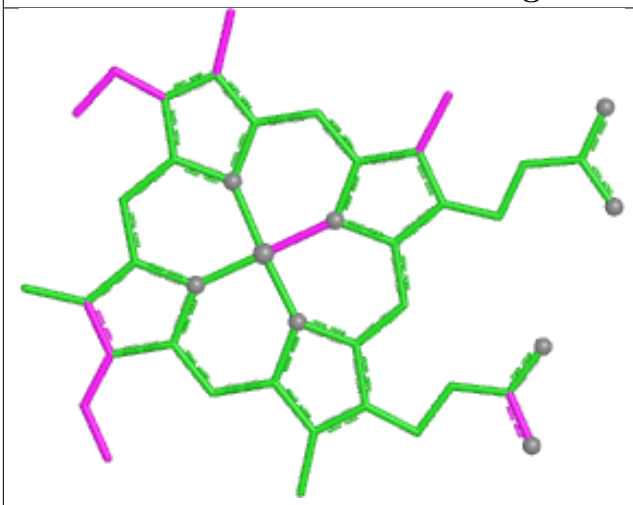


Torsions

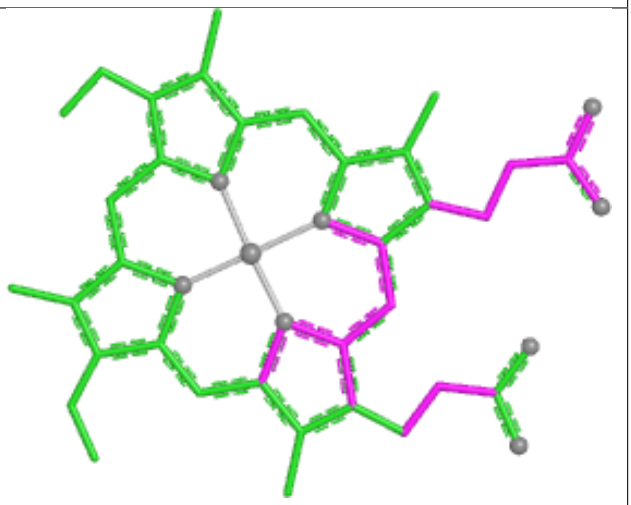


Rings

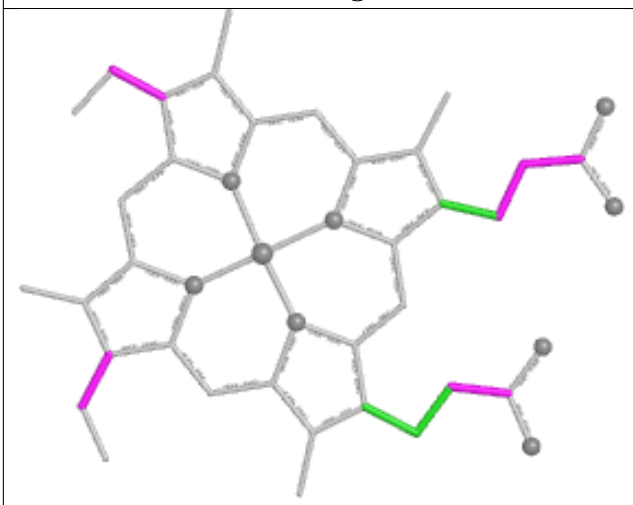
Ligand HEC C 602



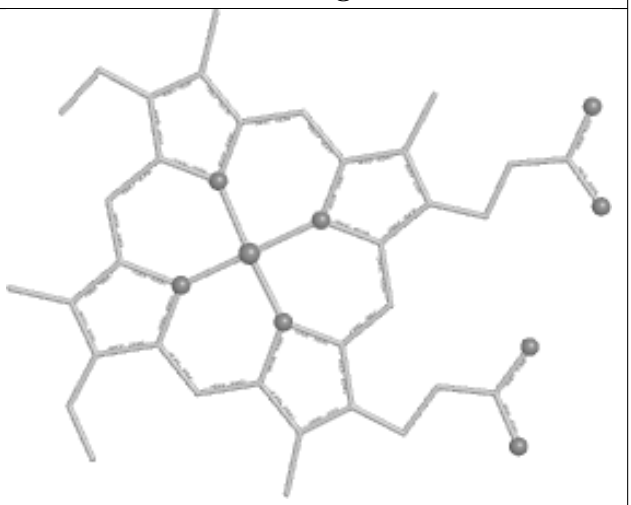
Bond lengths



Bond angles

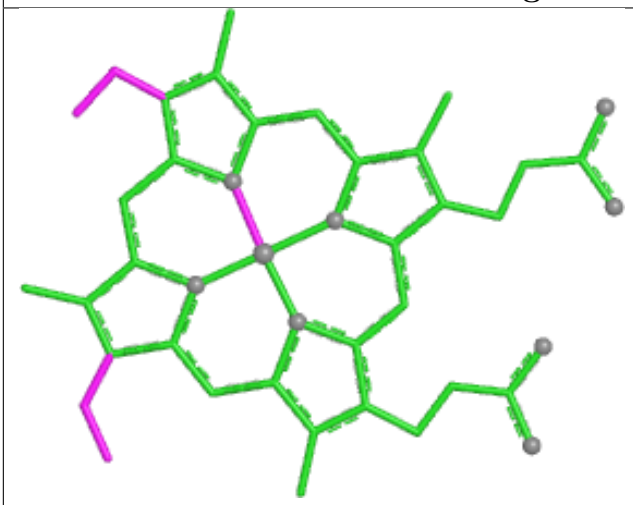


Torsions

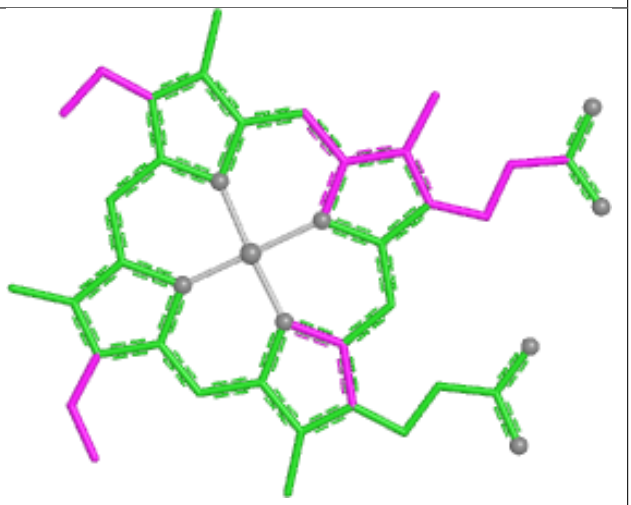


Rings

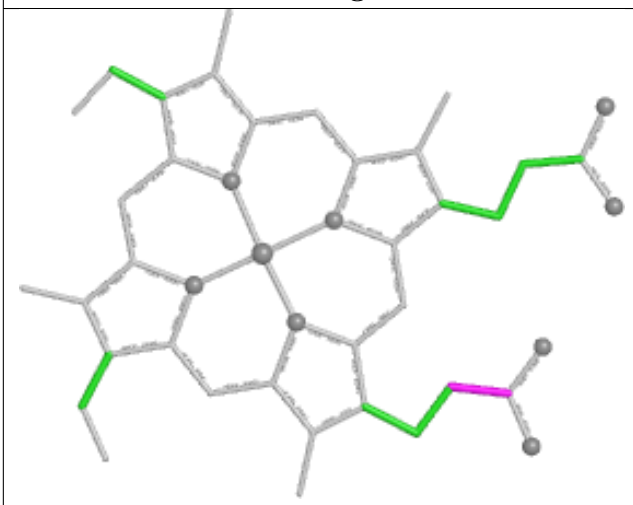
Ligand HEC B 603



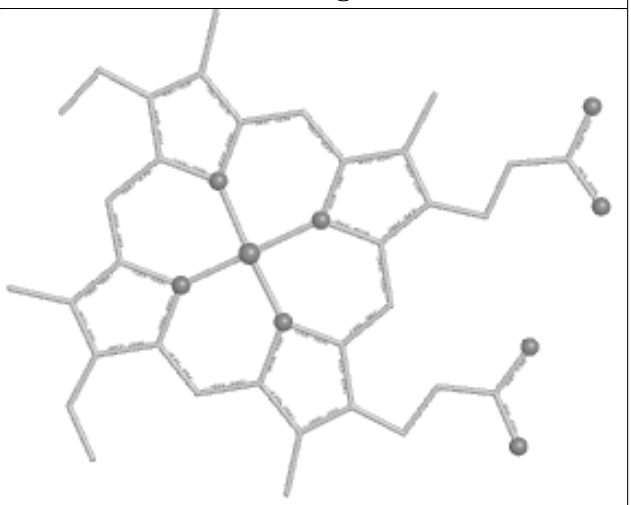
Bond lengths



Bond angles

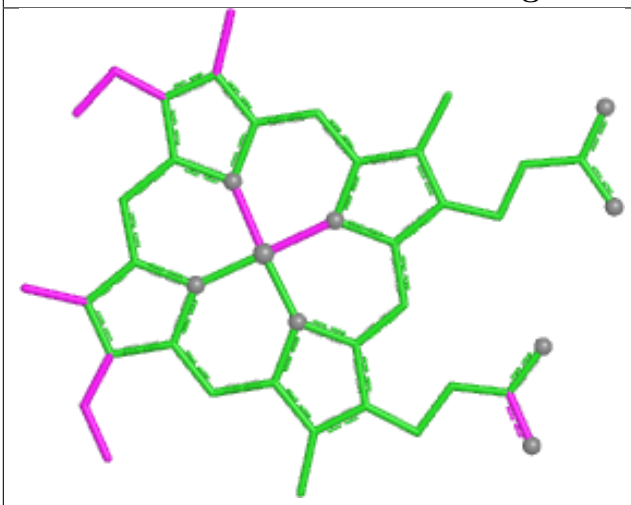


Torsions

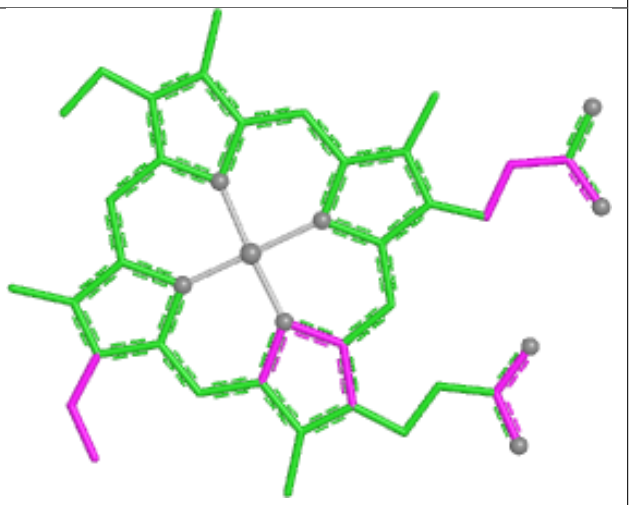


Rings

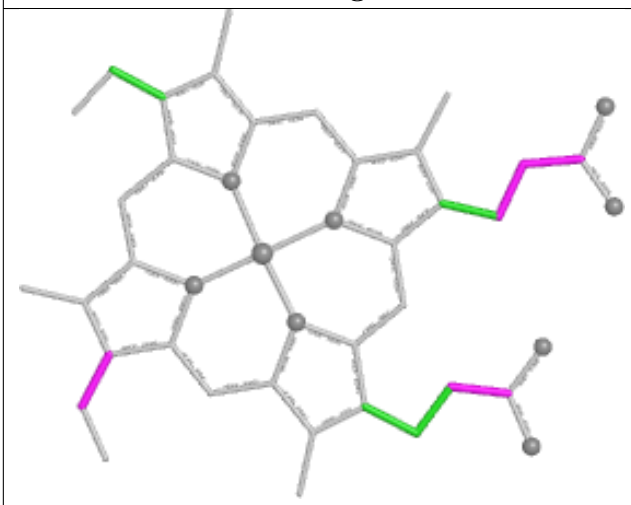
Ligand HEC D 602



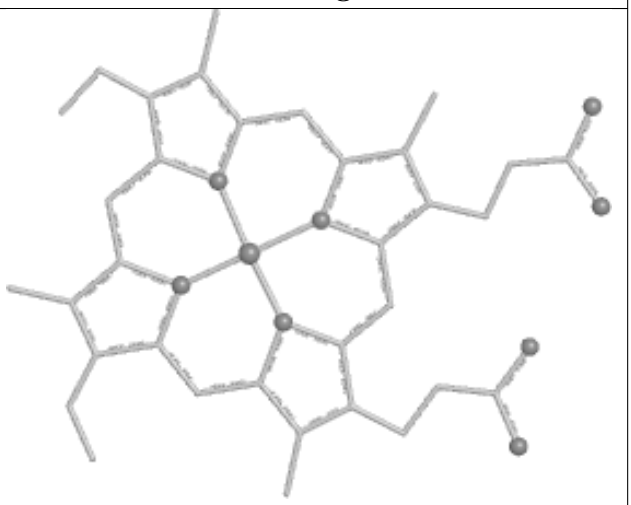
Bond lengths



Bond angles

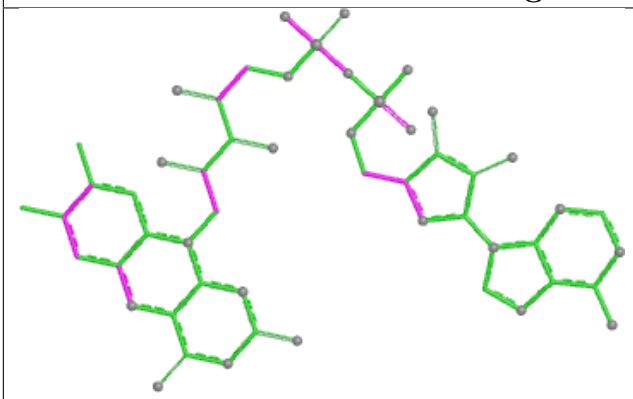


Torsions

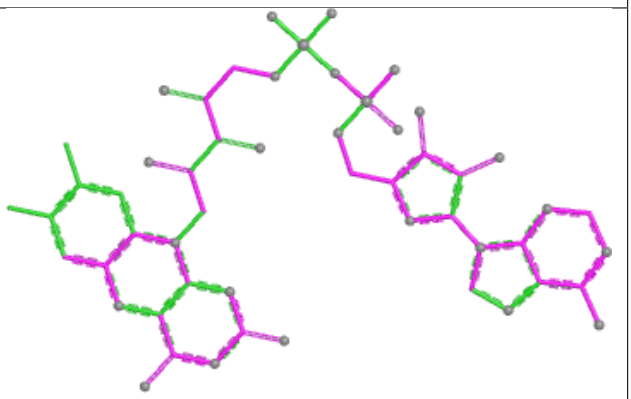


Rings

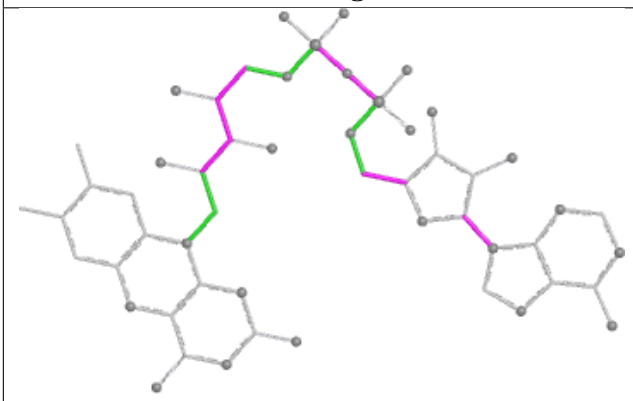
Ligand FAD C 800



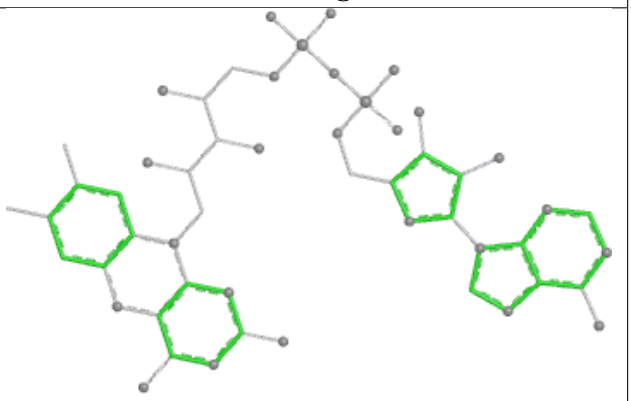
Bond lengths



Bond angles

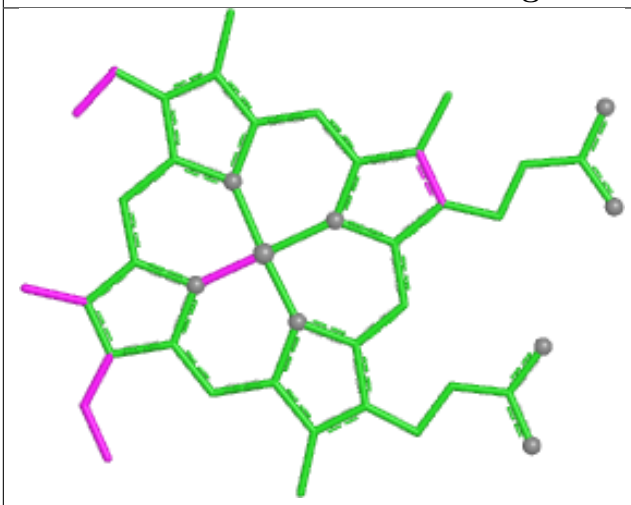


Torsions

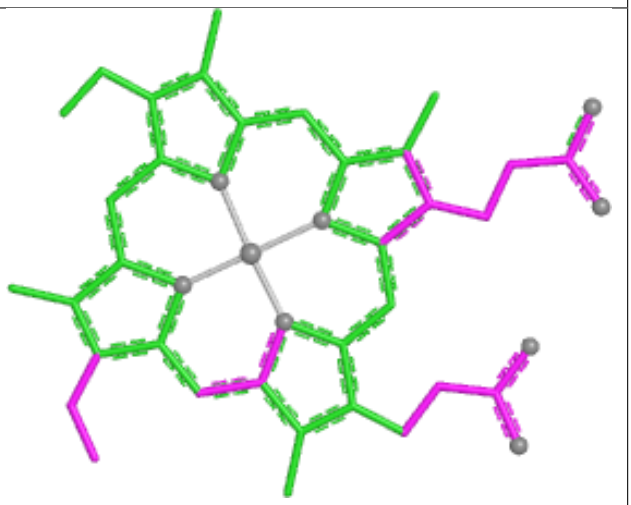


Rings

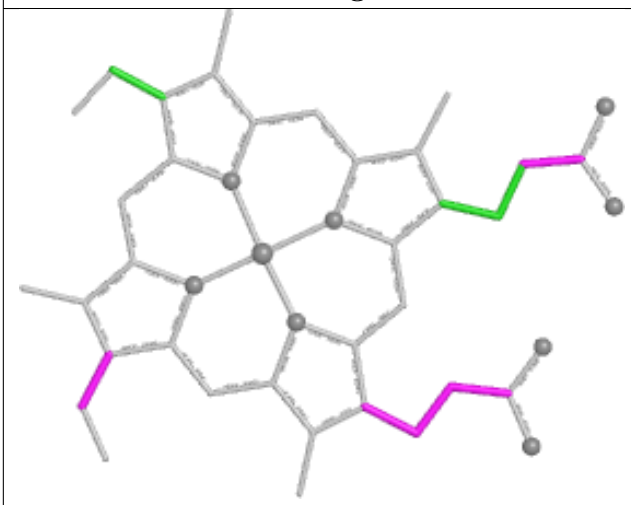
Ligand HEC D 601



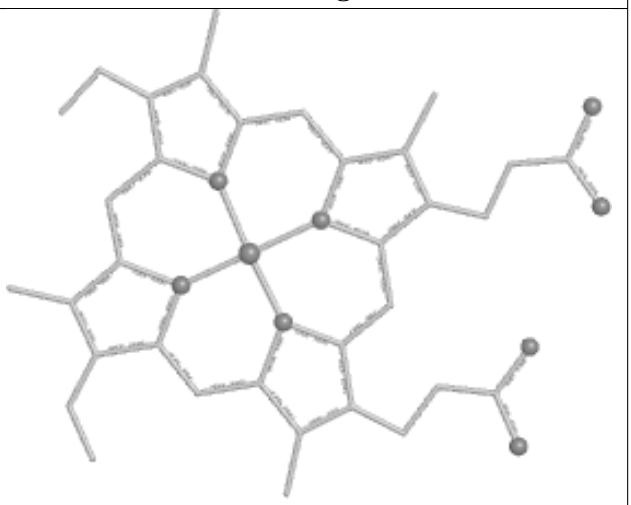
Bond lengths



Bond angles

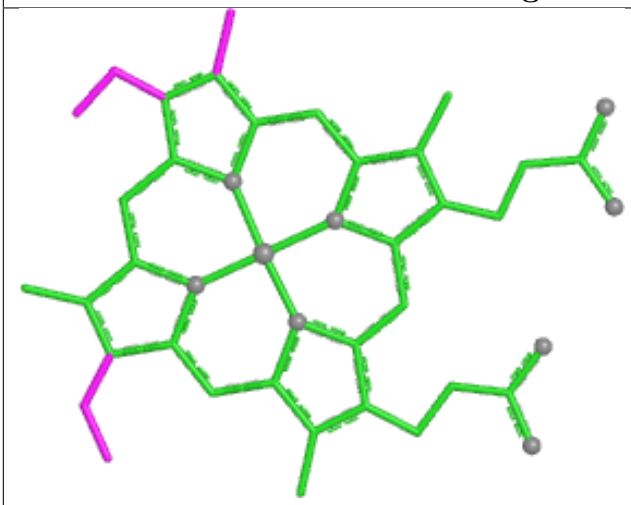


Torsions



Rings

Ligand HEC D 604



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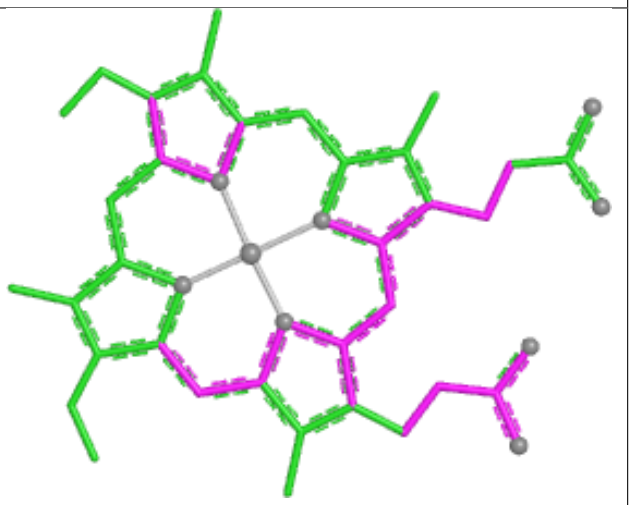

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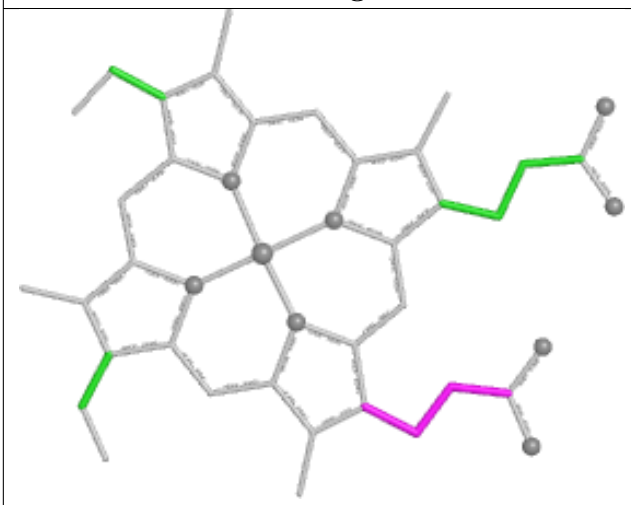

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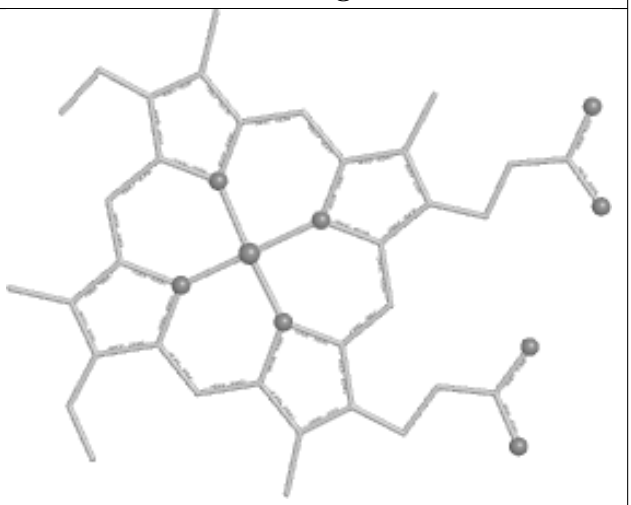
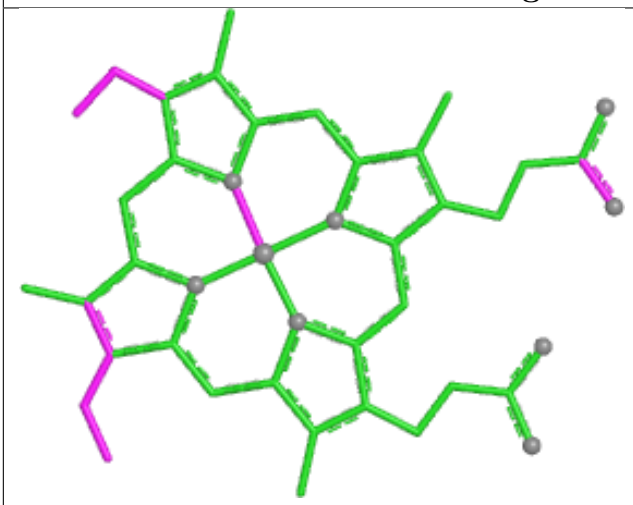


Rings

Ligand HEC A 603



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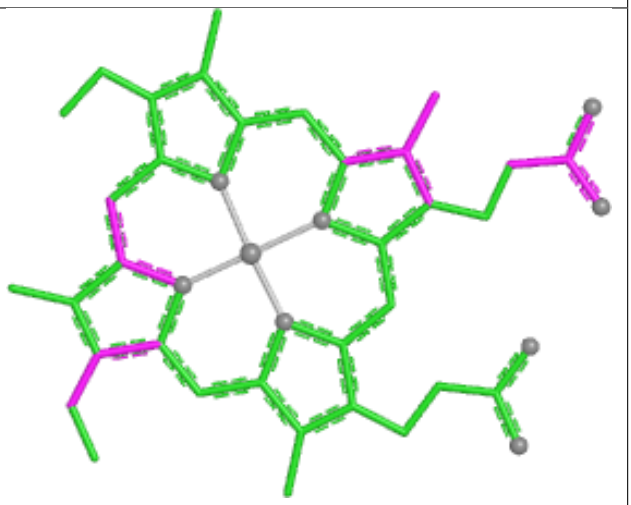

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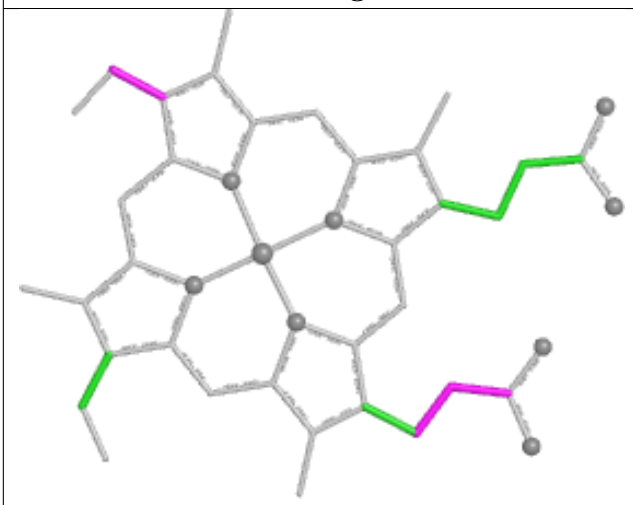

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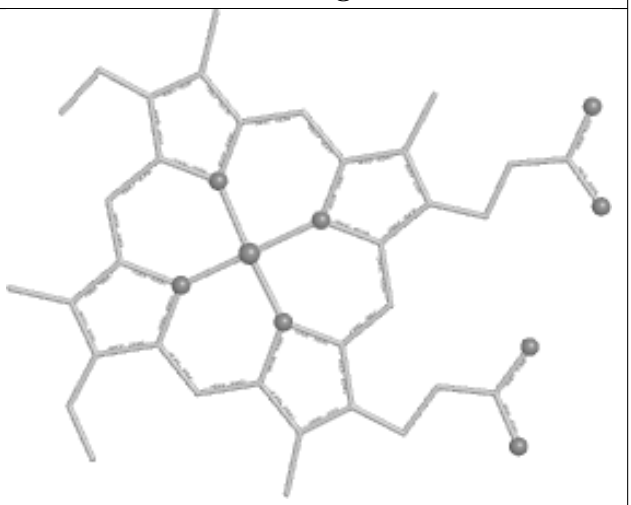

Rings

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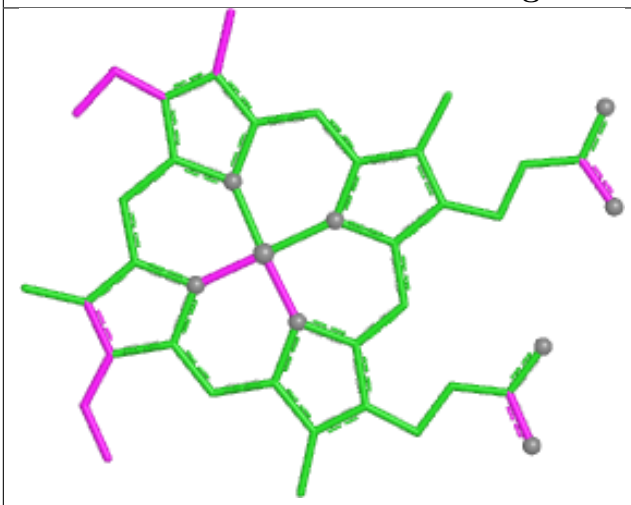

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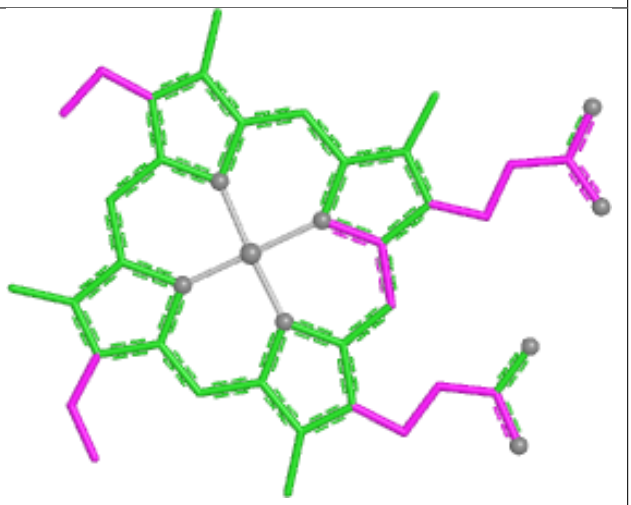
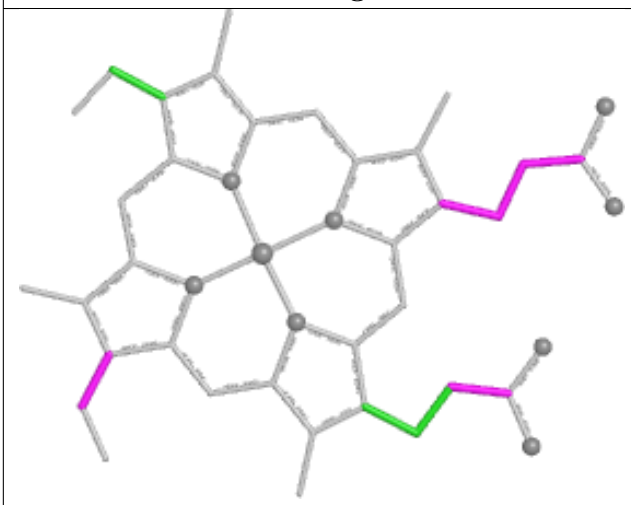


Bond angles



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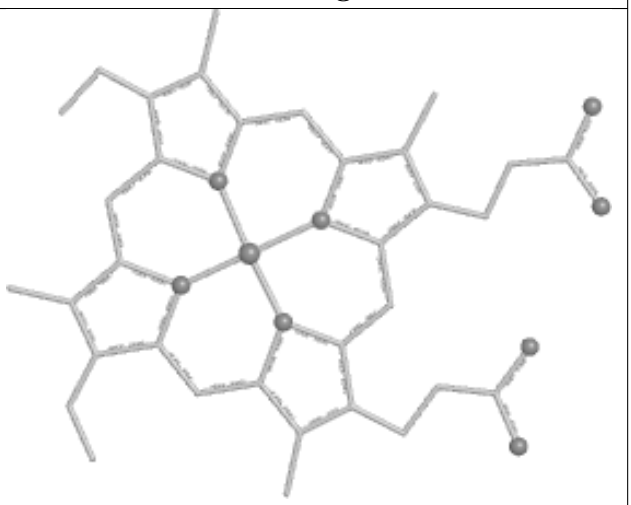
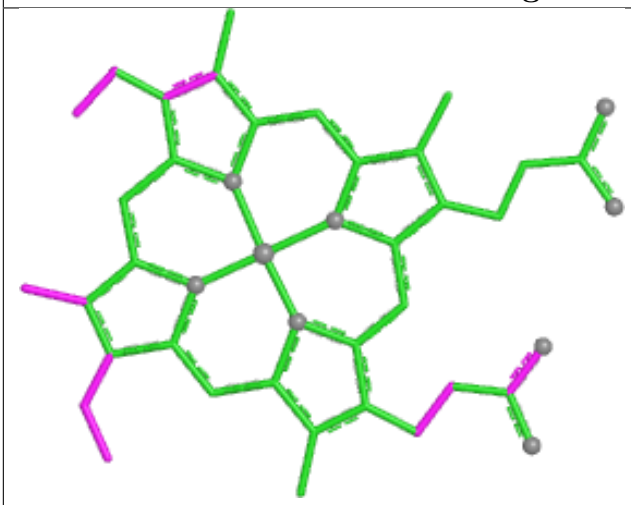


Rings

Ligand HEC A 601



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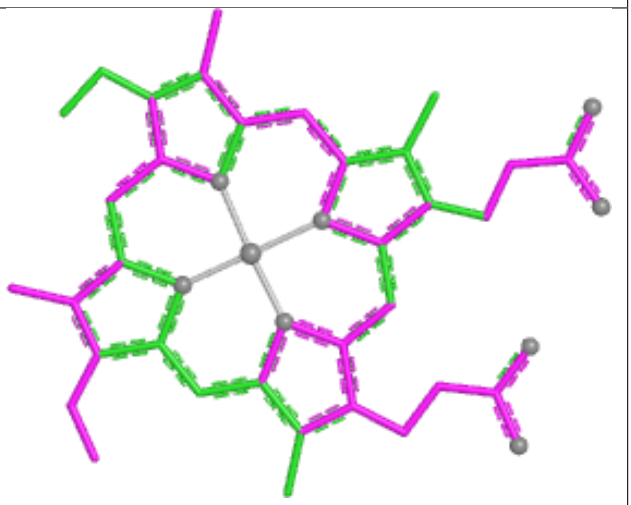

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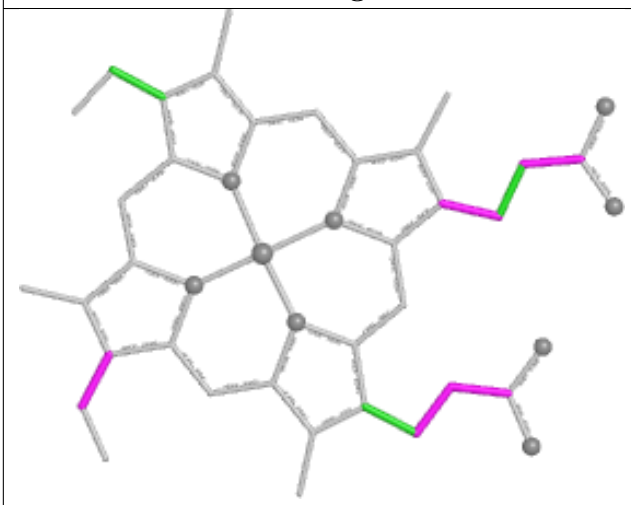

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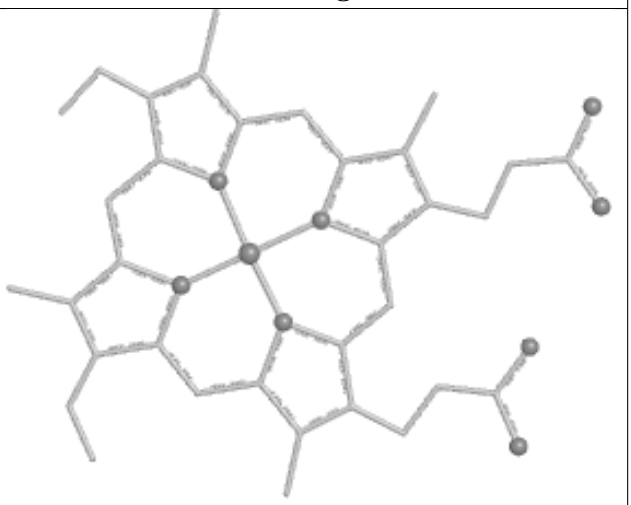
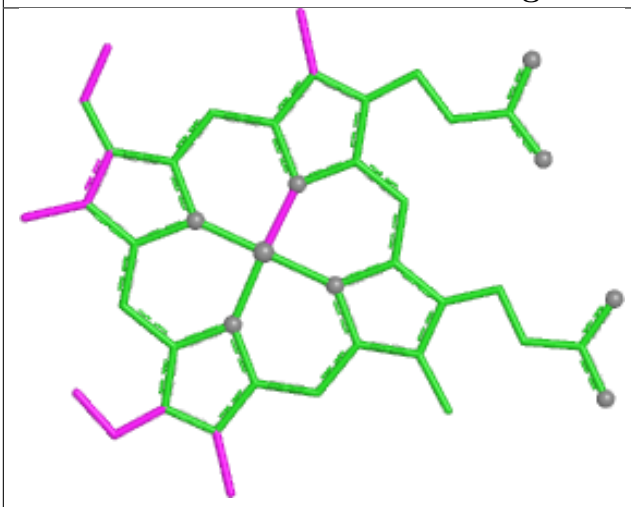


Rings

Ligand HEC A 604



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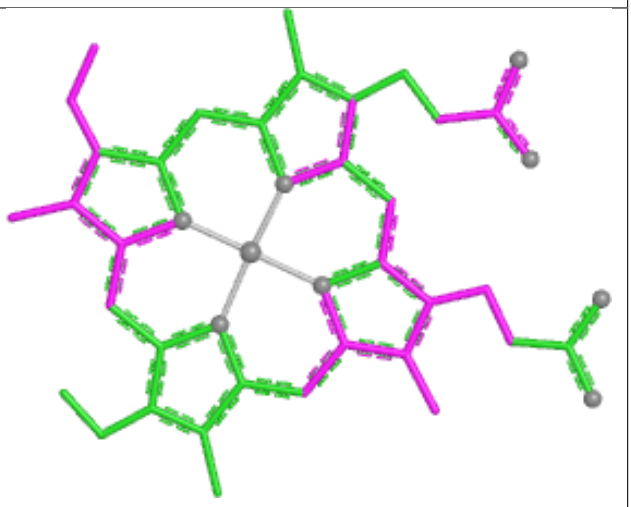

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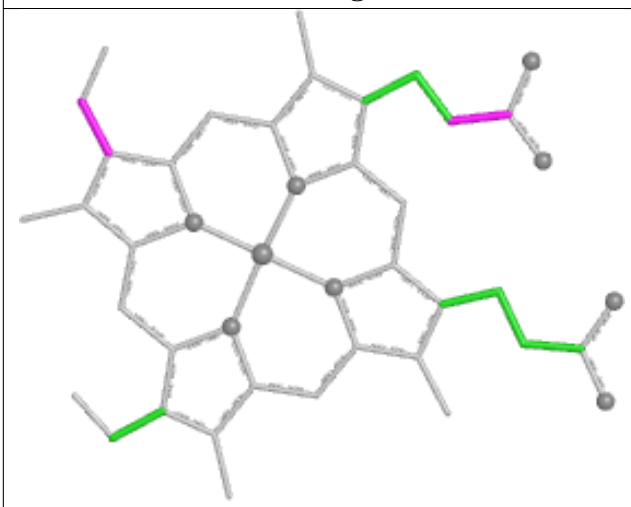

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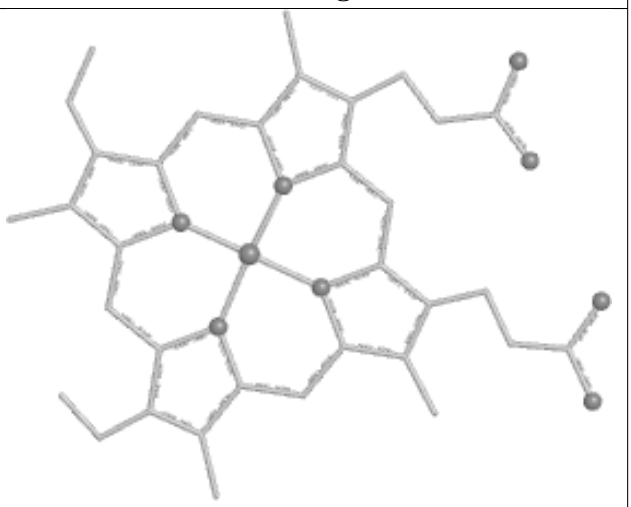
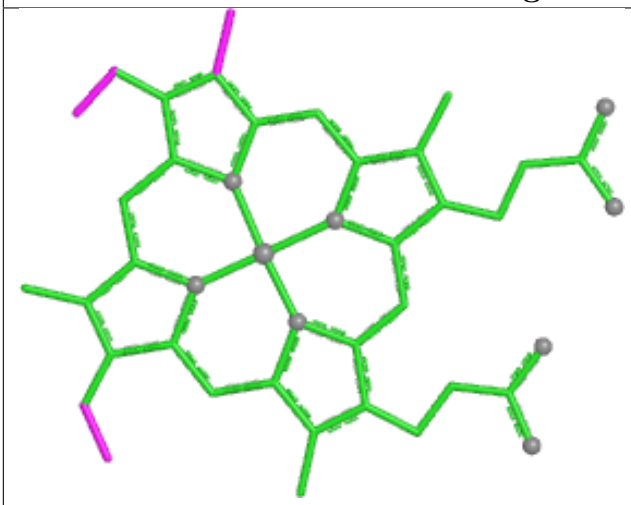


Rings

Ligand HEC B 602



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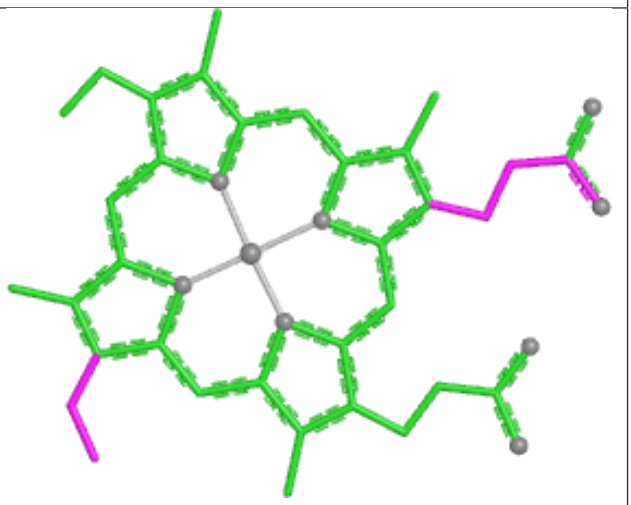

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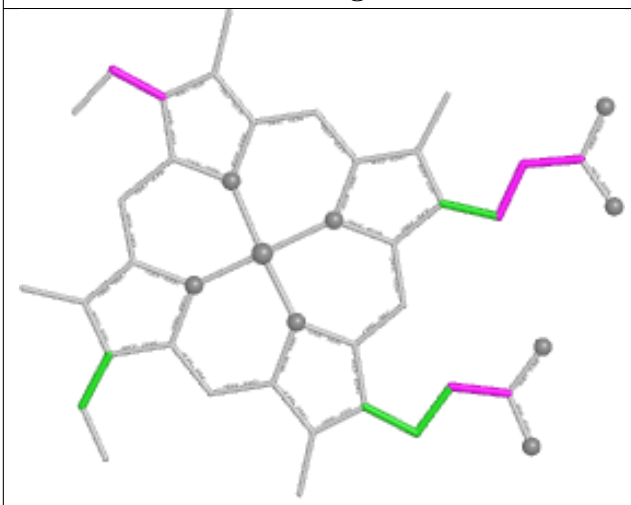

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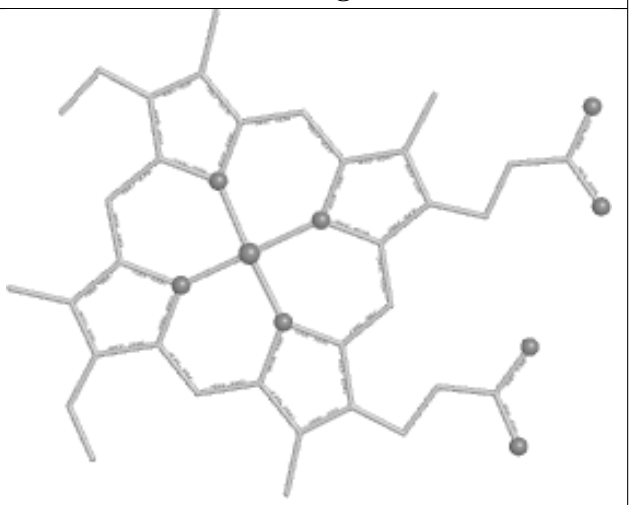
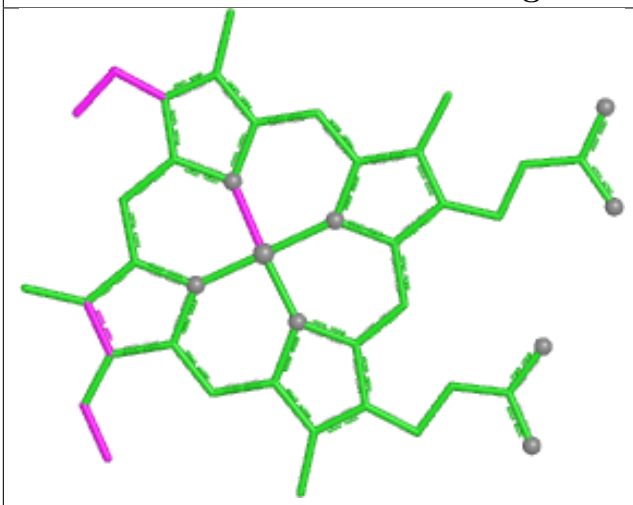


Rings

Ligand HEC C 603



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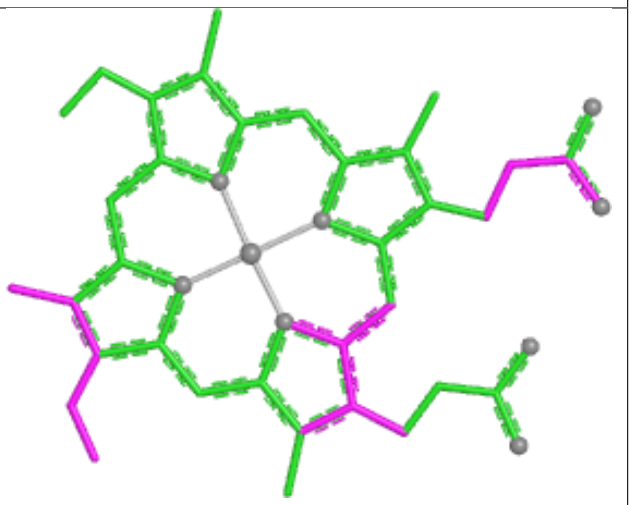
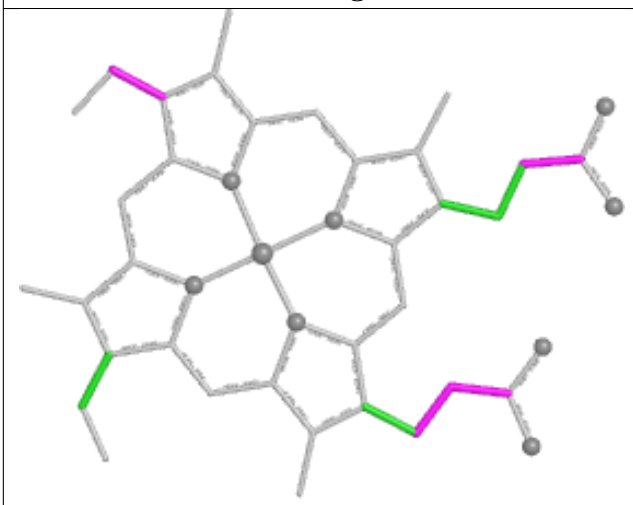


Bond angles



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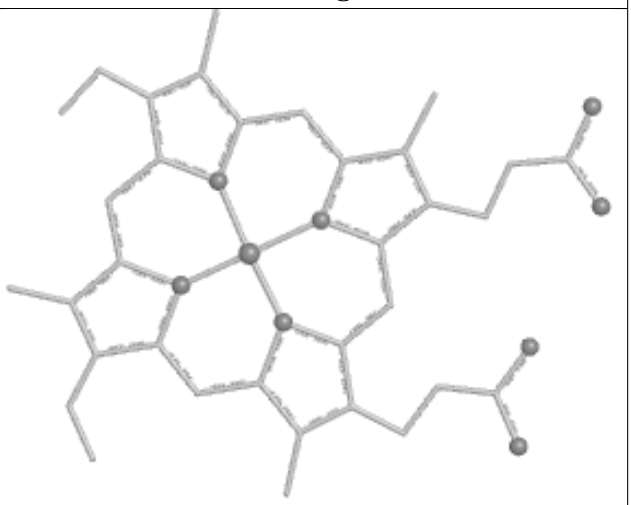

Rings

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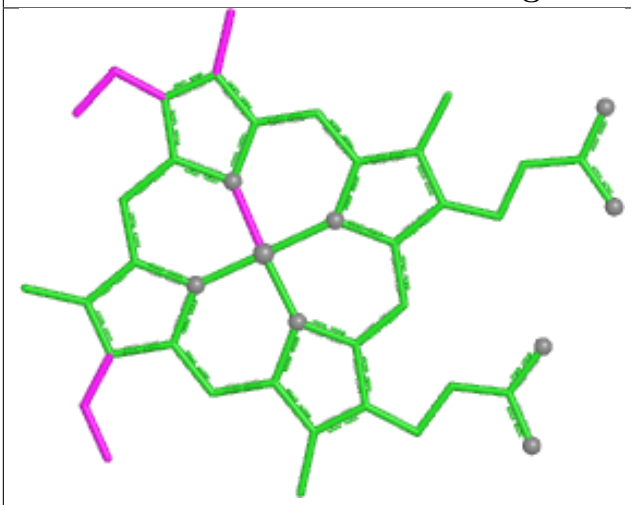

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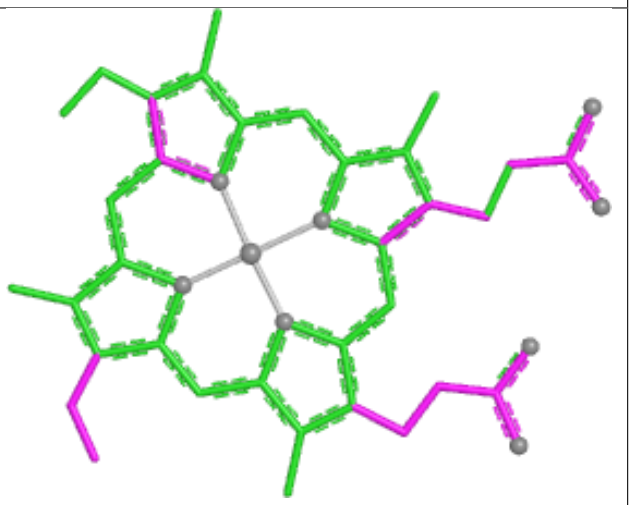
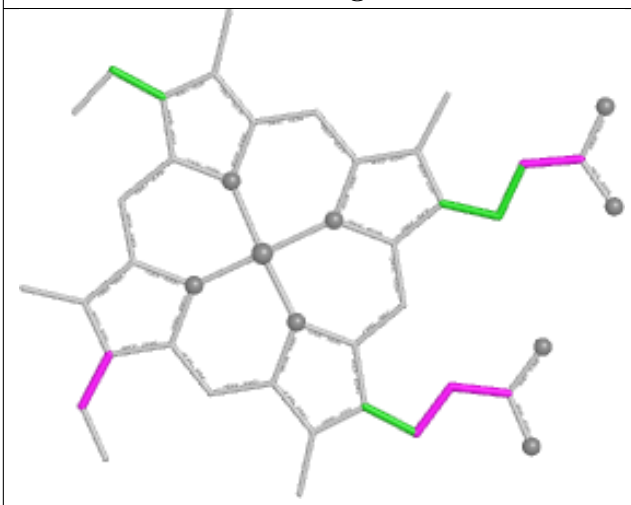


Bond angles



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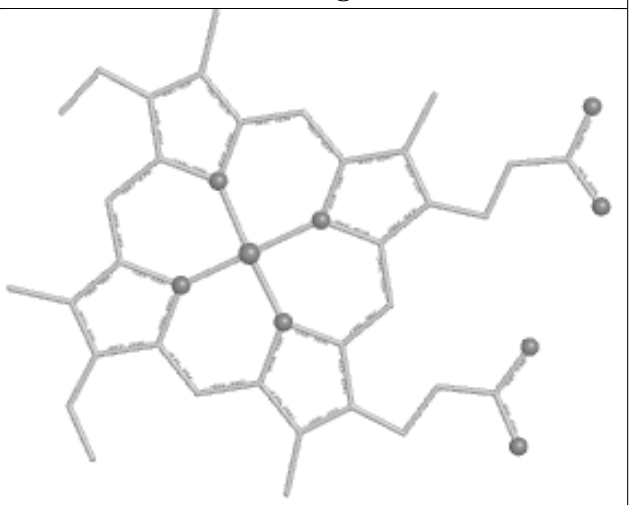
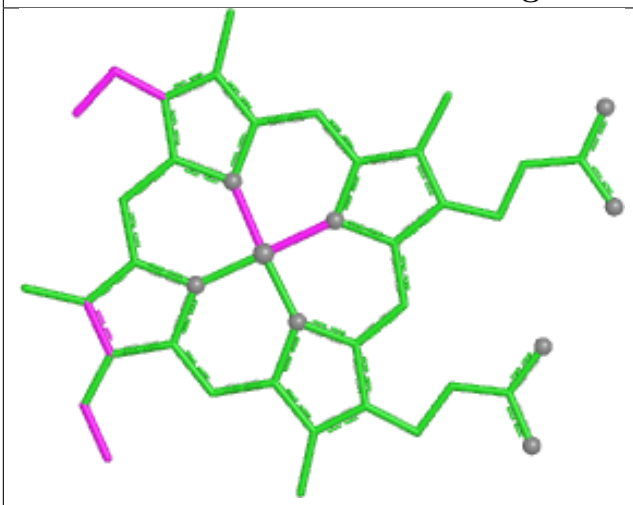


Rings

Ligand HEC D 603



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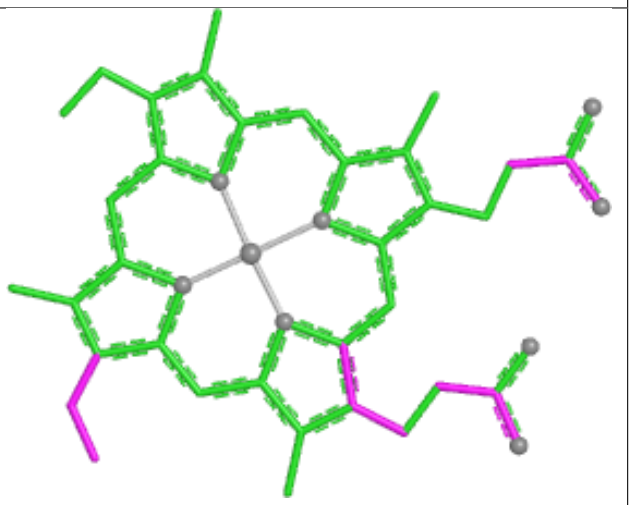
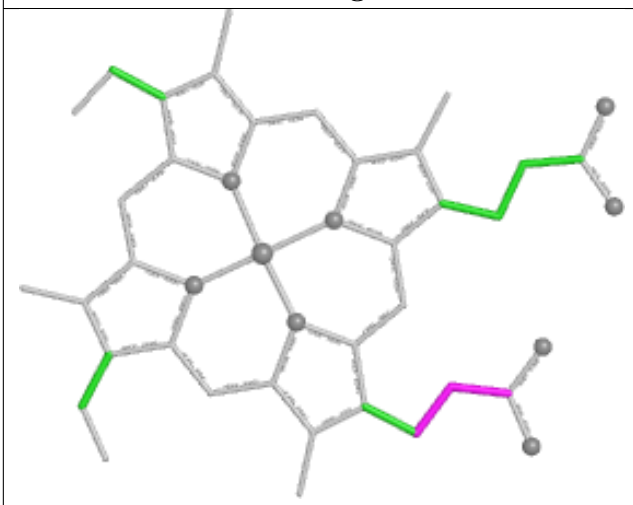


Bond angles



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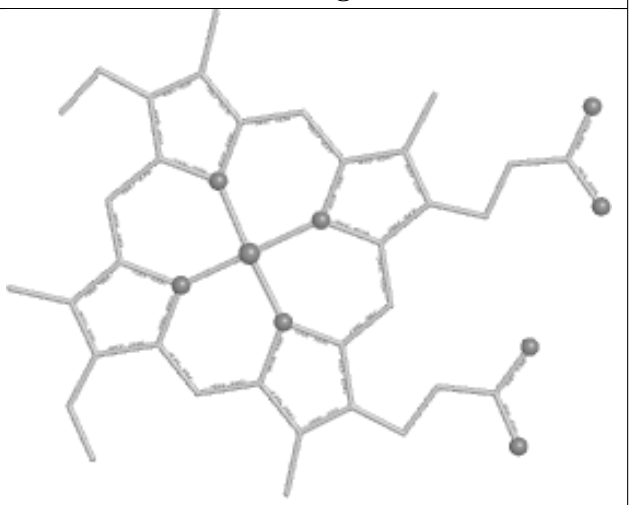
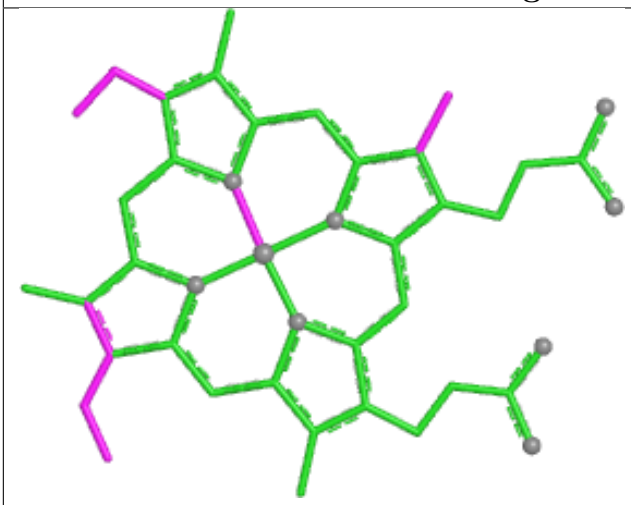


Rings

Ligand HEC B 601



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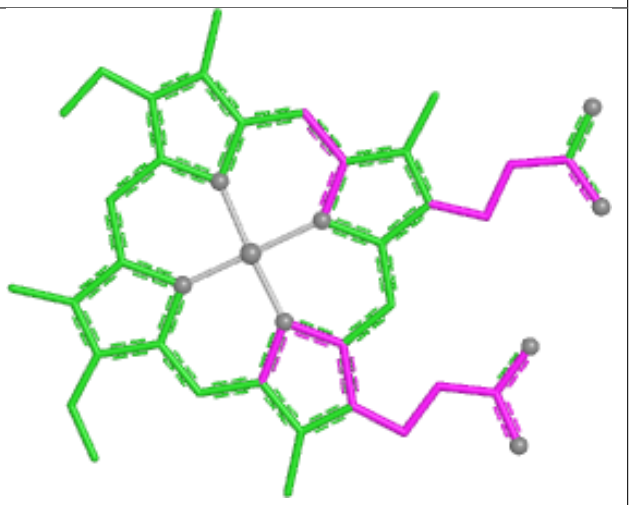
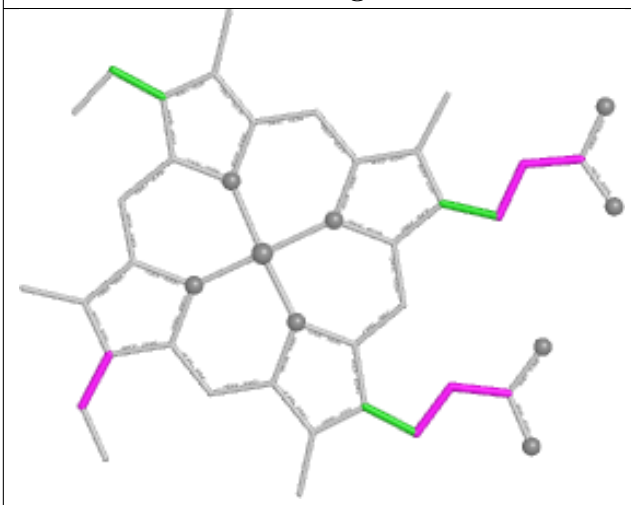


Bond angles



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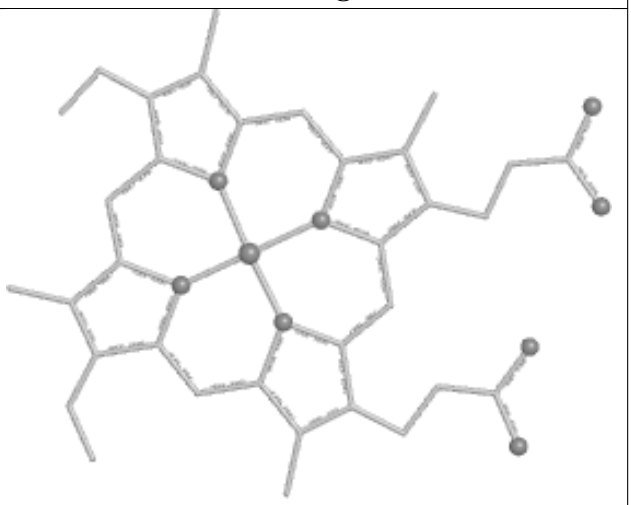
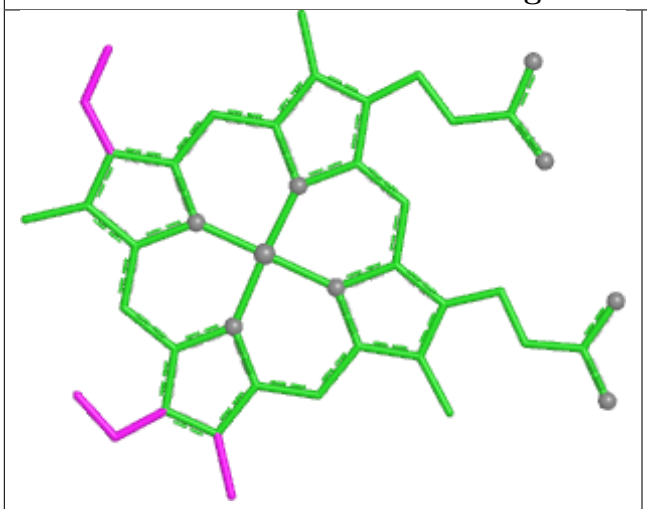


Rings

Ligand HEC B 604



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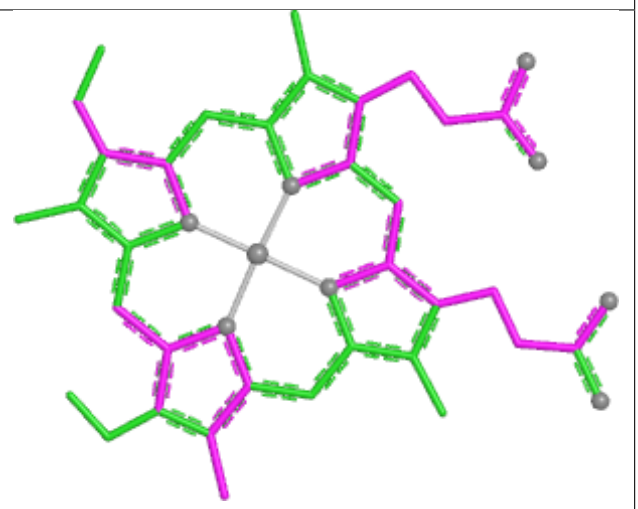
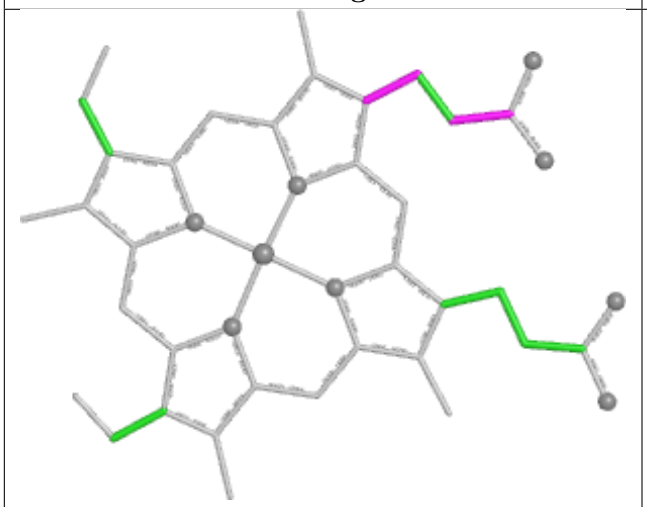


Bond angles



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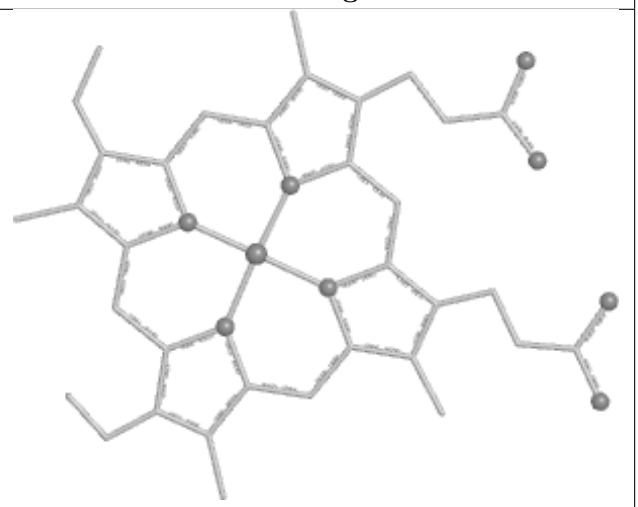
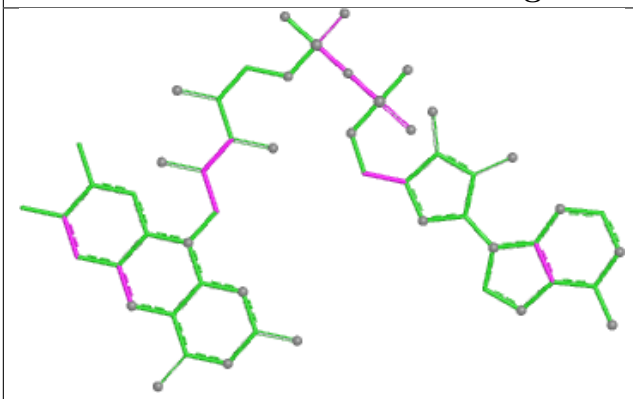


Rings

Ligand FAD D 900



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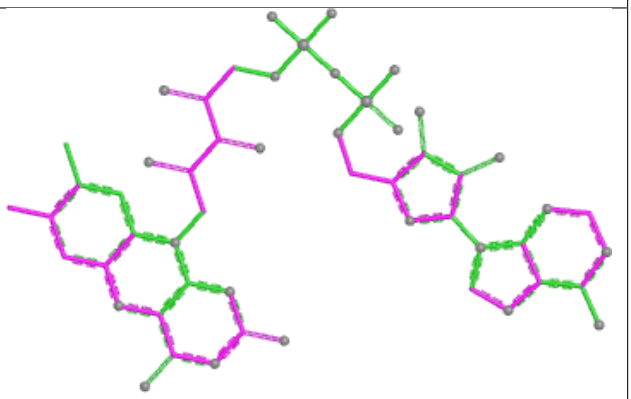
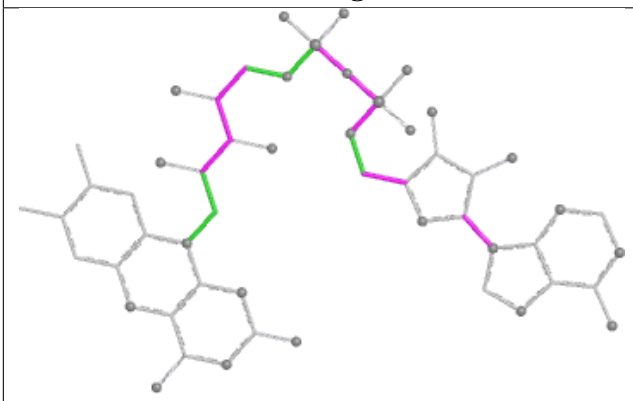


Bond angles



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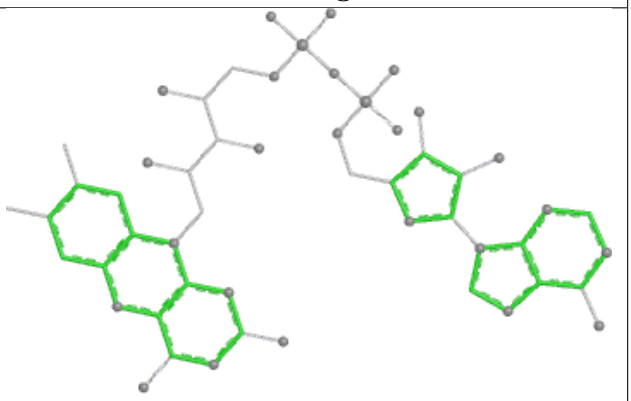
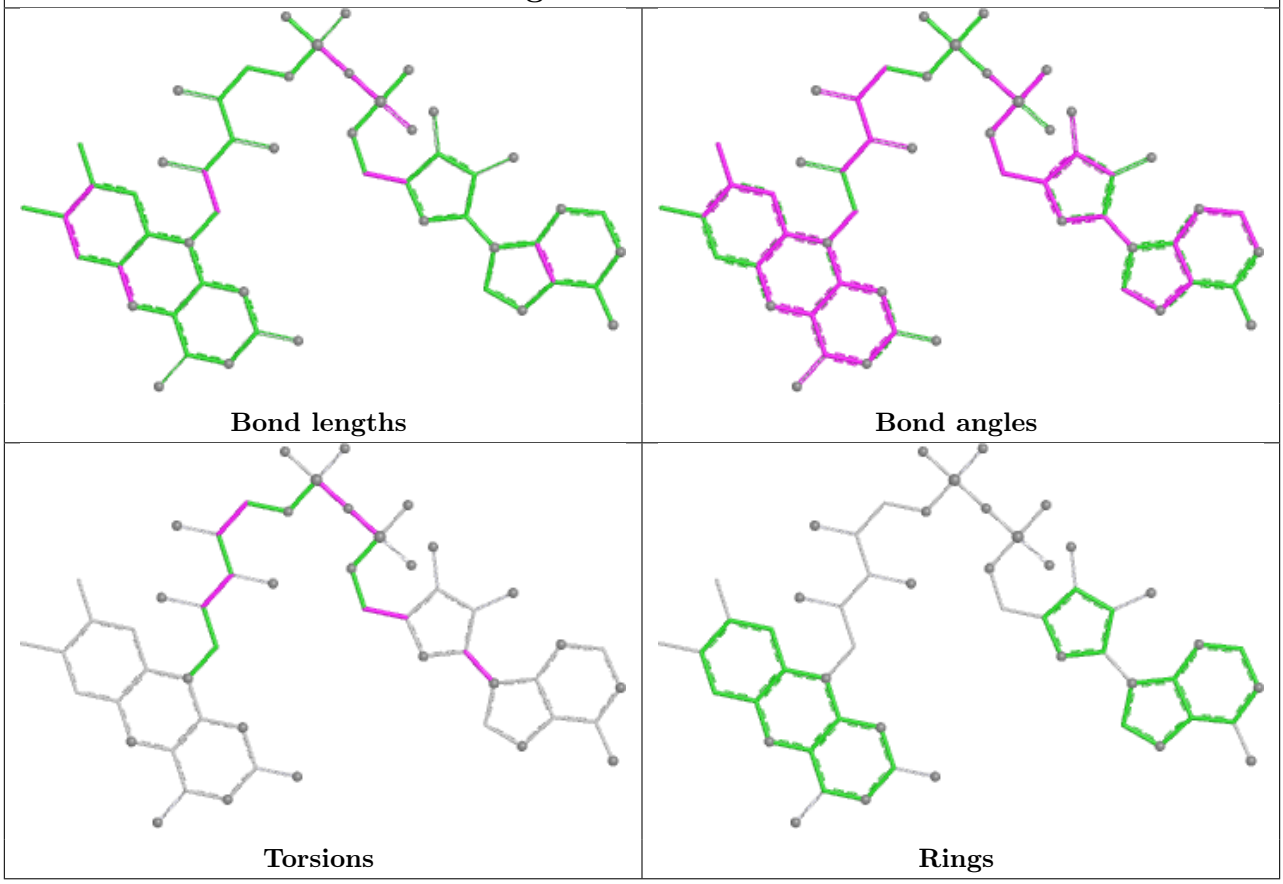


Rings

Ligand FAD B 700



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.