



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 06:03 AM EDT

PDB ID : 1D4E / pdb_00001d4e
Title : CRYSTAL STRUCTURE OF THE FLAVOCYTOCHROME C FUMARATE
REDUCTASE OF SHEWANELLA PUTREFACIENS STRAIN MR-1 COM-
PLEXED WITH FUMARATE
Authors : Leys, D.; Tsapin, A.S.; Meyer, T.E.; Cusanovich, M.A.; Van Beeumen, J.J.
Deposited on : 1999-10-03
Resolution : 2.80 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 ⓘ 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 ⓘ](#)) 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

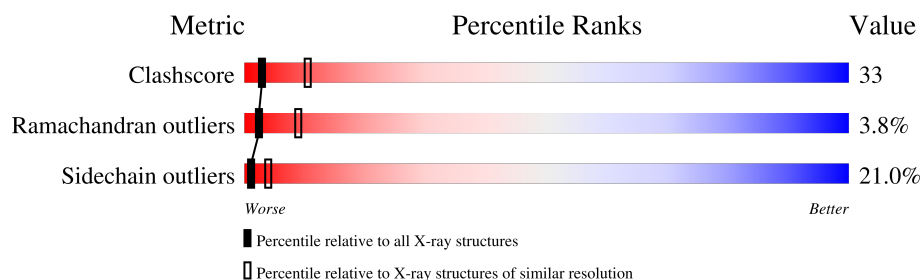
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

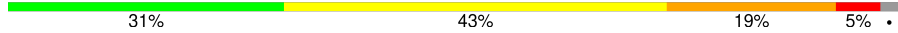
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	572	

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	604	X	-	-	-
3	FAD	A	600	X	-	-	-
4	FUM	A	700	-	-	X	-

2 Entry composition [i](#)

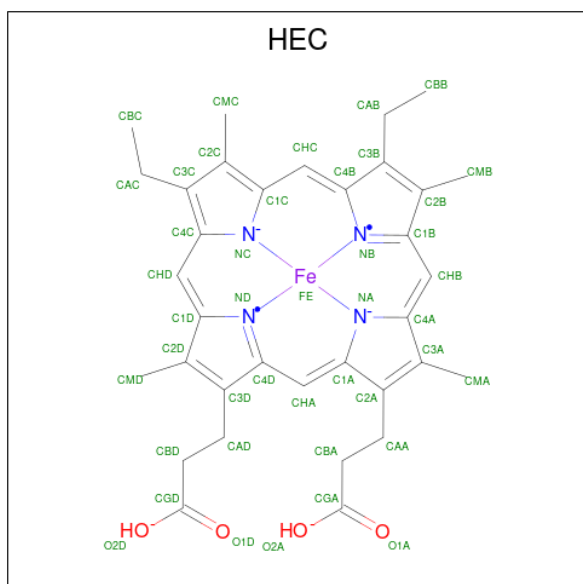
There are 5 unique types of molecules in this entry. The entry contains 4254 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

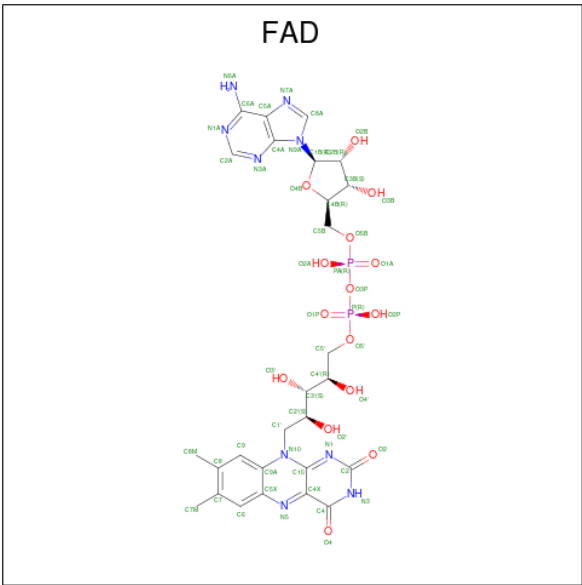
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	560	Total	C	N	O	S	0	0	0
			3965	2462	710	774	19			

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



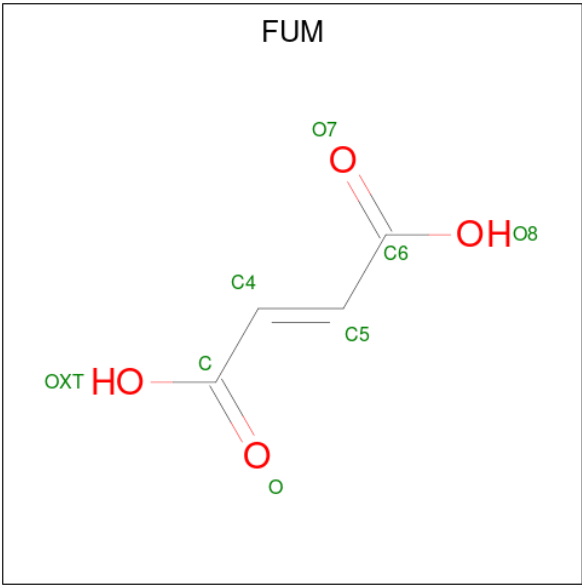
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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		

- Molecule 4 is FUMARIC ACID (CCD ID: FUM) (formula: C₄H₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	4	4		

- Molecule 5 is water.

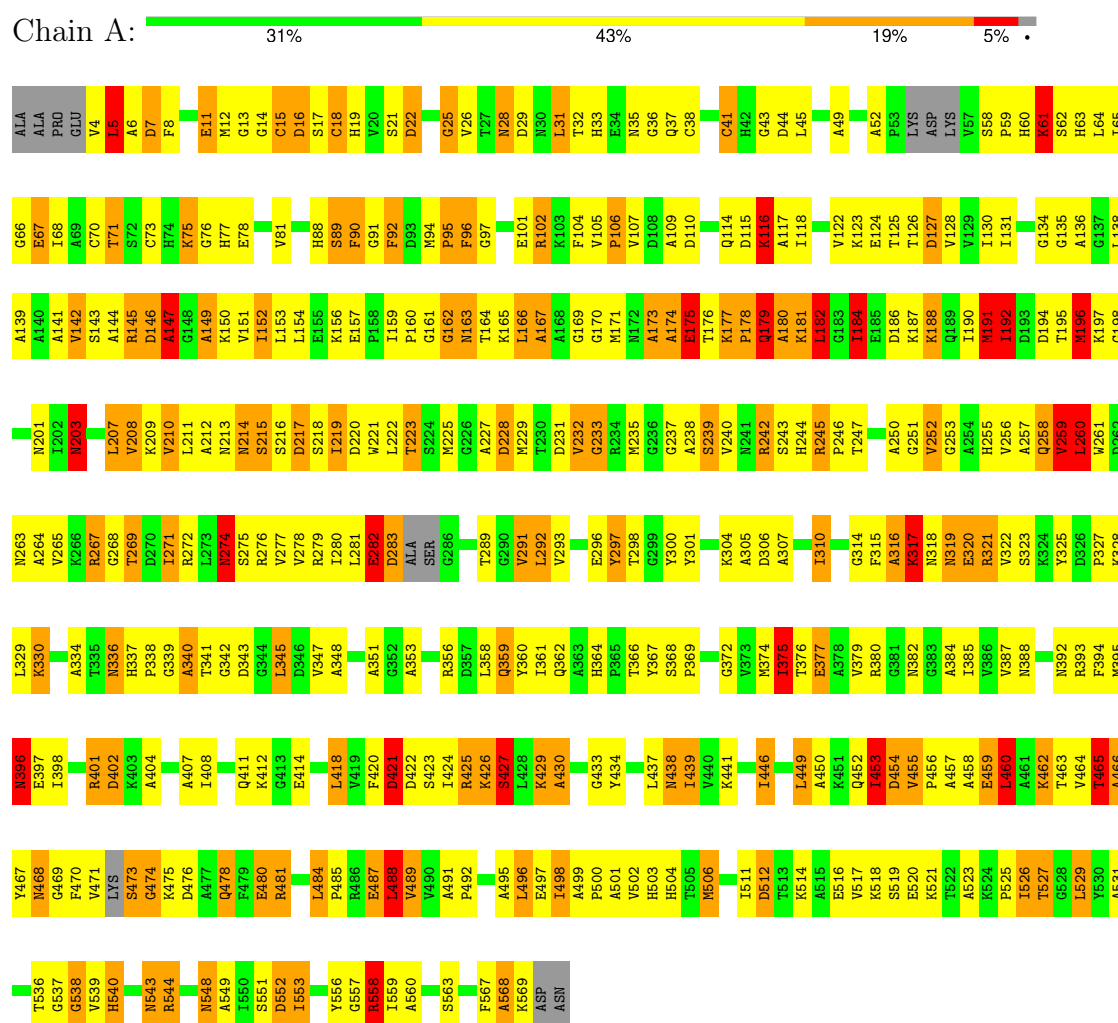
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total	O	0	0
			56	56		

3 Residue-property plots

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



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	73.08Å 73.08Å 216.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.80)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.243 , 0.311	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4254	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.88	0/4029	2.59	333/5478 (6.1%)

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	2

There are no bond length outliers.

All (333) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	GLU	CA-C-N	16.39	151.47	120.99
1	A	175	GLU	C-N-CA	16.39	151.47	120.99
1	A	468	ASN	CA-CB-CG	-14.37	98.23	112.60
1	A	491	ALA	CA-C-O	-13.95	105.52	120.87
1	A	318	ASN	OD1-CG-ND2	12.66	135.26	122.60
1	A	362	GLN	OE1-CD-NE2	-12.53	110.07	122.60
1	A	174	ALA	CA-C-O	12.40	134.92	120.66
1	A	220	ASP	CA-CB-CG	12.40	125.00	112.60
1	A	426	LYS	CA-C-O	-12.10	107.12	120.92
1	A	375	ILE	N-CA-CB	11.74	127.78	111.82
1	A	144	ALA	CA-C-O	11.60	133.00	120.82
1	A	283	ASP	CA-C-O	11.00	139.50	120.80
1	A	558	ARG	CD-NE-CZ	10.75	139.45	124.40
1	A	385	ILE	CA-C-O	-10.73	109.36	121.92
1	A	274	ASN	OD1-CG-ND2	10.50	133.10	122.60
1	A	281	LEU	CA-C-N	10.44	137.95	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	LEU	C-N-CA	10.44	137.95	121.66
1	A	282	GLU	CB-CG-CD	10.36	130.20	112.60
1	A	438	ASN	CA-CB-CG	10.32	122.92	112.60
1	A	499	ALA	CB-CA-C	10.26	124.42	110.37
1	A	512	ASP	CA-CB-CG	10.12	122.72	112.60
1	A	122	VAL	N-CA-CB	9.89	127.54	111.23
1	A	203	ASN	CA-CB-CG	9.77	122.37	112.60
1	A	281	LEU	CA-C-O	9.56	131.14	120.43
1	A	149	ALA	N-CA-C	9.50	124.52	110.17
1	A	15	CYS	CA-C-N	9.45	133.33	120.38
1	A	15	CYS	C-N-CA	9.45	133.33	120.38
1	A	22	ASP	CA-CB-CG	9.40	122.00	112.60
1	A	316	ALA	CA-C-O	-9.37	111.62	121.55
1	A	161	GLY	N-CA-C	9.24	128.15	115.30
1	A	92	PHE	CA-C-O	-9.24	111.08	121.89
1	A	454	ASP	CA-CB-CG	9.22	121.82	112.60
1	A	184	ILE	N-CA-CB	9.19	121.97	111.21
1	A	418	LEU	N-CA-CB	9.11	123.35	109.97
1	A	263	ASN	OD1-CG-ND2	9.09	131.69	122.60
1	A	77	HIS	CA-CB-CG	-9.04	104.76	113.80
1	A	356	ARG	NE-CZ-NH1	-8.83	112.67	121.50
1	A	446	ILE	CA-C-O	-8.80	111.79	120.95
1	A	31	LEU	N-CA-CB	-8.72	98.96	112.13
1	A	527	THR	CA-C-O	8.70	130.82	120.81
1	A	169	GLY	N-CA-C	8.60	129.68	115.66
1	A	19	HIS	CA-CB-CG	-8.55	105.25	113.80
1	A	376	THR	N-CA-C	8.49	122.21	110.24
1	A	128	VAL	N-CA-CB	-8.39	100.88	111.46
1	A	13	GLY	N-CA-C	8.29	128.91	115.73
1	A	214	ASN	OD1-CG-ND2	-8.26	114.34	122.60
1	A	178	PRO	CA-C-N	8.16	137.13	121.54
1	A	178	PRO	C-N-CA	8.16	137.13	121.54
1	A	487	GLU	N-CA-C	8.13	122.48	112.23
1	A	144	ALA	O-C-N	-8.10	113.73	122.07
1	A	452	GLN	CA-C-O	8.04	128.94	120.42
1	A	43	GLY	CA-C-O	8.00	129.93	122.57
1	A	267	ARG	NE-CZ-NH2	8.00	126.40	119.20
1	A	421	ASP	N-CA-C	7.94	122.16	110.17
1	A	551	SER	CA-C-O	-7.83	111.55	120.24
1	A	465	THR	N-CA-CB	7.80	121.33	110.01
1	A	401	ARG	CD-NE-CZ	7.74	135.23	124.40
1	A	496	LEU	CA-C-O	-7.72	111.34	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	GLY	CA-C-O	7.71	128.20	120.64
1	A	163	ASN	CA-CB-CG	7.69	120.29	112.60
1	A	459	GLU	CB-CG-CD	7.62	125.55	112.60
1	A	179	GLN	CB-CG-CD	7.55	125.44	112.60
1	A	552	ASP	CA-CB-CG	7.53	120.13	112.60
1	A	88	HIS	CA-CB-CG	7.51	121.31	113.80
1	A	320	GLU	CB-CG-CD	7.51	125.37	112.60
1	A	421	ASP	N-CA-CB	-7.51	98.42	110.51
1	A	503	HIS	N-CA-C	7.47	123.12	113.18
1	A	128	VAL	N-CA-C	7.38	118.51	107.80
1	A	147	ALA	N-CA-C	-7.38	95.08	110.80
1	A	421	ASP	CA-CB-CG	-7.36	105.24	112.60
1	A	191	MET	CA-CB-CG	7.35	128.80	114.10
1	A	321	ARG	NE-CZ-NH2	7.33	125.80	119.20
1	A	117	ALA	CA-C-O	-7.31	110.39	119.38
1	A	247	THR	N-CA-C	7.30	120.97	110.10
1	A	292	LEU	CA-C-N	7.30	132.13	122.93
1	A	292	LEU	C-N-CA	7.30	132.13	122.93
1	A	360	TYR	CA-C-N	7.29	133.02	123.11
1	A	360	TYR	C-N-CA	7.29	133.02	123.11
1	A	519	SER	CA-C-O	-7.29	112.75	121.05
1	A	135	GLY	CA-C-O	-7.27	113.26	120.75
1	A	422	ASP	CA-C-O	7.27	128.32	119.31
1	A	5	LEU	CA-C-O	-7.26	110.13	120.51
1	A	251	GLY	CA-C-N	7.24	132.51	120.64
1	A	251	GLY	C-N-CA	7.24	132.51	120.64
1	A	455	VAL	N-CA-CB	7.22	121.31	111.21
1	A	213	ASN	CB-CG-ND2	-7.21	105.58	116.40
1	A	242	ARG	NE-CZ-NH2	7.15	125.64	119.20
1	A	149	ALA	CA-C-O	7.15	131.17	121.88
1	A	452	GLN	CA-C-N	7.14	132.35	120.64
1	A	452	GLN	C-N-CA	7.14	132.35	120.64
1	A	36	GLY	N-CA-C	-7.06	104.31	112.50
1	A	196	MET	CB-CA-C	7.05	122.63	110.79
1	A	178	PRO	CB-CA-C	-7.00	100.01	111.56
1	A	314	GLY	N-CA-C	7.00	123.43	112.31
1	A	382	ASN	OD1-CG-ND2	-6.98	115.62	122.60
1	A	147	ALA	CA-C-O	6.97	130.48	120.51
1	A	263	ASN	CA-CB-CG	-6.96	105.64	112.60
1	A	61	LYS	CA-CB-CG	6.95	127.99	114.10
1	A	95	PRO	CA-C-O	-6.94	113.52	121.36
1	A	160	PRO	N-CA-C	6.93	121.56	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	VAL	N-CA-CB	6.92	119.95	110.54
1	A	214	ASN	N-CA-C	-6.90	104.75	113.72
1	A	319	ASN	CA-C-O	-6.88	112.06	119.97
1	A	177	LYS	CA-C-N	6.88	128.44	119.84
1	A	177	LYS	C-N-CA	6.88	128.44	119.84
1	A	152	ILE	CB-CG1-CD1	6.86	128.20	113.80
1	A	492	PRO	N-CA-CB	6.84	110.13	102.60
1	A	130	ILE	CA-C-O	-6.84	113.21	120.39
1	A	201	ASN	CA-C-O	-6.83	112.47	119.78
1	A	328	LYS	CA-C-N	6.82	132.12	120.72
1	A	328	LYS	C-N-CA	6.82	132.12	120.72
1	A	143	SER	N-CA-C	6.81	119.28	111.11
1	A	321	ARG	NE-CZ-NH1	-6.80	114.69	121.50
1	A	446	ILE	CB-CG1-CD1	-6.80	99.52	113.80
1	A	181	LYS	CA-C-O	-6.79	110.79	120.51
1	A	353	ALA	O-C-N	-6.75	115.16	122.85
1	A	456	PRO	CA-C-O	6.73	128.70	121.03
1	A	551	SER	O-C-N	6.72	130.97	122.23
1	A	259	VAL	CA-C-O	-6.71	113.97	120.95
1	A	341	THR	CA-CB-OG1	-6.71	99.54	109.60
1	A	127	ASP	CA-C-N	6.70	131.82	123.12
1	A	127	ASP	C-N-CA	6.70	131.82	123.12
1	A	11	GLU	CB-CG-CD	6.69	123.98	112.60
1	A	291	VAL	N-CA-CB	-6.67	101.24	111.05
1	A	92	PHE	CA-C-N	-6.67	113.85	122.79
1	A	92	PHE	C-N-CA	-6.67	113.85	122.79
1	A	258	GLN	OE1-CD-NE2	6.66	129.26	122.60
1	A	499	ALA	O-C-N	-6.66	115.88	121.54
1	A	214	ASN	CB-CG-ND2	6.65	126.38	116.40
1	A	491	ALA	O-C-N	6.64	128.63	121.60
1	A	422	ASP	CA-CB-CG	-6.63	105.97	112.60
1	A	553	ILE	N-CA-CB	6.60	118.27	110.55
1	A	239	SER	CA-C-O	6.57	123.56	119.55
1	A	325	TYR	CB-CA-C	-6.56	98.04	109.07
1	A	421	ASP	CB-CA-C	-6.55	98.49	111.60
1	A	543	ASN	CA-CB-CG	-6.55	106.05	112.60
1	A	251	GLY	O-C-N	-6.54	116.30	123.49
1	A	164	THR	CA-C-N	6.53	131.04	120.60
1	A	164	THR	C-N-CA	6.53	131.04	120.60
1	A	317	LYS	N-CA-CB	6.50	121.48	110.49
1	A	11	GLU	N-CA-C	-6.49	103.32	111.11
1	A	491	ALA	N-CA-C	6.49	119.54	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	540	HIS	CA-CB-CG	-6.44	107.36	113.80
1	A	16	ASP	N-CA-CB	-6.43	100.41	110.06
1	A	217	ASP	CA-C-O	-6.42	114.03	120.90
1	A	556	TYR	CA-CB-CG	-6.42	102.35	113.90
1	A	207	LEU	O-C-N	-6.41	115.17	122.09
1	A	527	THR	N-CA-C	6.39	119.55	109.96
1	A	382	ASN	CA-CB-CG	6.39	118.99	112.60
1	A	526	ILE	N-CA-C	-6.38	100.53	109.21
1	A	489	VAL	O-C-N	-6.38	114.60	122.57
1	A	377	GLU	CA-C-O	6.37	127.20	119.49
1	A	67	GLU	CB-CG-CD	6.36	123.41	112.60
1	A	143	SER	CA-CB-OG	-6.36	98.39	111.10
1	A	237	GLY	N-CA-C	6.35	123.47	115.21
1	A	264	ALA	O-C-N	6.34	129.38	122.15
1	A	106	PRO	CA-C-O	6.34	128.57	121.34
1	A	44	ASP	CA-CB-CG	6.31	118.91	112.60
1	A	362	GLN	O-C-N	6.29	130.36	123.13
1	A	552	ASP	CA-C-O	-6.29	114.22	120.82
1	A	196	MET	CA-C-O	6.27	127.26	120.55
1	A	222	LEU	CB-CA-C	6.26	120.82	110.81
1	A	368	SER	CA-C-N	6.26	125.48	118.97
1	A	368	SER	C-N-CA	6.26	125.48	118.97
1	A	318	ASN	CA-C-O	-6.26	114.57	121.58
1	A	104	PHE	CA-C-N	-6.25	117.89	123.33
1	A	104	PHE	C-N-CA	-6.25	117.89	123.33
1	A	356	ARG	NE-CZ-NH2	6.25	124.82	119.20
1	A	233	GLY	CA-C-N	6.25	131.08	122.77
1	A	233	GLY	C-N-CA	6.25	131.08	122.77
1	A	372	GLY	CA-C-O	6.23	127.32	119.72
1	A	474	GLY	N-CA-C	6.21	127.90	113.18
1	A	11	GLU	CA-CB-CG	6.20	126.50	114.10
1	A	551	SER	N-CA-CB	6.19	119.42	110.20
1	A	536	THR	N-CA-CB	6.17	120.18	110.56
1	A	227	ALA	N-CA-C	6.16	118.66	110.53
1	A	242	ARG	NE-CZ-NH1	-6.16	115.34	121.50
1	A	147	ALA	CB-CA-C	6.15	122.67	110.42
1	A	33	HIS	CA-CB-CG	-6.14	107.66	113.80
1	A	462	LYS	CA-C-O	-6.10	114.42	120.82
1	A	536	THR	CB-CA-C	-6.10	99.73	109.80
1	A	487	GLU	CA-C-O	-6.07	112.62	119.79
1	A	122	VAL	CA-C-N	6.06	129.98	120.89
1	A	122	VAL	C-N-CA	6.06	129.98	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	ALA	N-CA-C	6.04	118.41	110.08
1	A	217	ASP	CA-CB-CG	-6.04	106.56	112.60
1	A	232	VAL	CB-CA-C	-6.01	102.50	110.98
1	A	484	LEU	CA-C-N	6.00	125.39	118.85
1	A	484	LEU	C-N-CA	6.00	125.39	118.85
1	A	32	THR	CA-CB-OG1	-6.00	100.60	109.60
1	A	453	ILE	N-CA-CB	-5.99	98.20	111.50
1	A	526	ILE	CB-CA-C	5.99	119.84	111.34
1	A	457	ALA	N-CA-C	5.98	117.47	111.07
1	A	336	ASN	CA-C-O	-5.97	114.90	121.89
1	A	369	PRO	CA-C-O	5.95	128.65	120.03
1	A	396	ASN	CA-C-O	5.94	126.94	120.58
1	A	374	MET	CA-C-O	-5.93	115.34	121.87
1	A	489	VAL	N-CA-CB	-5.92	101.46	111.23
1	A	208	VAL	CA-C-N	5.91	130.46	120.88
1	A	208	VAL	C-N-CA	5.91	130.46	120.88
1	A	18	CYS	N-CA-C	5.91	120.54	112.68
1	A	426	LYS	CB-CA-C	5.90	119.11	109.90
1	A	263	ASN	CA-C-N	-5.90	111.92	120.29
1	A	263	ASN	C-N-CA	-5.90	111.92	120.29
1	A	523	ALA	CA-C-O	5.88	128.92	120.51
1	A	457	ALA	O-C-N	5.88	128.12	122.07
1	A	15	CYS	CA-C-O	5.85	126.45	119.60
1	A	14	GLY	N-CA-C	5.83	117.45	111.56
1	A	468	ASN	N-CA-CB	-5.83	101.25	109.94
1	A	264	ALA	CA-C-O	-5.83	114.24	120.42
1	A	278	VAL	CA-C-O	5.83	125.27	119.97
1	A	489	VAL	CA-C-N	5.82	131.02	123.11
1	A	489	VAL	C-N-CA	5.82	131.02	123.11
1	A	537	GLY	CA-C-O	5.81	126.64	120.94
1	A	367	TYR	CA-C-O	-5.81	114.57	121.66
1	A	245	ARG	CA-CB-CG	5.80	125.71	114.10
1	A	11	GLU	CB-CA-C	5.79	120.07	110.81
1	A	228	ASP	CA-CB-CG	-5.78	106.82	112.60
1	A	279	ARG	O-C-N	5.78	130.27	122.59
1	A	127	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	214	ASN	CB-CA-C	5.75	119.22	109.55
1	A	232	VAL	N-CA-C	5.75	117.28	108.71
1	A	316	ALA	O-C-N	-5.75	115.74	122.81
1	A	173	ALA	N-CA-CB	5.75	121.45	111.39
1	A	506	MET	CB-CA-C	-5.73	98.24	110.32
1	A	353	ALA	CA-C-O	5.72	128.56	121.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	THR	CA-C-O	-5.71	111.64	119.12
1	A	427	SER	N-CA-CB	5.68	120.08	110.49
1	A	208	VAL	O-C-N	-5.67	115.48	122.57
1	A	89	SER	CB-CA-C	5.66	120.16	111.95
1	A	425	ARG	CD-NE-CZ	5.65	132.31	124.40
1	A	480	GLU	N-CA-C	5.63	121.39	113.56
1	A	228	ASP	CB-CA-C	-5.63	103.21	111.77
1	A	317	LYS	CA-C-N	-5.61	113.36	122.34
1	A	317	LYS	C-N-CA	-5.61	113.36	122.34
1	A	150	LYS	CB-CA-C	5.61	118.78	109.53
1	A	323	SER	N-CA-C	-5.60	105.27	111.71
1	A	65	ILE	CB-CA-C	-5.60	103.18	111.19
1	A	134	GLY	O-C-N	-5.59	117.83	122.92
1	A	265	VAL	CA-C-N	5.58	127.69	120.44
1	A	265	VAL	C-N-CA	5.58	127.69	120.44
1	A	487	GLU	CA-CB-CG	-5.57	102.95	114.10
1	A	293	VAL	CB-CA-C	-5.57	103.26	110.84
1	A	167	ALA	N-CA-CB	5.56	118.73	109.56
1	A	182	LEU	CA-C-O	5.54	125.00	118.90
1	A	297	TYR	CA-CB-CG	-5.54	103.92	113.90
1	A	60	HIS	N-CA-C	-5.53	105.89	113.30
1	A	229	MET	N-CA-CB	-5.52	101.44	110.11
1	A	418	LEU	N-CA-C	-5.50	102.13	110.28
1	A	538	GLY	O-C-N	-5.50	116.69	122.52
1	A	36	GLY	CA-C-O	-5.49	115.08	121.00
1	A	117	ALA	N-CA-C	5.48	119.23	112.54
1	A	402	ASP	CA-C-O	-5.47	114.75	120.55
1	A	223	THR	O-C-N	-5.47	116.32	122.12
1	A	65	ILE	O-C-N	5.46	128.44	122.76
1	A	552	ASP	O-C-N	5.45	127.69	122.07
1	A	136	ALA	O-C-N	5.44	127.97	122.09
1	A	492	PRO	CA-C-N	5.44	130.81	122.93
1	A	492	PRO	C-N-CA	5.44	130.81	122.93
1	A	293	VAL	O-C-N	-5.43	117.00	123.03
1	A	171	MET	CA-C-O	-5.42	114.36	120.32
1	A	421	ASP	CA-C-O	-5.41	114.84	121.88
1	A	144	ALA	CA-C-N	5.41	127.53	120.28
1	A	144	ALA	C-N-CA	5.41	127.53	120.28
1	A	166	LEU	N-CA-C	-5.41	106.68	113.28
1	A	142	VAL	N-CA-CB	5.39	120.13	111.23
1	A	81	VAL	CB-CA-C	-5.39	101.16	110.65
1	A	7	ASP	N-CA-C	-5.39	104.83	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	544	ARG	CD-NE-CZ	5.38	131.94	124.40
1	A	485	PRO	N-CA-C	5.36	120.58	113.40
1	A	260	LEU	CA-C-O	-5.34	112.69	119.31
1	A	321	ARG	O-C-N	-5.34	116.57	122.07
1	A	548	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	A	310	ILE	N-CA-CB	5.34	118.08	111.41
1	A	466	ALA	CA-C-O	-5.34	115.19	120.90
1	A	146	ASP	CA-CB-CG	-5.33	107.27	112.60
1	A	336	ASN	O-C-N	5.33	128.92	122.68
1	A	276	ARG	CD-NE-CZ	-5.32	116.95	124.40
1	A	537	GLY	O-C-N	-5.32	117.16	123.18
1	A	366	THR	N-CA-C	5.32	116.04	108.54
1	A	214	ASN	CA-CB-CG	5.32	117.92	112.60
1	A	375	ILE	CA-CB-CG2	5.31	119.52	110.50
1	A	568	ALA	CA-C-O	-5.29	112.94	120.51
1	A	107	VAL	CA-C-N	5.28	130.77	122.11
1	A	107	VAL	C-N-CA	5.28	130.77	122.11
1	A	272	ARG	NE-CZ-NH2	-5.28	114.45	119.20
1	A	276	ARG	N-CA-CB	-5.28	102.26	110.55
1	A	92	PHE	N-CA-C	-5.28	102.94	110.59
1	A	65	ILE	CA-C-O	-5.26	115.76	121.92
1	A	427	SER	CA-C-O	-5.25	113.00	120.51
1	A	267	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	A	75	LYS	CG-CD-CE	5.24	123.35	111.30
1	A	260	LEU	N-CA-CB	5.22	118.90	110.40
1	A	267	ARG	CA-C-O	-5.22	113.05	120.51
1	A	563	SER	CA-C-O	5.22	126.48	120.90
1	A	503	HIS	CA-CB-CG	5.21	119.02	113.80
1	A	425	ARG	CG-CD-NE	5.21	123.47	112.00
1	A	41	CYS	CA-C-N	-5.20	113.99	122.26
1	A	41	CYS	C-N-CA	-5.20	113.99	122.26
1	A	271	ILE	CB-CA-C	-5.19	104.48	110.91
1	A	330	LYS	N-CA-CB	5.18	117.93	109.69
1	A	25	GLY	N-CA-C	5.17	119.38	112.65
1	A	19	HIS	CB-CG-CD2	5.17	137.92	131.20
1	A	81	VAL	CA-C-N	-5.17	113.38	120.71
1	A	81	VAL	C-N-CA	-5.17	113.38	120.71
1	A	179	GLN	O-C-N	5.16	129.45	122.59
1	A	498	ILE	CA-C-O	-5.15	116.53	121.63
1	A	304	LYS	N-CA-CB	5.15	118.57	110.23
1	A	96	PHE	CA-C-N	5.13	131.47	121.41
1	A	96	PHE	C-N-CA	5.13	131.47	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	ASP	N-CA-C	-5.13	106.70	113.12
1	A	201	ASN	N-CA-C	5.12	119.38	113.38
1	A	481	ARG	NH1-CZ-NH2	5.12	125.95	119.30
1	A	90	PHE	N-CA-CB	-5.11	102.43	110.46
1	A	283	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	429	LYS	O-C-N	-5.11	115.75	122.39
1	A	156	LYS	O-C-N	5.10	129.60	122.36
1	A	307	ALA	CA-C-O	-5.10	115.14	121.06
1	A	430	ALA	CA-C-O	-5.10	115.12	120.63
1	A	548	ASN	N-CA-CB	-5.10	102.69	110.33
1	A	242	ARG	N-CA-C	5.09	121.19	112.99
1	A	460	LEU	CA-C-O	5.08	125.93	120.55
1	A	439	ILE	CB-CA-C	-5.07	104.91	111.20
1	A	173	ALA	O-C-N	5.07	129.15	123.48
1	A	280	ILE	CA-C-O	-5.06	114.59	121.02
1	A	334	ALA	O-C-N	-5.05	116.34	123.11
1	A	116	LYS	CA-C-O	-5.04	115.52	121.07
1	A	462	LYS	N-CA-C	-5.03	105.69	111.07
1	A	58	SER	O-C-N	5.02	126.38	121.66
1	A	67	GLU	CA-C-O	-5.01	115.04	120.81
1	A	247	THR	CA-C-O	5.01	126.63	120.92
1	A	233	GLY	CA-C-O	5.01	129.28	120.57
1	A	485	PRO	CB-CA-C	-5.00	105.05	112.55

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	VAL	Mainchain
1	A	421	ASP	Mainchain

5.2 Too-close contacts ⓘ

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	3965	0	3738	252	0
2	A	172	0	122	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	53	0	31	10	0
4	A	8	0	1	7	0
5	A	56	0	0	5	0
All	All	4254	0	3892	263	0

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 33.

All (263) 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)
3:A:600:FAD:C1'	3:A:600:FAD:C2'	1.80	1.53
1:A:18:CYS:SG	2:A:603:HEC:CAC	2.02	1.47
1:A:15:CYS:SG	2:A:603:HEC:CAB	2.03	1.46
1:A:73:CYS:SG	2:A:602:HEC:HAC	1.54	1.44
1:A:73:CYS:SG	2:A:602:HEC:CAC	2.07	1.42
1:A:41:CYS:SG	2:A:604:HEC:CAC	2.14	1.35
1:A:41:CYS:SG	2:A:604:HEC:HAC	1.73	1.26
1:A:412:LYS:H	1:A:412:LYS:HD2	1.29	0.96
1:A:395:MET:HE2	1:A:407:ALA:HB3	1.50	0.94
1:A:41:CYS:HG	2:A:604:HEC:HAC	1.19	0.90
1:A:392:ASN:HD22	1:A:393:ARG:H	1.23	0.86
1:A:246:PRO:HG2	1:A:250:ALA:HB3	1.55	0.86
1:A:35:ASN:HD21	1:A:71:THR:H	1.26	0.82
1:A:145:ARG:HD2	1:A:268:GLY:H	1.45	0.81
1:A:49:ALA:HB1	1:A:61:LYS:HD3	1.63	0.81
1:A:393:ARG:HD3	1:A:478:GLN:HE22	1.48	0.78
1:A:392:ASN:ND2	1:A:393:ARG:H	1.81	0.77
1:A:468:ASN:ND2	1:A:487:GLU:HG2	2.00	0.77
1:A:154:LEU:HD23	1:A:275:SER:HB3	1.67	0.76
1:A:245:ARG:HB2	1:A:246:PRO:HD2	1.68	0.76
1:A:114:GLN:O	1:A:118:ILE:HG13	1.87	0.74
1:A:322:VAL:HG22	1:A:361:ILE:HD13	1.66	0.74
1:A:453:ILE:HG23	1:A:455:VAL:HG13	1.68	0.73
1:A:319:ASN:HD21	1:A:330:LYS:HA	1.51	0.73
1:A:337:HIS:HB2	1:A:338:PRO:HD2	1.69	0.73
3:A:600:FAD:C1'	3:A:600:FAD:C3'	2.65	0.73
1:A:514:LYS:HD3	1:A:516:GLU:OE2	1.89	0.73
1:A:170:GLY:HA3	1:A:243:SER:OG	1.89	0.73
1:A:434:TYR:HB3	1:A:439:ILE:HD11	1.72	0.72
1:A:377:GLU:N	4:A:700:FUM:O	2.17	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:GLY:O	1:A:543:ASN:HB3	1.90	0.71
1:A:388:ASN:HD22	1:A:412:LYS:HZ3	1.39	0.70
1:A:28:ASN:HD22	1:A:28:ASN:H	1.39	0.70
1:A:142:VAL:HG11	1:A:225:MET:HE1	1.74	0.70
1:A:235:MET:CE	4:A:700:FUM:H5	2.21	0.69
1:A:146:ASP:O	1:A:147:ALA:HB3	1.93	0.68
1:A:235:MET:HE1	4:A:700:FUM:C	2.24	0.68
1:A:467:TYR:CZ	1:A:484:LEU:HD23	2.27	0.68
1:A:388:ASN:ND2	1:A:412:LYS:HZ3	1.91	0.68
1:A:359:GLN:N	1:A:359:GLN:HE21	1.92	0.67
3:A:600:FAD:C1'	3:A:600:FAD:O2'	2.41	0.67
1:A:41:CYS:SG	2:A:604:HEC:C3C	2.82	0.67
1:A:66:GLY:H	1:A:258:GLN:HE22	1.40	0.67
1:A:245:ARG:HB2	1:A:246:PRO:CD	2.25	0.66
1:A:517:VAL:HB	1:A:529:LEU:HD13	1.77	0.65
1:A:393:ARG:HH11	1:A:478:GLN:NE2	1.95	0.65
1:A:359:GLN:HE21	1:A:359:GLN:H	1.43	0.64
1:A:252:VAL:O	1:A:256:VAL:HG23	1.98	0.63
1:A:345:LEU:HD11	1:A:358:LEU:HD21	1.80	0.63
1:A:426:LYS:O	1:A:427:SER:HB3	1.96	0.63
1:A:465:THR:O	1:A:468:ASN:HB2	1.99	0.63
1:A:467:TYR:OH	1:A:484:LEU:HD23	1.98	0.63
1:A:393:ARG:HD3	1:A:478:GLN:NE2	2.14	0.62
1:A:235:MET:HE3	4:A:700:FUM:H5	1.81	0.62
1:A:364:HIS:O	1:A:500:PRO:HA	2.00	0.62
1:A:190:ILE:O	1:A:194:ASP:OD1	2.18	0.62
1:A:8:PHE:O	1:A:11:GLU:HG2	2.00	0.61
1:A:504:HIS:CD2	1:A:544:ARG:HE	2.18	0.61
1:A:188:LYS:O	1:A:191:MET:HB3	2.00	0.61
1:A:146:ASP:O	1:A:147:ALA:CB	2.49	0.61
1:A:394:PHE:HE1	1:A:395:MET:HE3	1.66	0.61
1:A:167:ALA:HB3	1:A:253:GLY:CA	2.31	0.60
2:A:602:HEC:HBD1	2:A:602:HEC:HMD3	1.83	0.60
3:A:600:FAD:C2'	3:A:600:FAD:N10	2.59	0.60
1:A:28:ASN:HD22	1:A:28:ASN:N	1.99	0.60
1:A:395:MET:HE2	1:A:407:ALA:CB	2.27	0.60
1:A:18:CYS:SG	2:A:603:HEC:C3C	2.90	0.60
1:A:316:ALA:O	1:A:317:LYS:CB	2.46	0.60
1:A:567:PHE:O	1:A:568:ALA:HB3	2.02	0.59
1:A:235:MET:HE1	4:A:700:FUM:OXT	2.02	0.59
1:A:163:ASN:HD21	1:A:336:ASN:ND2	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LYS:HG3	1:A:166:LEU:HD23	1.83	0.59
1:A:337:HIS:HB2	1:A:338:PRO:CD	2.32	0.59
1:A:170:GLY:HA2	1:A:244:HIS:O	2.02	0.59
1:A:392:ASN:HD22	1:A:393:ARG:N	1.97	0.59
1:A:506:MET:HG3	1:A:540:HIS:HB2	1.85	0.59
1:A:453:ILE:HD11	1:A:495:ALA:CB	2.34	0.58
1:A:106:PRO:HG2	1:A:109:ALA:HB2	1.84	0.58
1:A:15:CYS:SG	2:A:603:HEC:C3B	2.91	0.58
1:A:469:GLY:O	1:A:470:PHE:C	2.44	0.57
1:A:394:PHE:CE1	1:A:395:MET:HE3	2.38	0.57
1:A:377:GLU:CB	4:A:700:FUM:O	2.52	0.57
1:A:395:MET:CE	1:A:407:ALA:HB3	2.30	0.57
1:A:177:LYS:O	1:A:179:GLN:N	2.37	0.57
1:A:411:GLN:O	1:A:412:LYS:C	2.48	0.57
1:A:167:ALA:HB3	1:A:253:GLY:HA3	1.87	0.57
1:A:393:ARG:HH11	1:A:478:GLN:HE21	1.52	0.57
1:A:433:GLY:HA3	2:A:601:HEC:HBA2	1.87	0.56
1:A:421:ASP:HB3	1:A:424:ILE:H	1.70	0.56
1:A:73:CYS:SG	2:A:602:HEC:C3C	2.93	0.56
1:A:214:ASN:O	1:A:215:SER:C	2.48	0.56
1:A:348:ALA:O	1:A:351:ALA:HB3	2.06	0.55
1:A:228:ASP:N	1:A:255:HIS:NE2	2.47	0.55
1:A:388:ASN:ND2	1:A:412:LYS:NZ	2.54	0.55
1:A:127:ASP:HB2	1:A:149:ALA:HB1	1.89	0.55
1:A:182:LEU:HD13	1:A:184:ILE:HD11	1.89	0.55
3:A:600:FAD:H1'1	3:A:600:FAD:O3'	2.06	0.55
1:A:453:ILE:CG2	1:A:455:VAL:HG13	2.37	0.54
1:A:62:SER:HB3	2:A:601:HEC:HBB3	1.89	0.54
1:A:166:LEU:HD21	2:A:601:HEC:HBC2	1.90	0.54
1:A:255:HIS:O	1:A:259:VAL:HG13	2.06	0.54
1:A:359:GLN:H	1:A:359:GLN:NE2	2.06	0.54
1:A:412:LYS:H	1:A:412:LYS:CD	2.09	0.54
3:A:600:FAD:C1'	3:A:600:FAD:O3'	2.56	0.54
1:A:450:ALA:HB1	1:A:455:VAL:O	2.08	0.54
1:A:154:LEU:HD12	1:A:154:LEU:N	2.23	0.54
1:A:559:ILE:O	1:A:560:ALA:C	2.50	0.54
1:A:196:MET:CE	1:A:203:ASN:HB2	2.38	0.53
1:A:329:LEU:O	1:A:330:LYS:C	2.50	0.53
1:A:426:LYS:O	1:A:427:SER:CB	2.57	0.53
1:A:127:ASP:CB	1:A:149:ALA:HB1	2.39	0.52
1:A:102:ARG:NH2	1:A:157:GLU:OE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:THR:HG21	1:A:208:VAL:HG13	1.92	0.52
1:A:380:ARG:HA	1:A:384:ALA:HB3	1.92	0.51
1:A:131:ILE:HD11	1:A:277:VAL:HG11	1.92	0.51
1:A:421:ASP:HB2	1:A:424:ILE:HG12	1.92	0.51
1:A:151:VAL:HB	1:A:269:THR:HG23	1.92	0.51
1:A:179:GLN:O	1:A:180:ALA:C	2.53	0.51
1:A:407:ALA:O	1:A:411:GLN:HG2	2.10	0.51
1:A:498:ILE:HD12	1:A:498:ILE:O	2.10	0.51
1:A:141:ALA:O	1:A:145:ARG:HB2	2.11	0.51
1:A:190:ILE:HD12	1:A:190:ILE:H	1.76	0.51
1:A:217:ASP:O	1:A:218:SER:C	2.54	0.51
1:A:175:GLU:OE2	1:A:187:LYS:HA	2.10	0.51
1:A:392:ASN:ND2	1:A:393:ARG:N	2.56	0.51
1:A:145:ARG:HG2	1:A:151:VAL:HG23	1.92	0.51
1:A:467:TYR:O	1:A:471:VAL:HG23	2.11	0.50
1:A:142:VAL:HG11	1:A:225:MET:CE	2.38	0.50
1:A:4:VAL:O	1:A:5:LEU:C	2.51	0.50
1:A:45:LEU:HG	2:A:602:HEC:HBB2	1.93	0.50
1:A:511:ILE:HD12	1:A:512:ASP:O	2.12	0.50
1:A:300:TYR:O	1:A:301:TYR:HB3	2.11	0.50
1:A:59:PRO:HD3	1:A:92:PHE:CE2	2.46	0.50
1:A:166:LEU:O	1:A:167:ALA:C	2.54	0.50
1:A:449:LEU:HD13	1:A:453:ILE:HD12	1.92	0.50
1:A:145:ARG:HD2	1:A:268:GLY:N	2.22	0.49
1:A:337:HIS:CE1	1:A:339:GLY:HA3	2.47	0.49
1:A:343:ASP:HB2	5:A:704:HOH:O	2.13	0.49
1:A:511:ILE:HA	1:A:516:GLU:O	2.11	0.49
1:A:29:ASP:O	1:A:274:ASN:ND2	2.41	0.49
1:A:228:ASP:O	1:A:246:PRO:HA	2.13	0.49
1:A:558:ARG:HH11	1:A:558:ARG:HG2	1.77	0.49
1:A:568:ALA:O	1:A:569:LYS:C	2.56	0.49
1:A:221:TRP:CZ2	1:A:558:ARG:HG3	2.47	0.49
1:A:166:LEU:CD2	2:A:601:HEC:HBC2	2.43	0.49
1:A:412:LYS:HD2	1:A:412:LYS:N	2.13	0.49
1:A:480:GLU:O	1:A:481:ARG:C	2.55	0.49
1:A:252:VAL:HG12	1:A:256:VAL:HG23	1.94	0.48
1:A:310:ILE:O	1:A:531:ALA:HA	2.13	0.48
1:A:105:VAL:HG13	1:A:106:PRO:HD2	1.94	0.48
1:A:429:LYS:O	1:A:430:ALA:C	2.54	0.48
1:A:315:PHE:O	1:A:316:ALA:C	2.55	0.48
1:A:481:ARG:HD3	1:A:484:LEU:HG	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ARG:CB	1:A:246:PRO:CD	2.91	0.48
1:A:90:PHE:HB2	5:A:747:HOH:O	2.15	0.47
1:A:115:ASP:O	1:A:116:LYS:C	2.57	0.47
1:A:196:MET:HE3	1:A:203:ASN:HB2	1.96	0.47
1:A:7:ASP:O	1:A:8:PHE:C	2.56	0.47
1:A:66:GLY:H	1:A:258:GLN:NE2	2.12	0.47
1:A:557:GLY:O	1:A:558:ARG:C	2.58	0.47
1:A:215:SER:O	1:A:216:SER:C	2.57	0.47
1:A:106:PRO:HG2	1:A:109:ALA:CB	2.44	0.46
1:A:162:GLY:O	1:A:165:LYS:HG2	2.15	0.46
1:A:173:ALA:O	1:A:242:ARG:HD3	2.16	0.46
1:A:245:ARG:CB	1:A:246:PRO:HD2	2.44	0.46
1:A:379:VAL:HG11	1:A:418:LEU:HD13	1.97	0.46
1:A:37:GLN:O	1:A:38:CYS:C	2.58	0.46
1:A:377:GLU:HB2	4:A:700:FUM:O	2.16	0.46
1:A:517:VAL:CB	1:A:529:LEU:HD13	2.44	0.46
1:A:238:ALA:HB2	5:A:712:HOH:O	2.15	0.46
1:A:420:PHE:HE1	1:A:496:LEU:HD11	1.81	0.46
1:A:404:ALA:O	1:A:408:ILE:HG13	2.16	0.46
1:A:506:MET:HE3	1:A:543:ASN:HA	1.97	0.46
1:A:145:ARG:HG2	1:A:151:VAL:CG2	2.47	0.45
1:A:221:TRP:CH2	1:A:558:ARG:HG3	2.51	0.45
1:A:316:ALA:O	1:A:317:LYS:HB3	2.16	0.45
1:A:437:LEU:O	1:A:438:ASN:HB2	2.15	0.45
1:A:487:GLU:O	1:A:488:LEU:HB2	2.16	0.45
1:A:186:ASP:OD1	1:A:187:LYS:N	2.49	0.45
1:A:256:VAL:O	1:A:257:ALA:C	2.58	0.45
1:A:395:MET:HE1	1:A:404:ALA:O	2.17	0.45
1:A:25:GLY:H	2:A:603:HEC:CHB	2.29	0.45
1:A:219:ILE:HD13	1:A:244:HIS:CD2	2.52	0.45
1:A:375:ILE:O	1:A:375:ILE:HG13	2.16	0.45
1:A:296:GLU:HG2	1:A:297:TYR:CE2	2.52	0.45
1:A:449:LEU:HD11	1:A:495:ALA:HB2	1.97	0.45
1:A:342:GLY:O	1:A:343:ASP:C	2.60	0.44
1:A:163:ASN:OD1	1:A:336:ASN:HA	2.17	0.44
1:A:245:ARG:HA	1:A:252:VAL:HG22	1.98	0.44
1:A:549:ALA:O	1:A:553:ILE:HG23	2.18	0.44
1:A:420:PHE:HE1	1:A:496:LEU:CD1	2.30	0.44
1:A:458:ALA:O	1:A:462:LYS:HG3	2.17	0.44
3:A:600:FAD:O2'	3:A:600:FAD:C9	2.65	0.44
3:A:600:FAD:O2'	3:A:600:FAD:C9A	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ALA:HA	1:A:260:LEU:HD22	1.99	0.44
1:A:433:GLY:CA	2:A:601:HEC:HBA2	2.48	0.44
1:A:567:PHE:O	1:A:568:ALA:CB	2.64	0.44
1:A:90:PHE:O	1:A:91:GLY:C	2.59	0.44
1:A:170:GLY:HA2	1:A:252:VAL:HG21	2.00	0.44
1:A:380:ARG:HD2	1:A:397:GLU:O	2.17	0.44
1:A:402:ASP:HB3	5:A:735:HOH:O	2.18	0.44
1:A:126:THR:OG1	1:A:127:ASP:N	2.51	0.44
1:A:141:ALA:O	1:A:142:VAL:C	2.60	0.44
1:A:315:PHE:CD1	1:A:321:ARG:HG2	2.53	0.44
1:A:35:ASN:ND2	1:A:70:CYS:N	2.66	0.44
1:A:151:VAL:HG12	1:A:152:ILE:N	2.32	0.44
1:A:289:THR:O	1:A:305:ALA:O	2.36	0.43
1:A:467:TYR:CE2	1:A:484:LEU:HD23	2.52	0.43
1:A:421:ASP:CB	1:A:424:ILE:HG12	2.49	0.43
2:A:604:HEC:HHA	2:A:604:HEC:HAA1	1.90	0.43
1:A:8:PHE:HE2	2:A:604:HEC:HHA	1.83	0.43
1:A:239:SER:O	1:A:240:VAL:C	2.60	0.43
1:A:468:ASN:OD1	1:A:487:GLU:O	2.36	0.43
1:A:501:ALA:O	1:A:502:VAL:C	2.62	0.43
3:A:600:FAD:H3B	5:A:701:HOH:O	2.19	0.42
1:A:196:MET:O	1:A:197:LYS:C	2.60	0.42
1:A:453:ILE:HD11	1:A:495:ALA:HB1	2.01	0.42
1:A:469:GLY:O	1:A:473:SER:HB2	2.19	0.42
1:A:63:HIS:O	1:A:64:LEU:C	2.61	0.42
1:A:127:ASP:O	1:A:305:ALA:HB1	2.19	0.42
1:A:207:LEU:O	1:A:209:LYS:N	2.53	0.42
1:A:4:VAL:O	1:A:6:ALA:N	2.53	0.42
1:A:35:ASN:HD22	1:A:70:CYS:H	1.66	0.42
1:A:138:LEU:HD13	1:A:261:TRP:HA	2.02	0.42
1:A:538:GLY:O	1:A:539:VAL:C	2.59	0.42
1:A:191:MET:HE3	1:A:191:MET:HB2	1.85	0.42
1:A:462:LYS:O	1:A:463:THR:C	2.62	0.42
1:A:94:MET:O	1:A:95:PRO:C	2.63	0.42
1:A:94:MET:HA	1:A:95:PRO:HD2	1.84	0.42
1:A:466:ALA:O	1:A:467:TYR:C	2.62	0.42
1:A:191:MET:HG2	1:A:212:ALA:CA	2.50	0.42
1:A:396:ASN:OD1	1:A:396:ASN:C	2.63	0.42
1:A:174:ALA:O	1:A:175:GLU:CB	2.68	0.41
1:A:460:LEU:O	1:A:464:VAL:HG23	2.19	0.41
1:A:109:ALA:O	1:A:110:ASP:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:GLU:O	1:A:488:LEU:CB	2.68	0.41
1:A:517:VAL:O	1:A:525:PRO:HA	2.20	0.41
1:A:306:ASP:CB	1:A:568:ALA:HB2	2.50	0.41
1:A:437:LEU:O	1:A:438:ASN:CB	2.68	0.41
1:A:282:GLU:H	1:A:282:GLU:HG3	1.22	0.41
1:A:336:ASN:HD22	1:A:340:ALA:CB	2.32	0.41
1:A:138:LEU:O	1:A:139:ALA:C	2.62	0.41
1:A:232:VAL:HG12	1:A:233:GLY:N	2.35	0.41
1:A:437:LEU:HD11	2:A:601:HEC:HAA1	2.00	0.41
1:A:153:LEU:HD23	1:A:153:LEU:C	2.46	0.41
1:A:196:MET:CE	1:A:196:MET:HA	2.51	0.41
1:A:421:ASP:H	1:A:424:ILE:HG12	1.86	0.41
1:A:71:THR:HG21	2:A:603:HEC:HMD2	2.03	0.41
1:A:453:ILE:HG22	1:A:455:VAL:H	1.85	0.41
1:A:470:PHE:HB3	1:A:476:ASP:HA	2.02	0.41
1:A:4:VAL:HA	1:A:96:PHE:HB3	2.03	0.41
1:A:63:HIS:CD2	2:A:601:HEC:NA	2.89	0.41
1:A:402:ASP:N	1:A:402:ASP:OD1	2.50	0.41
1:A:252:VAL:H	1:A:252:VAL:HG23	1.57	0.41
1:A:558:ARG:O	1:A:559:ILE:C	2.62	0.41
1:A:63:HIS:HE1	2:A:601:HEC:NC	2.18	0.40
1:A:191:MET:O	1:A:192:ILE:C	2.62	0.40
1:A:317:LYS:HD3	1:A:337:HIS:O	2.22	0.40
1:A:343:ASP:HB3	3:A:600:FAD:H61A	1.86	0.40
1:A:35:ASN:ND2	1:A:70:CYS:H	2.19	0.40
1:A:231:ASP:O	1:A:245:ARG:HG2	2.20	0.40
1:A:315:PHE:C	1:A:316:ALA:O	2.60	0.40
1:A:208:VAL:O	1:A:208:VAL:HG12	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	552/572 (96%)	470 (85%)	61 (11%)	21 (4%)	2 9

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	MET
1	A	175	GLU
1	A	178	PRO
1	A	181	LYS
1	A	474	GLY
1	A	5	LEU
1	A	147	ALA
1	A	180	ALA
1	A	215	SER
1	A	317	LYS
1	A	427	SER
1	A	489	VAL
1	A	97	GLY
1	A	521	LYS
1	A	179	GLN
1	A	340	ALA
1	A	488	LEU
1	A	192	ILE
1	A	162	GLY
1	A	76	GLY
1	A	327	PRO

5.3.2 Protein sidechains ⓘ

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	377/429 (88%)	298 (79%)	79 (21%)	1 4

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	17	SER
1	A	21	SER
1	A	22	ASP
1	A	26	VAL
1	A	28	ASN
1	A	31	LEU
1	A	61	LYS
1	A	67	GLU
1	A	68	ILE
1	A	71	THR
1	A	75	LYS
1	A	78	GLU
1	A	89	SER
1	A	101	GLU
1	A	102	ARG
1	A	116	LYS
1	A	123	LYS
1	A	124	GLU
1	A	125	THR
1	A	145	ARG
1	A	159	ILE
1	A	175	GLU
1	A	176	THR
1	A	182	LEU
1	A	184	ILE
1	A	188	LYS
1	A	191	MET
1	A	192	ILE
1	A	196	MET
1	A	203	ASN
1	A	210	VAL
1	A	211	LEU
1	A	219	ILE
1	A	223	THR
1	A	252	VAL
1	A	259	VAL
1	A	260	LEU
1	A	267	ARG
1	A	269	THR
1	A	271	ILE
1	A	274	ASN
1	A	282	GLU

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Mol	Chain	Res	Type
1	A	283	ASP
1	A	291	VAL
1	A	292	LEU
1	A	320	GLU
1	A	345	LEU
1	A	347	VAL
1	A	359	GLN
1	A	375	ILE
1	A	387	VAL
1	A	396	ASN
1	A	398	ILE
1	A	401	ARG
1	A	414	GLU
1	A	423	SER
1	A	425	ARG
1	A	441	LYS
1	A	446	ILE
1	A	449	LEU
1	A	453	ILE
1	A	454	ASP
1	A	459	GLU
1	A	460	LEU
1	A	465	THR
1	A	473	SER
1	A	475	LYS
1	A	478	GLN
1	A	488	LEU
1	A	497	GLU
1	A	518	LYS
1	A	520	GLU
1	A	526	ILE
1	A	527	THR
1	A	529	LEU
1	A	548	ASN
1	A	552	ASP
1	A	558	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	35	ASN

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Mol	Chain	Res	Type
1	A	114	GLN
1	A	172	ASN
1	A	189	GLN
1	A	213	ASN
1	A	258	GLN
1	A	319	ASN
1	A	336	ASN
1	A	359	GLN
1	A	382	ASN
1	A	388	ASN
1	A	392	ASN
1	A	411	GLN
1	A	468	ASN
1	A	478	GLN
1	A	548	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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
2	HEC	A	601	1	50,50,50	1.42	6 (12%)	68,82,82	1.56	16 (23%)
2	HEC	A	604	1	50,50,50	1.34	7 (14%)	68,82,82	2.02	18 (26%)
2	HEC	A	602	1	50,50,50	1.35	7 (14%)	68,82,82	1.36	9 (13%)
3	FAD	A	600	-	58,58,58	3.11	9 (15%)	85,89,89	3.21	41 (48%)
2	HEC	A	603	1	50,50,50	1.37	6 (12%)	68,82,82	1.39	9 (13%)
4	FUM	A	700	-	7,7,7	2.71	2 (28%)	8,8,8	1.61	2 (25%)

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
2	HEC	A	601	1	1/1/3/7	2/14/54/54	-
2	HEC	A	604	1	1/1/3/7	7/14/54/54	-
2	HEC	A	602	1	1/1/3/7	5/14/54/54	-
3	FAD	A	600	-	2/2/9/9	11/34/50/50	0/6/6/6
2	HEC	A	603	1	-	6/14/54/54	-
4	FUM	A	700	-	-	2/5/5/5	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	FAD	C1'-C2'	20.18	1.80	1.52
3	A	600	FAD	C5B-C4B	6.91	1.72	1.51
4	A	700	FUM	C5-C6	5.23	1.61	1.48
2	A	601	HEC	CBC-CAC	-4.12	1.34	1.51
3	A	600	FAD	P-O3P	-4.06	1.55	1.59
2	A	603	HEC	CBC-CAC	-4.00	1.34	1.51
2	A	601	HEC	CBB-CAB	-3.96	1.34	1.51
4	A	700	FUM	C4-C	3.83	1.57	1.48
2	A	603	HEC	CBB-CAB	-3.80	1.35	1.51
3	A	600	FAD	C5'-C4'	-3.51	1.47	1.51
2	A	604	HEC	CBC-CAC	-3.47	1.36	1.51
2	A	602	HEC	CBC-CAC	-3.34	1.37	1.51
2	A	602	HEC	CBB-CAB	-3.29	1.37	1.51
2	A	602	HEC	CAB-C3B	2.94	1.58	1.51
2	A	604	HEC	CBB-CAB	-2.89	1.39	1.51
2	A	604	HEC	FE-ND	2.75	2.03	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	FAD	C5X-N5	-2.70	1.34	1.39
2	A	601	HEC	C3C-C2C	-2.59	1.32	1.38
3	A	600	FAD	O4'-C4'	-2.52	1.38	1.43
2	A	602	HEC	FE-NA	2.47	2.03	1.95
2	A	601	HEC	CMC-C2C	2.47	1.55	1.50
2	A	603	HEC	FE-NB	2.44	2.02	1.94
2	A	604	HEC	C3C-C2C	-2.38	1.32	1.38
2	A	604	HEC	CMC-C2C	2.37	1.55	1.50
3	A	600	FAD	PA-O2A	-2.34	1.44	1.55
2	A	601	HEC	CAC-C3C	2.33	1.57	1.51
2	A	603	HEC	CMB-C2B	2.27	1.55	1.50
2	A	601	HEC	FE-NC	2.22	2.02	1.95
2	A	602	HEC	O1D-CGD	2.20	1.29	1.22
2	A	602	HEC	CMA-C3A	2.17	1.55	1.50
2	A	604	HEC	CAB-C3B	2.16	1.56	1.51
2	A	603	HEC	CAC-C3C	2.09	1.56	1.51
3	A	600	FAD	P-O1P	-2.08	1.43	1.50
2	A	602	HEC	CAC-C3C	2.07	1.56	1.51
2	A	603	HEC	CAB-C3B	2.06	1.56	1.51
3	A	600	FAD	PA-O3P	-2.03	1.57	1.59
2	A	604	HEC	CMD-C2D	2.00	1.54	1.50

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	FAD	C5B-C4B-C3B	-11.58	73.52	115.21
3	A	600	FAD	O4B-C1B-N9A	-8.73	91.33	108.09
3	A	600	FAD	O5B-C5B-C4B	8.39	137.58	108.99
3	A	600	FAD	O4B-C4B-C5B	7.84	134.46	109.33
2	A	604	HEC	CBD-CAD-C3D	7.32	132.76	112.53
3	A	600	FAD	O4B-C1B-C2B	-6.58	92.53	106.62
2	A	604	HEC	CBA-CAA-C2A	6.55	130.64	112.53
3	A	600	FAD	C4A-N9A-C8A	5.85	111.88	105.74
3	A	600	FAD	C4-N3-C2	-5.19	116.43	125.64
3	A	600	FAD	C1'-N10-C9A	5.02	130.38	120.63
3	A	600	FAD	C9-C9A-N10	4.67	128.13	121.85
3	A	600	FAD	C4'-C3'-C2'	-4.59	105.93	113.57
3	A	600	FAD	C4-C4X-N5	4.43	124.32	118.21
3	A	600	FAD	C9A-C5X-N5	-4.37	117.81	122.45
3	A	600	FAD	O4'-C4'-C3'	-4.23	99.35	109.25
3	A	600	FAD	C5X-C9A-N10	-3.87	114.47	117.97
3	A	600	FAD	O5'-C5'-C4'	3.87	119.68	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	FAD	O2B-C2B-C3B	3.76	123.86	111.82
3	A	600	FAD	N9A-C8A-N7A	-3.68	108.71	113.94
3	A	600	FAD	C6-C5X-C9A	3.65	124.06	119.05
3	A	600	FAD	C4B-O4B-C1B	-3.60	101.53	109.47
2	A	604	HEC	O1D-CGD-CBD	-3.56	111.79	123.09
2	A	603	HEC	CHB-C4A-NA	3.50	128.26	124.45
3	A	600	FAD	O3'-C3'-C4'	3.48	116.83	108.93
2	A	604	HEC	O2A-CGA-O1A	3.45	132.22	123.33
3	A	600	FAD	O2'-C2'-C1'	-3.42	96.14	110.20
2	A	603	HEC	CMA-C3A-C4A	-3.37	118.80	124.73
3	A	600	FAD	C5A-C4A-N9A	-3.36	102.15	105.81
3	A	600	FAD	C10-C4X-N5	-3.25	118.16	124.81
2	A	604	HEC	CHD-C1D-ND	-3.25	120.35	124.37
2	A	604	HEC	CAA-CBA-CGA	-3.18	105.23	113.67
4	A	700	FUM	O8-C6-O7	3.17	129.15	122.70
3	A	600	FAD	N6A-C6A-N1A	3.14	125.38	118.38
2	A	601	HEC	CBD-CAD-C3D	3.14	121.22	112.53
2	A	604	HEC	CAA-C2A-C1A	-3.13	118.50	124.85
2	A	601	HEC	CHA-C1A-C2A	3.11	129.78	124.86
2	A	601	HEC	C3C-C4C-NC	-3.09	106.72	110.15
2	A	601	HEC	CAD-C3D-C4D	-3.06	119.36	124.70
2	A	602	HEC	CMC-C2C-C1C	-3.04	120.79	125.42
3	A	600	FAD	C4X-C4-N3	3.02	120.94	113.25
2	A	604	HEC	CAA-C2A-C3A	2.99	133.47	127.87
2	A	603	HEC	CMA-C3A-C2A	2.99	134.22	126.15
3	A	600	FAD	C5A-C4A-N3A	2.98	130.81	126.72
3	A	600	FAD	O2A-PA-O3P	2.93	115.21	107.27
2	A	604	HEC	O1A-CGA-CBA	-2.91	113.85	123.09
2	A	603	HEC	CHA-C1A-NA	-2.82	121.38	124.45
2	A	601	HEC	CHB-C1B-NB	2.79	127.43	124.42
3	A	600	FAD	C5X-N5-C4X	2.77	122.58	118.09
3	A	600	FAD	C9-C8-C7	2.77	123.75	119.69
2	A	601	HEC	CMC-C2C-C3C	2.75	131.45	125.62
2	A	601	HEC	C4C-C3C-C2C	2.70	111.04	106.87
2	A	602	HEC	O2A-CGA-O1A	2.69	130.25	123.33
3	A	600	FAD	C2B-C1B-N9A	-2.65	106.72	113.30
3	A	600	FAD	C10-N1-C2	2.65	122.58	116.85
2	A	604	HEC	CHA-C4D-ND	-2.62	121.60	124.42
2	A	603	HEC	CBC-CAC-C3C	2.61	119.51	112.42
3	A	600	FAD	C5A-N7A-C8A	2.58	107.51	103.45
2	A	602	HEC	CBD-CAD-C3D	2.56	119.60	112.53
2	A	601	HEC	CHA-C1A-NA	-2.54	121.69	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	FAD	O4B-C4B-C3B	-2.53	100.14	105.15
2	A	602	HEC	C3D-C4D-ND	-2.52	107.92	110.35
3	A	600	FAD	C2A-N1A-C6A	2.51	122.86	118.73
2	A	602	HEC	CBA-CAA-C2A	-2.51	105.59	112.53
4	A	700	FUM	O7-C6-C5	-2.49	113.42	121.06
3	A	600	FAD	C4X-C10-N10	2.47	120.02	116.48
2	A	601	HEC	C1D-ND-C4D	2.45	108.11	105.21
3	A	600	FAD	C2A-N3A-C4A	-2.45	105.85	111.83
2	A	603	HEC	C3D-C4D-ND	-2.44	108.00	110.35
2	A	604	HEC	O2D-CGD-O1D	2.43	129.57	123.33
2	A	603	HEC	O2D-CGD-O1D	2.40	129.51	123.33
2	A	602	HEC	CMC-C2C-C3C	2.40	130.71	125.62
3	A	600	FAD	C4A-N9A-C1B	-2.36	121.12	126.63
2	A	604	HEC	C1C-CHC-C4B	-2.35	120.72	126.25
2	A	601	HEC	CAD-C3D-C2D	2.34	132.24	127.87
2	A	601	HEC	C2D-C1D-ND	-2.32	107.17	109.84
2	A	603	HEC	CHA-C1A-C2A	2.31	128.52	124.86
2	A	602	HEC	CHC-C4B-NB	2.31	127.23	124.37
2	A	601	HEC	C3D-C4D-ND	-2.31	108.12	110.35
2	A	604	HEC	CMD-C2D-C1D	-2.30	121.44	125.03
2	A	604	HEC	CAB-C3B-C4B	2.28	127.75	124.79
3	A	600	FAD	O2-C2-N1	-2.27	118.02	121.80
2	A	603	HEC	C4A-CHB-C1B	-2.27	121.20	126.02
2	A	602	HEC	CHA-C4D-ND	2.25	126.84	124.42
3	A	600	FAD	O4-C4-N3	-2.21	115.97	120.11
2	A	604	HEC	CHC-C1C-NC	2.18	127.81	123.86
3	A	600	FAD	C6-C7-C8	-2.17	116.50	119.69
2	A	601	HEC	CMB-C2B-C1B	-2.16	121.66	125.03
2	A	604	HEC	CBB-CAB-C3B	2.16	118.27	112.42
2	A	601	HEC	CAB-C3B-C2B	-2.12	123.66	127.56
2	A	602	HEC	CAA-C2A-C1A	-2.10	120.58	124.85
2	A	601	HEC	C4A-CHB-C1B	-2.09	121.58	126.02
3	A	600	FAD	C6-C5X-N5	-2.08	114.99	118.44
2	A	604	HEC	CHB-C1B-C2B	2.05	128.26	125.03
2	A	601	HEC	CMB-C2B-C3B	2.02	131.62	126.15
2	A	604	HEC	CBC-CAC-C3C	2.02	117.89	112.42

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	HEC	NA
2	A	602	HEC	NA

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Mol	Chain	Res	Type	Atom
2	A	604	HEC	NA
3	A	600	FAD	C3'
3	A	600	FAD	C4'

All (33) torsion outliers are listed below:

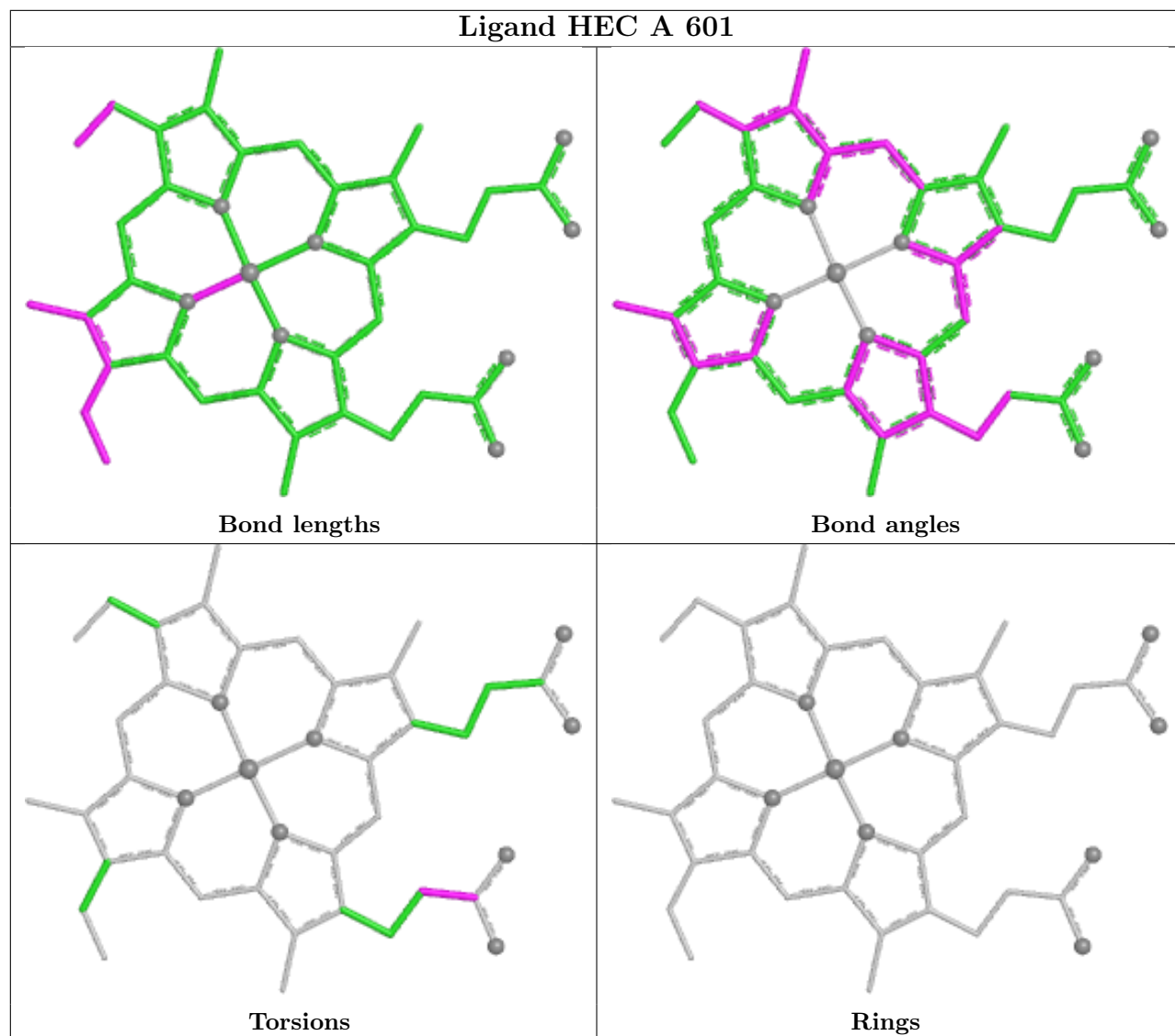
Mol	Chain	Res	Type	Atoms
2	A	602	HEC	C2D-C3D-CAD-CBD
2	A	602	HEC	C4D-C3D-CAD-CBD
2	A	604	HEC	C1A-C2A-CAA-CBA
3	A	600	FAD	C3B-C4B-C5B-O5B
3	A	600	FAD	C1'-C2'-C3'-O3'
3	A	600	FAD	C1'-C2'-C3'-C4'
3	A	600	FAD	C3'-C4'-C5'-O5'
3	A	600	FAD	O4'-C4'-C5'-O5'
3	A	600	FAD	PA-O3P-P-O5'
4	A	700	FUM	OXT-C-C4-C5
4	A	700	FUM	O-C-C4-C5
2	A	604	HEC	C3A-C2A-CAA-CBA
2	A	603	HEC	C2A-CAA-CBA-CGA
2	A	604	HEC	C4C-C3C-CAC-CBC
3	A	600	FAD	O4B-C4B-C5B-O5B
2	A	604	HEC	C2C-C3C-CAC-CBC
2	A	602	HEC	C4C-C3C-CAC-CBC
2	A	602	HEC	C2C-C3C-CAC-CBC
2	A	603	HEC	C3D-CAD-CBD-CGD
3	A	600	FAD	P-O3P-PA-O1A
3	A	600	FAD	P-O3P-PA-O2A
3	A	600	FAD	C5B-O5B-PA-O2A
3	A	600	FAD	C2B-C1B-N9A-C8A
2	A	603	HEC	CAD-CBD-CGD-O1D
2	A	603	HEC	CAA-CBA-CGA-O1A
2	A	603	HEC	CAA-CBA-CGA-O2A
2	A	603	HEC	CAD-CBD-CGD-O2D
2	A	604	HEC	CAA-CBA-CGA-O1A
2	A	601	HEC	CAD-CBD-CGD-O2D
2	A	601	HEC	CAD-CBD-CGD-O1D
2	A	604	HEC	CAA-CBA-CGA-O2A
2	A	604	HEC	C4B-C3B-CAB-CBB
2	A	602	HEC	CAA-CBA-CGA-O2A

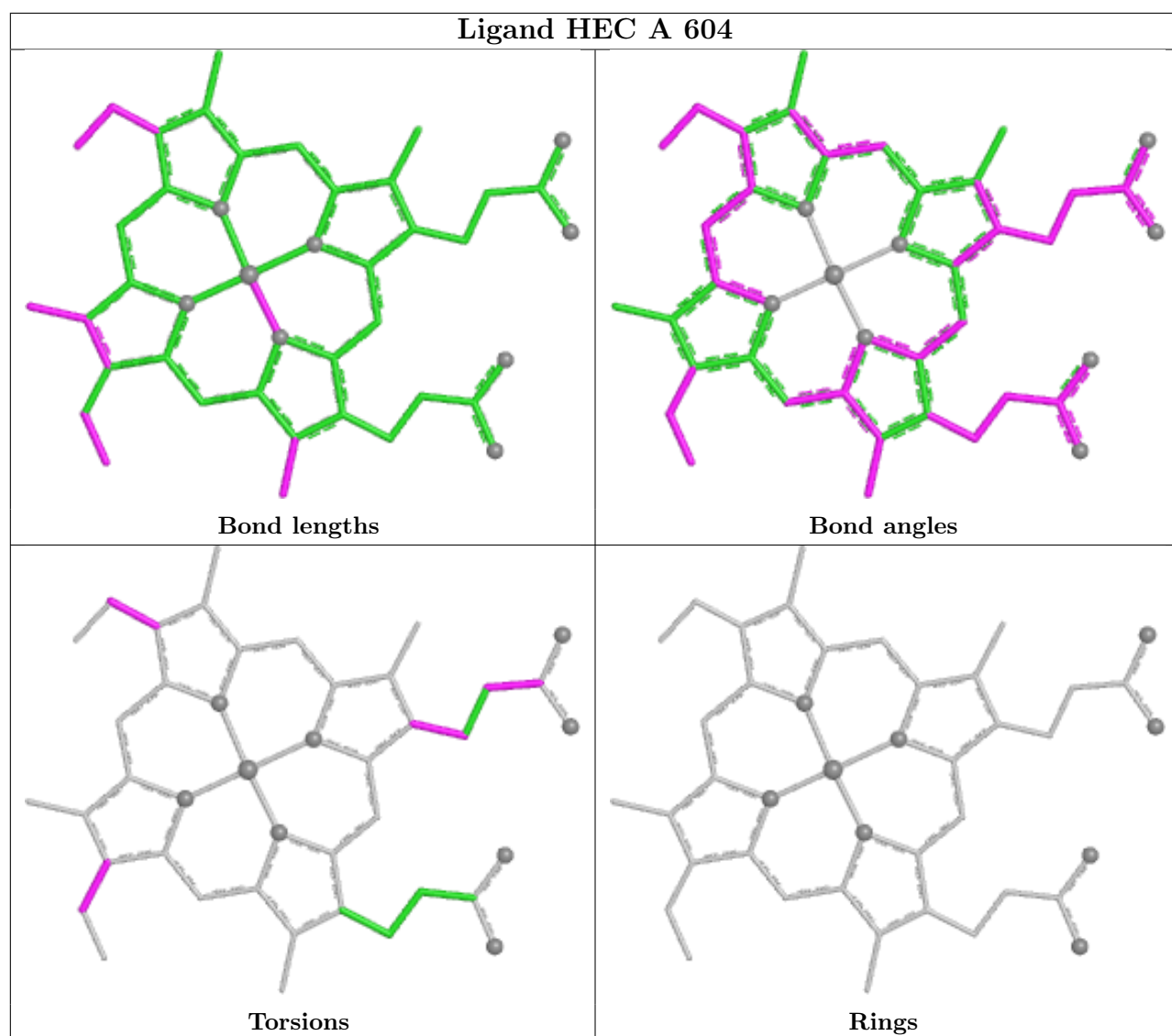
There are no ring outliers.

6 monomers are involved in 42 short contacts:

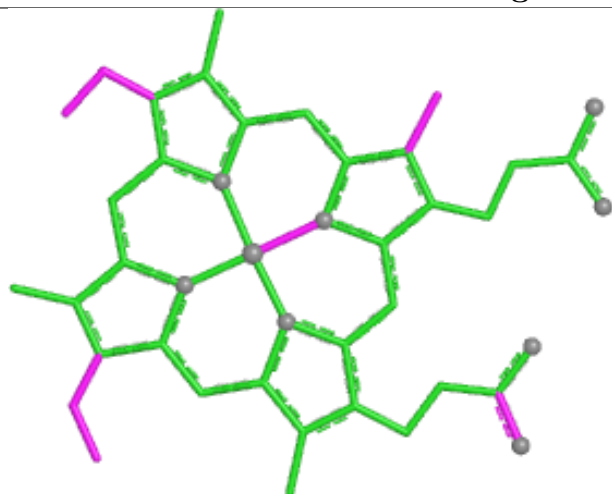
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEC	8	0
2	A	604	HEC	6	0
2	A	602	HEC	5	0
3	A	600	FAD	10	0
2	A	603	HEC	6	0
4	A	700	FUM	7	0

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 than 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.

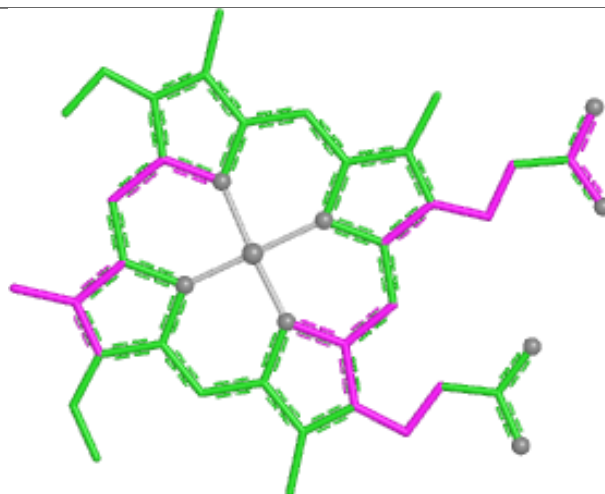




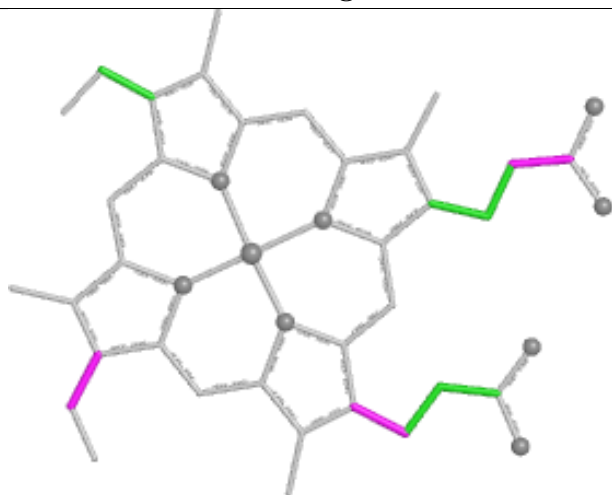
Ligand HEC A 602



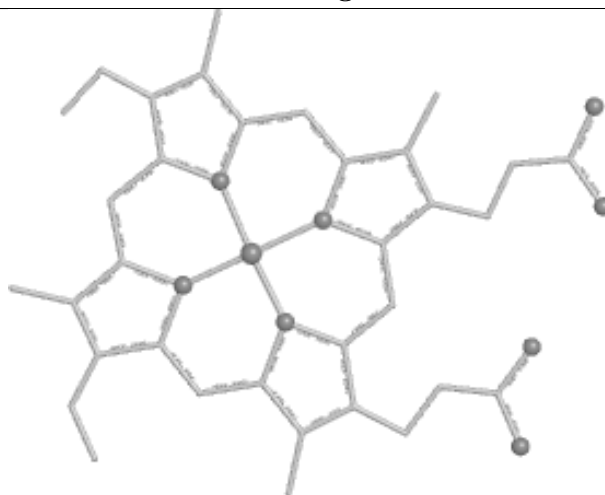
Bond lengths



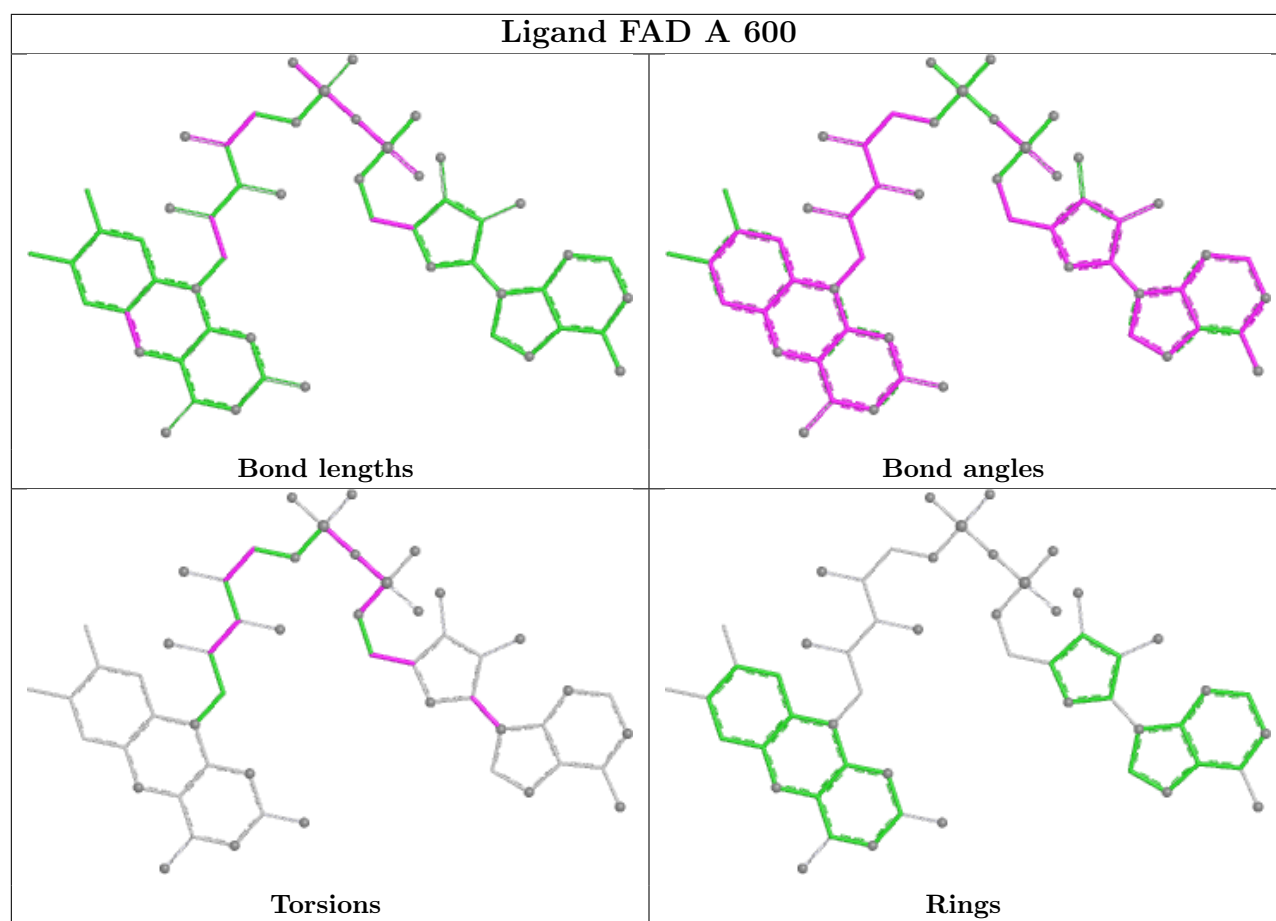
Bond angles

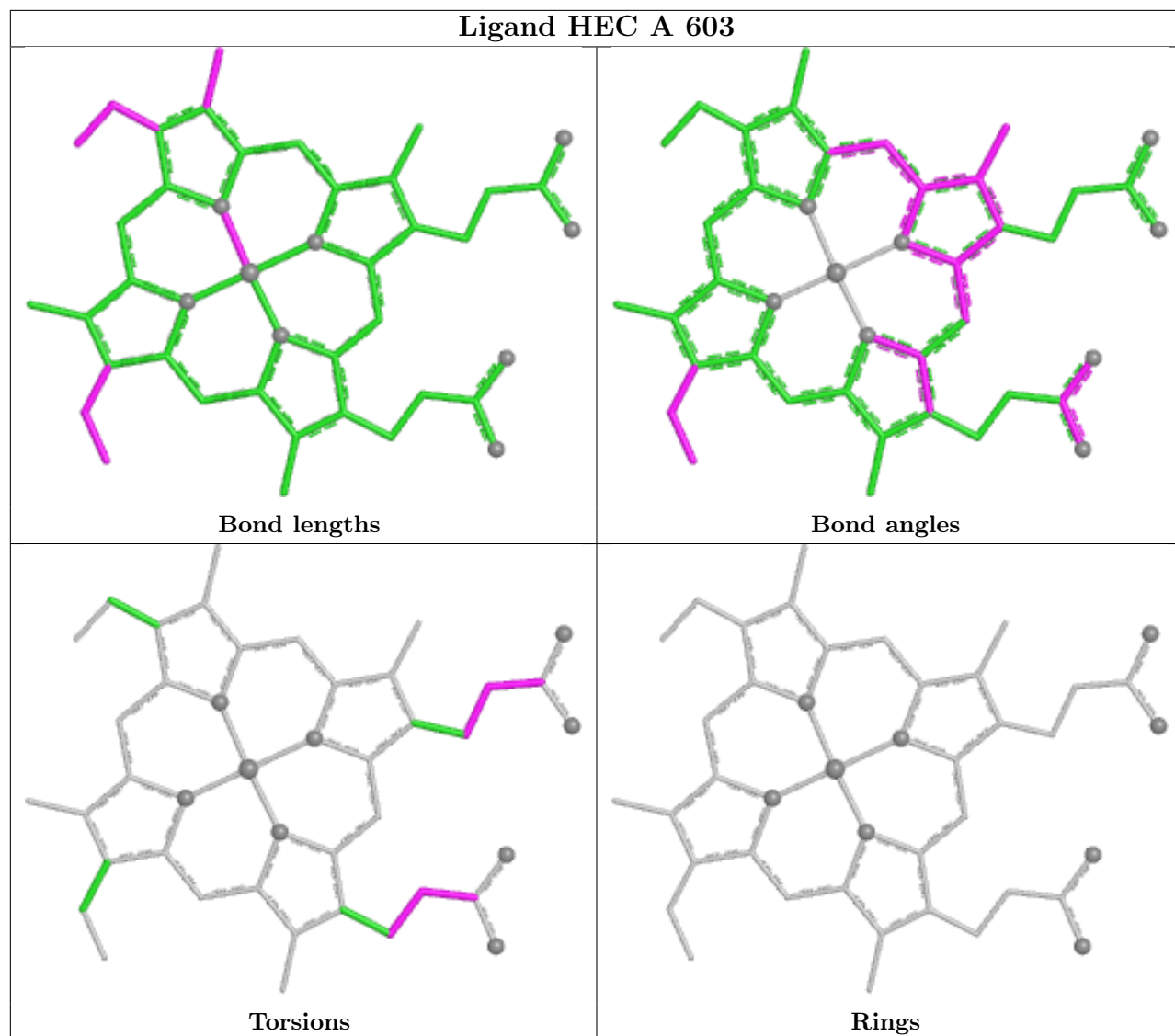


Torsions



Rings





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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.