



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 09:08 AM EDT

PDB ID : 1FCD / pdb_00001fcd
Title : THE STRUCTURE OF FLAVOCYTOCHROME C SULFIDE DEHYDROGENASE FROM A PURPLE PHOTOTROPHIC BACTERIUM CHROMATIUM VINOSUM AT 2.5 ANGSTROMS RESOLUTION
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Deposited on : 1994-08-18
Resolution : 2.53 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

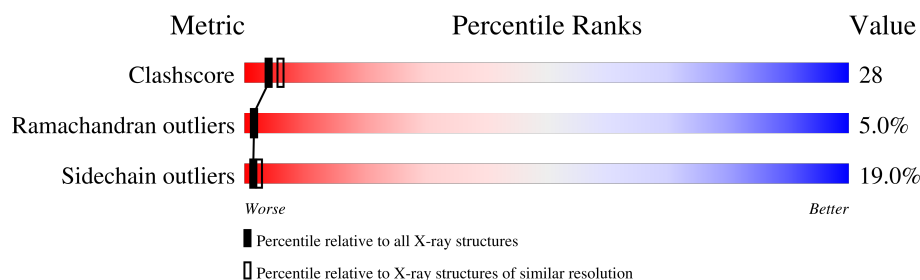
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)

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	401	
1	B	401	
2	C	174	
2	D	174	

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
3	FAD	A	699	X	-	-	-
3	FAD	B	699	X	-	-	-
4	HEC	C	901	X	-	-	-
4	HEC	C	902	X	-	-	-
4	HEC	D	901	X	-	-	-
4	HEC	D	902	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9002 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 SULFIDE DEHYDROGENASE (FLAVIN-BINDING SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3018	1918	505	584	11			
1	B	401	Total	C	N	O	S	0	0	0
			3018	1918	505	584	11			

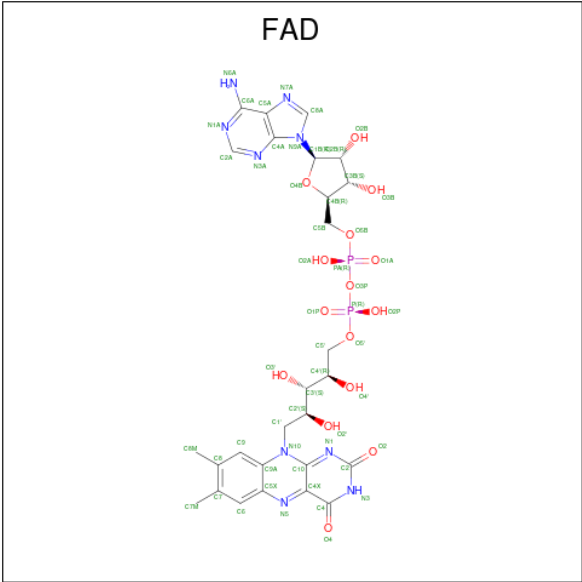
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	MET	LYS	conflict	UNP Q06530
A	296	SER	CYS	conflict	UNP Q06530
A	321	VAL	ALA	conflict	UNP Q06530
B	182	MET	LYS	conflict	UNP Q06530
B	296	SER	CYS	conflict	UNP Q06530
B	321	VAL	ALA	conflict	UNP Q06530

- Molecule 2 is a protein called FLAVOCYTOCHROME C SULFIDE DEHYDROGENASE (CYTOCHROME SUBUNIT).

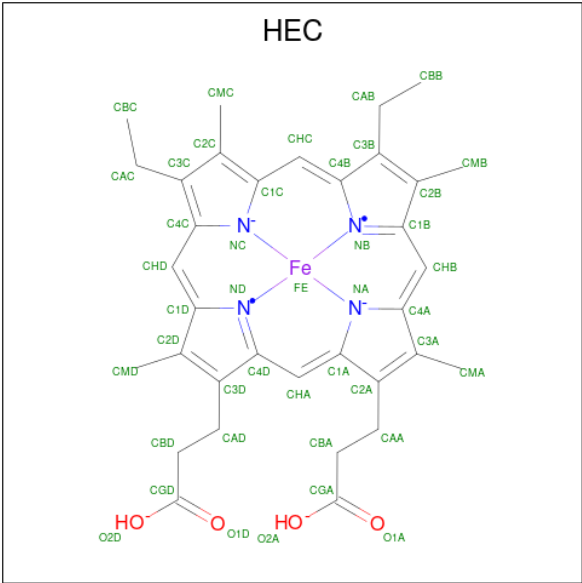
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	174	Total	C	N	O	S	0	0	0
			1344	842	225	264	13			
2	D	174	Total	C	N	O	S	0	0	0
			1344	842	225	264	13			

- 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 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

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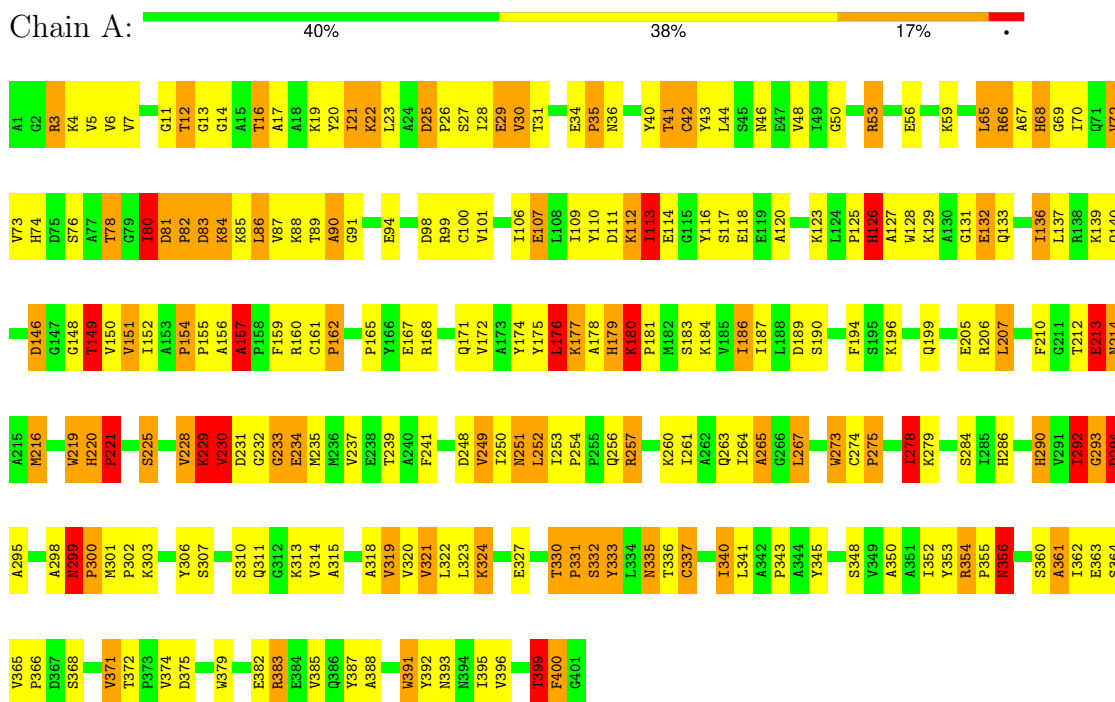
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

3 Residue-property plots

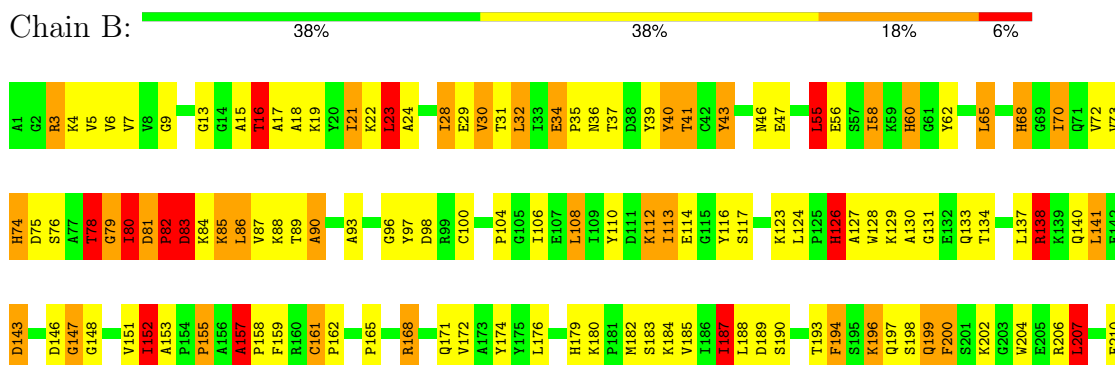
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

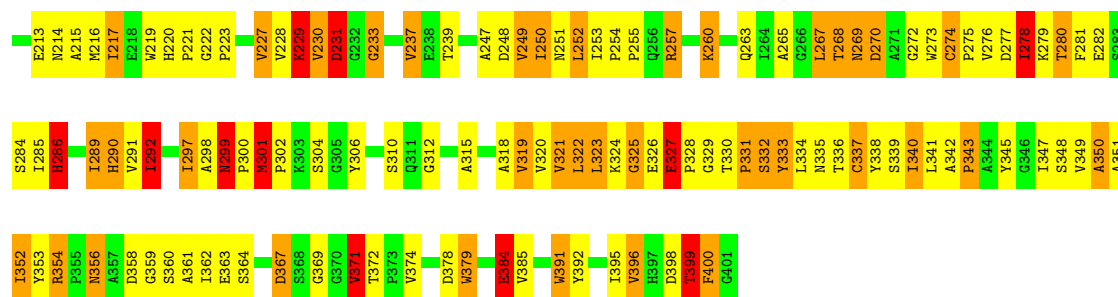
Note EDS was not executed.

- Molecule 1: FLAVOCYTOCHROME C SULFIDE DEHYDROGENASE (FLAVIN-BINDING SUBUNIT)



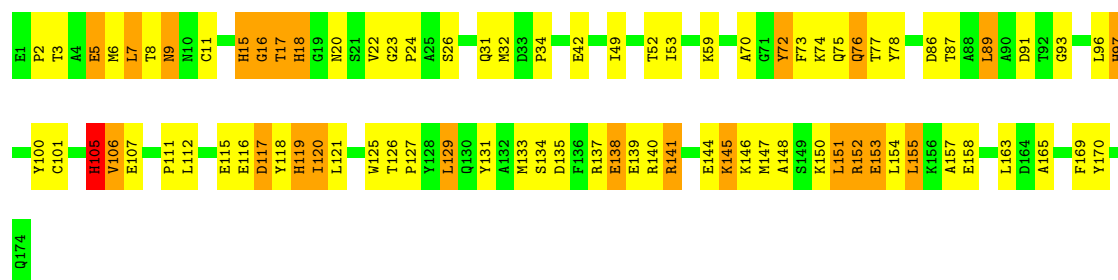
- Molecule 1: FLAVOCYTOCHROME C SULFIDE DEHYDROGENASE (FLAVIN-BINDING SUBUNIT)





- Molecule 2: FLAVOCYTOCHROME C SULFIDE DEHYDROGENASE (CYTOCHROME SUBUNIT)

Chain C: 52% 34% 13%



- Molecule 2: FLAVOCYTOCHROME C SULFIDE DEHYDROGENASE (CYTOCHROME SUBUNIT)

Chain D: 47% 37% 11% 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.60Å 84.60Å 106.40Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.53	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.53)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.237 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9002	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: HEC, 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	1.22	15/3093 (0.5%)	2.12	129/4209 (3.1%)
1	B	1.25	14/3093 (0.5%)	2.08	130/4209 (3.1%)
2	C	1.06	2/1374 (0.1%)	1.92	39/1847 (2.1%)
2	D	1.15	5/1374 (0.4%)	1.97	47/1847 (2.5%)
All	All	1.20	36/8934 (0.4%)	2.05	345/12112 (2.8%)

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	4
1	B	0	2
2	C	0	1
All	All	0	7

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	399	THR	C-O	-14.64	1.05	1.24
2	D	30	ALA	C-O	-13.83	1.07	1.23
1	B	400	PHE	N-CA	12.11	1.60	1.46
1	A	399	THR	C-O	-11.28	1.09	1.24
1	A	400	PHE	CA-C	10.39	1.67	1.52
1	A	340	ILE	CA-CB	9.58	1.65	1.54
1	B	340	ILE	CA-CB	8.60	1.64	1.54
1	B	230	VAL	CA-CB	8.48	1.66	1.54
1	A	337	CYS	CA-CB	8.20	1.64	1.53
1	A	180	LYS	C-O	-7.11	1.15	1.24
1	B	371	VAL	CA-CB	6.77	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	15	HIS	CG-CD2	6.54	1.43	1.35
1	A	230	VAL	CA-CB	6.52	1.63	1.54
1	B	233	GLY	CA-C	6.42	1.60	1.51
1	A	400	PHE	N-CA	6.39	1.54	1.46
2	D	53	ILE	CA-CB	6.17	1.62	1.54
2	D	15	HIS	CG-CD2	6.05	1.42	1.35
1	A	187	ILE	CA-CB	5.97	1.61	1.54
1	B	7	VAL	CA-CB	5.95	1.61	1.53
2	D	31	GLN	N-CA	5.92	1.55	1.46
1	A	40	TYR	CA-CB	-5.88	1.45	1.53
1	A	154	PRO	CA-CB	-5.83	1.46	1.54
1	B	187	ILE	CA-CB	5.82	1.61	1.54
1	A	136	ILE	CA-CB	5.59	1.60	1.54
1	A	391	TRP	NE1-CE2	-5.52	1.31	1.37
1	B	152	ILE	CA-CB	5.49	1.61	1.54
1	A	379	TRP	NE1-CE2	-5.38	1.31	1.37
1	B	16	THR	C-N	-5.26	1.26	1.33
1	B	220	HIS	CA-C	-5.22	1.48	1.52
1	B	391	TRP	NE1-CE2	-5.20	1.31	1.37
1	A	186	ILE	CA-CB	5.18	1.61	1.54
2	D	14	CYS	CA-CB	-5.17	1.45	1.53
1	B	229	LYS	N-CA	-5.12	1.39	1.46
1	B	79	GLY	C-N	-5.06	1.27	1.33
2	C	125	TRP	NE1-CE2	-5.05	1.31	1.37
1	A	220	HIS	CA-CB	5.01	1.59	1.53

All (345) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	400	PHE	CA-C-O	-31.73	77.56	119.12
1	B	126	HIS	CA-CB-CG	15.80	129.60	113.80
1	A	180	LYS	O-C-N	-15.02	104.05	121.32
2	D	18	HIS	CA-CB-CG	14.58	128.38	113.80
1	B	399	THR	O-C-N	-14.42	101.08	122.28
1	A	41	THR	N-CA-C	12.77	125.19	111.28
1	A	399	THR	O-C-N	-12.08	106.52	122.59
1	A	159	PHE	CA-CB-CG	11.48	125.28	113.80
1	A	189	ASP	CA-CB-CG	11.45	124.05	112.60
1	B	112	LYS	N-CA-C	-11.24	100.10	114.04
1	B	286	HIS	CA-CB-CG	10.99	124.79	113.80
2	D	15	HIS	CB-CG-ND1	-10.90	106.35	122.70
1	A	292	ILE	O-C-N	10.85	134.42	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	159	PHE	CA-CB-CG	10.65	124.45	113.80
1	A	214	ASN	N-CA-C	-10.25	89.87	109.24
2	D	105	HIS	CA-CB-CG	-10.18	103.62	113.80
1	A	46	ASN	OD1-CG-ND2	-10.00	112.60	122.60
1	A	36	ASN	N-CA-C	9.92	124.22	109.24
1	B	126	HIS	O-C-N	-9.87	111.31	123.05
2	D	15	HIS	CG-CD2-NE2	-9.84	97.36	107.20
1	B	323	LEU	O-C-N	-9.80	109.56	122.59
2	D	15	HIS	ND1-CG-CD2	9.80	115.90	106.10
1	A	234	GLU	N-CA-C	-9.76	101.38	113.28
1	B	126	HIS	CB-CG-CD2	-9.65	118.65	131.20
1	B	179	HIS	CA-CB-CG	9.57	123.37	113.80
1	B	41	THR	N-CA-C	9.41	122.50	111.02
1	A	230	VAL	O-C-N	9.22	134.10	122.57
1	A	225	SER	N-CA-CB	-9.04	95.78	110.42
1	A	230	VAL	CA-C-O	8.86	131.85	120.78
1	B	237	VAL	N-CA-CB	-8.71	100.32	112.52
1	B	143	ASP	CB-CA-C	-8.56	98.47	111.73
2	C	18	HIS	CB-CG-CD2	-8.53	120.11	131.20
1	A	251	ASN	OD1-CG-ND2	-8.46	114.14	122.60
2	D	114	ASP	N-CA-C	-8.35	91.38	107.57
1	B	230	VAL	CG1-CB-CG2	-8.30	92.53	110.80
1	B	126	HIS	N-CA-C	-8.25	94.08	108.20
1	B	93	ALA	N-CA-C	8.25	120.96	110.24
2	C	15	HIS	CG-CD2-NE2	-8.24	98.96	107.20
2	D	103	LYS	N-CA-C	-8.19	93.35	110.80
1	B	384	GLU	CA-CB-CG	-8.19	97.72	114.10
1	B	73	VAL	N-CA-C	-8.18	95.32	107.51
2	D	144	GLU	CB-CA-C	8.18	124.11	109.64
1	A	299	ASN	O-C-N	-8.16	111.94	121.32
2	C	18	HIS	CG-CD2-NE2	-8.10	99.10	107.20
1	A	74	HIS	CB-CG-CD2	-8.03	120.77	131.20
1	B	80	ILE	N-CA-C	-7.96	96.85	108.23
1	A	290	HIS	CA-CB-CG	-7.94	105.86	113.80
2	C	15	HIS	ND1-CG-CD2	7.92	114.02	106.10
1	B	280	THR	N-CA-C	-7.91	96.34	109.24
1	B	229	LYS	CA-C-O	-7.85	111.06	120.32
2	D	15	HIS	CA-CB-CG	7.82	121.62	113.80
1	A	46	ASN	CB-CG-ND2	7.82	128.13	116.40
2	D	105	HIS	CB-CG-CD2	-7.76	121.11	131.20
1	B	269	ASN	OD1-CG-ND2	-7.70	114.90	122.60
1	B	273	TRP	CG-CD2-CE3	7.67	141.57	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	LYS	N-CA-C	-7.67	97.39	109.50
2	C	119	HIS	CA-CB-CG	-7.66	106.14	113.80
1	B	269	ASN	CA-CB-CG	7.62	120.22	112.60
1	B	290	HIS	CB-CG-CD2	-7.60	121.32	131.20
2	C	18	HIS	ND1-CG-CD2	7.57	113.67	106.10
1	B	68	HIS	CB-CG-CD2	-7.54	121.39	131.20
1	A	113	ILE	N-CA-CB	-7.54	105.11	112.65
1	A	220	HIS	CA-C-N	7.53	129.25	119.84
1	A	220	HIS	C-N-CA	7.53	129.25	119.84
2	D	102	GLU	N-CA-C	-7.45	98.43	109.15
1	B	286	HIS	CB-CG-CD2	-7.43	121.55	131.20
1	B	162	PRO	N-CA-C	7.38	119.70	110.70
1	A	72	VAL	N-CA-CB	-7.34	104.26	111.89
1	A	5	VAL	N-CA-C	-7.33	97.92	108.48
2	D	65	ASP	CA-CB-CG	7.31	119.91	112.60
1	B	16	THR	O-C-N	-7.31	112.87	122.59
2	D	15	HIS	N-CA-C	-7.30	96.36	108.34
1	A	207	LEU	N-CA-C	7.30	122.55	112.04
1	B	221	PRO	N-CA-C	7.27	122.62	111.57
2	C	75	GLN	OE1-CD-NE2	-7.23	115.37	122.60
1	A	292	ILE	CA-C-N	7.20	135.51	121.41
1	A	292	ILE	C-N-CA	7.20	135.51	121.41
2	C	52	THR	N-CA-C	-7.20	103.47	112.90
1	A	230	VAL	CG1-CB-CG2	-7.15	95.06	110.80
1	B	41	THR	N-CA-CB	-7.15	98.95	109.82
1	B	34	GLU	CA-C-N	7.14	126.98	119.05
1	B	34	GLU	C-N-CA	7.14	126.98	119.05
2	D	18	HIS	CG-CD2-NE2	-7.12	100.08	107.20
1	A	286	HIS	CG-CD2-NE2	-7.09	100.11	107.20
1	A	251	ASN	CA-CB-CG	7.08	119.68	112.60
1	B	379	TRP	CG-CD2-CE3	7.04	140.94	133.90
1	A	113	ILE	CB-CA-C	7.04	118.34	111.23
2	D	22	VAL	N-CA-C	-7.04	99.84	109.55
1	B	157	ALA	CA-C-O	-7.04	110.52	120.16
1	B	126	HIS	CA-C-O	-7.02	113.24	120.54
1	A	400	PHE	N-CA-C	-7.00	104.73	113.20
1	B	179	HIS	CB-CG-CD2	-6.98	122.12	131.20
1	B	228	VAL	CA-C-O	6.97	130.08	121.92
1	B	228	VAL	O-C-N	6.95	129.99	122.76
1	B	213	GLU	CB-CG-CD	6.95	124.41	112.60
1	B	82	PRO	O-C-N	6.90	131.95	122.64
1	B	79	GLY	O-C-N	6.86	131.61	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	PRO	N-CA-C	6.81	119.01	110.70
1	A	78	THR	N-CA-CB	-6.81	100.73	110.81
1	A	337	CYS	CA-CB-SG	6.81	130.06	114.40
1	A	131	GLY	CA-C-N	6.80	129.29	120.44
1	A	131	GLY	C-N-CA	6.80	129.29	120.44
2	C	15	HIS	CB-CG-ND1	-6.78	112.53	122.70
2	D	18	HIS	ND1-CG-CD2	6.78	112.88	106.10
1	A	273	TRP	CG-CD2-CE3	6.72	140.62	133.90
1	A	148	GLY	N-CA-C	6.70	123.62	115.31
1	B	210	PHE	N-CA-C	6.66	122.29	111.37
1	B	9	GLY	O-C-N	-6.65	112.79	122.30
1	B	43	TYR	CB-CA-C	-6.65	100.17	110.81
1	A	212	THR	N-CA-C	6.63	120.47	112.38
1	B	323	LEU	CA-C-O	6.61	129.96	120.51
1	B	248	ASP	CA-CB-CG	6.61	119.21	112.60
1	B	60	HIS	CB-CG-CD2	-6.58	122.64	131.20
1	B	194	PHE	CA-CB-CG	6.57	120.37	113.80
1	B	187	ILE	CB-CG1-CD1	-6.56	100.02	113.80
2	C	119	HIS	ND1-CG-CD2	6.55	112.66	106.10
2	C	73	PHE	CA-CB-CG	-6.53	107.27	113.80
2	C	6	MET	N-CA-C	-6.51	103.87	110.97
2	D	121	LEU	N-CA-C	-6.49	104.78	114.64
1	A	194	PHE	CA-CB-CG	6.46	120.26	113.80
2	D	10	ASN	OD1-CG-ND2	-6.43	116.17	122.60
1	B	74	HIS	CA-CB-CG	6.43	120.23	113.80
1	B	340	ILE	CB-CA-C	6.39	118.69	110.96
1	B	274	CYS	CA-C-N	6.38	126.75	119.93
1	B	274	CYS	C-N-CA	6.38	126.75	119.93
1	A	225	SER	CB-CA-C	6.37	122.22	110.11
1	A	41	THR	N-CA-CB	-6.33	100.81	110.12
1	A	152	ILE	O-C-N	-6.33	116.36	123.20
1	A	286	HIS	ND1-CG-CD2	6.31	112.41	106.10
1	B	379	TRP	CB-CG-CD1	-6.30	117.45	126.90
1	A	98	ASP	N-CA-C	-6.29	103.71	112.45
1	A	249	VAL	CA-C-O	-6.29	113.92	120.27
2	C	119	HIS	CG-CD2-NE2	-6.26	100.94	107.20
2	C	120	ILE	N-CA-CB	-6.24	101.77	110.13
1	B	273	TRP	CB-CG-CD1	-6.22	117.57	126.90
1	B	217	ILE	N-CA-C	-6.22	99.25	108.45
1	A	251	ASN	CB-CG-ND2	6.21	125.72	116.40
1	A	225	SER	CA-CB-OG	6.20	123.50	111.10
2	D	21	SER	N-CA-C	6.19	119.49	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	72	TYR	CA-C-O	-6.18	114.33	120.82
1	B	126	HIS	CB-CG-ND1	6.18	131.97	122.70
1	A	273	TRP	CB-CG-CD1	-6.16	117.66	126.90
1	A	81	ASP	O-C-N	6.16	128.40	121.32
1	B	367	ASP	CA-CB-CG	6.16	118.75	112.60
1	A	68	HIS	N-CA-CB	-6.15	102.09	110.95
1	B	193	THR	N-CA-CB	-6.15	100.12	110.83
1	A	286	HIS	CB-CG-CD2	-6.14	123.22	131.20
2	C	119	HIS	CB-CG-CD2	-6.14	123.22	131.20
1	B	292	ILE	CB-CG1-CD1	-6.14	100.91	113.80
2	C	26	SER	CA-C-N	6.13	125.89	119.76
2	C	26	SER	C-N-CA	6.13	125.89	119.76
1	B	179	HIS	CG-CD2-NE2	-6.12	101.08	107.20
2	D	97	HIS	CB-CG-CD2	-6.10	123.28	131.20
1	B	39	TYR	N-CA-C	-6.09	98.97	108.90
1	B	189	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	68	HIS	CA-CB-CG	6.07	119.87	113.80
1	A	324	LYS	O-C-N	-6.05	114.92	122.24
1	A	111	ASP	CA-CB-CG	6.05	118.65	112.60
1	A	340	ILE	N-CA-C	-6.05	99.70	108.17
1	A	126	HIS	O-C-N	-6.03	115.02	122.68
1	B	233	GLY	O-C-N	-6.03	114.86	122.70
1	B	214	ASN	CB-CG-ND2	6.03	125.44	116.40
2	D	119	HIS	CG-CD2-NE2	-6.00	101.20	107.20
1	A	59	LYS	O-C-N	-6.00	116.20	123.16
1	B	152	ILE	N-CA-C	-5.96	99.89	108.53
1	B	290	HIS	CG-CD2-NE2	-5.95	101.25	107.20
1	B	278	ILE	N-CA-CB	-5.91	102.51	110.54
1	A	265	ALA	N-CA-C	5.90	118.67	111.82
1	B	16	THR	CA-C-O	5.89	128.93	120.51
1	B	179	HIS	N-CA-C	-5.89	98.26	110.80
2	C	105	HIS	CB-CG-CD2	-5.88	123.55	131.20
2	C	157	ALA	N-CA-C	-5.87	105.61	112.89
2	C	5	GLU	CA-CB-CG	-5.85	102.39	114.10
1	B	339	SER	O-C-N	-5.85	116.49	123.27
1	A	356	ASN	O-C-N	5.84	130.66	122.77
2	D	131	TYR	N-CA-C	-5.83	104.56	111.03
1	B	98	ASP	N-CA-C	-5.83	105.83	113.12
1	B	194	PHE	N-CA-C	5.80	118.00	109.24
2	D	90	ALA	N-CA-C	5.80	117.61	111.28
1	A	229	LYS	N-CA-CB	-5.80	100.68	110.49
1	B	161	CYS	CA-C-N	5.80	126.35	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	CYS	C-N-CA	5.80	126.35	120.38
1	A	228	VAL	O-C-N	5.79	128.78	122.76
1	A	149	THR	CA-CB-OG1	-5.79	100.92	109.60
2	C	15	HIS	CA-CB-CG	5.78	119.58	113.80
1	A	73	VAL	N-CA-CB	-5.78	104.21	111.31
2	C	106	VAL	N-CA-C	5.77	121.35	109.34
2	C	105	HIS	CA-CB-CG	-5.76	108.03	113.80
1	A	278	ILE	N-CA-C	5.74	118.27	111.09
1	B	220	HIS	CG-CD2-NE2	-5.74	101.46	107.20
2	D	79	GLN	N-CA-C	-5.74	98.36	108.69
1	B	231	ASP	N-CA-CB	-5.71	102.12	111.66
1	B	128	TRP	CE2-CD2-CG	-5.71	100.35	107.20
1	A	241	PHE	CA-CB-CG	5.69	119.49	113.80
1	A	118	GLU	CB-CG-CD	5.69	122.27	112.60
2	C	11	CYS	N-CA-C	-5.68	106.39	113.38
1	A	213	GLU	N-CA-C	5.67	122.88	110.80
1	B	185	VAL	N-CA-C	-5.66	100.32	108.53
1	B	276	VAL	N-CA-CB	-5.65	101.91	112.36
1	A	73	VAL	CB-CA-C	5.65	118.42	111.25
1	B	269	ASN	N-CA-C	-5.64	102.41	110.59
1	B	337	CYS	CA-CB-SG	5.64	127.37	114.40
1	A	248	ASP	CA-CB-CG	5.64	118.24	112.60
1	B	290	HIS	ND1-CG-CD2	5.63	111.73	106.10
1	A	131	GLY	O-C-N	5.63	130.01	122.70
1	B	123	LYS	CA-C-O	5.62	124.99	118.97
1	A	180	LYS	CA-C-N	-5.60	112.84	119.84
1	A	180	LYS	C-N-CA	-5.60	112.84	119.84
1	A	41	THR	O-C-N	-5.58	116.20	122.12
1	B	237	VAL	CB-CA-C	5.58	119.09	110.82
2	D	144	GLU	O-C-N	-5.57	115.69	122.82
1	B	378	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	400	PHE	N-CA-CB	-5.56	101.41	110.42
2	D	119	HIS	ND1-CG-CD2	5.56	111.66	106.10
2	D	21	SER	CA-CB-OG	-5.56	99.99	111.10
1	A	146	ASP	CA-CB-CG	5.55	118.15	112.60
1	B	204	TRP	CG-CD2-CE3	5.55	139.45	133.90
1	B	273	TRP	CE2-CD2-CG	-5.54	100.55	107.20
1	A	36	ASN	CA-CB-CG	5.53	118.12	112.60
2	D	68	LYS	O-C-N	5.52	127.83	122.09
1	A	148	GLY	CA-C-O	-5.52	110.32	119.15
1	B	200	PHE	N-CA-C	-5.52	105.18	111.14
1	B	152	ILE	CB-CG1-CD1	-5.50	102.24	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	GLU	CA-C-O	5.49	128.37	120.51
1	B	214	ASN	OD1-CG-ND2	-5.49	117.11	122.60
1	B	372	THR	CA-CB-OG1	-5.49	101.37	109.60
1	A	299	ASN	CB-CA-C	5.48	120.96	110.17
1	A	90	ALA	N-CA-C	5.48	122.46	110.80
1	A	253	ILE	CA-C-N	5.47	126.01	120.38
1	A	253	ILE	C-N-CA	5.47	126.01	120.38
2	D	119	HIS	N-CA-C	-5.46	99.38	108.34
1	A	126	HIS	CB-CG-CD2	-5.46	124.10	131.20
1	B	34	GLU	CB-CG-CD	5.46	121.87	112.60
1	A	216	MET	N-CA-CB	-5.45	102.42	110.49
1	A	354	ARG	NE-CZ-NH2	5.45	124.11	119.20
1	B	347	ILE	CB-CG1-CD1	-5.45	102.36	113.80
1	A	157	ALA	CA-C-O	-5.45	112.70	120.16
1	B	40	TYR	N-CA-C	-5.44	100.32	109.07
1	B	78	THR	O-C-N	5.43	127.86	122.10
2	C	9	ASN	CA-CB-CG	5.42	118.02	112.60
1	B	354	ARG	NE-CZ-NH2	5.42	124.08	119.20
2	D	21	SER	CA-C-O	5.42	126.55	120.70
1	A	112	LYS	CA-C-N	-5.42	117.81	122.96
1	A	112	LYS	C-N-CA	-5.42	117.81	122.96
1	A	231	ASP	CA-CB-CG	-5.41	107.19	112.60
1	B	151	VAL	N-CA-CB	5.41	118.87	111.41
1	B	323	LEU	CA-C-N	-5.40	114.79	122.41
1	B	323	LEU	C-N-CA	-5.40	114.79	122.41
2	D	119	HIS	CB-CG-CD2	-5.40	124.18	131.20
1	B	379	TRP	CE2-CD2-CG	-5.39	100.73	107.20
1	A	187	ILE	N-CA-C	-5.38	100.58	108.11
2	C	141	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	A	228	VAL	CB-CA-C	-5.37	103.51	111.19
1	B	56	GLU	N-CA-CB	-5.37	102.23	110.01
1	B	68	HIS	CG-CD2-NE2	-5.35	101.85	107.20
1	A	149	THR	N-CA-C	5.35	122.19	110.80
1	B	257	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	B	70	ILE	CA-C-N	-5.31	115.71	122.77
1	B	70	ILE	C-N-CA	-5.31	115.71	122.77
2	C	140	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	A	107	GLU	O-C-N	-5.28	116.86	123.04
2	C	15	HIS	ND1-CE1-NE2	5.28	113.68	108.40
1	A	335	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	A	213	GLU	O-C-N	5.27	129.60	122.59
1	A	219	TRP	CE2-CD2-CG	-5.27	100.87	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	ASP	O-C-N	5.27	129.60	122.59
2	C	153	GLU	CB-CA-C	-5.27	102.51	110.83
1	A	220	HIS	CB-CG-CD2	-5.27	124.35	131.20
1	B	147	GLY	N-CA-C	-5.27	108.36	115.21
2	C	75	GLN	CG-CD-NE2	5.26	124.29	116.40
2	C	116	GLU	CA-C-N	5.26	131.58	121.54
2	C	116	GLU	C-N-CA	5.26	131.58	121.54
1	A	126	HIS	CG-CD2-NE2	-5.24	101.96	107.20
1	B	280	THR	CA-C-O	-5.24	114.72	120.43
1	A	81	ASP	CA-C-N	5.24	126.39	119.84
1	A	81	ASP	C-N-CA	5.24	126.39	119.84
2	D	125	TRP	CG-CD2-CE3	5.23	139.13	133.90
1	A	333	TYR	N-CA-C	-5.23	101.41	109.52
1	A	179	HIS	O-C-N	5.23	129.21	122.20
2	D	6	MET	N-CA-C	-5.23	105.27	110.97
1	A	273	TRP	CE2-CD2-CG	-5.22	100.94	107.20
1	B	187	ILE	CB-CA-C	5.21	118.34	110.63
1	A	375	ASP	CA-CB-CG	5.21	117.81	112.60
2	D	124	GLN	N-CA-C	-5.21	102.81	110.52
2	D	65	ASP	N-CA-C	-5.21	105.50	111.07
1	B	214	ASN	CA-CB-CG	5.20	117.80	112.60
2	D	15	HIS	CG-ND1-CE1	-5.20	100.46	109.30
1	A	66	ARG	NE-CZ-NH2	5.19	123.87	119.20
2	D	97	HIS	CG-CD2-NE2	-5.19	102.01	107.20
2	C	97	HIS	CB-CG-CD2	-5.19	124.45	131.20
1	A	257	ARG	O-C-N	-5.18	116.76	122.72
1	B	138	ARG	NE-CZ-NH2	5.18	123.86	119.20
2	D	140	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	A	278	ILE	CA-CB-CG1	-5.18	101.60	110.40
1	A	234	GLU	CA-C-N	5.17	129.90	122.35
1	A	234	GLU	C-N-CA	5.17	129.90	122.35
2	C	137	ARG	NE-CZ-NH2	5.16	123.85	119.20
1	B	43	TYR	CA-CB-CG	5.16	123.19	113.90
1	B	129	LYS	CA-C-N	-5.16	113.24	122.32
1	B	129	LYS	C-N-CA	-5.16	113.24	122.32
2	D	114	ASP	CA-CB-CG	5.16	117.76	112.60
1	B	128	TRP	CD1-CG-CD2	5.15	114.54	106.30
1	A	256	GLN	CA-C-O	-5.14	115.62	121.58
1	B	90	ALA	N-CA-C	-5.13	103.37	110.35
2	D	170	TYR	CA-C-N	5.13	127.47	120.54
2	D	170	TYR	C-N-CA	5.13	127.47	120.54
2	C	152	ARG	NE-CZ-NH2	5.13	123.81	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	117	ASP	N-CA-C	5.12	121.70	110.80
2	D	15	HIS	ND1-CE1-NE2	5.12	113.52	108.40
2	D	97	HIS	ND1-CG-CD2	5.11	111.21	106.10
2	D	116	GLU	CA-CB-CG	5.11	124.33	114.10
1	B	193	THR	CA-CB-OG1	-5.11	101.94	109.60
1	B	342	ALA	CA-C-N	5.10	125.14	119.32
1	B	342	ALA	C-N-CA	5.10	125.14	119.32
1	B	331	PRO	O-C-N	5.09	129.51	122.64
2	D	30	ALA	CA-C-O	-5.08	115.07	120.92
1	A	22	LYS	O-C-N	5.08	127.30	122.07
1	B	168	ARG	N-CA-C	-5.08	105.44	110.97
1	A	340	ILE	CB-CA-C	5.07	118.39	110.83
1	B	37	THR	CA-CB-OG1	-5.07	101.99	109.60
2	C	105	HIS	ND1-CE1-NE2	5.07	113.47	108.40
1	B	350	ALA	O-C-N	-5.07	116.00	122.94
1	B	199	GLN	OE1-CD-NE2	-5.06	117.54	122.60
2	D	145	LYS	N-CA-C	5.06	117.53	111.71
1	A	162	PRO	O-C-N	-5.05	115.50	121.46
1	A	221	PRO	N-CA-C	5.05	122.88	112.47
2	C	17	THR	N-CA-C	-5.05	102.57	110.10
1	A	125	PRO	N-CA-C	5.05	121.64	111.69
1	A	275	PRO	N-CA-C	5.04	119.12	110.95
1	A	348	SER	CA-C-O	-5.04	115.84	121.23
1	A	332	SER	N-CA-C	-5.04	100.83	109.24
1	B	207	LEU	N-CA-C	5.03	119.29	112.04
1	A	219	TRP	CG-CD2-CE3	5.03	138.93	133.90
1	B	249	VAL	O-C-N	-5.03	117.85	123.03
1	A	74	HIS	CG-CD2-NE2	-5.03	102.17	107.20
1	A	161	CYS	CA-C-N	5.03	125.56	120.38
1	A	161	CYS	C-N-CA	5.03	125.56	120.38
1	A	30	VAL	CA-C-O	5.02	125.61	120.39
1	A	205	GLU	O-C-N	5.02	127.24	122.07
1	B	356	ASN	O-C-N	5.02	129.31	122.48
1	B	274	CYS	N-CA-C	5.02	117.46	108.47
1	B	46	ASN	CB-CG-ND2	5.01	123.92	116.40
1	A	167	GLU	N-CA-C	-5.01	105.90	111.36
1	A	199	GLN	OE1-CD-NE2	-5.01	117.59	122.60
2	D	141	ARG	NE-CZ-NH2	5.00	123.70	119.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	HIS	Sidechain
1	A	220	HIS	Sidechain
1	A	400	PHE	Mainchain,Peptide
1	B	60	HIS	Sidechain
1	B	68	HIS	Sidechain
2	C	105	HIS	Sidechain

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	3018	0	2953	174	0
1	B	3018	0	2954	210	0
2	C	1344	0	1282	57	0
2	D	1344	0	1282	63	0
3	A	53	0	30	7	0
3	B	53	0	30	2	0
4	C	86	0	60	2	0
4	D	86	0	60	7	0
All	All	9002	0	8651	494	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 28.

All (494) 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:A:180:LYS:NZ	1:A:180:LYS:HA	1.25	1.51
1:A:293:GLY:HA3	1:A:311:GLN:HE22	1.09	1.15
1:B:300:PRO:O	1:B:301:MET:HB2	1.47	1.11
1:A:293:GLY:HA3	1:A:311:GLN:NE2	1.70	1.06
1:B:19:LYS:O	1:B:23:LEU:HB2	1.55	1.06
1:B:81:ASP:HB3	1:B:82:PRO:CD	1.86	1.05
1:A:180:LYS:NZ	1:A:180:LYS:CA	2.20	1.04
1:B:299:ASN:HB3	1:B:300:PRO:HD2	1.37	1.04
1:A:298:ALA:O	1:A:299:ASN:O	1.75	1.02
1:B:81:ASP:HB3	1:B:82:PRO:HD3	1.41	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ASP:OD1	1:A:25:ASP:O	1.79	1.00
1:B:298:ALA:O	1:B:300:PRO:O	1.81	0.97
1:A:299:ASN:O	1:A:301:MET:N	1.99	0.96
1:B:17:ALA:O	1:B:21:ILE:HB	1.66	0.94
1:B:82:PRO:C	1:B:84:LYS:H	1.75	0.90
1:B:80:ILE:O	1:B:81:ASP:HB2	1.69	0.90
2:C:145:LYS:H	2:C:145:LYS:HD3	1.37	0.89
1:B:299:ASN:HB3	1:B:300:PRO:CD	2.02	0.89
1:A:88:LYS:HG3	1:A:94:GLU:HG2	1.54	0.89
1:B:15:ALA:HB3	1:B:399:THR:HG22	1.56	0.86
1:A:180:LYS:HA	1:A:180:LYS:HZ3	1.06	0.86
1:B:290:HIS:NE2	1:B:319:VAL:HG23	1.91	0.86
1:B:153:ALA:HB1	1:B:227:VAL:HG11	1.57	0.86
1:A:180:LYS:CA	1:A:180:LYS:HZ2	1.86	0.85
2:D:145:LYS:HD3	2:D:145:LYS:N	1.90	0.85
1:A:146:ASP:OD1	1:A:179:HIS:O	1.95	0.85
1:A:180:LYS:HA	1:A:180:LYS:HZ2	1.05	0.83
1:B:16:THR:HG22	1:B:17:ALA:N	1.91	0.83
1:B:22:LYS:HZ3	1:B:29:GLU:HA	1.44	0.83
1:A:53:ARG:HB2	1:A:53:ARG:HH11	1.44	0.83
1:B:299:ASN:CG	1:B:362:ILE:H	1.86	0.82
2:D:143:MET:HE1	2:D:151:LEU:HD22	1.61	0.82
1:A:293:GLY:CA	1:A:311:GLN:HE22	1.92	0.82
1:A:180:LYS:CA	1:A:180:LYS:HZ3	1.89	0.82
2:C:145:LYS:HD3	2:C:145:LYS:N	1.91	0.82
1:B:290:HIS:CD2	1:B:319:VAL:HG23	2.14	0.81
1:B:260:LYS:H	1:B:260:LYS:HD2	1.44	0.80
1:B:299:ASN:HD21	1:B:361:ALA:HA	1.46	0.80
1:A:22:LYS:HE2	1:A:69:GLY:HA3	1.63	0.79
1:B:3:ARG:NH2	1:B:323:LEU:HB3	1.99	0.78
1:B:17:ALA:HB1	1:B:21:ILE:CD1	2.15	0.77
1:A:109:ILE:HD11	1:A:257:ARG:HD2	1.66	0.77
2:D:145:LYS:HD3	2:D:145:LYS:H	1.49	0.77
1:B:112:LYS:HG3	1:B:255:PRO:HG2	1.65	0.77
1:B:290:HIS:HE2	1:B:319:VAL:HG23	1.45	0.77
1:B:84:LYS:O	1:B:85:LYS:HB3	1.85	0.76
1:B:299:ASN:OD1	1:B:361:ALA:HB1	1.86	0.76
1:A:213:GLU:HG2	1:B:223:PRO:HD3	1.67	0.76
1:B:80:ILE:O	1:B:81:ASP:CB	2.32	0.76
1:B:19:LYS:O	1:B:23:LEU:CB	2.33	0.75
1:B:82:PRO:C	1:B:84:LYS:N	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ILE:CG2	1:A:30:VAL:HG21	2.16	0.75
1:B:321:VAL:HG11	1:B:328:PRO:HA	1.69	0.75
2:C:18:HIS:HB3	2:C:76:GLN:HG2	1.69	0.74
1:A:19:LYS:O	1:A:23:LEU:HB2	1.87	0.73
1:B:100:CYS:HB3	1:B:289:ILE:HG23	1.69	0.73
2:D:146:LYS:HE3	2:D:146:LYS:H	1.54	0.73
2:C:145:LYS:H	2:C:145:LYS:CD	1.96	0.72
1:B:81:ASP:O	1:B:83:ASP:N	2.22	0.72
1:A:99:ARG:HH11	1:A:290:HIS:HE1	1.36	0.72
1:B:81:ASP:CB	1:B:82:PRO:CD	2.63	0.72
1:A:150:VAL:HG13	1:A:249:VAL:HB	1.72	0.72
1:A:315:ALA:O	1:A:319:VAL:HG13	1.90	0.71
1:B:148:GLY:O	1:B:183:SER:HB3	1.90	0.71
1:B:22:LYS:NZ	1:B:29:GLU:HA	2.04	0.71
2:D:31:GLN:HB2	2:D:76:GLN:O	1.91	0.70
1:A:331:PRO:HD2	1:A:355:PRO:HG3	1.72	0.70
1:B:83:ASP:N	1:B:83:ASP:OD1	2.23	0.70
1:A:382:GLU:O	1:A:385:VAL:HG12	1.91	0.69
1:B:292:ILE:HD11	1:B:315:ALA:CB	2.22	0.69
1:B:279:LYS:NZ	1:B:329:GLY:O	2.25	0.69
1:A:298:ALA:C	1:A:299:ASN:O	2.35	0.69
1:A:146:ASP:CG	1:A:179:HIS:O	2.36	0.69
2:C:138:GLU:O	2:C:139:GLU:HB2	1.93	0.69
1:B:34:GLU:O	1:B:74:HIS:HA	1.92	0.69
1:B:392:TYR:O	1:B:396:VAL:HB	1.92	0.69
1:B:32:LEU:HD23	1:B:72:VAL:HG23	1.74	0.68
1:B:15:ALA:O	1:B:16:THR:C	2.35	0.68
1:A:260:LYS:H	1:A:260:LYS:HD2	1.58	0.68
1:B:260:LYS:H	1:B:260:LYS:CD	2.07	0.68
1:B:141:LEU:HD21	1:B:172:VAL:HG13	1.76	0.67
1:A:313:LYS:HD3	2:C:9:ASN:HB3	1.75	0.67
1:B:334:LEU:HD12	1:B:352:ILE:HD13	1.77	0.67
1:A:301:MET:HE2	1:A:362:ILE:HD13	1.75	0.67
1:B:81:ASP:CB	1:B:82:PRO:HD3	2.21	0.67
1:B:131:GLY:HA2	1:B:134:THR:OG1	1.95	0.67
1:B:110:TYR:HB3	1:B:117:SER:HA	1.77	0.67
1:A:299:ASN:HB2	1:A:362:ILE:HB	1.78	0.66
1:B:275:PRO:HG2	1:B:285:ILE:HD11	1.76	0.66
1:A:66:ARG:C	1:A:68:HIS:H	2.03	0.66
1:A:250:ILE:HD12	1:A:252:LEU:HD23	1.77	0.66
1:A:265:ALA:HB3	1:A:267:LEU:HD22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ARG:HD3	3:A:699:FAD:H9	1.78	0.65
1:A:350:ALA:HB2	2:C:53:ILE:HD11	1.77	0.65
1:B:79:GLY:O	1:B:88:LYS:N	2.28	0.65
1:B:301:MET:HE2	1:B:362:ILE:HD13	1.79	0.65
1:B:81:ASP:HB3	1:B:82:PRO:HD2	1.76	0.65
1:A:19:LYS:HG3	1:A:20:TYR:N	2.11	0.65
1:A:319:VAL:O	1:A:323:LEU:N	2.24	0.65
1:B:252:LEU:O	1:B:254:PRO:HD3	1.95	0.65
1:B:17:ALA:O	1:B:21:ILE:CB	2.44	0.65
2:C:97:HIS:HD1	2:C:101:CYS:HB2	1.61	0.64
1:B:297:ILE:HG22	1:B:297:ILE:O	1.96	0.64
1:A:300:PRO:HD2	1:A:362:ILE:O	1.98	0.64
1:B:80:ILE:HG22	1:B:265:ALA:HB2	1.79	0.64
1:B:280:THR:HG22	1:B:318:ALA:HB1	1.80	0.64
2:C:24:PRO:O	2:C:127:PRO:HG2	1.98	0.64
2:D:136:PHE:CE1	2:D:141:ARG:HD3	2.32	0.64
1:A:65:LEU:O	1:A:68:HIS:HB3	1.97	0.64
2:D:145:LYS:H	2:D:145:LYS:CD	2.11	0.64
1:B:331:PRO:HA	2:D:6:MET:HE3	1.79	0.63
1:B:108:LEU:HD13	1:B:126:HIS:NE2	2.14	0.63
1:A:221:PRO:O	1:A:225:SER:HB3	1.99	0.63
2:D:49:ILE:HG13	2:D:141:ARG:HG3	1.81	0.63
1:A:319:VAL:CG2	1:A:320:VAL:N	2.61	0.63
2:D:1:GLU:HG2	2:D:2:PRO:HD2	1.81	0.63
2:D:146:LYS:HG2	4:D:902:HEC:HBC3	1.81	0.63
1:B:356:ASN:CG	1:B:363:GLU:HB3	2.24	0.62
2:C:49:ILE:HG23	2:C:141:ARG:HG2	1.81	0.62
1:A:19:LYS:HA	1:A:70:ILE:HD11	1.80	0.62
2:D:153:GLU:HB3	2:D:154:LEU:HD12	1.81	0.62
1:A:156:ALA:HB2	1:A:190:SER:HB2	1.82	0.62
1:A:176:LEU:HB3	1:A:216:MET:HE2	1.80	0.62
1:B:153:ALA:CB	1:B:227:VAL:HG11	2.27	0.62
1:A:99:ARG:HH11	1:A:290:HIS:CE1	2.17	0.62
1:A:180:LYS:HD2	1:A:180:LYS:N	2.15	0.61
1:A:365:VAL:HG13	1:A:368:SER:OG	2.00	0.61
1:A:84:LYS:O	1:A:86:LEU:HD23	1.99	0.61
1:B:112:LYS:CG	1:B:255:PRO:HG2	2.30	0.61
2:D:27:PRO:HG3	2:D:128:TYR:CD1	2.35	0.61
1:B:153:ALA:HB1	1:B:227:VAL:CG1	2.27	0.61
1:B:358:ASP:O	1:B:360:SER:N	2.33	0.61
2:D:126:THR:O	2:D:130:GLN:HG3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ILE:HG22	1:B:265:ALA:CB	2.30	0.60
2:D:20:ASN:HD21	2:D:78:TYR:HA	1.66	0.60
1:B:85:LYS:O	1:B:96:GLY:HA2	2.01	0.60
1:A:25:ASP:OD1	1:A:25:ASP:C	2.45	0.60
1:B:17:ALA:HB1	1:B:21:ILE:HG13	1.84	0.60
1:B:168:ARG:HH11	1:B:251:ASN:HD21	1.48	0.60
1:B:5:VAL:O	1:B:30:VAL:HA	2.01	0.60
2:D:55:GLY:O	2:D:59:LYS:HG3	2.02	0.60
1:A:319:VAL:O	1:A:323:LEU:HB2	2.02	0.60
1:B:130:ALA:O	1:B:134:THR:HG23	2.02	0.60
2:C:111:PRO:HB3	2:C:120:ILE:HD12	1.82	0.59
1:A:11:GLY:O	1:A:12:THR:C	2.45	0.59
1:A:11:GLY:O	1:A:13:GLY:N	2.35	0.59
2:C:89:LEU:HD23	2:C:165:ALA:HA	1.84	0.59
1:A:114:GLU:N	1:A:229:LYS:HA	2.17	0.59
1:B:78:THR:OG1	1:B:90:ALA:HB2	2.02	0.59
1:B:6:VAL:HG11	1:B:87:VAL:HG21	1.85	0.59
1:B:28:ILE:HD12	1:B:323:LEU:HD21	1.85	0.59
1:B:65:LEU:O	1:B:70:ILE:HG12	2.03	0.59
1:B:304:SER:HA	3:B:699:FAD:H1'2	1.85	0.59
1:B:351:ALA:O	1:B:352:ILE:O	2.21	0.59
1:A:80:ILE:HG21	1:A:265:ALA:HB1	1.85	0.58
1:B:85:LYS:O	1:B:85:LYS:HG2	2.01	0.58
1:B:300:PRO:HD2	1:B:362:ILE:O	2.03	0.58
2:D:156:LYS:HZ2	2:D:163:LEU:HD21	1.68	0.58
1:A:301:MET:HE2	1:A:362:ILE:CD1	2.33	0.58
1:B:40:TYR:HD2	1:B:58:ILE:HG22	1.69	0.58
1:B:5:VAL:HG23	1:B:30:VAL:HB	1.85	0.58
2:D:141:ARG:HG2	2:D:142:PRO:HD2	1.86	0.57
1:B:299:ASN:CB	1:B:362:ILE:HB	2.34	0.57
1:A:7:VAL:HG22	1:A:101:VAL:HB	1.87	0.57
1:A:53:ARG:HB2	1:A:53:ARG:NH1	2.17	0.57
1:A:179:HIS:O	1:A:180:LYS:HB2	2.05	0.57
1:B:302:PRO:HG2	1:B:335:ASN:OD1	2.03	0.57
1:A:356:ASN:HB2	1:A:363:GLU:HB2	1.87	0.56
1:A:183:SER:O	1:A:184:LYS:HG3	2.05	0.56
1:A:302:PRO:HG2	1:A:335:ASN:ND2	2.20	0.56
1:A:206:ARG:HD2	1:A:345:TYR:HE2	1.69	0.56
1:B:274:CYS:SG	1:B:291:VAL:HG11	2.46	0.56
1:B:17:ALA:HB1	1:B:21:ILE:CG1	2.36	0.56
2:D:38:VAL:O	2:D:42:GLU:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:151:LEU:C	2:C:151:LEU:HD22	2.31	0.56
1:B:299:ASN:CB	1:B:300:PRO:CD	2.80	0.56
1:B:16:THR:HG22	1:B:17:ALA:H	1.70	0.56
1:A:87:VAL:O	1:A:94:GLU:HA	2.06	0.55
1:B:126:HIS:O	1:B:126:HIS:ND1	2.39	0.55
2:C:153:GLU:HB2	2:C:154:LEU:HD12	1.86	0.55
2:D:100:TYR:HE2	2:D:154:LEU:HB3	1.71	0.55
1:A:21:ILE:CG2	1:A:22:LYS:N	2.70	0.55
1:B:112:LYS:CB	1:B:255:PRO:HG2	2.37	0.55
1:B:114:GLU:H	1:B:229:LYS:HA	1.72	0.55
1:B:282:GLU:HG3	1:B:290:HIS:CE1	2.41	0.55
1:A:327:GLU:O	1:A:327:GLU:HG3	2.07	0.55
2:C:5:GLU:HG3	2:C:72:TYR:CE2	2.41	0.55
1:B:157:ALA:HB1	1:B:158:PRO:HD3	1.89	0.55
1:A:117:SER:H	1:A:120:ALA:HB3	1.72	0.54
1:B:227:VAL:HA	1:B:239:THR:HA	1.89	0.54
1:B:292:ILE:HD11	1:B:315:ALA:HB3	1.87	0.54
2:D:95:LYS:HG3	2:D:96:LEU:N	2.21	0.54
2:D:33:ASP:OD2	2:D:117:ASP:HA	2.07	0.54
1:A:293:GLY:CA	1:A:311:GLN:NE2	2.58	0.54
2:D:114:ASP:O	2:D:116:GLU:HG2	2.07	0.54
1:A:228:VAL:O	1:A:230:VAL:N	2.40	0.54
2:C:31:GLN:HG3	2:C:76:GLN:O	2.07	0.54
1:B:114:GLU:O	1:B:230:VAL:HA	2.07	0.54
1:B:324:LYS:O	1:B:325:GLY:C	2.51	0.54
1:A:12:THR:HA	1:A:399:THR:HG21	1.89	0.53
1:A:383:ARG:HH11	1:A:383:ARG:CG	2.21	0.53
2:D:32:MET:HE1	4:D:901:HEC:HBA2	1.88	0.53
2:C:20:ASN:HD21	2:C:78:TYR:HA	1.73	0.53
1:B:4:LYS:HD3	1:B:29:GLU:HB3	1.89	0.53
1:B:279:LYS:NZ	1:B:279:LYS:HB3	2.24	0.53
1:B:85:LYS:O	1:B:85:LYS:CG	2.56	0.53
1:B:21:ILE:HD11	1:B:319:VAL:HG11	1.89	0.53
1:B:229:LYS:O	1:B:230:VAL:HG23	2.09	0.53
1:B:321:VAL:HG13	1:B:326:GLU:O	2.08	0.53
1:B:13:GLY:O	1:B:16:THR:HB	2.08	0.53
1:B:147:GLY:HA2	1:B:182:MET:O	2.08	0.53
2:D:27:PRO:HG3	2:D:128:TYR:CE1	2.43	0.53
1:A:171:GLN:O	1:A:174:TYR:HB3	2.08	0.52
1:B:257:ARG:HB2	1:B:272:GLY:O	2.10	0.52
1:B:326:GLU:O	1:B:327:GLU:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:TYR:HD1	1:B:353:TYR:HB2	1.74	0.52
1:A:229:LYS:O	1:A:230:VAL:HG23	2.09	0.52
2:D:97:HIS:NE2	2:D:102:GLU:HG2	2.24	0.52
2:C:93:GLY:HA3	2:C:169:PHE:HB2	1.92	0.52
2:C:86:ASP:HB3	2:C:89:LEU:HB2	1.90	0.52
1:B:260:LYS:O	1:B:263:GLN:HB2	2.10	0.52
1:B:300:PRO:O	1:B:301:MET:CB	2.34	0.52
1:B:278:ILE:HD12	1:B:362:ILE:HD12	1.91	0.52
1:A:307:SER:O	1:A:311:GLN:HG3	2.10	0.52
1:A:393:ASN:HD22	2:C:24:PRO:HD3	1.75	0.52
1:A:343:PRO:O	1:A:385:VAL:HG21	2.10	0.51
1:A:151:VAL:HA	1:A:186:ILE:O	2.10	0.51
1:B:171:GLN:O	1:B:174:TYR:HB3	2.10	0.51
1:B:306:TYR:HB3	1:B:335:ASN:HD22	1.75	0.51
2:C:134:SER:O	2:C:138:GLU:HB2	2.09	0.51
1:B:15:ALA:HA	1:B:18:ALA:HB3	1.92	0.51
1:B:196:LYS:HB3	1:B:371:VAL:HG21	1.93	0.51
1:B:87:VAL:HG23	1:B:97:TYR:HD2	1.75	0.51
1:A:298:ALA:O	1:A:299:ASN:C	2.53	0.51
1:A:86:LEU:HD12	1:A:94:GLU:HB3	1.93	0.51
1:B:318:ALA:O	1:B:322:LEU:HB2	2.10	0.51
2:D:136:PHE:CZ	2:D:141:ARG:HD3	2.45	0.51
1:A:21:ILE:HG22	1:A:22:LYS:N	2.26	0.51
2:C:111:PRO:HD3	2:C:120:ILE:HG13	1.92	0.50
2:C:121:LEU:O	2:C:170:TYR:HB3	2.11	0.50
2:D:100:TYR:CE2	2:D:154:LEU:HB3	2.45	0.50
1:A:260:LYS:H	1:A:260:LYS:CD	2.23	0.50
1:A:17:ALA:O	1:A:21:ILE:HB	2.11	0.50
1:A:80:ILE:O	1:A:81:ASP:C	2.54	0.50
1:B:17:ALA:HB1	1:B:21:ILE:HD12	1.91	0.50
1:A:101:VAL:HG22	1:A:290:HIS:HB2	1.93	0.50
1:A:306:TYR:HD2	1:A:391:TRP:HE1	1.54	0.50
1:B:55:LEU:HD21	1:B:131:GLY:HA2	1.93	0.50
2:D:82:LYS:HA	2:D:174:GLN:NE2	2.27	0.50
2:C:2:PRO:HB2	2:C:7:LEU:HD13	1.94	0.49
2:D:104:CYS:O	2:D:106:VAL:HG23	2.12	0.49
1:A:3:ARG:HB2	1:A:28:ILE:HG12	1.94	0.49
1:A:300:PRO:O	1:A:302:PRO:HD3	2.12	0.49
1:B:190:SER:C	1:B:222:GLY:HA3	2.37	0.49
1:A:132:GLU:H	1:A:132:GLU:CD	2.20	0.49
1:A:360:SER:O	1:A:361:ALA:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:SER:HB3	2:D:56:ARG:HH22	1.77	0.49
2:D:156:LYS:NZ	2:D:163:LEU:HD21	2.27	0.49
1:A:3:ARG:HE	1:A:3:ARG:HA	1.76	0.49
1:B:207:LEU:HD21	1:B:345:TYR:CD2	2.48	0.49
2:C:34:PRO:HD3	2:C:74:LYS:HD3	1.92	0.49
1:B:5:VAL:HG21	1:B:21:ILE:CD1	2.43	0.49
1:B:13:GLY:O	1:B:16:THR:CB	2.60	0.49
1:B:65:LEU:HD13	1:B:400:PHE:HA	1.94	0.49
1:A:50:GLY:HA3	1:A:171:GLN:HE21	1.76	0.49
1:A:250:ILE:CD1	1:A:252:LEU:HD23	2.41	0.49
1:B:292:ILE:HD11	1:B:315:ALA:HB2	1.94	0.49
1:B:332:SER:O	2:D:10:ASN:ND2	2.38	0.49
2:D:12:ALA:HA	2:D:15:HIS:O	2.13	0.49
2:D:111:PRO:HD3	2:D:120:ILE:HG23	1.94	0.49
1:B:16:THR:CG2	1:B:17:ALA:N	2.60	0.49
2:D:144:GLU:HG2	4:D:902:HEC:HBD2	1.95	0.49
1:A:149:THR:HA	1:A:184:LYS:O	2.13	0.49
1:A:294:ASP:HB2	3:A:699:FAD:O2P	2.13	0.49
1:A:387:TYR:OH	2:C:131:TYR:HD2	1.95	0.49
1:B:343:PRO:O	1:B:385:VAL:HG21	2.12	0.49
2:D:100:TYR:O	2:D:150:LYS:HG2	2.12	0.48
1:B:268:THR:HG23	1:B:269:ASN:O	2.13	0.48
1:A:48:VAL:HA	1:A:53:ARG:O	2.13	0.48
2:D:18:HIS:HB2	2:D:76:GLN:HG3	1.94	0.48
1:A:82:PRO:O	1:A:84:LYS:N	2.46	0.48
1:A:318:ALA:O	1:A:322:LEU:CB	2.62	0.48
2:D:96:LEU:HD23	2:D:155:LEU:HD21	1.96	0.48
2:D:98:ASP:HA	2:D:102:GLU:HB2	1.96	0.48
2:C:107:GLU:HB3	2:C:112:LEU:HD11	1.96	0.48
1:B:124:LEU:HD22	1:B:250:ILE:HG12	1.94	0.48
1:A:126:HIS:HB3	1:A:254:PRO:HD2	1.96	0.48
2:C:150:LYS:HD3	2:C:154:LEU:HD22	1.96	0.48
1:B:113:ILE:HG12	1:B:116:TYR:HB2	1.96	0.48
1:B:260:LYS:CD	1:B:260:LYS:N	2.76	0.48
1:A:126:HIS:CG	1:A:126:HIS:O	2.66	0.47
1:A:126:HIS:NE2	1:A:133:GLN:NE2	2.62	0.47
1:A:279:LYS:HE2	1:A:279:LYS:HB3	1.75	0.47
1:B:227:VAL:HG13	1:B:227:VAL:O	2.13	0.47
1:B:326:GLU:HG2	1:B:327:GLU:OE2	2.14	0.47
2:D:97:HIS:ND1	2:D:101:CYS:HB2	2.29	0.47
1:A:35:PRO:HD2	3:A:699:FAD:N3A	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:VAL:O	1:A:100:CYS:HA	2.13	0.47
1:A:257:ARG:HG3	1:A:263:GLN:HE22	1.78	0.47
1:B:16:THR:HG23	1:B:312:GLY:HA2	1.95	0.47
1:B:108:LEU:HD22	1:B:126:HIS:CD2	2.48	0.47
2:C:120:ILE:O	2:C:121:LEU:HD12	2.14	0.47
2:D:144:GLU:HA	2:D:144:GLU:OE1	2.13	0.47
2:D:148:ALA:O	2:D:152:ARG:HB3	2.15	0.47
1:B:336:THR:HG22	1:B:350:ALA:HA	1.96	0.47
1:A:42:CYS:SG	3:A:699:FAD:HM71	2.54	0.47
2:C:22:VAL:HG12	2:C:23:GLY:H	1.78	0.47
1:A:136:ILE:HG22	1:A:140:GLN:OE1	2.15	0.47
1:A:365:VAL:HG13	1:A:368:SER:HG	1.79	0.47
1:A:365:VAL:O	1:A:368:SER:OG	2.31	0.47
1:B:152:ILE:O	1:B:187:ILE:HA	2.15	0.47
1:B:108:LEU:HD13	1:B:126:HIS:CE1	2.49	0.47
1:B:157:ALA:CB	1:B:158:PRO:HD3	2.44	0.47
1:B:187:ILE:HG23	1:B:219:TRP:HA	1.95	0.47
1:B:23:LEU:O	1:B:24:ALA:C	2.57	0.47
1:B:15:ALA:CB	1:B:399:THR:HG22	2.36	0.47
1:B:277:ASP:O	1:B:281:PHE:HA	2.14	0.47
1:A:160:ARG:HG3	3:A:699:FAD:H1'1	1.95	0.46
2:C:148:ALA:O	2:C:152:ARG:N	2.44	0.46
2:D:16:GLY:HA3	2:D:20:ASN:O	2.15	0.46
1:A:176:LEU:HD12	1:A:176:LEU:HA	1.77	0.46
1:A:274:CYS:SG	1:A:295:ALA:O	2.72	0.46
1:B:55:LEU:HD21	1:B:131:GLY:CA	2.44	0.46
1:B:202:LYS:HE3	1:B:206:ARG:HH12	1.79	0.46
1:B:391:TRP:O	1:B:395:ILE:HG22	2.16	0.46
2:D:15:HIS:HA	2:D:21:SER:OG	2.15	0.46
1:B:127:ALA:HA	1:B:133:GLN:HG2	1.98	0.46
1:A:16:THR:O	1:A:20:TYR:HB2	2.15	0.46
1:A:65:LEU:C	1:A:68:HIS:HB3	2.41	0.46
2:C:31:GLN:HB2	2:C:78:TYR:HB2	1.96	0.46
1:B:267:LEU:CD1	1:B:286:HIS:HD2	2.28	0.46
1:B:79:GLY:HA3	1:B:88:LYS:HB3	1.98	0.46
1:B:334:LEU:HD12	1:B:352:ILE:CD1	2.44	0.46
1:A:35:PRO:HD3	1:A:76:SER:HA	1.97	0.46
1:A:89:THR:O	1:A:91:GLY:N	2.49	0.46
1:B:215:ALA:HB1	1:B:217:ILE:O	2.15	0.46
1:B:290:HIS:CD2	1:B:319:VAL:CG2	2.92	0.46
1:A:19:LYS:O	1:A:23:LEU:CB	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ALA:O	1:B:16:THR:O	2.33	0.46
1:B:35:PRO:HD2	3:B:699:FAD:N3A	2.31	0.46
1:B:268:THR:HG23	1:B:272:GLY:HA2	1.96	0.46
1:B:336:THR:HA	1:B:349:VAL:O	2.15	0.46
2:C:97:HIS:ND1	2:C:101:CYS:HB2	2.31	0.45
1:A:180:LYS:HZ3	1:A:180:LYS:N	2.14	0.45
2:C:148:ALA:O	2:C:151:LEU:N	2.48	0.45
1:B:282:GLU:HA	1:B:290:HIS:ND1	2.31	0.45
2:D:43:GLY:C	2:D:49:ILE:HG22	2.42	0.45
1:A:25:ASP:O	1:A:27:SER:N	2.49	0.45
2:C:105:HIS:CE1	2:C:119:HIS:HB2	2.52	0.45
1:B:40:TYR:CD2	1:B:131:GLY:HA3	2.50	0.45
1:B:80:ILE:HD11	1:B:100:CYS:SG	2.56	0.45
1:A:260:LYS:O	1:A:264:ILE:HG13	2.16	0.45
1:B:78:THR:HB	1:B:90:ALA:N	2.32	0.45
2:D:150:LYS:HE2	2:D:154:LEU:HD22	1.98	0.45
2:C:145:LYS:N	2:C:145:LYS:CD	2.61	0.45
1:A:80:ILE:HG21	1:A:265:ALA:CB	2.47	0.45
1:A:385:VAL:O	1:A:388:ALA:HB3	2.17	0.45
1:B:336:THR:HG21	4:D:901:HEC:CBC	2.47	0.45
2:D:34:PRO:HA	2:D:70:ALA:HB1	1.98	0.45
1:A:101:VAL:CG1	1:A:292:ILE:HD11	2.46	0.45
1:A:318:ALA:O	1:A:322:LEU:HB2	2.16	0.44
3:A:699:FAD:H5'2	3:A:699:FAD:O2A	2.17	0.44
1:B:299:ASN:CB	1:B:300:PRO:HD2	2.27	0.44
1:A:392:TYR:O	1:A:396:VAL:HG13	2.18	0.44
1:B:336:THR:HG22	1:B:350:ALA:CB	2.47	0.44
2:D:144:GLU:HG3	4:D:902:HEC:HMD3	2.00	0.44
1:B:35:PRO:HB3	1:B:76:SER:OG	2.18	0.44
1:B:247:ALA:HB3	1:B:250:ILE:HG22	1.99	0.44
1:B:319:VAL:HG12	1:B:320:VAL:N	2.33	0.44
1:B:194:PHE:HE1	1:B:200:PHE:CD2	2.35	0.44
1:B:267:LEU:HD11	1:B:289:ILE:HD12	1.99	0.44
1:A:383:ARG:HH11	1:A:383:ARG:HG2	1.82	0.44
1:A:107:GLU:HA	1:A:260:LYS:NZ	2.33	0.44
1:A:310:SER:O	1:A:313:LYS:HB2	2.18	0.44
2:C:144:GLU:HG2	2:C:146:LYS:CE	2.48	0.44
1:B:28:ILE:HD12	1:B:323:LEU:CD2	2.47	0.44
1:B:299:ASN:CG	1:B:362:ILE:HB	2.42	0.44
1:A:278:ILE:HD12	1:A:362:ILE:CD1	2.47	0.44
2:C:5:GLU:HA	2:C:8:THR:OG1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:111:PRO:HA	2:C:118:TYR:CE2	2.53	0.44
1:A:232:GLY:C	1:A:234:GLU:H	2.25	0.44
1:B:22:LYS:HD2	1:B:22:LYS:HA	1.73	0.44
1:A:319:VAL:HG22	1:A:320:VAL:H	1.82	0.43
2:C:126:THR:HB	2:C:127:PRO:HD3	1.98	0.43
1:A:319:VAL:HG22	1:A:320:VAL:N	2.32	0.43
1:A:356:ASN:ND2	1:A:363:GLU:HB3	2.32	0.43
1:A:371:VAL:O	1:A:372:THR:C	2.60	0.43
1:A:42:CYS:SG	3:A:699:FAD:C7M	3.06	0.43
1:A:274:CYS:HA	1:A:275:PRO:HD2	1.74	0.43
1:A:314:VAL:O	1:A:318:ALA:HB2	2.18	0.43
1:A:126:HIS:CD2	1:A:126:HIS:H	2.37	0.43
1:A:175:TYR:O	1:A:178:ALA:N	2.37	0.43
1:B:4:LYS:HA	1:B:29:GLU:O	2.18	0.43
1:B:75:ASP:OD2	1:B:89:THR:HG22	2.18	0.43
2:D:95:LYS:HG3	2:D:96:LEU:H	1.84	0.43
1:A:292:ILE:HG22	1:A:311:GLN:HB3	2.00	0.43
2:C:150:LYS:O	2:C:155:LEU:N	2.46	0.43
1:B:13:GLY:O	1:B:16:THR:OG1	2.34	0.43
1:B:18:ALA:HA	1:B:30:VAL:HG21	1.99	0.43
1:B:87:VAL:HG23	1:B:97:TYR:CD2	2.54	0.43
1:B:231:ASP:HB2	1:B:237:VAL:HG23	2.00	0.43
1:B:369:GLY:HA2	2:D:56:ARG:HB3	2.00	0.43
1:A:11:GLY:O	1:A:14:GLY:N	2.51	0.43
1:A:273:TRP:CZ2	1:A:303:LYS:HE3	2.53	0.43
1:B:299:ASN:HB2	1:B:362:ILE:HB	1.99	0.43
1:B:319:VAL:O	1:B:323:LEU:HD13	2.17	0.43
2:D:31:GLN:CB	2:D:76:GLN:O	2.65	0.43
2:C:100:TYR:CE1	2:C:154:LEU:HB3	2.53	0.43
2:C:133:MET:HG2	2:C:163:LEU:HD22	2.00	0.43
1:A:82:PRO:HB2	1:A:83:ASP:H	1.38	0.43
2:C:22:VAL:HG12	2:C:23:GLY:N	2.34	0.43
1:A:292:ILE:HG22	1:A:311:GLN:CB	2.49	0.43
2:C:16:GLY:HA3	2:C:20:ASN:O	2.18	0.43
1:B:338:TYR:HE1	1:B:384:GLU:HG2	1.84	0.43
1:B:379:TRP:HH2	2:D:50:ALA:HB1	1.84	0.43
2:D:103:LYS:HE3	4:D:902:HEC:HMC1	2.00	0.43
4:D:902:HEC:HBC2	4:D:902:HEC:HH2	2.01	0.43
1:A:176:LEU:HB3	1:A:216:MET:CE	2.47	0.43
1:A:180:LYS:N	1:A:180:LYS:CD	2.81	0.43
1:B:3:ARG:CZ	1:B:323:LEU:HB3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PRO:HG3	1:A:165:PRO:HB3	2.00	0.42
2:C:147:MET:HB2	4:C:902:HEC:C4C	2.49	0.42
1:A:4:LYS:HA	1:A:29:GLU:O	2.19	0.42
1:A:114:GLU:O	1:A:230:VAL:HA	2.19	0.42
2:C:78:TYR:CD2	2:C:120:ILE:HD11	2.55	0.42
1:B:278:ILE:HG23	1:B:362:ILE:HG13	2.02	0.42
1:A:7:VAL:HA	1:A:101:VAL:O	2.19	0.42
2:C:34:PRO:HA	2:C:70:ALA:HB1	2.00	0.42
2:D:105:HIS:CE1	2:D:119:HIS:HB2	2.54	0.42
1:A:319:VAL:HG23	1:A:320:VAL:N	2.33	0.42
1:B:155:PRO:HD3	1:B:253:ILE:HB	2.01	0.42
1:B:348:SER:O	1:B:371:VAL:HG23	2.20	0.42
2:D:112:LEU:HD12	2:D:118:TYR:HB3	2.02	0.42
1:B:343:PRO:O	1:B:385:VAL:HG11	2.19	0.42
1:A:172:VAL:HG12	1:A:176:LEU:HD22	2.00	0.42
1:B:146:ASP:CG	1:B:180:LYS:HB3	2.45	0.42
1:A:106:ILE:O	1:A:106:ILE:HG13	2.19	0.42
1:A:127:ALA:HB3	1:A:168:ARG:NH2	2.35	0.41
2:C:72:TYR:CD1	2:C:72:TYR:C	2.98	0.41
1:B:17:ALA:CB	1:B:21:ILE:HG13	2.49	0.41
1:B:19:LYS:HE2	1:B:398:ASP:O	2.19	0.41
1:B:194:PHE:O	1:B:197:GLN:HB2	2.19	0.41
1:B:356:ASN:ND2	1:B:363:GLU:HB3	2.35	0.41
2:D:61:TYR:HB2	2:D:66:PHE:CE1	2.55	0.41
1:A:176:LEU:C	1:A:178:ALA:N	2.77	0.41
1:B:84:LYS:O	1:B:85:LYS:CB	2.60	0.41
1:B:138:ARG:HD3	1:B:138:ARG:C	2.45	0.41
1:B:187:ILE:HG21	1:B:187:ILE:HD13	1.83	0.41
1:A:21:ILE:HG22	1:A:22:LYS:H	1.85	0.41
1:A:110:TYR:HD1	1:A:116:TYR:CD2	2.39	0.41
1:B:199:GLN:N	1:B:199:GLN:OE1	2.52	0.41
1:A:66:ARG:HD3	1:A:72:VAL:HB	2.01	0.41
1:A:113:ILE:HG23	1:A:116:TYR:HB2	2.02	0.41
1:A:233:GLY:HA2	1:A:235:MET:SD	2.61	0.41
2:C:129:LEU:HD12	2:C:129:LEU:HA	1.88	0.41
2:C:135:ASP:HB3	2:C:141:ARG:HG3	2.02	0.41
1:B:85:LYS:HD2	1:B:86:LEU:HD22	2.01	0.41
1:B:152:ILE:HD11	1:B:165:PRO:HB3	2.02	0.41
2:D:143:MET:O	2:D:144:GLU:C	2.61	0.41
1:A:156:ALA:O	1:A:157:ALA:HB3	2.21	0.41
1:A:175:TYR:O	1:A:177:LYS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:TYR:HB3	1:A:362:ILE:HG23	2.02	0.41
1:A:354:ARG:HH21	1:A:366:PRO:CD	2.33	0.41
2:C:144:GLU:HG2	2:C:146:LYS:NZ	2.35	0.41
1:B:62:TYR:N	1:B:62:TYR:CD1	2.88	0.41
1:B:334:LEU:CB	2:D:10:ASN:HB3	2.51	0.41
2:C:53:ILE:HD13	4:C:901:HEC:HBC2	2.01	0.41
1:B:85:LYS:HG2	1:B:97:TYR:H	1.85	0.41
1:B:206:ARG:HE	1:B:345:TYR:HE2	1.69	0.41
1:B:126:HIS:O	1:B:126:HIS:CG	2.74	0.41
1:A:356:ASN:ND2	1:A:363:GLU:CB	2.83	0.41
1:A:393:ASN:ND2	2:C:24:PRO:HD3	2.34	0.41
1:B:321:VAL:HG11	1:B:328:PRO:CA	2.44	0.41
1:B:324:LYS:HA	1:B:324:LYS:HD2	1.88	0.41
2:D:37:PHE:CD1	2:D:70:ALA:HB2	2.56	0.41
2:D:53:ILE:HA	2:D:56:ARG:HD3	2.02	0.41
1:A:21:ILE:HG21	1:A:30:VAL:HG21	2.01	0.41
1:A:219:TRP:CZ3	1:A:221:PRO:HG3	2.56	0.41
1:A:320:VAL:CG1	1:A:321:VAL:N	2.83	0.41
1:B:267:LEU:HD12	1:B:286:HIS:CD2	2.55	0.41
2:D:20:ASN:ND2	2:D:79:GLN:H	2.19	0.41
1:A:19:LYS:HG3	1:A:20:TYR:HD1	1.87	0.40
1:B:140:GLN:HE21	1:B:249:VAL:HG13	1.87	0.40
1:B:146:ASP:OD1	1:B:180:LYS:HB3	2.21	0.40
1:A:391:TRP:O	1:A:395:ILE:HG22	2.21	0.40
1:B:17:ALA:CA	1:B:21:ILE:HG13	2.51	0.40
1:A:318:ALA:O	1:A:322:LEU:HB3	2.21	0.40
1:A:330:THR:HA	1:A:331:PRO:HD3	1.93	0.40
2:C:126:THR:N	2:C:127:PRO:HD2	2.36	0.40
1:B:268:THR:CG2	1:B:272:GLY:HA2	2.51	0.40
2:C:3:THR:HG22	2:C:5:GLU:H	1.87	0.40
1:A:175:TYR:C	1:A:177:LYS:N	2.79	0.40
2:C:155:LEU:O	2:C:158:GLU:HB2	2.21	0.40
2:D:95:LYS:HE3	2:D:96:LEU:HD12	2.04	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	399/401 (100%)	330 (83%)	41 (10%)	28 (7%)	1	0
1	B	399/401 (100%)	328 (82%)	51 (13%)	20 (5%)	1	1
2	C	172/174 (99%)	144 (84%)	24 (14%)	4 (2%)	5	7
2	D	172/174 (99%)	151 (88%)	16 (9%)	5 (3%)	3	5
All	All	1142/1150 (99%)	953 (84%)	132 (12%)	57 (5%)	1	1

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	82	PRO
1	A	85	LYS
1	A	90	ALA
1	A	149	THR
1	A	157	ALA
1	A	213	GLU
1	A	221	PRO
1	A	229	LYS
1	A	230	VAL
1	A	293	GLY
1	A	294	ASP
1	A	299	ASN
1	A	361	ALA
2	C	106	VAL
2	C	115	GLU
2	C	117	ASP
1	B	16	THR
1	B	81	ASP
1	B	157	ALA
1	B	233	GLY
1	B	301	MET

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Mol	Chain	Res	Type
1	B	325	GLY
1	B	327	GLU
2	D	16	GLY
2	D	59	LYS
2	D	103	LYS
1	A	80	ILE
1	A	83	ASP
1	A	181	PRO
1	A	399	THR
1	B	23	LEU
1	B	267	LEU
1	B	299	ASN
1	B	352	ILE
1	B	359	GLY
1	A	176	LEU
1	A	233	GLY
1	A	331	PRO
2	D	115	GLU
1	A	26	PRO
1	A	35	PRO
1	A	67	ALA
1	A	210	PHE
1	A	300	PRO
1	B	55	LEU
1	B	82	PRO
1	B	270	ASP
2	D	10	ASN
1	A	180	LYS
1	B	260	LYS
1	A	155	PRO
1	B	161	CYS
1	B	286	HIS
1	B	227	VAL
2	C	16	GLY
1	B	155	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	313/313 (100%)	253 (81%)	60 (19%)	1	2
1	B	313/313 (100%)	243 (78%)	70 (22%)	1	1
2	C	138/138 (100%)	121 (88%)	17 (12%)	4	9
2	D	138/138 (100%)	114 (83%)	24 (17%)	2	3
All	All	902/902 (100%)	731 (81%)	171 (19%)	1	2

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	16	THR
1	A	21	ILE
1	A	25	ASP
1	A	29	GLU
1	A	31	THR
1	A	34	GLU
1	A	41	THR
1	A	42	CYS
1	A	43	TYR
1	A	44	LEU
1	A	53	ARG
1	A	56	GLU
1	A	65	LEU
1	A	78	THR
1	A	80	ILE
1	A	84	LYS
1	A	86	LEU
1	A	112	LYS
1	A	113	ILE
1	A	123	LYS
1	A	128	TRP
1	A	132	GLU
1	A	137	LEU
1	A	139	LYS
1	A	151	VAL
1	A	162	PRO
1	A	176	LEU
1	A	177	LYS
1	A	180	LYS
1	A	196	LYS

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Mol	Chain	Res	Type
1	A	207	LEU
1	A	214	ASN
1	A	221	PRO
1	A	237	VAL
1	A	239	THR
1	A	251	ASN
1	A	252	LEU
1	A	261	ILE
1	A	267	LEU
1	A	278	ILE
1	A	284	SER
1	A	292	ILE
1	A	294	ASP
1	A	319	VAL
1	A	321	VAL
1	A	324	LYS
1	A	330	THR
1	A	332	SER
1	A	333	TYR
1	A	336	THR
1	A	337	CYS
1	A	340	ILE
1	A	341	LEU
1	A	352	ILE
1	A	356	ASN
1	A	364	SER
1	A	371	VAL
1	A	374	VAL
1	A	383	ARG
2	C	7	LEU
2	C	15	HIS
2	C	17	THR
2	C	32	MET
2	C	42	GLU
2	C	59	LYS
2	C	76	GLN
2	C	77	THR
2	C	87	THR
2	C	89	LEU
2	C	91	ASP
2	C	96	LEU
2	C	129	LEU

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Mol	Chain	Res	Type
2	C	138	GLU
2	C	145	LYS
2	C	151	LEU
2	C	155	LEU
1	B	3	ARG
1	B	21	ILE
1	B	23	LEU
1	B	28	ILE
1	B	30	VAL
1	B	31	THR
1	B	32	LEU
1	B	36	ASN
1	B	41	THR
1	B	43	TYR
1	B	47	GLU
1	B	55	LEU
1	B	58	ILE
1	B	65	LEU
1	B	78	THR
1	B	80	ILE
1	B	83	ASP
1	B	85	LYS
1	B	86	LEU
1	B	104	PRO
1	B	106	ILE
1	B	108	LEU
1	B	113	ILE
1	B	126	HIS
1	B	137	LEU
1	B	138	ARG
1	B	141	LEU
1	B	143	ASP
1	B	152	ILE
1	B	176	LEU
1	B	184	LYS
1	B	187	ILE
1	B	188	LEU
1	B	196	LYS
1	B	198	SER
1	B	207	LEU
1	B	216	MET
1	B	229	LYS

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Mol	Chain	Res	Type
1	B	231	ASP
1	B	250	ILE
1	B	252	LEU
1	B	268	THR
1	B	270	ASP
1	B	278	ILE
1	B	284	SER
1	B	289	ILE
1	B	292	ILE
1	B	297	ILE
1	B	299	ASN
1	B	301	MET
1	B	310	SER
1	B	319	VAL
1	B	321	VAL
1	B	322	LEU
1	B	327	GLU
1	B	330	THR
1	B	332	SER
1	B	333	TYR
1	B	337	CYS
1	B	340	ILE
1	B	341	LEU
1	B	343	PRO
1	B	354	ARG
1	B	364	SER
1	B	367	ASP
1	B	371	VAL
1	B	374	VAL
1	B	384	GLU
1	B	396	VAL
1	B	399	THR
2	D	15	HIS
2	D	18	HIS
2	D	24	PRO
2	D	28	SER
2	D	79	GLN
2	D	84	SER
2	D	92	THR
2	D	96	LEU
2	D	98	ASP
2	D	102	GLU

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Mol	Chain	Res	Type
2	D	103	LYS
2	D	107	GLU
2	D	114	ASP
2	D	117	ASP
2	D	121	LEU
2	D	133	MET
2	D	139	GLU
2	D	141	ARG
2	D	146	LYS
2	D	150	LYS
2	D	155	LEU
2	D	156	LYS
2	D	166	LEU
2	D	173	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	171	GLN
1	A	256	GLN
1	A	263	GLN
1	A	290	HIS
1	A	311	GLN
1	A	356	ASN
2	C	20	ASN
2	C	76	GLN
1	B	46	ASN
1	B	60	HIS
1	B	140	GLN
1	B	171	GLN
1	B	220	HIS
1	B	251	ASN
1	B	263	GLN
1	B	286	HIS
1	B	309	ASN
1	B	335	ASN
2	D	9	ASN
2	D	20	ASN
2	D	79	GLN
2	D	130	GLN

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	$\# Z > 2$
3	FAD	A	699	1	58,58,58	1.32	9 (15%)	85,89,89	1.30	7 (8%)
4	HEC	D	901	2	50,50,50	1.13	3 (6%)	68,82,82	1.20	7 (10%)
4	HEC	C	901	2	50,50,50	0.92	0	68,82,82	1.00	1 (1%)
3	FAD	B	699	1	58,58,58	1.58	12 (20%)	85,89,89	1.24	5 (5%)
4	HEC	D	902	2	50,50,50	1.07	3 (6%)	68,82,82	1.16	4 (5%)
4	HEC	C	902	2	50,50,50	0.95	3 (6%)	68,82,82	0.96	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	699	1	3/3/9/9	10/34/50/50	0/6/6/6
4	HEC	D	901	2	1/1/3/7	4/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEC	C	901	2	1/1/3/7	5/14/54/54	-
3	FAD	B	699	1	3/3/9/9	6/34/50/50	0/6/6/6
4	HEC	D	902	2	1/1/3/7	8/14/54/54	-
4	HEC	C	902	2	1/1/3/7	5/14/54/54	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	699	FAD	P-O3P	6.35	1.66	1.59
3	B	699	FAD	C10-N10	3.68	1.45	1.37
3	A	699	FAD	C10-N10	3.57	1.45	1.37
3	A	699	FAD	C2'-C3'	-2.90	1.48	1.53
3	B	699	FAD	C4X-N5	2.84	1.36	1.30
3	A	699	FAD	C5'-C4'	-2.77	1.48	1.51
3	A	699	FAD	C4X-N5	2.68	1.36	1.30
3	B	699	FAD	C4'-C3'	-2.57	1.48	1.53
4	D	902	HEC	O2A-CGA	-2.53	1.22	1.30
3	A	699	FAD	O2'-C2'	-2.52	1.38	1.43
4	D	901	HEC	C4B-C3B	2.50	1.49	1.45
3	B	699	FAD	C6-C7	-2.48	1.36	1.39
3	B	699	FAD	C2'-C3'	-2.46	1.49	1.53
3	A	699	FAD	C1'-C2'	-2.38	1.49	1.52
3	B	699	FAD	C5'-C4'	2.36	1.55	1.51
3	B	699	FAD	C2A-N1A	-2.35	1.29	1.33
3	B	699	FAD	C8M-C8	2.30	1.55	1.51
4	D	902	HEC	C4B-NB	-2.29	1.36	1.40
4	D	901	HEC	C1A-C2A	2.26	1.49	1.45
4	D	902	HEC	CBD-CGD	2.19	1.55	1.50
4	D	901	HEC	C1C-NC	-2.19	1.35	1.39
3	B	699	FAD	PA-O3P	2.18	1.61	1.59
4	C	902	HEC	C4B-NB	-2.16	1.36	1.40
3	B	699	FAD	C5A-C4A	-2.14	1.35	1.39
4	C	902	HEC	C1D-ND	-2.10	1.36	1.40
3	B	699	FAD	C10-N1	2.09	1.37	1.33
3	A	699	FAD	C6-C7	-2.08	1.36	1.39
3	A	699	FAD	C4X-C10	-2.07	1.38	1.44
3	A	699	FAD	C9-C8	-2.05	1.36	1.39
4	C	902	HEC	O2D-CGD	-2.02	1.24	1.30

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	699	FAD	C9A-C5X-N5	5.28	128.06	122.45
3	A	699	FAD	O4B-C1B-C2B	-4.58	96.80	106.62
3	A	699	FAD	C9A-C5X-N5	4.28	126.99	122.45
3	A	699	FAD	O4'-C4'-C3'	3.80	118.14	109.25
3	B	699	FAD	C5X-N5-C4X	-3.69	112.12	118.09
4	D	902	HEC	CAC-C3C-C4C	3.55	129.80	124.91
4	D	902	HEC	CBD-CAD-C3D	3.11	121.12	112.53
3	A	699	FAD	C5X-N5-C4X	-2.94	113.33	118.09
4	D	901	HEC	C3B-C4B-NB	2.89	113.34	110.17
3	B	699	FAD	O3'-C3'-C2'	2.82	115.34	108.93
4	D	901	HEC	C2B-C1B-NB	2.66	112.98	109.90
4	D	902	HEC	CAC-C3C-C2C	-2.50	122.93	126.89
4	D	901	HEC	CBB-CAB-C3B	2.49	119.17	112.42
3	A	699	FAD	C4-C4X-N5	-2.48	114.78	118.21
3	B	699	FAD	C6-C5X-N5	-2.46	114.36	118.44
4	C	901	HEC	O2D-CGD-CBD	2.34	121.38	114.00
4	D	902	HEC	C3B-C4B-NB	2.30	112.69	110.17
3	B	699	FAD	O2A-PA-O3P	2.25	113.35	107.27
4	D	901	HEC	CHA-C1A-NA	-2.11	122.15	124.45
3	A	699	FAD	C6-C5X-N5	-2.09	114.97	118.44
4	D	901	HEC	C4B-NB-C1B	-2.08	102.75	105.21
4	D	901	HEC	C2A-C1A-NA	2.06	112.31	110.32
3	A	699	FAD	O4B-C4B-C5B	2.04	115.86	109.33
4	D	901	HEC	C4B-C3B-C2B	-2.00	103.97	106.89

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	699	FAD	C3'
3	A	699	FAD	C4'
3	A	699	FAD	C2'
3	B	699	FAD	C3'
3	B	699	FAD	C4'
3	B	699	FAD	C2'
4	C	901	HEC	NA
4	C	902	HEC	NA
4	D	901	HEC	NA
4	D	902	HEC	NA

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	699	FAD	C5B-O5B-PA-O1A

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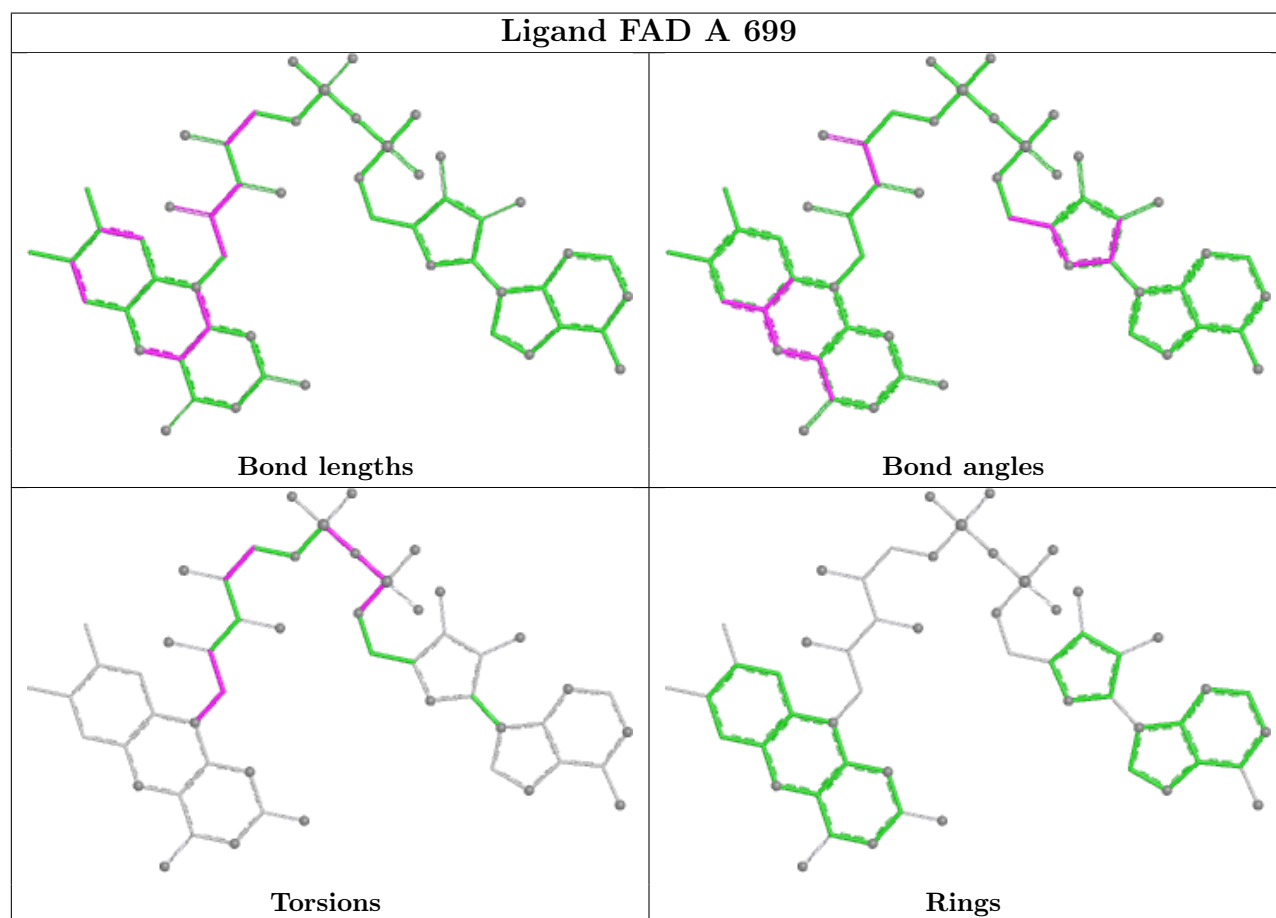
Mol	Chain	Res	Type	Atoms
3	A	699	FAD	C5B-O5B-PA-O3P
3	A	699	FAD	C2'-C1'-N10-C10
3	A	699	FAD	N10-C1'-C2'-O2'
3	A	699	FAD	N10-C1'-C2'-C3'
3	A	699	FAD	C3'-C4'-C5'-O5'
3	A	699	FAD	O4'-C4'-C5'-O5'
3	A	699	FAD	PA-O3P-P-O5'
3	B	699	FAD	N10-C1'-C2'-O2'
3	B	699	FAD	O4'-C4'-C5'-O5'
4	D	901	HEC	C4C-C3C-CAC-CBC
4	D	901	HEC	C2C-C3C-CAC-CBC
4	D	902	HEC	C2C-C3C-CAC-CBC
3	B	699	FAD	O3'-C3'-C4'-O4'
4	C	901	HEC	C4C-C3C-CAC-CBC
3	B	699	FAD	O3'-C3'-C4'-C5'
4	C	902	HEC	C2C-C3C-CAC-CBC
3	B	699	FAD	C3'-C4'-C5'-O5'
4	D	902	HEC	C4C-C3C-CAC-CBC
4	C	901	HEC	C2C-C3C-CAC-CBC
3	A	699	FAD	C5B-O5B-PA-O2A
4	D	902	HEC	C1A-C2A-CAA-CBA
4	D	901	HEC	CAD-CBD-CGD-O1D
4	C	902	HEC	CAA-CBA-CGA-O1A
4	C	901	HEC	CAD-CBD-CGD-O1D
4	C	902	HEC	CAA-CBA-CGA-O2A
4	D	901	HEC	CAD-CBD-CGD-O2D
4	C	901	HEC	CAD-CBD-CGD-O2D
4	D	902	HEC	CAA-CBA-CGA-O2A
4	D	902	HEC	CAD-CBD-CGD-O1D
4	D	902	HEC	CAA-CBA-CGA-O1A
4	D	902	HEC	CAD-CBD-CGD-O2D
4	C	902	HEC	CAD-CBD-CGD-O2D
3	B	699	FAD	O4B-C4B-C5B-O5B
4	C	902	HEC	CAD-CBD-CGD-O1D
4	D	902	HEC	C3A-C2A-CAA-CBA
3	A	699	FAD	P-O3P-PA-O2A
4	C	901	HEC	C3D-CAD-CBD-CGD

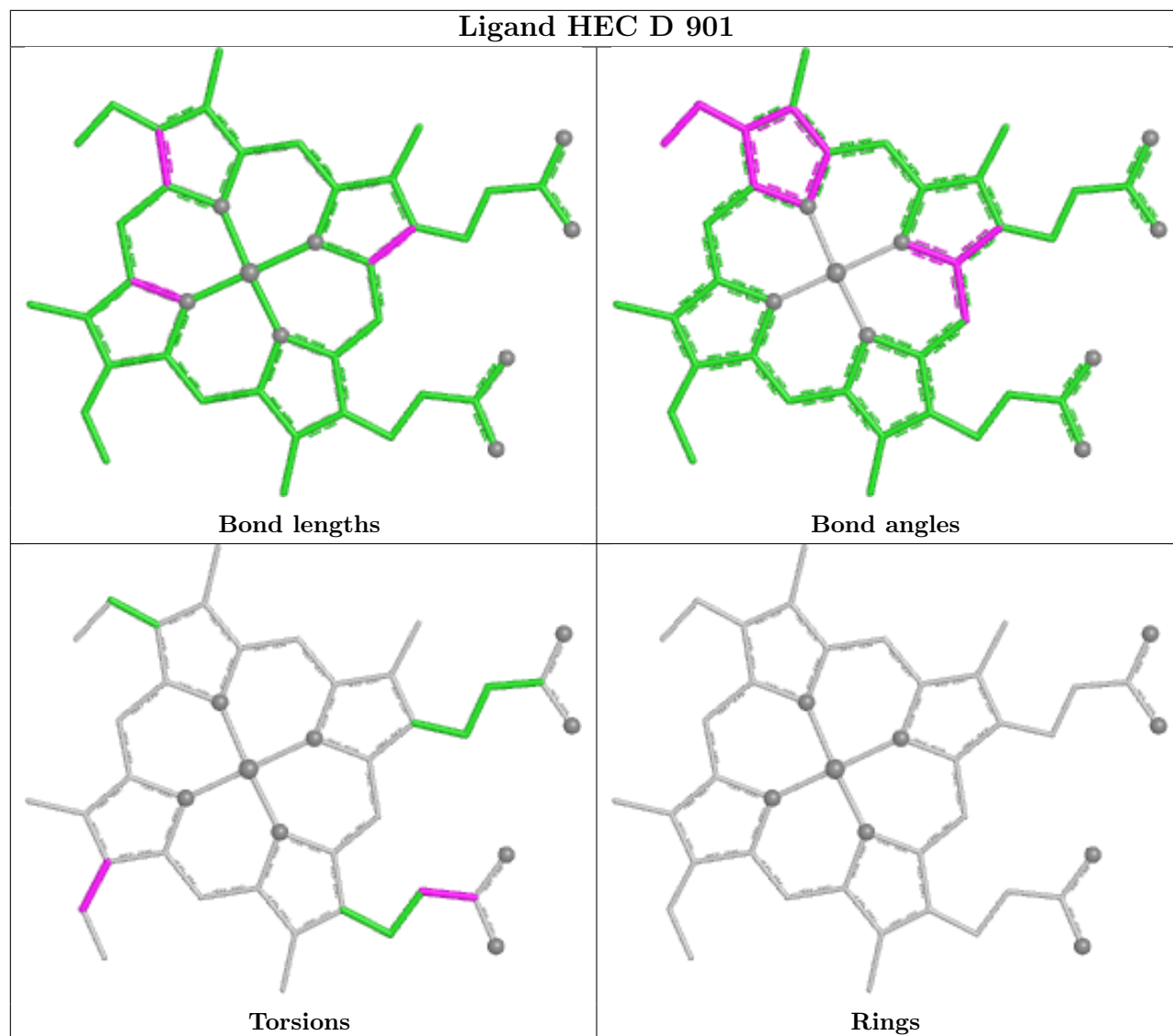
There are no ring outliers.

6 monomers are involved in 18 short contacts:

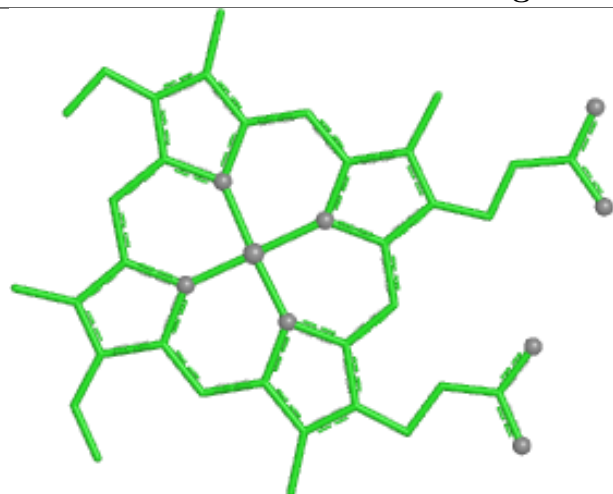
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	699	FAD	7	0
4	D	901	HEC	2	0
4	C	901	HEC	1	0
3	B	699	FAD	2	0
4	D	902	HEC	5	0
4	C	902	HEC	1	0

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.

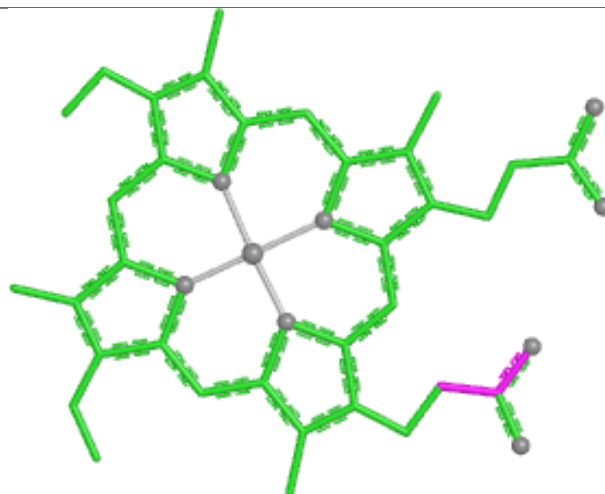




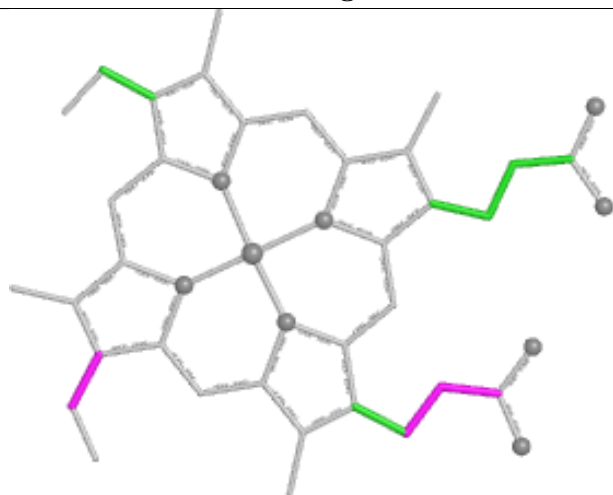
Ligand HEC C 901



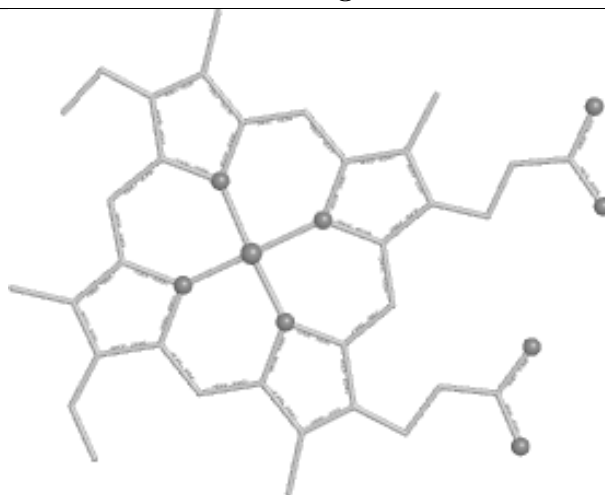
Bond lengths



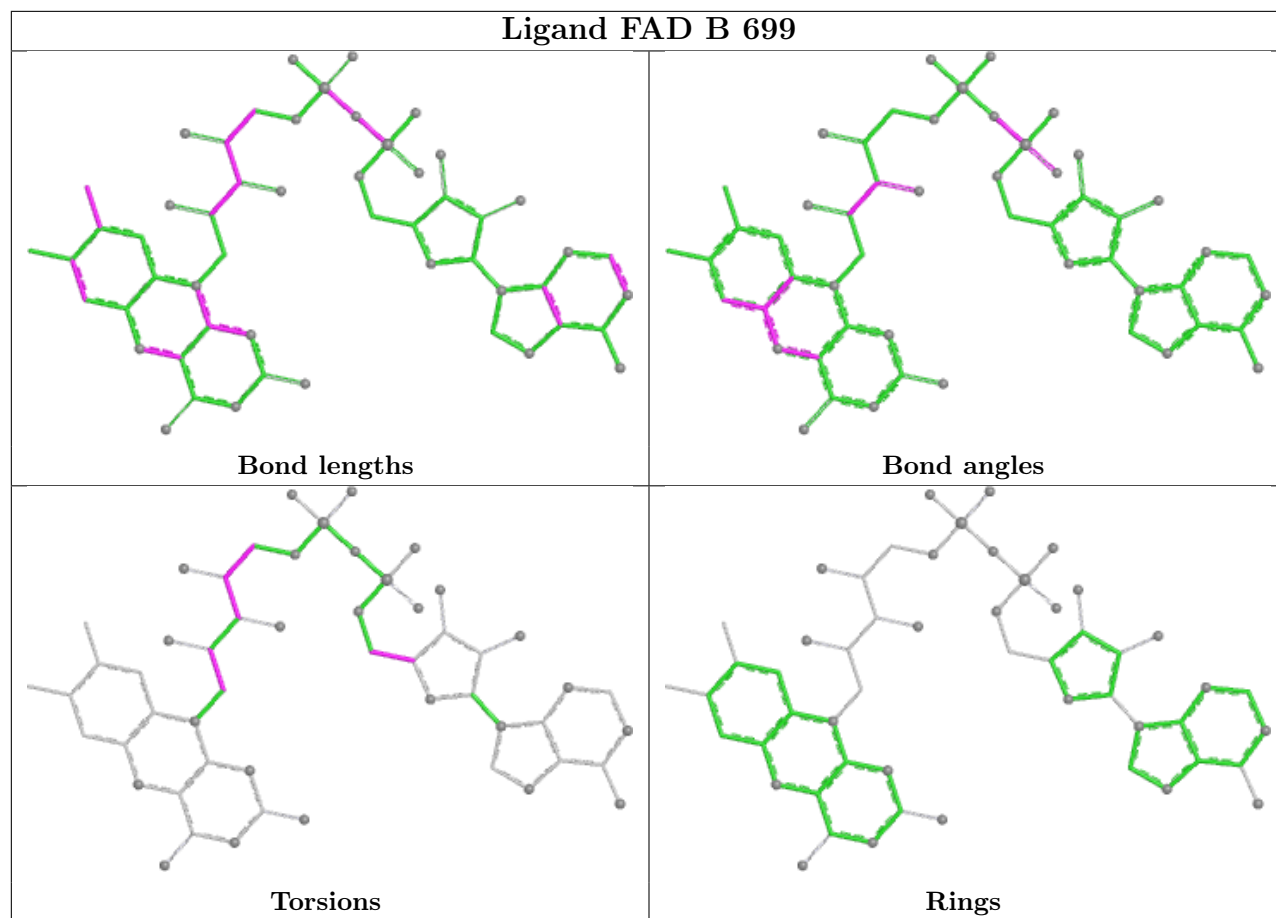
Bond angles

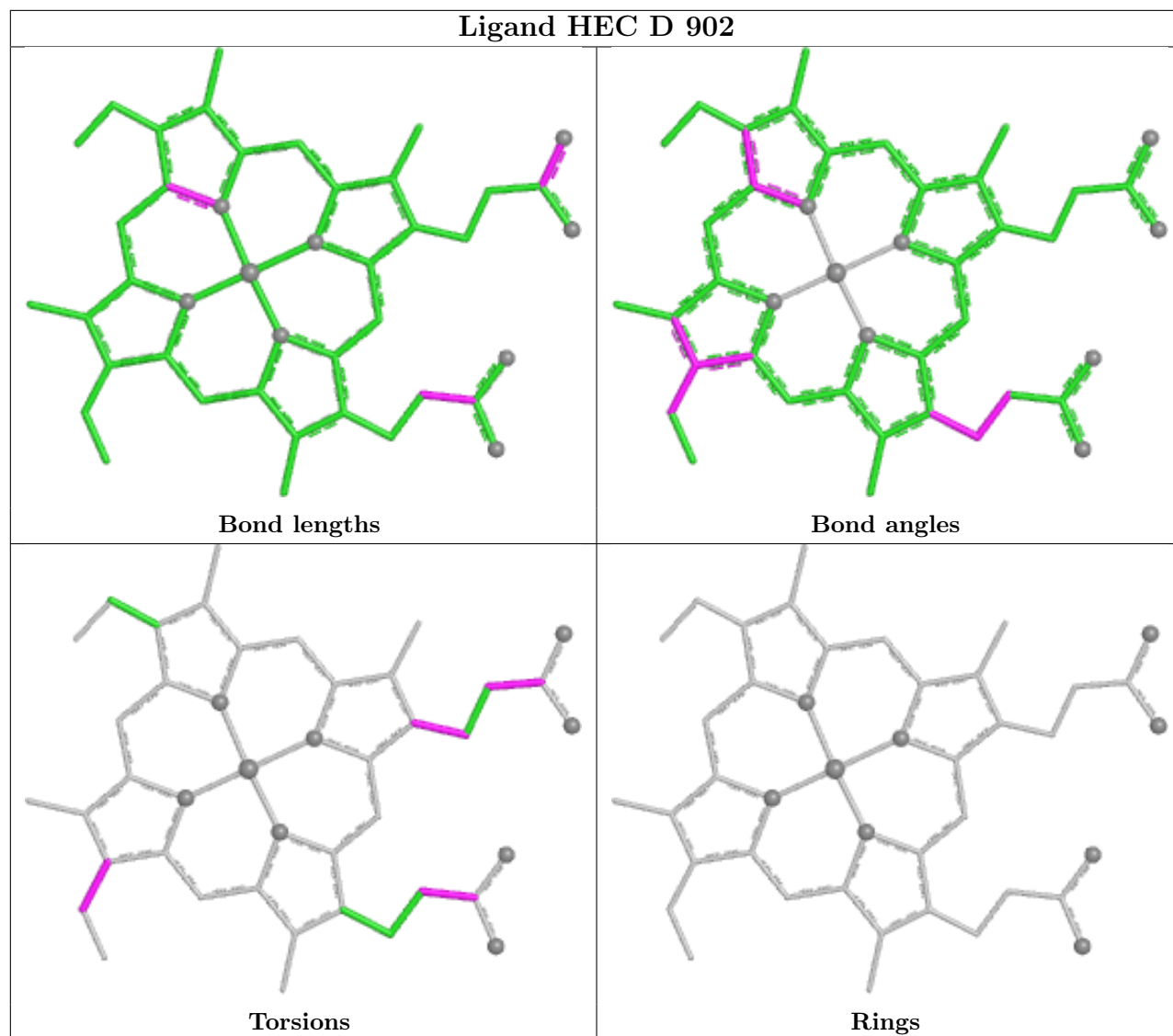


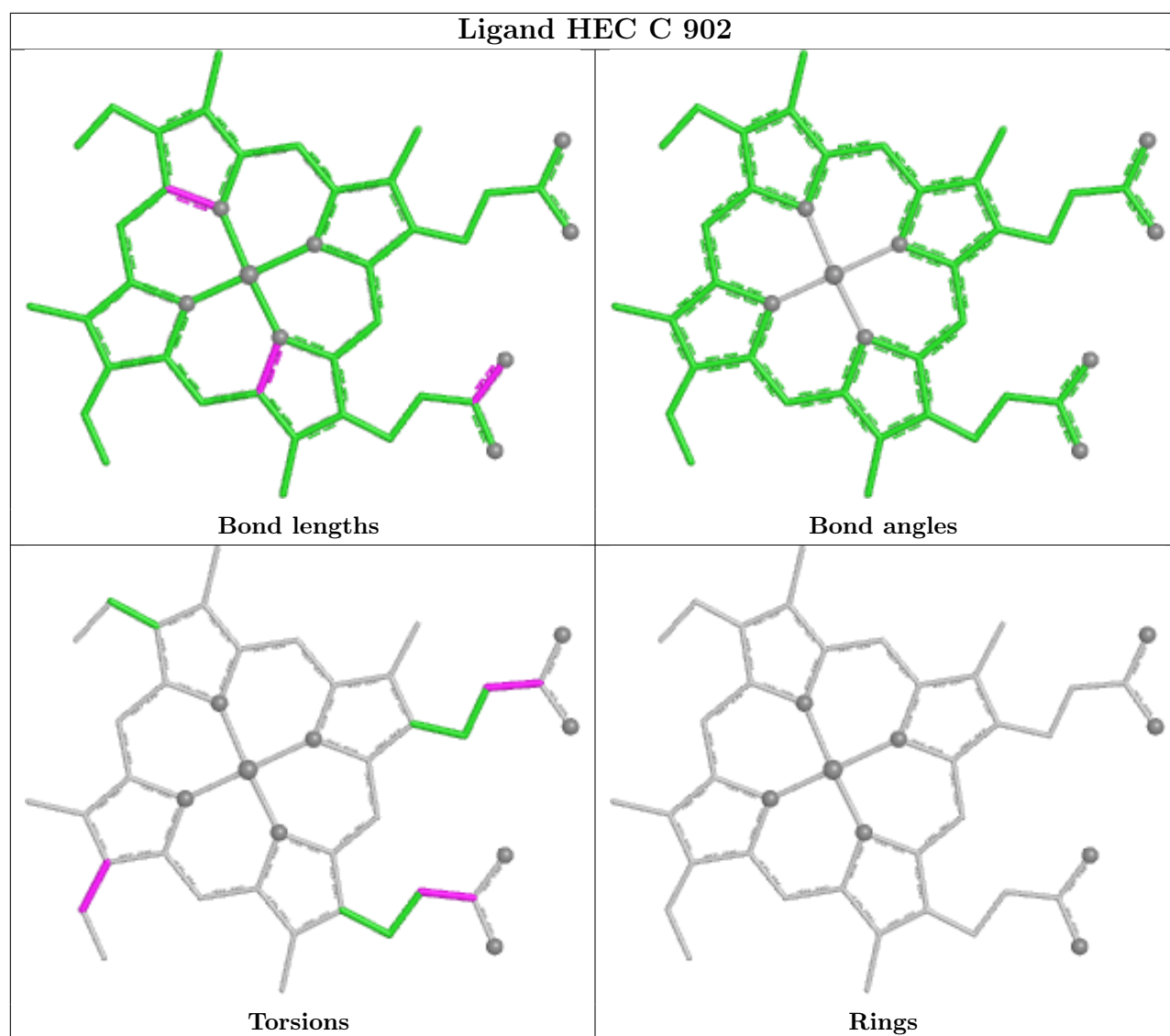
Torsions



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.