



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:39 AM UTC

PDB ID : 3RN0 / pdb_00003rn0
Title : Crystal Structure of the W199K-MauG/pre-Methylamine Dehydrogenase Complex
Authors : Jensen, L.M.R.; Wilmot, C.M.
Deposited on : 2011-04-21
Resolution : 1.91 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

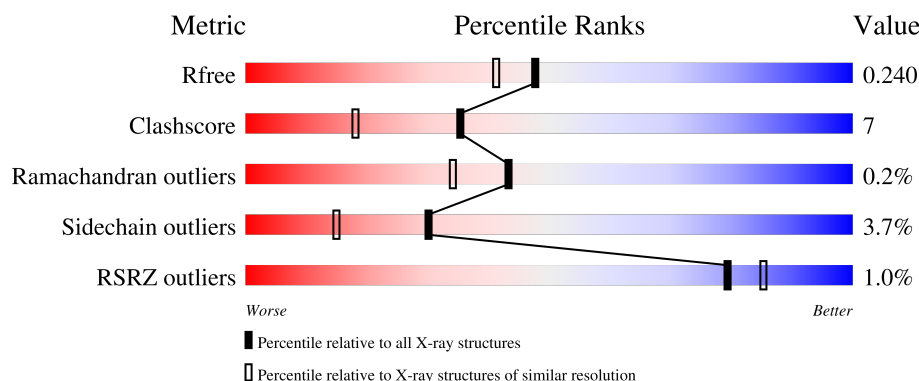
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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))
R_{free}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	373	2% 74% 18% • 5%
1	B	373	2% 76% 17% •• 5%
2	C	137	2% 66% 24% • 9%
2	E	137	2% 71% 18% • 9%
3	D	386	2% 77% 19% ••

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Mol	Chain	Length	Quality of chain
3	F	386	 80%16% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	0AF	C	57	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14657 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 Methylamine utilization protein MauG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	2	0
			2741	1710	491	529	11			
1	B	355	Total	C	N	O	S	0	1	0
			2746	1712	494	529	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	LYS	TRP	engineered mutation	UNP Q51658
A	368	HIS	-	expression tag	UNP Q51658
A	369	HIS	-	expression tag	UNP Q51658
A	370	HIS	-	expression tag	UNP Q51658
A	371	HIS	-	expression tag	UNP Q51658
A	372	HIS	-	expression tag	UNP Q51658
A	373	HIS	-	expression tag	UNP Q51658
B	199	LYS	TRP	engineered mutation	UNP Q51658
B	368	HIS	-	expression tag	UNP Q51658
B	369	HIS	-	expression tag	UNP Q51658
B	370	HIS	-	expression tag	UNP Q51658
B	371	HIS	-	expression tag	UNP Q51658
B	372	HIS	-	expression tag	UNP Q51658
B	373	HIS	-	expression tag	UNP Q51658

- Molecule 2 is a protein called Methylamine dehydrogenase light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	125	Total	C	N	O	S	0	1	0
			957	592	161	190	14			
2	E	125	Total	C	N	O	S	0	1	0
			957	592	161	190	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	HIS	-	expression tag	UNP A1BBA0
C	133	HIS	-	expression tag	UNP A1BBA0
C	134	HIS	-	expression tag	UNP A1BBA0
C	135	HIS	-	expression tag	UNP A1BBA0
C	136	HIS	-	expression tag	UNP A1BBA0
C	137	HIS	-	expression tag	UNP A1BBA0
E	132	HIS	-	expression tag	UNP A1BBA0
E	133	HIS	-	expression tag	UNP A1BBA0
E	134	HIS	-	expression tag	UNP A1BBA0
E	135	HIS	-	expression tag	UNP A1BBA0
E	136	HIS	-	expression tag	UNP A1BBA0
E	137	HIS	-	expression tag	UNP A1BBA0

- Molecule 3 is a protein called Methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	376	Total	C	N	O	S	0	1	0
			2931	1858	505	560	8			
3	F	376	Total	C	N	O	S	0	0	0
			2923	1853	502	560	8			

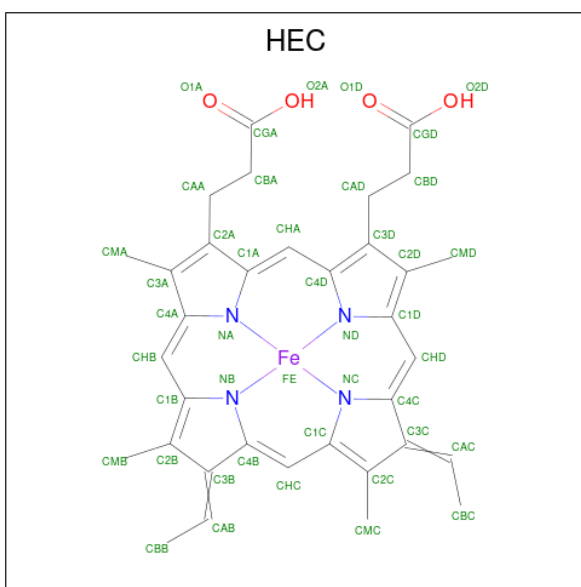
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

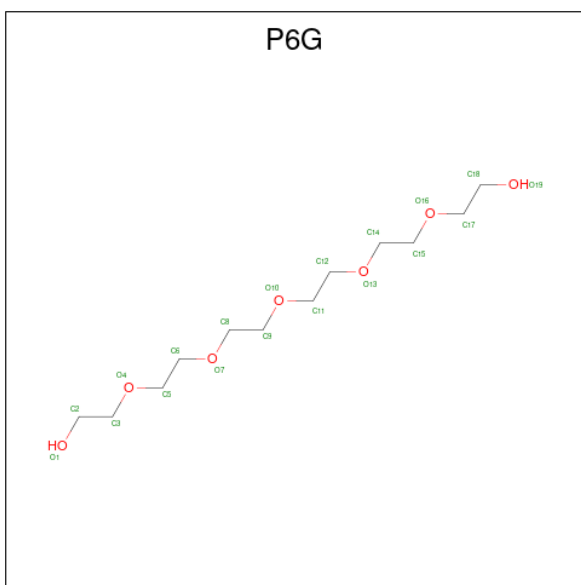
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Na	0	0
			2	2		
5	B	2	Total	Na	0	0
			2	2		

- Molecule 6 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



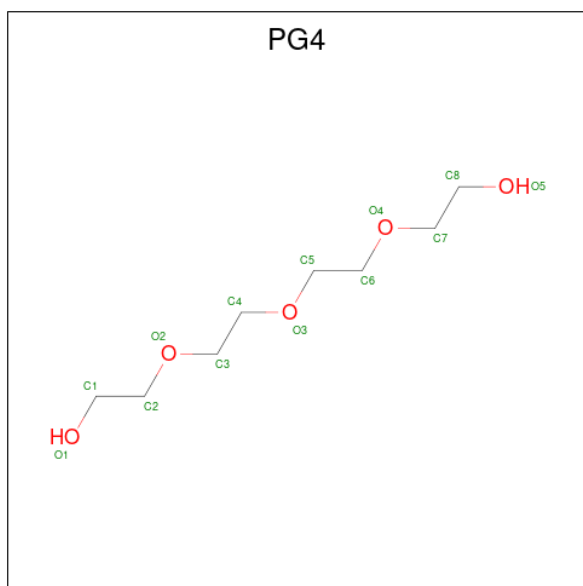
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 7 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $\text{C}_{12}\text{H}_{26}\text{O}_7$).



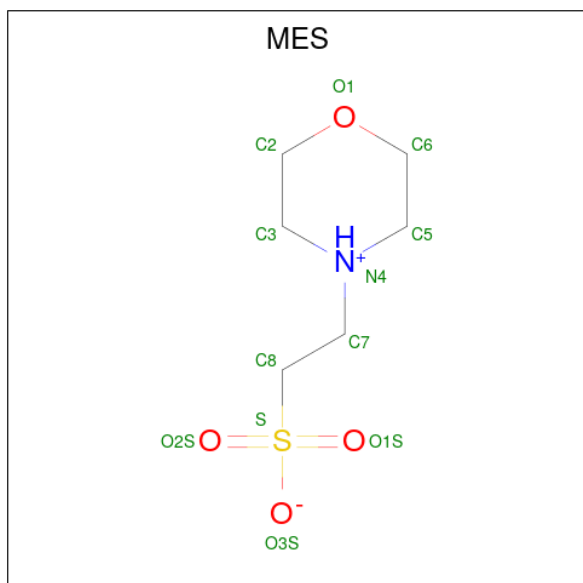
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			19	12	7		

- Molecule 8 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	C	O	0	0
			13	8	5		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

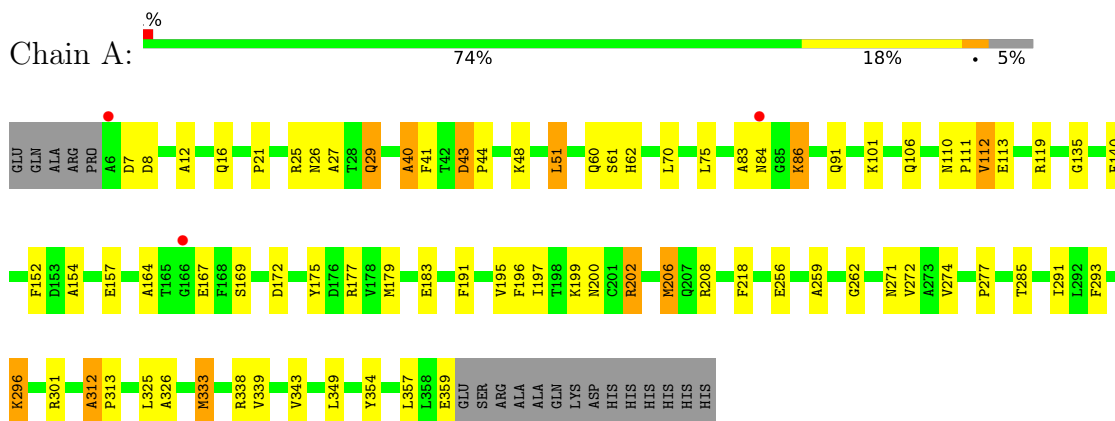
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	206	Total	O	0	0
			206	206		
10	B	265	Total	O	0	0
			265	265		
10	C	83	Total	O	0	0
			83	83		
10	D	223	Total	O	0	0
			223	223		
10	E	89	Total	O	0	0
			89	89		
10	F	314	Total	O	0	0
			314	314		

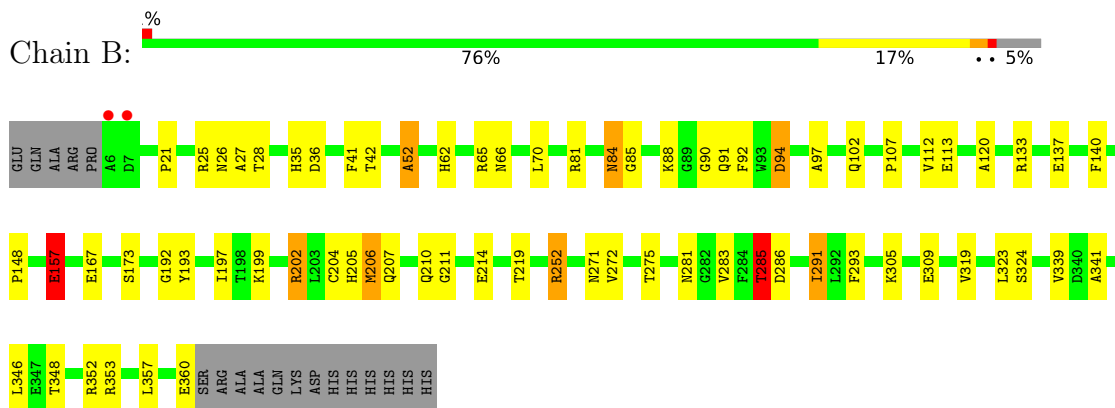
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

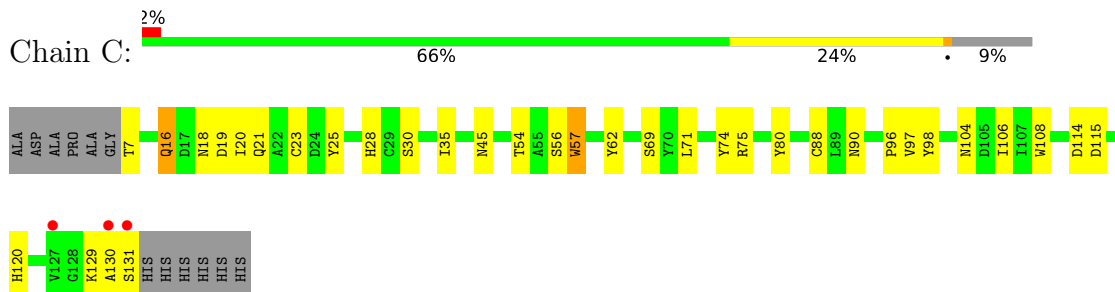
• Molecule 1: Methylamine utilization protein MauG



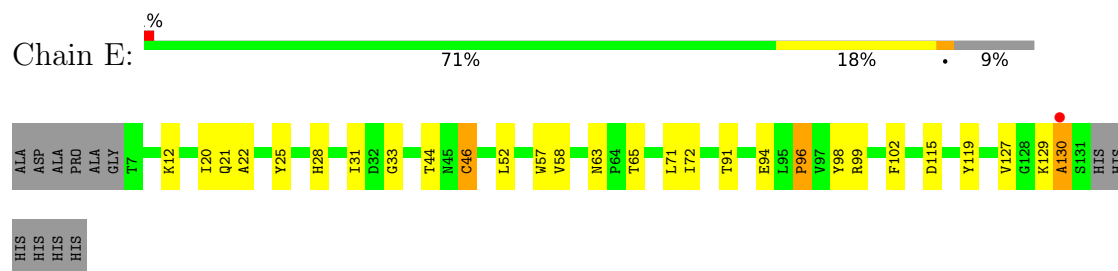
• Molecule 1: Methylamine utilization protein MauG



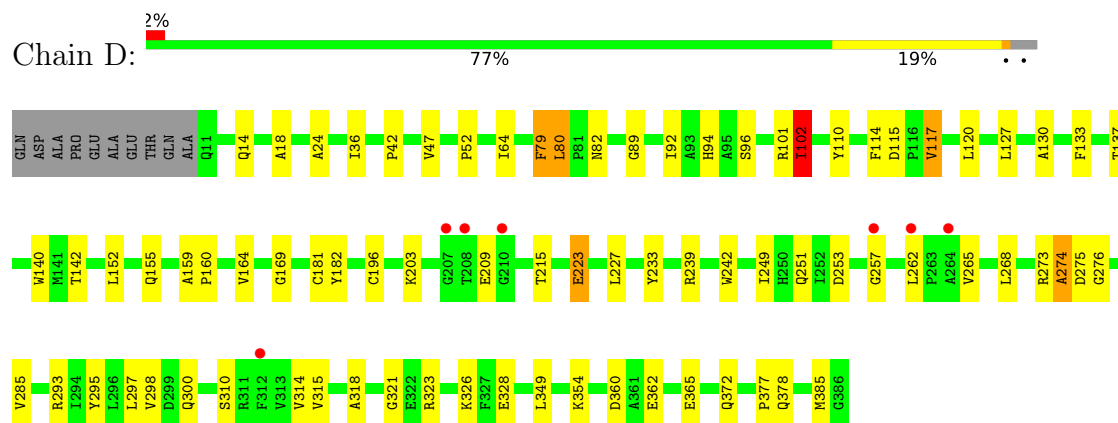
• Molecule 2: Methylamine dehydrogenase light chain



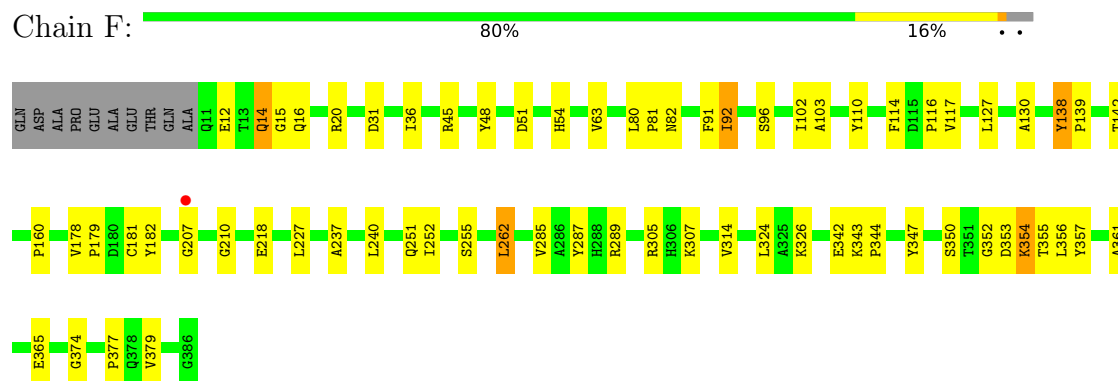
- Molecule 2: Methylamine dehydrogenase light chain



- Molecule 3: Methylamine dehydrogenase heavy chain



- Molecule 3: Methylamine dehydrogenase heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.53Å 83.52Å 107.78Å 109.94° 91.54° 105.78°	Depositor
Resolution (Å)	39.58 – 1.91 39.58 – 1.91	Depositor EDS
% Data completeness (in resolution range)	86.4 (39.58-1.91) 86.8 (39.58-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.173 , 0.230 0.190 , 0.240	Depositor DCC
R_{free} test set	5868 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14657	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, MES, PG4, CA, OAF, NA, P6G

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	2/2809 (0.1%)	1.27	22/3809 (0.6%)
1	B	1.45	12/2811 (0.4%)	1.32	16/3811 (0.4%)
2	C	1.24	2/969 (0.2%)	1.24	3/1323 (0.2%)
2	E	1.51	6/969 (0.6%)	1.41	3/1323 (0.2%)
3	D	1.23	6/3011 (0.2%)	1.20	8/4102 (0.2%)
3	F	1.46	10/3000 (0.3%)	1.26	6/4088 (0.1%)
All	All	1.35	38/13569 (0.3%)	1.27	58/18456 (0.3%)

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
2	C	1	0

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	272	VAL	CA-CB	7.88	1.64	1.54
3	F	80	LEU	N-CA	7.54	1.51	1.46
3	F	285	VAL	C-O	7.08	1.30	1.24
1	B	97	ALA	CA-CB	6.95	1.64	1.53
1	B	90	GLY	N-CA	6.91	1.52	1.45
3	D	80	LEU	C-O	6.74	1.27	1.23
3	F	287	TYR	N-CA	-6.45	1.38	1.46
1	B	206	MET	CA-C	-6.41	1.44	1.52
3	F	138	TYR	C-O	-6.34	1.19	1.25
2	E	31	ILE	CA-CB	6.27	1.61	1.54
2	E	22	ALA	CA-CB	6.21	1.64	1.53
3	D	79	PHE	C-O	6.08	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	63	ASN	N-CA	-6.07	1.39	1.46
1	B	157	GLU	N-CA	-6.04	1.39	1.46
3	D	102	ILE	C-O	-6.01	1.17	1.24
2	C	20	ILE	CA-CB	5.93	1.61	1.54
3	F	103	ALA	CA-CB	5.87	1.62	1.53
3	F	81	PRO	CA-C	5.85	1.59	1.52
1	A	164	ALA	CA-CB	5.84	1.62	1.53
3	F	355	THR	CA-C	-5.76	1.45	1.52
1	A	40	ALA	CA-CB	5.58	1.61	1.53
3	F	130	ALA	CA-CB	5.56	1.57	1.52
1	B	252	ARG	CD-NE	-5.55	1.38	1.46
2	E	99	ARG	C-O	-5.55	1.18	1.24
1	B	324	SER	N-CA	5.50	1.53	1.46
2	C	35	ILE	CA-CB	5.49	1.60	1.54
3	F	357	TYR	CA-C	-5.48	1.46	1.52
1	B	52	ALA	CA-CB	-5.46	1.44	1.53
1	B	94	ASP	N-CA	5.46	1.52	1.46
3	D	120	LEU	C-O	-5.44	1.16	1.24
2	E	52	LEU	CA-CB	5.31	1.60	1.53
1	B	52	ALA	C-O	-5.21	1.18	1.24
2	E	96	PRO	CA-C	5.20	1.58	1.52
1	B	319	VAL	C-O	5.19	1.30	1.24
3	D	24	ALA	CA-CB	5.18	1.61	1.53
3	F	379	VAL	C-O	5.07	1.29	1.24
1	B	291	ILE	N-CA	5.04	1.52	1.46
3	D	18	ALA	CA-C	5.01	1.59	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	46	CYS	CA-C-N	10.10	126.93	119.66
2	E	46	CYS	C-N-CA	10.10	126.93	119.66
1	B	252	ARG	NE-CZ-NH2	-9.12	111.00	119.20
1	A	200	ASN	N-CA-C	8.19	122.38	112.38
1	B	206	MET	CG-SD-CE	-8.14	83.00	100.90
3	F	127	LEU	CA-C-N	-8.10	112.38	120.31
3	F	127	LEU	C-N-CA	-8.10	112.38	120.31
1	A	312	ALA	CA-C-N	-7.30	112.44	119.89
1	A	312	ALA	C-N-CA	-7.30	112.44	119.89
1	B	62	HIS	CA-C-N	-7.29	115.05	122.27
1	B	62	HIS	C-N-CA	-7.29	115.05	122.27
3	D	115	ASP	CA-C-N	-7.02	112.85	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	115	ASP	C-N-CA	-7.02	112.85	121.00
1	A	325	LEU	N-CA-C	6.96	119.75	111.33
3	F	210	GLY	N-CA-C	-6.95	104.49	111.85
1	A	169	SER	CA-C-N	-6.86	113.14	120.47
1	A	169	SER	C-N-CA	-6.86	113.14	120.47
3	F	352	GLY	N-CA-C	-6.64	104.27	112.77
3	D	274	ALA	N-CA-C	-6.49	96.97	110.80
1	A	43	ASP	CA-C-N	6.49	126.11	119.56
1	A	43	ASP	C-N-CA	6.49	126.11	119.56
1	A	262	GLY	N-CA-C	-6.29	106.41	115.27
1	A	195	VAL	N-CA-C	-6.20	104.46	110.72
1	A	339	VAL	N-CA-C	-6.16	104.74	110.53
3	D	285	VAL	N-CA-C	6.08	117.51	108.46
1	B	36	ASP	CA-C-N	6.01	127.36	119.84
1	B	36	ASP	C-N-CA	6.01	127.36	119.84
1	B	193	TYR	N-CA-C	-5.98	104.84	111.36
1	B	271	ASN	N-CA-C	5.72	120.07	113.38
1	A	326	ALA	N-CA-C	-5.71	104.96	111.07
3	F	63	VAL	N-CA-C	-5.61	100.31	108.17
1	B	252	ARG	NE-CZ-NH1	5.56	127.06	121.50
1	B	252	ARG	CA-C-N	-5.56	114.03	119.76
1	B	252	ARG	C-N-CA	-5.56	114.03	119.76
1	A	106	GLN	CA-C-N	-5.55	113.18	119.28
1	A	106	GLN	C-N-CA	-5.55	113.18	119.28
1	A	75	LEU	CA-CB-CG	-5.52	96.98	116.30
1	B	211	GLY	N-CA-C	-5.51	102.83	112.53
2	C	104	ASN	N-CA-C	5.47	120.65	112.94
1	B	207	GLN	N-CA-C	5.47	116.92	111.07
3	F	324	LEU	N-CA-C	-5.46	106.75	113.41
2	C	45	ASN	N-CA-C	5.40	117.89	109.52
3	D	130	ALA	CA-C-N	-5.34	114.42	120.89
3	D	130	ALA	C-N-CA	-5.34	114.42	120.89
1	A	29	GLN	N-CA-C	5.33	117.18	108.55
1	A	199	LYS	N-CA-C	-5.31	102.15	110.17
3	D	249	ILE	N-CA-C	5.28	115.59	107.77
1	A	259	ALA	N-CA-C	5.28	118.82	112.38
2	C	54	THR	N-CA-C	-5.25	107.04	113.50
1	A	167	GLU	N-CA-C	5.24	116.99	111.28
1	A	274	VAL	N-CA-C	-5.19	107.92	112.90
2	E	127	VAL	N-CA-C	5.19	119.50	113.42
1	A	40	ALA	N-CA-C	-5.12	104.83	111.74
3	D	169	GLY	N-CA-C	-5.12	108.62	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	293	PHE	N-CA-C	-5.06	105.76	111.28
1	B	285	THR	N-CA-CB	-5.04	102.67	110.13
1	A	301	ARG	N-CA-C	5.02	115.38	109.60
1	B	339	VAL	N-CA-C	-5.00	105.52	110.62

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	57	0AF	CA

There are no planarity outliers.

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	2741	0	2624	38	0
1	B	2746	0	2629	43	0
2	C	957	0	863	26	0
2	E	957	0	864	16	0
3	D	2931	0	2821	50	0
3	F	2923	0	2808	36	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	86	0	60	3	0
6	B	86	0	61	6	0
7	F	19	0	26	4	0
8	F	13	0	18	1	0
9	F	12	0	12	0	0
10	A	206	0	0	4	0
10	B	265	0	0	9	0
10	C	83	0	0	2	0
10	D	223	0	0	6	0
10	E	89	0	0	0	0
10	F	314	0	0	4	0
All	All	14657	0	12786	194	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 7.

All (194) 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:B:204:CYS:SG	6:B:600:HEC:CAC	2.02	1.47
3:D:52:PRO:HG2	3:D:378:GLN:HE21	1.16	1.05
3:F:207:GLY:HA3	10:F:1052:HOH:O	1.61	1.00
1:B:204:CYS:SG	6:B:600:HEC:HAC	2.01	0.95
1:A:48:LYS:H	1:A:62:HIS:HE1	1.17	0.91
1:B:107:PRO:HG3	10:B:1182:HOH:O	1.68	0.91
10:C:1121:HOH:O	3:F:36:ILE:HD11	1.69	0.91
3:D:314:VAL:HG12	3:D:326:LYS:HG3	1.55	0.88
3:D:52:PRO:HG2	3:D:378:GLN:NE2	1.89	0.88
1:B:197:ILE:O	1:B:202:ARG:HD3	1.74	0.86
1:B:204:CYS:SG	6:B:600:HEC:C3C	2.64	0.86
1:A:48:LYS:H	1:A:62:HIS:CE1	1.97	0.82
3:F:218:GLU:HG2	7:F:387:P6G:H31	1.66	0.76
1:B:204:CYS:SG	6:B:600:HEC:CBC	2.73	0.76
1:B:210:GLN:HE22	2:E:44:THR:HG21	1.51	0.75
1:A:113:GLU:HG2	6:A:500:HEC:HBC2	1.71	0.72
3:F:218:GLU:HG2	7:F:387:P6G:C3	2.20	0.71
3:F:255:SER:HA	8:F:388:PG4:H32	1.72	0.71
3:D:14:GLN:HE21	2:E:21:GLN:HE22	1.37	0.70
3:D:360:ASP:OD1	3:D:362:GLU:HB3	1.92	0.70
1:B:352:ARG:HD2	10:B:1181:HOH:O	1.94	0.67
3:D:265:VAL:HG21	3:D:321:GLY:HA3	1.76	0.67
3:D:268:LEU:HD21	3:D:298:VAL:HG11	1.78	0.66
3:F:218:GLU:CG	7:F:387:P6G:H31	2.25	0.65
3:D:181:CYS:C	3:D:182:TYR:CD1	2.76	0.64
3:F:342:GLU:HA	10:F:870:HOH:O	1.99	0.63
2:C:16:GLN:HE22	2:C:19:ASP:H	1.47	0.63
2:C:16:GLN:NE2	2:C:18:ASN:H	1.97	0.62
3:F:12:GLU:OE1	3:F:20:ARG:NH1	2.32	0.62
2:C:56:SER:HB2	2:C:74:TYR:O	2.01	0.61
3:D:36:ILE:CD1	2:E:46:CYS:HB2	2.31	0.60
1:B:285:THR:HG22	1:B:286:ASP:OD1	2.01	0.60
2:C:16:GLN:C	2:C:16:GLN:HE21	2.08	0.60
3:F:347:TYR:HB3	3:F:356:LEU:HD11	1.83	0.60
2:C:21:GLN:HE22	3:F:14:GLN:HE21	1.50	0.59
2:C:21:GLN:HE22	3:F:14:GLN:NE2	2.00	0.59
3:D:295:TYR:CD2	3:D:315:VAL:HG22	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:237:ALA:HB2	3:F:289:ARG:HG3	1.84	0.58
2:C:18:ASN:O	3:F:16:GLN:HA	2.04	0.58
2:E:91:THR:HG21	3:F:307:LYS:HD2	1.87	0.57
1:A:110:ASN:OD1	1:A:111:PRO:HD2	2.04	0.57
1:B:202:ARG:HH11	1:B:202:ARG:HG2	1.70	0.57
3:D:265:VAL:CG2	3:D:321:GLY:HA3	2.34	0.56
3:D:36:ILE:HD12	2:E:46:CYS:HB2	1.88	0.56
3:F:365:GLU:HA	3:F:365:GLU:OE1	2.05	0.56
3:F:181:CYS:C	3:F:182:TYR:CD1	2.84	0.56
2:C:19:ASP:OD1	3:F:15:GLY:HA3	2.05	0.56
1:A:101:LYS:NZ	1:A:157:GLU:OE2	2.32	0.55
3:F:51:ASP:HA	3:F:377:PRO:HA	1.88	0.55
1:B:81:ARG:HD2	10:B:1180:HOH:O	2.05	0.55
1:A:196:PHE:HE2	1:A:206:MET:HE3	1.72	0.55
3:D:274:ALA:HB3	10:D:838:HOH:O	2.07	0.55
3:D:297:LEU:HD22	3:D:310:SER:HB2	1.89	0.54
3:D:181:CYS:HA	3:D:196:CYS:HA	1.89	0.54
3:F:240:LEU:HD23	3:F:252:ILE:HD13	1.90	0.54
2:C:16:GLN:HE21	2:C:18:ASN:H	1.57	0.53
1:B:202:ARG:HH11	1:B:202:ARG:CG	2.21	0.53
1:A:119:ARG:HG2	1:A:152:PHE:CG	2.44	0.53
1:B:42:THR:HG21	1:B:275:THR:HB	1.91	0.53
3:F:45:ARG:NH2	3:F:343:LYS:O	2.42	0.52
3:F:82:ASN:HB3	3:F:142:THR:HB	1.91	0.52
1:A:208:ARG:NH1	3:F:31:ASP:HB2	2.25	0.52
1:B:21:PRO:O	1:B:27:ALA:HA	2.09	0.52
3:D:155:GLN:NE2	10:D:632:HOH:O	2.41	0.52
3:F:54:HIS:HE1	10:F:595:HOH:O	1.93	0.52
1:A:60:GLN:O	1:A:62:HIS:HD2	1.93	0.51
1:A:218:PHE:CE1	1:A:349:LEU:HD22	2.45	0.51
3:D:251:GLN:HE22	3:D:318:ALA:HB1	1.75	0.51
1:B:210:GLN:NE2	2:E:44:THR:HG21	2.21	0.51
3:D:349:LEU:HD21	3:D:377:PRO:HB2	1.92	0.51
1:B:285:THR:HB	1:B:309:GLU:OE1	2.10	0.50
3:D:140:TRP:CE2	3:D:233:TYR:HB3	2.48	0.49
3:D:372:GLN:NE2	10:D:1077:HOH:O	2.27	0.49
3:F:354:LYS:HG2	3:F:374:GLY:O	2.13	0.49
1:A:26:ASN:ND2	10:A:819:HOH:O	2.43	0.49
1:B:81:ARG:HH11	1:B:85:GLY:HA2	1.77	0.49
3:D:203:LYS:HE3	3:D:257:GLY:O	2.12	0.49
3:D:293:ARG:HD2	3:D:295:TYR:OH	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ARG:HH11	1:A:26:ASN:HD21	1.61	0.48
1:A:333:MET:HE2	3:D:159:ALA:CB	2.44	0.48
1:B:291:ILE:HD11	1:B:346:LEU:HD12	1.95	0.48
3:D:92:ILE:HG13	3:D:114:PHE:HB2	1.96	0.48
1:A:51:LEU:HB3	1:A:277:PRO:HD3	1.95	0.48
2:C:25:TYR:HB3	2:C:28:HIS:CD2	2.49	0.47
1:A:272:VAL:HG21	6:A:600:HEC:HMA3	1.96	0.47
3:F:227:LEU:N	3:F:227:LEU:HD12	2.30	0.47
1:A:86:LYS:HG3	10:A:501:HOH:O	2.15	0.47
2:E:25:TYR:HB3	2:E:28:HIS:CD2	2.49	0.47
3:F:96:SER:HB3	3:F:110:TYR:CZ	2.50	0.47
1:A:175:TYR:CD2	1:A:175:TYR:C	2.93	0.46
2:C:23:CYS:SG	2:C:88[B]:CYS:HB2	2.56	0.46
2:E:94:GLU:HG2	2:E:102:PHE:O	2.16	0.46
1:A:271:ASN:O	1:A:272:VAL:C	2.58	0.46
3:D:96:SER:HB3	3:D:110:TYR:CZ	2.50	0.46
3:D:275:ASP:OD1	10:D:1136:HOH:O	2.21	0.46
3:D:253:ASP:HB2	3:D:262:LEU:CD1	2.46	0.46
3:D:79:PHE:O	3:D:80:LEU:C	2.58	0.46
3:F:344:PRO:HG2	3:F:361:ALA:HB3	1.97	0.46
1:A:12:ALA:O	1:A:16:GLN:HG2	2.15	0.46
2:C:56:SER:HB3	2:C:75:ARG:HD2	1.97	0.46
1:A:140:PHE:CE1	1:A:154:ALA:HB1	2.51	0.46
1:A:175:TYR:CE1	1:A:179:MET:HE3	2.51	0.45
1:A:312:ALA:O	1:A:313:PRO:C	2.56	0.45
3:D:47:VAL:HG13	3:D:64:ILE:HB	1.98	0.45
1:A:40:ALA:HA	1:A:354:TYR:CZ	2.50	0.45
3:D:82:ASN:HB3	3:D:142:THR:HB	1.97	0.45
2:C:62:TYR:HB2	10:C:1114:HOH:O	2.16	0.45
2:E:20:ILE:HG22	2:E:25:TYR:CZ	2.51	0.45
1:B:192:GLY:N	1:B:341:ALA:HB1	2.31	0.45
3:D:276:GLY:O	3:D:300:GLN:HA	2.16	0.45
1:B:88:LYS:NZ	10:B:758:HOH:O	2.50	0.45
3:F:48:TYR:CZ	3:F:92:ILE:HG21	2.52	0.45
3:D:239:ARG:HH11	3:D:251:GLN:NE2	2.15	0.45
2:E:96:PRO:HB2	2:E:98:TYR:CE1	2.52	0.45
3:F:350:SER:HB3	3:F:353:ASP:HB2	1.99	0.45
1:A:333:MET:HE2	3:D:159:ALA:HB2	1.99	0.44
7:F:387:P6G:H142	7:F:387:P6G:H171	1.57	0.44
3:D:227:LEU:HB3	3:D:242:TRP:NE1	2.33	0.44
2:C:88[B]:CYS:SG	2:C:90:ASN:ND2	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LYS:HD3	10:B:802:HOH:O	2.18	0.44
2:C:130:ALA:O	2:C:131:SER:CB	2.65	0.44
2:E:12:LYS:HE2	10:F:971:HOH:O	2.18	0.44
2:E:58:VAL:HA	2:E:72:ILE:O	2.18	0.44
3:D:265:VAL:HG21	3:D:321:GLY:CA	2.45	0.44
3:D:239:ARG:HD2	3:D:251:GLN:HE21	1.83	0.43
1:B:35:HIS:CE1	1:B:70:LEU:HD21	2.53	0.43
1:A:293:PHE:CE1	1:A:296:LYS:CD	3.02	0.43
2:C:129:LYS:O	2:C:130:ALA:C	2.61	0.43
3:F:91:PHE:HA	3:F:116:PRO:HD3	2.00	0.43
1:B:360:GLU:C	10:B:780:HOH:O	2.61	0.43
2:C:106:ILE:HG12	3:D:133:PHE:CZ	2.53	0.43
1:A:48:LYS:N	1:A:62:HIS:HE1	1.98	0.43
1:A:61:SER:HB3	1:A:112:VAL:HB	2.01	0.43
3:D:152:LEU:HD23	3:D:164:VAL:HA	2.00	0.43
1:B:173:SER:HB2	1:B:348:THR:O	2.18	0.43
2:C:57:OAF:CE3	2:C:108:TRP:CD1	3.02	0.43
3:D:273:ARG:HG2	10:D:643:HOH:O	2.19	0.43
3:D:137:THR:HA	10:D:389:HOH:O	2.19	0.42
1:A:135:GLY:HA2	10:A:1122:HOH:O	2.20	0.42
1:B:25:ARG:HD3	10:B:1124:HOH:O	2.19	0.42
1:B:133:ARG:O	1:B:137:GLU:HG3	2.19	0.42
2:E:129:LYS:O	2:E:130:ALA:HB2	2.18	0.42
3:F:92:ILE:HG12	3:F:114:PHE:HB2	2.00	0.42
1:B:84:ASN:OD1	1:B:84:ASN:N	2.52	0.42
1:B:113:GLU:HG2	6:B:500:HEC:HBC2	2.00	0.42
2:C:96:PRO:HB2	2:C:98:TYR:CE1	2.55	0.42
2:C:106:ILE:HG12	3:D:133:PHE:HZ	1.84	0.42
3:D:82:ASN:O	3:D:94:HIS:HA	2.20	0.42
3:D:182:TYR:CD1	3:D:182:TYR:N	2.87	0.42
1:B:202:ARG:CG	1:B:202:ARG:NH1	2.80	0.42
3:F:305:ARG:HA	3:F:305:ARG:HD2	1.89	0.42
1:B:65:ARG:HH12	1:B:94:ASP:CG	2.28	0.41
1:B:205:HIS:C	1:B:206:MET:HG2	2.44	0.41
1:B:252:ARG:HD3	10:B:811:HOH:O	2.20	0.41
1:A:197:ILE:O	1:A:202:ARG:HD2	2.20	0.41
2:C:80:TYR:HB2	2:C:120:HIS:HB2	2.02	0.41
3:D:101:ARG:C	3:D:102:ILE:HD12	2.44	0.41
1:A:83:ALA:N	10:A:1003:HOH:O	2.51	0.41
1:A:191:PHE:CZ	1:A:338:ARG:HG2	2.55	0.41
1:B:81:ARG:CD	10:B:1180:HOH:O	2.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:GLY:CA	1:B:341:ALA:HB1	2.51	0.41
3:D:326:LYS:HB3	3:D:326:LYS:HE2	1.84	0.41
2:C:56:SER:CB	2:C:74:TYR:O	2.67	0.41
3:D:297:LEU:HD23	3:D:297:LEU:HA	1.88	0.41
1:B:204:CYS:CB	6:B:600:HEC:C3C	2.98	0.41
2:E:129:LYS:O	2:E:130:ALA:CB	2.68	0.41
1:B:120:ALA:HA	1:B:148:PRO:HB3	2.02	0.41
1:B:140:PHE:HZ	1:B:157:GLU:HG2	1.85	0.41
1:A:21:PRO:O	1:A:27:ALA:HA	2.21	0.41
1:A:43:ASP:HA	1:A:44:PRO:HD2	1.65	0.41
3:F:251:GLN:O	3:F:262:LEU:HB2	2.20	0.41
1:B:281:ASN:OD1	1:B:283:VAL:HB	2.20	0.41
3:D:89:GLY:HA3	3:D:385:MET:HE3	2.03	0.41
3:D:253:ASP:HB2	3:D:262:LEU:HD11	2.02	0.41
3:F:178:VAL:HB	3:F:179:PRO:CD	2.50	0.41
3:F:314:VAL:HG12	3:F:326:LYS:HG3	2.03	0.41
2:C:97:VAL:HG23	2:C:106:ILE:HD11	2.02	0.41
1:A:172:ASP:O	1:A:177:ARG:NH1	2.54	0.40
1:B:41:PHE:HE2	1:B:353:ARG:HH21	1.69	0.40
1:B:91:GLN:O	1:B:92:PHE:HB2	2.21	0.40
2:C:16:GLN:NE2	2:C:16:GLN:C	2.78	0.40
2:C:114:ASP:O	2:C:115:ASP:HB2	2.21	0.40
3:F:138:TYR:O	3:F:139:PRO:C	2.62	0.40
1:A:291:ILE:HD12	1:A:343:VAL:HG23	2.02	0.40
1:B:52:ALA:O	1:B:66:ASN:HA	2.21	0.40
3:D:36:ILE:HD13	2:E:46:CYS:HB2	2.04	0.40
1:A:41:PHE:HB2	1:A:70:LEU:H	1.86	0.40
1:A:277:PRO:HB3	1:A:285:THR:HA	2.02	0.40
3:D:42:PRO:HD3	3:D:117:VAL:HG12	2.03	0.40
2:E:33:GLY:HA3	2:E:119:TYR:OH	2.22	0.40
1:A:91:GLN:HB3	6:A:500:HEC:HAA1	2.03	0.40
1:B:26:ASN:HB2	1:B:28:THR:HG23	2.04	0.40
1:B:199:LYS:O	1:B:202:ARG:NH1	2.54	0.40
2:C:16:GLN:NE2	2:C:19:ASP:H	2.15	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	354/373 (95%)	336 (95%)	18 (5%)	0	100	100
1	B	354/373 (95%)	341 (96%)	13 (4%)	0	100	100
2	C	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
2	E	123/137 (90%)	119 (97%)	3 (2%)	1 (1%)	16	6
3	D	375/386 (97%)	356 (95%)	17 (4%)	2 (0%)	24	14
3	F	374/386 (97%)	360 (96%)	13 (4%)	1 (0%)	36	26
All	All	1703/1792 (95%)	1633 (96%)	66 (4%)	4 (0%)	43	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	130	ALA
3	D	102	ILE
3	D	223	GLU
3	F	102	ILE

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	278/292 (95%)	263 (95%)	15 (5%)	20	7
1	B	278/292 (95%)	266 (96%)	12 (4%)	26	11
2	C	105/112 (94%)	100 (95%)	5 (5%)	23	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	105/112 (94%)	102 (97%)	3 (3%)	37	21
3	D	305/311 (98%)	295 (97%)	10 (3%)	33	17
3	F	304/311 (98%)	298 (98%)	6 (2%)	48	35
All	All	1375/1430 (96%)	1324 (96%)	51 (4%)	30	15

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	8	ASP
1	A	29	GLN
1	A	51	LEU
1	A	84	ASN
1	A	86	LYS
1	A	112	VAL
1	A	183	GLU
1	A	202	ARG
1	A	206	MET
1	A	256	GLU
1	A	296	LYS
1	A	333	MET
1	A	357	LEU
1	A	359	GLU
1	B	84	ASN
1	B	102	GLN
1	B	112	VAL
1	B	157	GLU
1	B	167	GLU
1	B	202	ARG
1	B	214	GLU
1	B	219	THR
1	B	285	THR
1	B	305	LYS
1	B	323	LEU
1	B	357	LEU
2	C	7	THR
2	C	16	GLN
2	C	30	SER
2	C	69	SER
2	C	71	LEU
3	D	117	VAL

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Mol	Chain	Res	Type
3	D	127	LEU
3	D	160	PRO
3	D	209	GLU
3	D	215	THR
3	D	223	GLU
3	D	323	ARG
3	D	328	GLU
3	D	354	LYS
3	D	365	GLU
2	E	65	THR
2	E	71	LEU
2	E	115	ASP
3	F	14	GLN
3	F	92	ILE
3	F	117	VAL
3	F	160	PRO
3	F	262	LEU
3	F	354	LYS

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	26	ASN
1	A	62	HIS
1	A	91	GLN
1	B	16	GLN
1	B	60	GLN
1	B	91	GLN
1	B	210	GLN
2	C	16	GLN
2	C	90	ASN
3	D	30	GLN
3	D	155	GLN
3	D	251	GLN
3	D	331	HIS
3	D	375	HIS
3	D	378	GLN
2	E	21	GLN
3	F	14	GLN
3	F	50	ASN
3	F	54	HIS
3	F	61	GLN

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Mol	Chain	Res	Type
3	F	300	GLN
3	F	375	HIS
3	F	378	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	0AF	C	57	2	15,16,17	1.57	3 (20%)	14,22,24	1.71	2 (14%)
2	0AF	E	57	2	15,16,17	2.43	8 (53%)	14,22,24	1.56	4 (28%)

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	0AF	C	57	2	1/1/1/2	1/5/6/8	0/2/2/2
2	0AF	E	57	2	-	1/5/6/8	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57	0AF	CD2-CE2	-5.49	1.34	1.41
2	C	57	0AF	CD2-CE2	-3.44	1.37	1.41
2	E	57	0AF	CD1-NE1	-3.23	1.32	1.37
2	E	57	0AF	CE2-NE1	-2.86	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57	0AF	CB-CA	-2.43	1.48	1.53
2	C	57	0AF	CA-N	-2.41	1.41	1.48
2	E	57	0AF	CZ3-CE3	2.29	1.42	1.38
2	E	57	0AF	CA-N	-2.28	1.41	1.48
2	E	57	0AF	CZ3-CH2	2.24	1.42	1.38
2	C	57	0AF	CB-CA	-2.23	1.49	1.53
2	E	57	0AF	CD1-CG	2.08	1.39	1.36

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	57	0AF	CG-CD1-NE1	-3.67	106.28	110.31
2	C	57	0AF	CE2-NE1-CD1	3.39	111.85	108.93
2	E	57	0AF	CB-CG-CD2	3.03	132.52	126.70
2	E	57	0AF	O1-CZ2-CH2	2.20	125.28	119.36
2	E	57	0AF	CH2-CZ3-CE3	-2.19	117.43	120.24
2	E	57	0AF	CB-CG-CD1	-2.17	122.73	126.97

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	57	0AF	CA

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	57	0AF	N-CA-CB-CG
2	C	57	0AF	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	57	0AF	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 for Mogul analysis.

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
8	PG4	F	388	-	12,12,12	0.54	0	11,11,11	0.36	0
6	HEC	B	600	1	46,50,50	2.78	15 (32%)	58,82,82	2.82	25 (43%)
9	MES	F	389	-	12,12,12	2.08	1 (8%)	15,16,16	3.19	8 (53%)
6	HEC	B	500	10,1	46,50,50	2.63	23 (50%)	58,82,82	2.32	23 (39%)
6	HEC	A	500	1	46,50,50	2.70	20 (43%)	58,82,82	2.53	13 (22%)
6	HEC	A	600	1	46,50,50	2.71	21 (45%)	58,82,82	2.45	21 (36%)
7	P6G	F	387	-	18,18,18	0.83	0	17,17,17	0.78	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
8	PG4	F	388	-	-	6/10/10/10	-
6	HEC	B	600	1	-	6/14/54/54	-
9	MES	F	389	-	-	4/6/14/14	0/1/1/1
6	HEC	B	500	10,1	-	6/14/54/54	-
6	HEC	A	500	1	-	5/14/54/54	-
6	HEC	A	600	1	-	4/14/54/54	-
7	P6G	F	387	-	-	5/16/16/16	-

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	389	MES	C8-S	-7.00	1.67	1.77
6	A	500	HEC	CHA-C1A	6.73	1.51	1.38
6	B	600	HEC	C4C-NC	-6.18	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	500	HEC	CHA-C1A	5.95	1.50	1.38
6	B	600	HEC	C4B-NB	-5.61	1.29	1.39
6	A	500	HEC	CHB-C4A	5.49	1.49	1.38
6	B	500	HEC	C4C-NC	-5.38	1.29	1.39
6	B	600	HEC	CAB-C3B	5.38	1.52	1.35
6	B	600	HEC	CHB-C4A	5.36	1.48	1.38
6	A	500	HEC	CAC-C3C	5.33	1.52	1.35
6	A	500	HEC	CAB-C3B	5.25	1.52	1.35
6	B	500	HEC	CAB-C3B	5.22	1.52	1.35
6	A	600	HEC	CAB-C3B	5.21	1.51	1.35
6	B	600	HEC	CHC-C4B	5.20	1.48	1.38
6	A	500	HEC	CHD-C4C	5.17	1.48	1.38
6	A	500	HEC	CHC-C4B	4.98	1.48	1.38
6	B	600	HEC	CAC-C3C	4.97	1.51	1.35
6	A	600	HEC	CHD-C4C	4.97	1.48	1.38
6	A	600	HEC	CHA-C1A	4.94	1.48	1.38
6	A	600	HEC	CHC-C4B	4.91	1.48	1.38
6	A	600	HEC	C1A-NA	-4.82	1.30	1.39
6	B	600	HEC	CHA-C1A	4.77	1.47	1.38
6	B	600	HEC	C4D-ND	-4.71	1.30	1.39
6	B	500	HEC	CAC-C3C	4.63	1.50	1.35
6	B	600	HEC	C1D-ND	-4.62	1.30	1.39
6	A	600	HEC	CAC-C3C	4.54	1.49	1.35
6	B	500	HEC	CHB-C4A	4.43	1.47	1.38
6	B	600	HEC	C4A-NA	-4.34	1.31	1.39
6	A	500	HEC	CHD-C1D	4.31	1.49	1.39
6	A	600	HEC	C1B-NB	-4.29	1.31	1.39
6	B	500	HEC	CHC-C4B	4.20	1.46	1.38
6	A	600	HEC	C4A-NA	-3.98	1.32	1.39
6	A	600	HEC	CHB-C4A	3.83	1.45	1.38
6	A	600	HEC	C4B-NB	-3.81	1.32	1.39
6	B	500	HEC	CHD-C4C	3.77	1.45	1.38
6	B	600	HEC	C1A-NA	-3.77	1.32	1.39
6	A	500	HEC	CHA-C4D	3.73	1.47	1.39
6	B	500	HEC	CHC-C1C	3.73	1.47	1.39
6	B	600	HEC	C1C-NC	-3.68	1.32	1.39
6	A	600	HEC	CHD-C1D	3.67	1.47	1.39
6	A	600	HEC	C1C-NC	-3.60	1.32	1.39
6	A	600	HEC	C1D-ND	-3.53	1.33	1.39
6	B	500	HEC	C4B-NB	-3.50	1.33	1.39
6	B	500	HEC	C1C-NC	-3.43	1.33	1.39
6	A	600	HEC	CHA-C4D	3.42	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	600	HEC	CHA-C4D	3.37	1.47	1.39
6	A	600	HEC	CHC-C1C	3.35	1.46	1.39
6	B	600	HEC	CHD-C4C	3.28	1.44	1.38
6	A	500	HEC	CHB-C1B	3.27	1.46	1.39
6	B	500	HEC	C1D-ND	-3.27	1.33	1.39
6	A	600	HEC	C4C-NC	-3.20	1.33	1.39
6	A	600	HEC	CHB-C1B	3.18	1.46	1.39
6	B	500	HEC	CHA-C4D	3.01	1.46	1.39
6	A	500	HEC	C4B-NB	-2.98	1.34	1.39
6	B	500	HEC	C4A-NA	-2.89	1.34	1.39
6	B	500	HEC	C3C-C4C	2.83	1.50	1.46
6	B	500	HEC	C4D-C3D	2.81	1.50	1.44
6	A	600	HEC	C4D-ND	-2.79	1.34	1.39
6	A	500	HEC	C1D-ND	-2.77	1.34	1.39
6	A	500	HEC	CHC-C1C	2.76	1.45	1.39
6	B	500	HEC	CHB-C1B	2.74	1.45	1.39
6	B	500	HEC	C1B-C2B	2.73	1.49	1.43
6	A	500	HEC	C1A-C2A	2.67	1.49	1.45
6	B	500	HEC	C4A-C3A	2.64	1.50	1.45
6	A	600	HEC	C1C-C2C	2.62	1.49	1.43
6	A	500	HEC	C3C-C4C	2.61	1.50	1.46
6	B	500	HEC	C1D-C2D	2.54	1.49	1.43
6	A	600	HEC	O2D-CGD	-2.53	1.22	1.30
6	B	500	HEC	CHD-C1D	2.51	1.45	1.39
6	A	500	HEC	C1A-NA	-2.40	1.35	1.39
6	A	500	HEC	C1B-C2B	2.38	1.48	1.43
6	A	500	HEC	C4D-C3D	2.34	1.49	1.44
6	A	500	HEC	C1C-NC	-2.34	1.35	1.39
6	B	500	HEC	C1A-NA	-2.31	1.35	1.39
6	A	600	HEC	O2A-CGA	-2.23	1.23	1.30
6	B	500	HEC	C1B-NB	-2.16	1.35	1.39
6	B	500	HEC	C3B-C4B	2.15	1.49	1.46
6	A	500	HEC	C1C-C2C	2.12	1.48	1.43
6	A	500	HEC	C4D-ND	-2.09	1.35	1.39
6	B	600	HEC	CHD-C1D	2.03	1.44	1.39

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	600	HEC	CBB-CAB-C3B	-12.39	102.67	127.43
6	A	500	HEC	CBB-CAB-C3B	-12.39	102.68	127.43
6	B	600	HEC	CBC-CAC-C3C	-8.79	109.86	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	600	HEC	CBB-CAB-C3B	-8.59	110.26	127.43
6	A	500	HEC	CBC-CAC-C3C	-7.90	111.64	127.43
6	B	500	HEC	CBB-CAB-C3B	-7.88	111.69	127.43
6	A	600	HEC	CBC-CAC-C3C	-7.43	112.59	127.43
9	F	389	MES	C2-C3-N4	-7.35	98.95	110.12
6	A	600	HEC	CBD-CAD-C3D	-5.43	97.51	112.53
6	B	500	HEC	C3D-C4D-ND	4.96	115.66	110.15
6	B	600	HEC	CBD-CAD-C3D	-4.95	98.84	112.53
9	F	389	MES	C7-N4-C5	4.26	122.59	111.24
9	F	389	MES	C6-C5-N4	-4.20	103.74	110.12
6	B	500	HEC	CBD-CAD-C3D	-4.16	101.02	112.53
6	A	600	HEC	CHB-C4A-NA	-4.11	119.98	124.45
6	A	600	HEC	C4A-C3A-C2A	-4.10	100.88	106.97
6	A	500	HEC	C2D-C1D-ND	4.05	116.63	110.14
9	F	389	MES	C7-N4-C3	3.92	121.68	111.24
6	B	500	HEC	CBC-CAC-C3C	-3.80	119.84	127.43
6	B	500	HEC	C2B-C1B-NB	3.70	116.07	110.14
6	B	600	HEC	CHD-C4C-NC	-3.68	120.45	124.45
6	B	500	HEC	CMC-C2C-C3C	3.67	135.19	126.55
6	A	500	HEC	C3D-C4D-ND	3.65	114.20	110.15
6	A	600	HEC	C2A-C1A-NA	3.60	113.80	110.32
6	A	600	HEC	C3A-C4A-NA	3.48	116.07	109.64
6	B	600	HEC	CMC-C2C-C3C	3.46	134.68	126.55
6	A	500	HEC	C1D-C2D-C3D	-3.43	102.88	106.82
6	B	500	HEC	C2D-C1D-ND	3.31	115.45	110.14
6	A	600	HEC	CMD-C2D-C3D	3.27	132.55	125.62
6	A	600	HEC	CMC-C2C-C3C	3.27	134.23	126.55
6	B	600	HEC	C3D-C4D-ND	3.24	113.75	110.15
6	B	600	HEC	CMA-C3A-C4A	3.22	130.41	124.73
9	F	389	MES	O2S-S-C8	3.17	111.52	106.73
9	F	389	MES	C5-N4-C3	3.17	115.67	108.84
6	B	600	HEC	CHB-C4A-NA	-3.17	121.01	124.45
6	B	500	HEC	CHD-C1D-ND	-3.14	118.17	123.86
6	A	600	HEC	C3D-C4D-ND	3.10	113.59	110.15
6	A	600	HEC	C1D-C2D-C3D	-3.08	103.29	106.82
6	B	500	HEC	C4D-C3D-C2D	-3.04	102.17	106.87
6	B	600	HEC	C2D-C1D-ND	3.03	115.00	110.14
6	B	500	HEC	C2A-C1A-NA	3.00	113.22	110.32
6	B	500	HEC	CHC-C4B-NB	-2.96	121.23	124.45
6	A	500	HEC	CMD-C2D-C3D	2.94	131.86	125.62
6	A	500	HEC	C2B-C1B-NB	2.91	114.81	110.14
9	F	389	MES	O1-C6-C5	-2.91	105.51	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	600	HEC	C2C-C1C-NC	2.90	114.78	110.14
6	B	600	HEC	C2A-C1A-NA	2.81	113.03	110.32
9	F	389	MES	O1S-S-C8	2.80	110.97	106.73
6	B	500	HEC	C4D-ND-C1D	-2.80	101.26	105.82
6	B	600	HEC	CAD-C3D-C4D	2.76	130.33	124.94
6	B	600	HEC	C4A-C3A-C2A	-2.74	102.91	106.97
6	B	500	HEC	C2C-C1C-NC	2.72	114.50	110.14
6	A	600	HEC	C2B-C1B-NB	2.68	114.43	110.14
6	A	600	HEC	CHC-C4B-NB	-2.67	121.54	124.45
6	B	500	HEC	CBA-CAA-C2A	-2.61	105.33	112.53
6	B	500	HEC	C4B-NB-C1B	-2.60	101.59	105.82
6	A	600	HEC	C2D-C1D-ND	2.57	114.27	110.14
6	B	600	HEC	C1D-C2D-C3D	-2.56	103.89	106.82
6	A	500	HEC	CHD-C4C-NC	-2.53	121.70	124.45
6	B	500	HEC	O2A-CGA-CBA	2.46	121.78	114.00
6	B	600	HEC	CBA-CAA-C2A	-2.46	105.74	112.53
6	A	600	HEC	CMC-C2C-C1C	-2.45	121.68	125.42
6	B	500	HEC	CHA-C1A-C2A	-2.44	121.01	124.86
6	B	500	HEC	O2D-CGD-CBD	2.44	121.72	114.00
6	B	500	HEC	CMC-C2C-C1C	-2.41	121.75	125.42
6	A	500	HEC	C4D-ND-C1D	-2.40	101.91	105.82
6	B	600	HEC	CHC-C1C-C2C	-2.39	120.48	127.43
6	A	500	HEC	CMB-C2B-C3B	2.38	132.15	126.55
6	B	600	HEC	O2A-CGA-O1A	-2.36	117.27	123.33
6	B	500	HEC	C1A-C2A-C3A	-2.29	104.10	107.11
6	B	600	HEC	C2B-C1B-NB	2.29	113.81	110.14
6	B	600	HEC	CAD-CBD-CGD	-2.28	107.61	113.67
6	B	500	HEC	CAD-C3D-C4D	2.27	129.38	124.94
6	B	500	HEC	O1A-CGA-CBA	-2.26	115.93	123.09
6	B	600	HEC	C3A-C4A-NA	2.25	113.80	109.64
6	A	600	HEC	CMA-C3A-C4A	2.21	128.62	124.73
6	A	600	HEC	CHB-C1B-C2B	-2.21	121.02	127.43
6	A	600	HEC	C2C-C1C-NC	2.18	113.63	110.14
6	B	600	HEC	CHB-C1B-C2B	-2.16	121.15	127.43
6	B	600	HEC	CAA-C2A-C3A	2.16	131.91	127.87
6	B	600	HEC	O2D-CGD-CBD	2.14	120.76	114.00
6	B	500	HEC	CHC-C1C-C2C	-2.14	121.22	127.43
6	A	500	HEC	C2A-C1A-NA	2.12	112.37	110.32
6	A	600	HEC	CBA-CAA-C2A	-2.11	106.69	112.53
6	A	500	HEC	CHA-C1A-NA	-2.07	122.20	124.45
6	A	600	HEC	CHD-C4C-NC	-2.05	122.22	124.45
6	B	600	HEC	CHA-C4D-ND	-2.05	120.15	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	600	HEC	CMC-C2C-C1C	-2.04	122.31	125.42
6	A	500	HEC	CHD-C1D-C2D	-2.03	121.53	127.43
6	A	600	HEC	CAA-C2A-C3A	2.00	131.62	127.87

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	500	HEC	C2B-C3B-CAB-CBB
6	A	500	HEC	C4B-C3B-CAB-CBB
6	A	500	HEC	C2C-C3C-CAC-CBC
6	A	500	HEC	C4C-C3C-CAC-CBC
6	A	600	HEC	C2B-C3B-CAB-CBB
6	A	600	HEC	C4B-C3B-CAB-CBB
6	A	600	HEC	C2C-C3C-CAC-CBC
6	A	600	HEC	C4C-C3C-CAC-CBC
6	B	500	HEC	C2B-C3B-CAB-CBB
6	B	500	HEC	C4B-C3B-CAB-CBB
6	B	500	HEC	C2C-C3C-CAC-CBC
6	B	500	HEC	C4C-C3C-CAC-CBC
6	B	600	HEC	C2B-C3B-CAB-CBB
6	B	600	HEC	C4B-C3B-CAB-CBB
6	B	600	HEC	C2C-C3C-CAC-CBC
6	B	600	HEC	C4C-C3C-CAC-CBC
9	F	389	MES	C7-C8-S-O1S
9	F	389	MES	C7-C8-S-O3S
7	F	387	P6G	C14-C15-O16-C17
8	F	388	PG4	O2-C3-C4-O3
7	F	387	P6G	O13-C14-C15-O16
7	F	387	P6G	O1-C2-C3-O4
7	F	387	P6G	O16-C17-C18-O19
8	F	388	PG4	O1-C1-C2-O2
9	F	389	MES	C7-C8-S-O2S
8	F	388	PG4	C3-C4-O3-C5
8	F	388	PG4	C8-C7-O4-C6
9	F	389	MES	C8-C7-N4-C5
8	F	388	PG4	C1-C2-O2-C3
6	A	500	HEC	CAD-CBD-CGD-O2D
7	F	387	P6G	C11-C12-O13-C14
6	B	500	HEC	CAA-CBA-CGA-O2A
6	B	600	HEC	CAD-CBD-CGD-O2D
6	B	600	HEC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
6	B	500	HEC	CAA-CBA-CGA-O1A
8	F	388	PG4	O3-C5-C6-O4

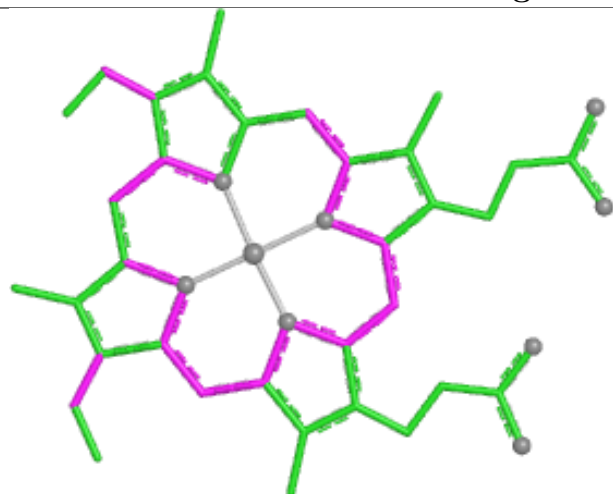
There are no ring outliers.

6 monomers are involved in 14 short contacts:

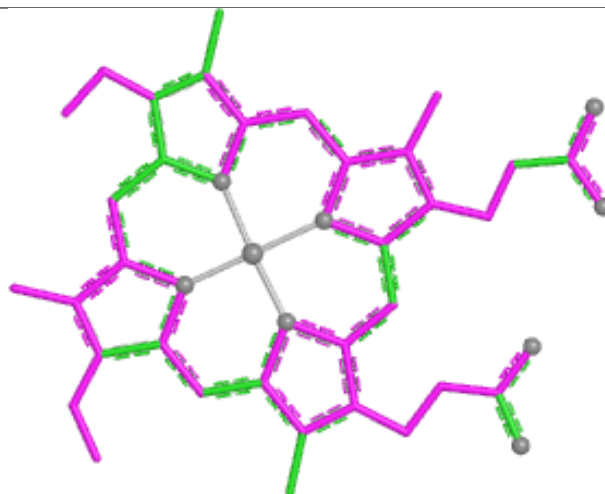
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	388	PG4	1	0
6	B	600	HEC	5	0
6	B	500	HEC	1	0
6	A	500	HEC	2	0
6	A	600	HEC	1	0
7	F	387	P6G	4	0

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.

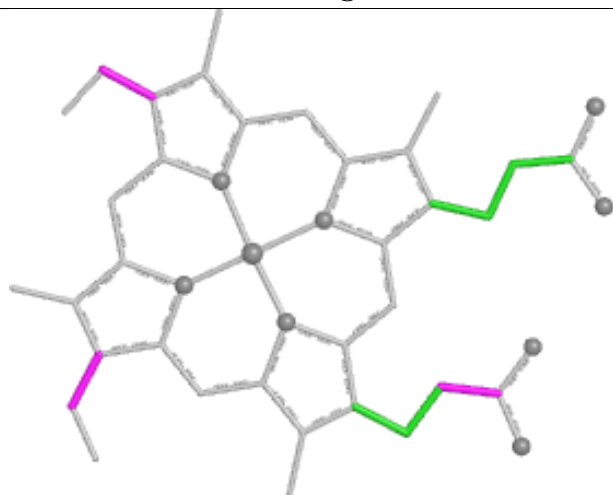
Ligand HEC B 600



Bond lengths



Bond angles

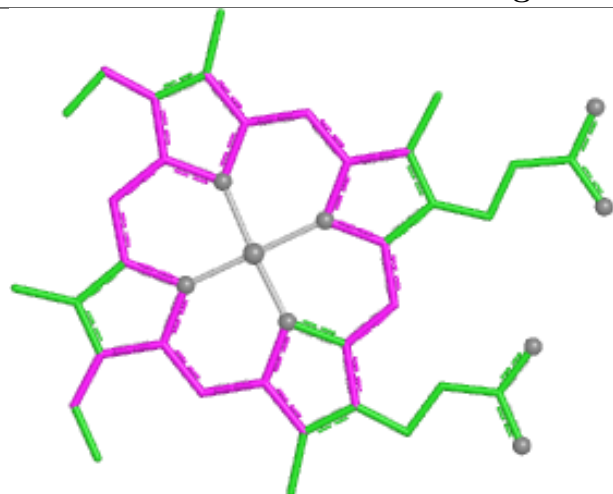


Torsions

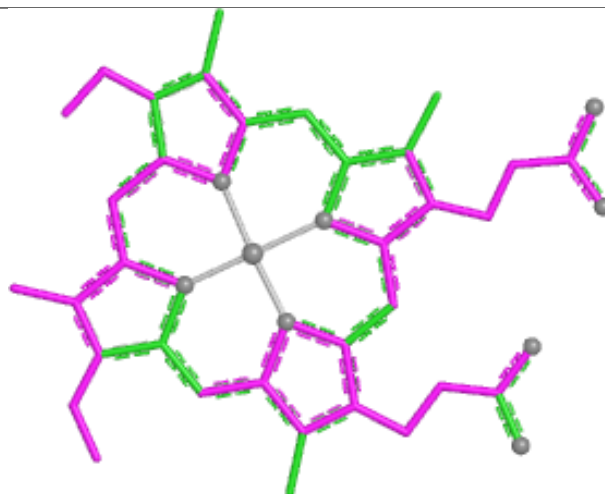


Rings

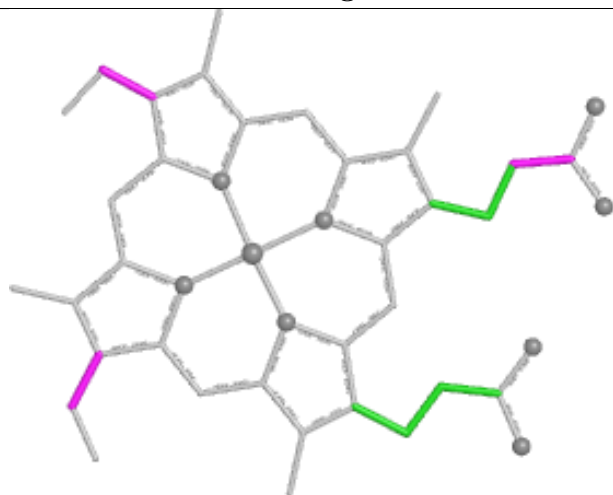
Ligand HEC B 500



Bond lengths



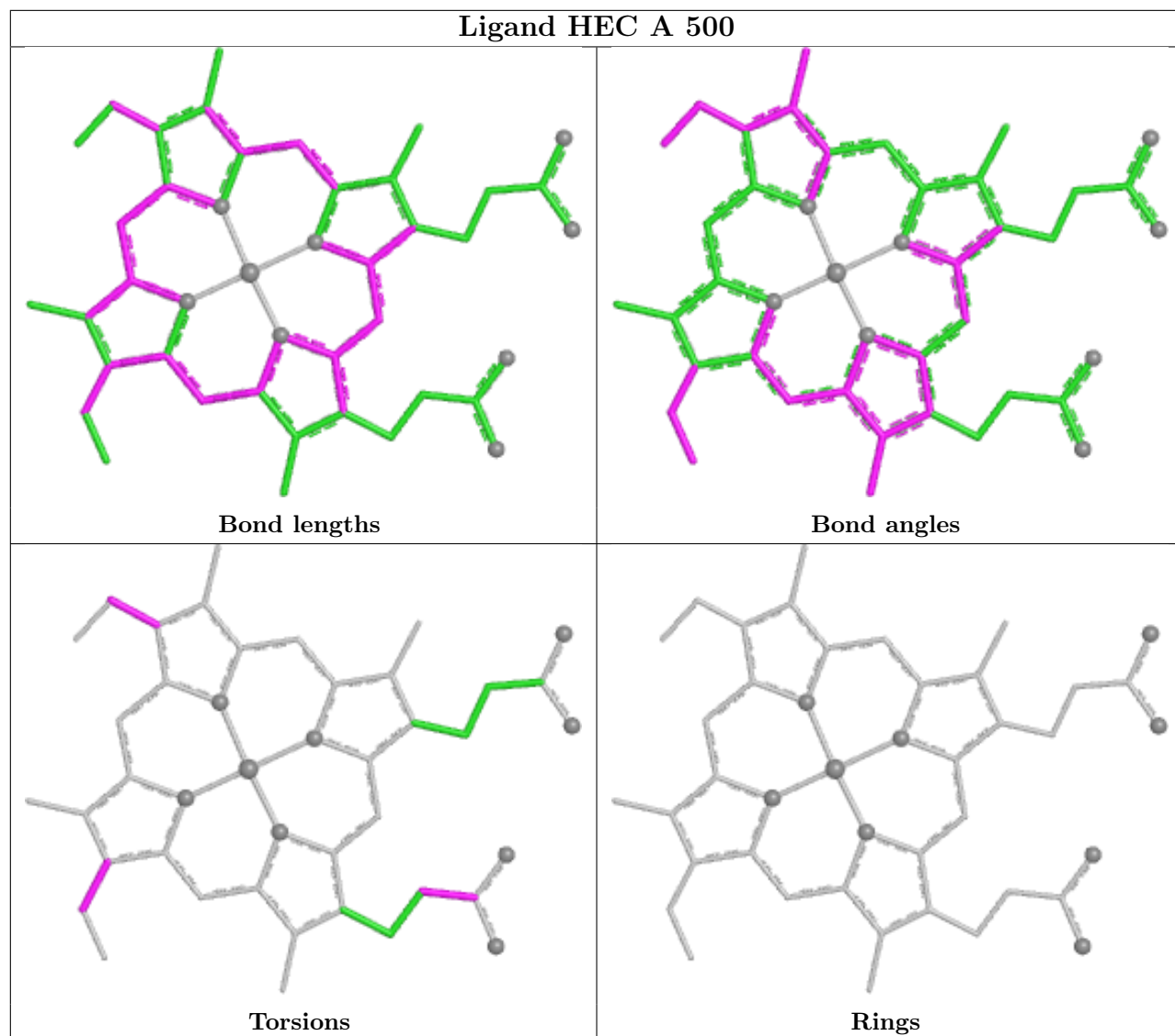
Bond angles

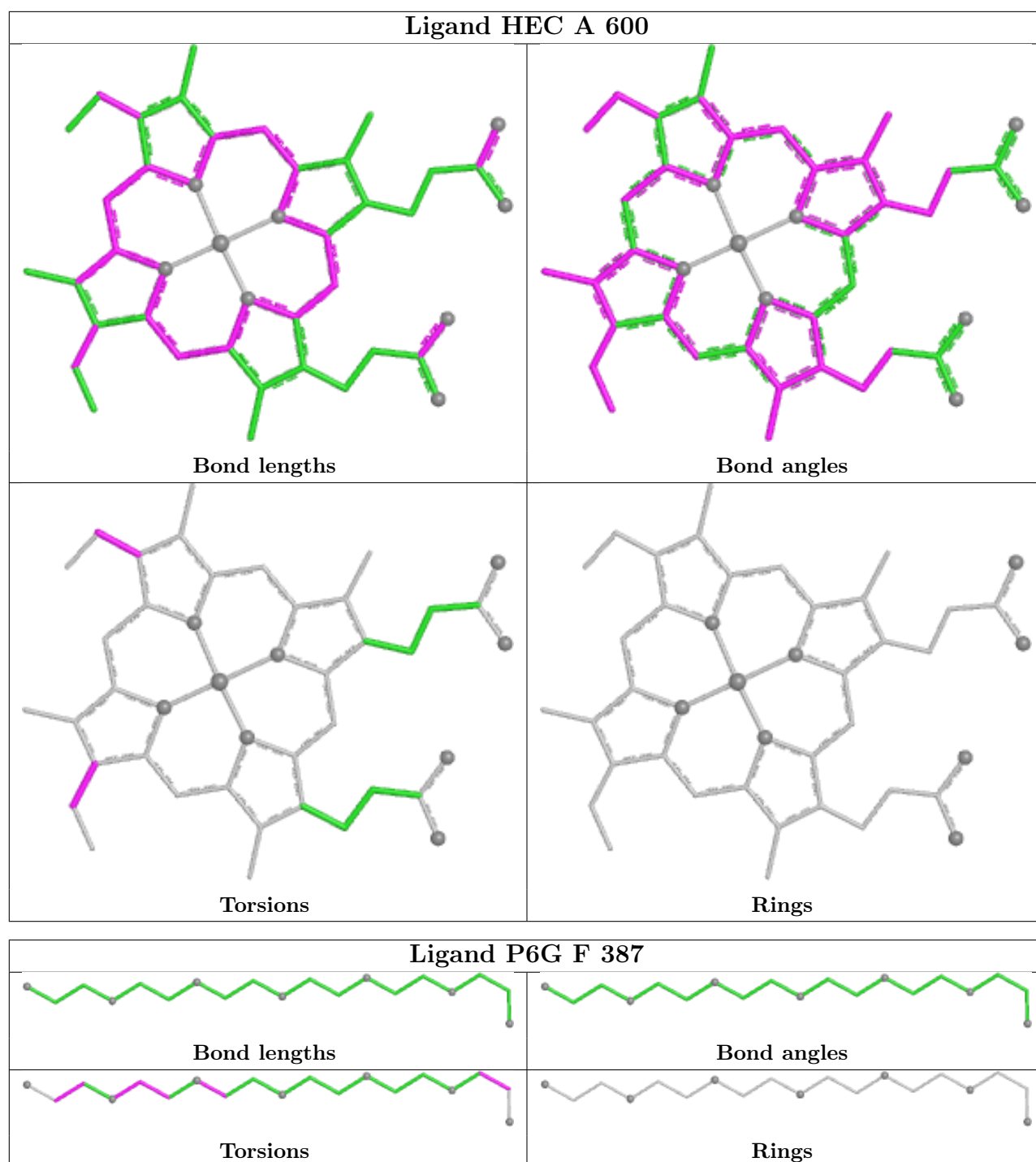


Torsions



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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	354/373 (94%)	0.23	3 (0%) 82 88	22, 37, 51, 70	2 (0%)
1	B	355/373 (95%)	-0.07	2 (0%) 85 89	16, 30, 47, 66	1 (0%)
2	C	124/137 (90%)	0.18	3 (2%) 59 66	23, 35, 52, 69	1 (0%)
2	E	124/137 (90%)	-0.13	1 (0%) 82 88	18, 26, 35, 60	1 (0%)
3	D	376/386 (97%)	0.28	7 (1%) 66 73	15, 40, 66, 77	1 (0%)
3	F	376/386 (97%)	-0.12	1 (0%) 90 93	19, 28, 45, 61	0
All	All	1709/1792 (95%)	0.07	17 (0%) 79 85	15, 33, 55, 77	6 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	ALA	3.5
1	A	166	GLY	3.3
2	C	130	ALA	2.9
2	E	130	ALA	2.9
1	A	6	ALA	2.7
3	D	262	LEU	2.6
3	D	208	THR	2.6
3	D	210	GLY	2.4
3	D	207	GLY	2.3
3	D	257	GLY	2.3
3	F	207	GLY	2.2
2	C	131	SER	2.2
1	A	84	ASN	2.1
3	D	264	ALA	2.1
1	B	7	ASP	2.1
3	D	312	PHE	2.0
2	C	127	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	0AF	C	57	15/16	0.92	0.10	32,35,36,38	0
2	0AF	E	57	15/16	0.94	0.07	21,25,27,27	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

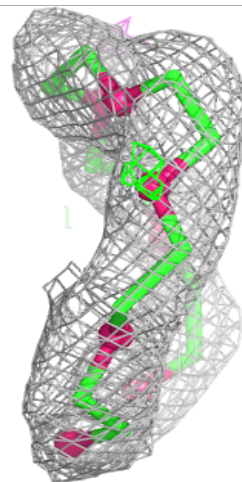
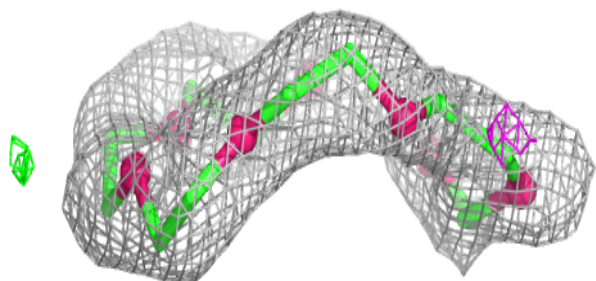
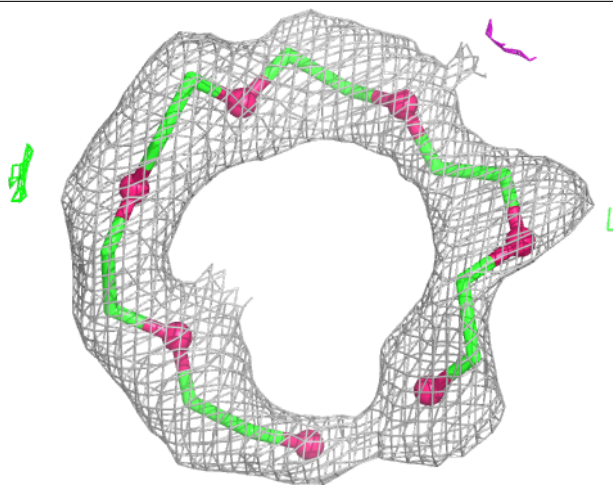
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NA	A	401	1/1	0.81	0.10	45,45,45,45	0
8	PG4	F	388	13/13	0.86	0.12	58,61,78,78	0
7	P6G	F	387	19/19	0.88	0.12	43,49,62,62	0
9	MES	F	389	12/12	0.88	0.17	20,33,37,37	12
5	NA	B	402	1/1	0.93	0.06	35,35,35,35	0
5	NA	B	401	1/1	0.93	0.10	41,41,41,41	0
5	NA	A	402	1/1	0.97	0.05	37,37,37,37	0
6	HEC	A	500	43/43	0.97	0.07	26,30,33,35	0
6	HEC	B	500	43/43	0.97	0.07	18,23,27,28	0
6	HEC	B	600	43/43	0.98	0.06	12,17,21,24	0
6	HEC	A	600	43/43	0.98	0.06	18,28,30,32	0
4	CA	B	400	1/1	0.99	0.02	20,20,20,20	0
4	CA	A	400	1/1	0.99	0.04	29,29,29,29	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

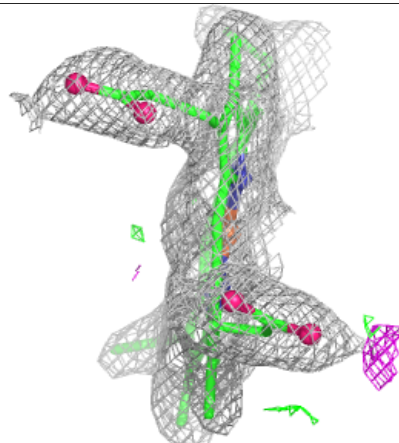
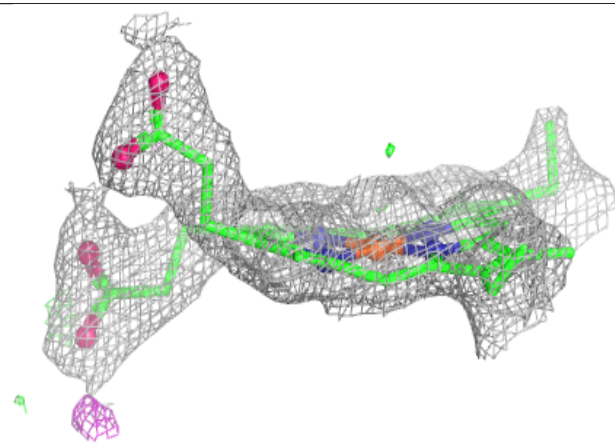
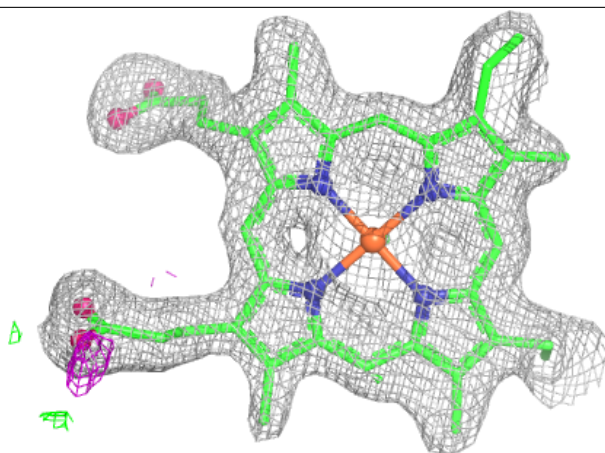
Electron density around P6G F 387:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



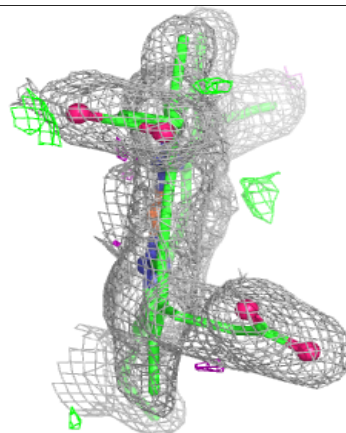
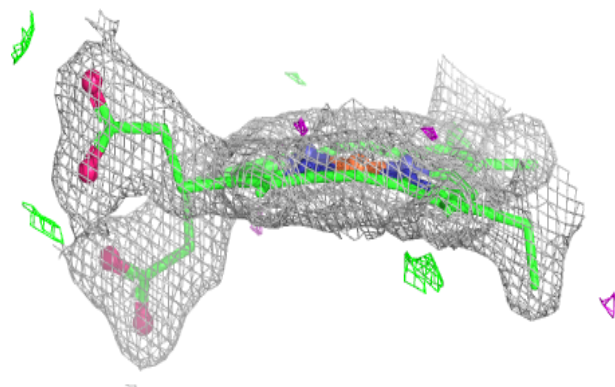
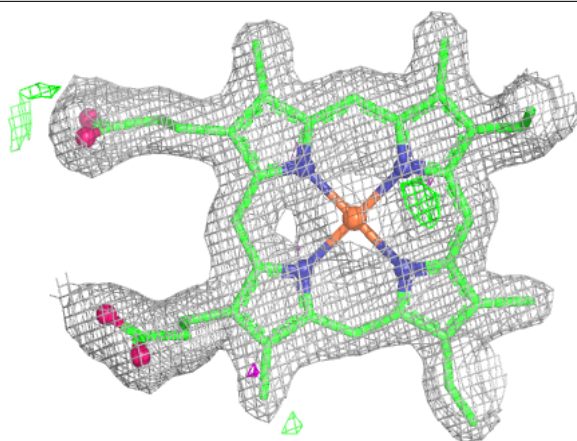
Electron density around HEC A 500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



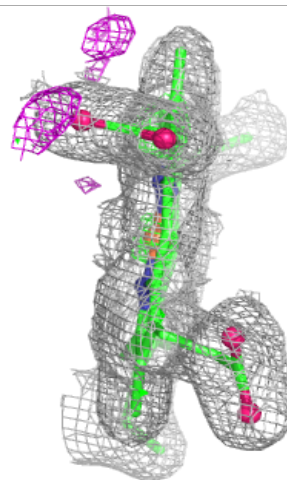
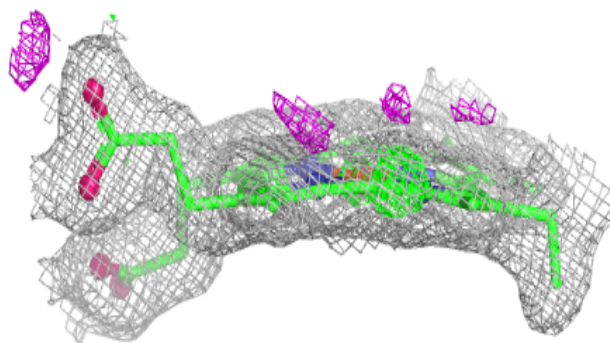
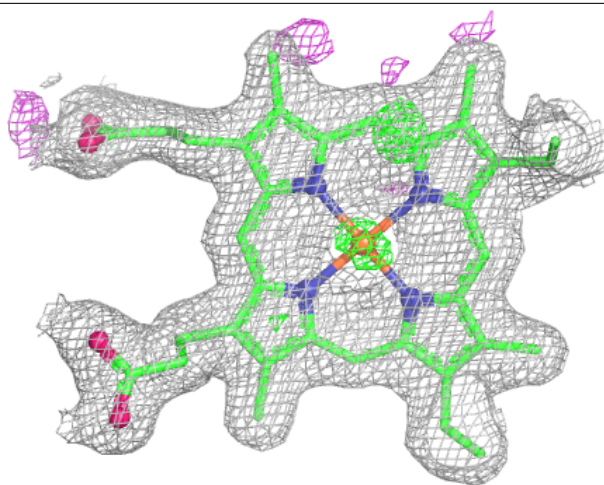
Electron density around HEC B 500:

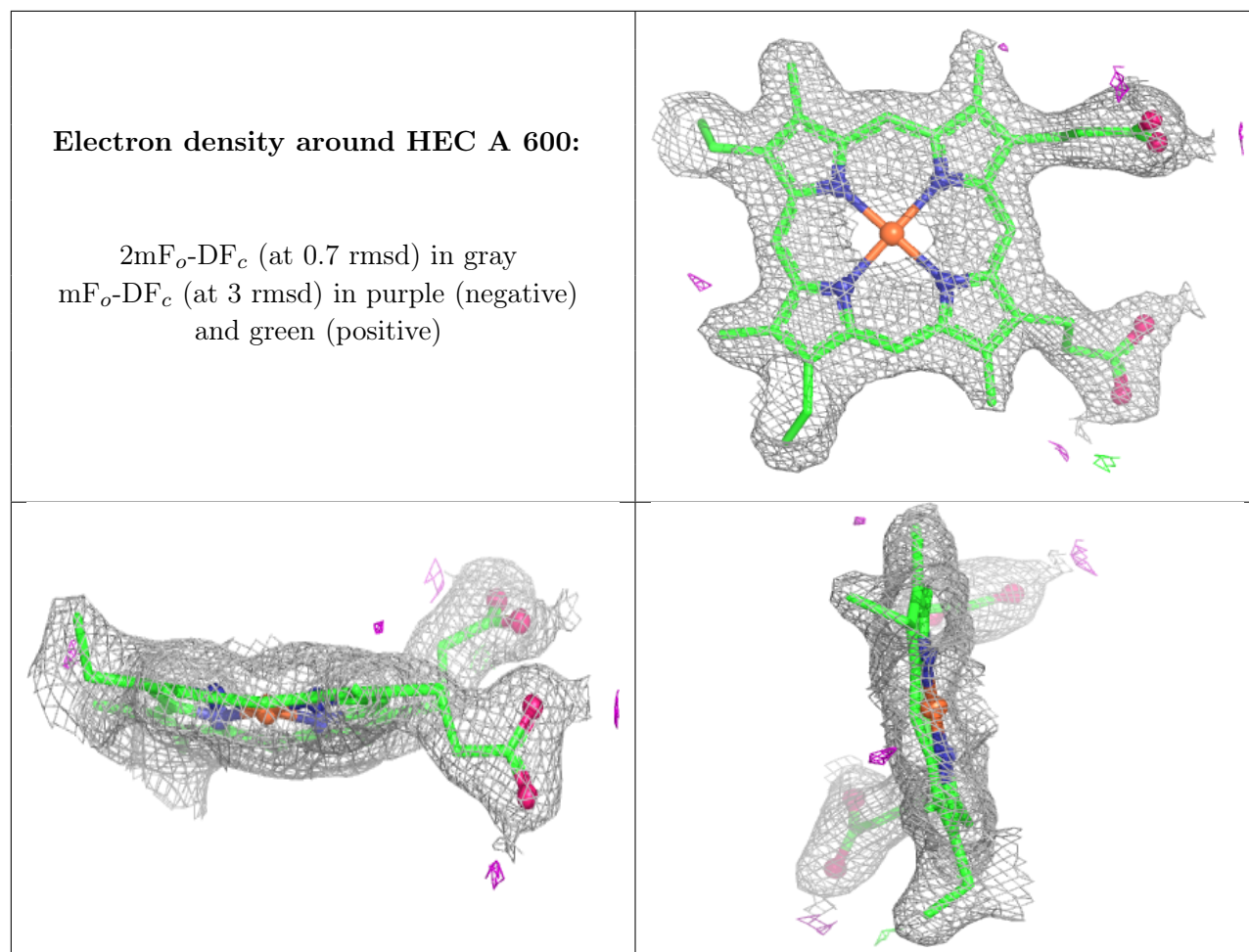
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC B 600:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.