



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:12 AM UTC

PDB ID : 3RUK / pdb_00003ruk
Title : Human Cytochrome P450 CYP17A1 in complex with Abiraterone
Authors : DeVore, N.M.; Scott, E.E.
Deposited on : 2011-05-05
Resolution : 2.60 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

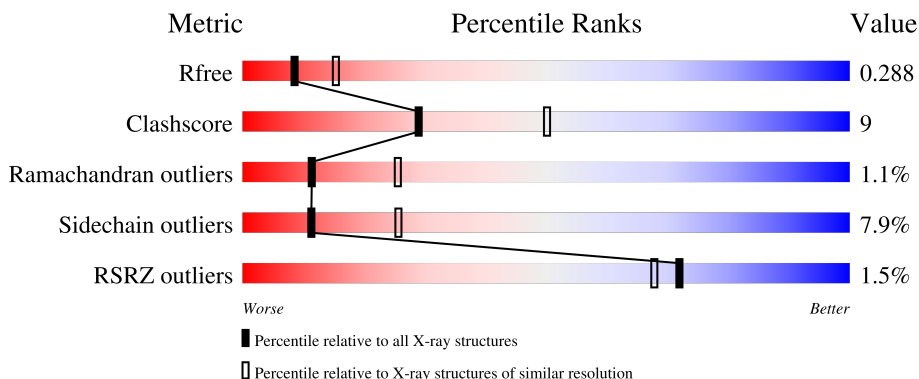
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	494	2% 73% 19% 6%
1	B	494	2% 73% 18% 6%
1	C	494	2% 68% 25% 5%
1	D	494	2% 70% 22% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15332 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 Steroid 17-alpha-hydroxylase/17,20 lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	2	0
			3710	2382	640	673	15			
1	B	465	Total	C	N	O	S	0	0	0
			3708	2380	641	672	15			
1	C	472	Total	C	N	O	S	0	0	0
			3752	2404	650	683	15			
1	D	473	Total	C	N	O	S	0	1	0
			3768	2414	654	685	15			

There are 36 discrepancies between the modelled and reference sequences:

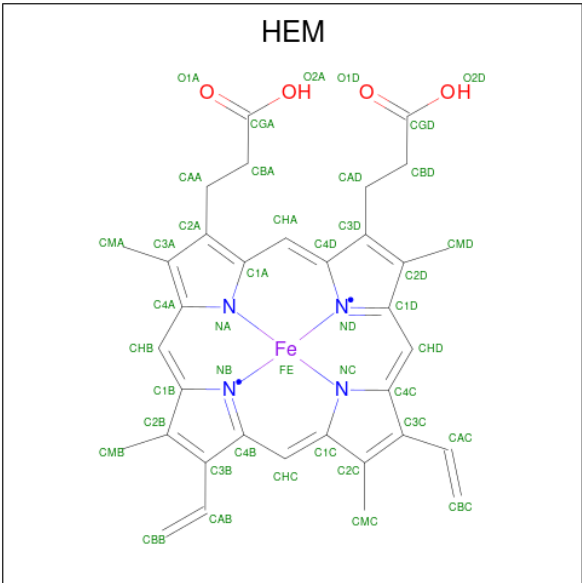
Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	expression tag	UNP P05093
A	20	ALA	-	expression tag	UNP P05093
A	21	LYS	-	expression tag	UNP P05093
A	22	LYS	-	expression tag	UNP P05093
A	23	THR	-	expression tag	UNP P05093
A	509	HIS	-	expression tag	UNP P05093
A	510	HIS	-	expression tag	UNP P05093
A	511	HIS	-	expression tag	UNP P05093
A	512	HIS	-	expression tag	UNP P05093
B	19	MET	-	expression tag	UNP P05093
B	20	ALA	-	expression tag	UNP P05093
B	21	LYS	-	expression tag	UNP P05093
B	22	LYS	-	expression tag	UNP P05093
B	23	THR	-	expression tag	UNP P05093
B	509	HIS	-	expression tag	UNP P05093
B	510	HIS	-	expression tag	UNP P05093
B	511	HIS	-	expression tag	UNP P05093
B	512	HIS	-	expression tag	UNP P05093
C	19	MET	-	expression tag	UNP P05093
C	20	ALA	-	expression tag	UNP P05093
C	21	LYS	-	expression tag	UNP P05093

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Chain	Residue	Modelled	Actual	Comment	Reference
C	22	LYS	-	expression tag	UNP P05093
C	23	THR	-	expression tag	UNP P05093
C	509	HIS	-	expression tag	UNP P05093
C	510	HIS	-	expression tag	UNP P05093
C	511	HIS	-	expression tag	UNP P05093
C	512	HIS	-	expression tag	UNP P05093
D	19	MET	-	expression tag	UNP P05093
D	20	ALA	-	expression tag	UNP P05093
D	21	LYS	-	expression tag	UNP P05093
D	22	LYS	-	expression tag	UNP P05093
D	23	THR	-	expression tag	UNP P05093
D	509	HIS	-	expression tag	UNP P05093
D	510	HIS	-	expression tag	UNP P05093
D	511	HIS	-	expression tag	UNP P05093
D	512	HIS	-	expression tag	UNP P05093

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



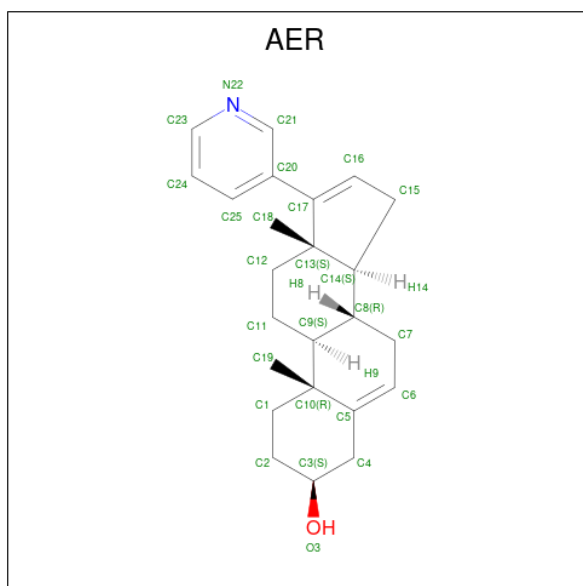
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

- Molecule 3 is Abiraterone (CCD ID: AER) (formula: $C_{24}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	24	1	1		
3	B	1	Total	C	N	O	0	0
			26	24	1	1		
3	C	1	Total	C	N	O	0	0
			26	24	1	1		
3	D	1	Total	C	N	O	0	0
			26	24	1	1		

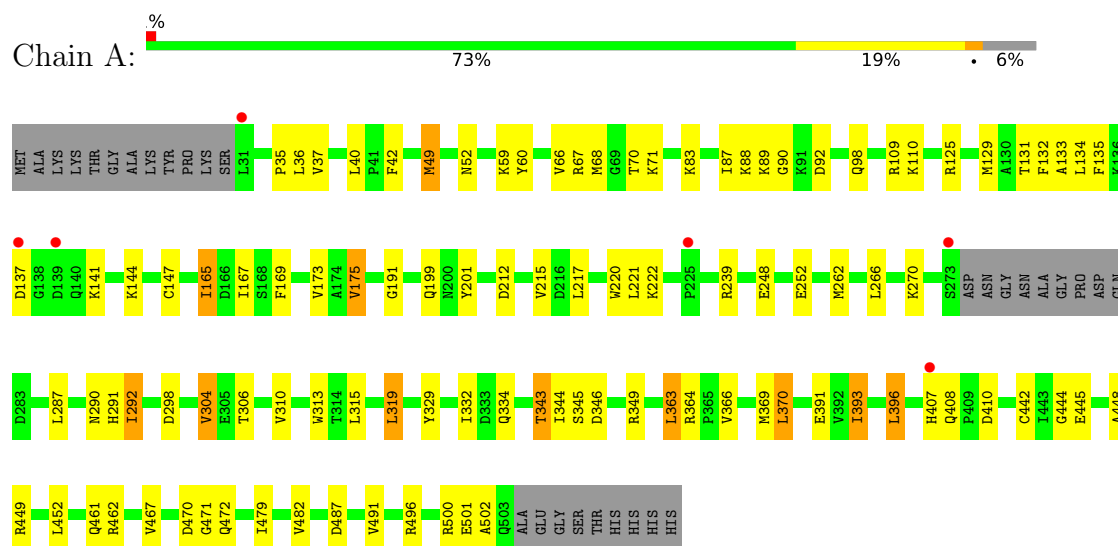
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	43	Total O 43 43	0	0
4	B	22	Total O 22 22	0	0
4	C	23	Total O 23 23	0	0
4	D	30	Total O 30 30	0	0

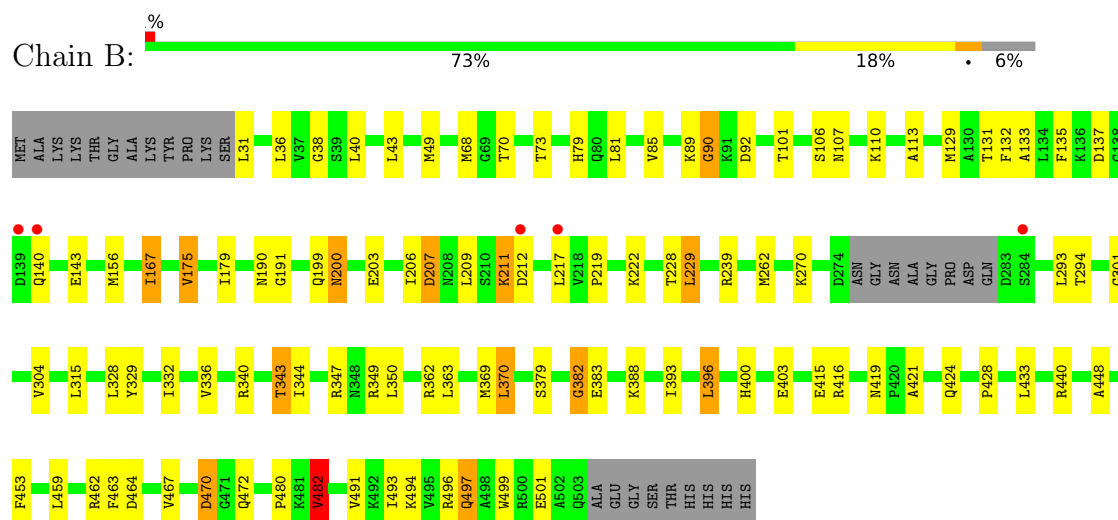
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Steroid 17-alpha-hydroxylase/17,20 lyase

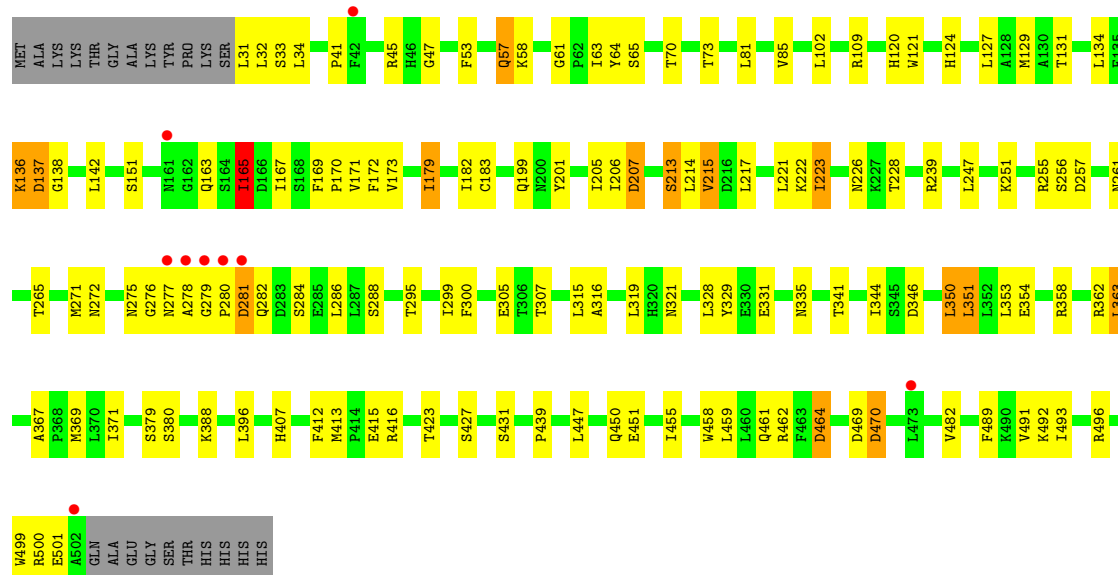


- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

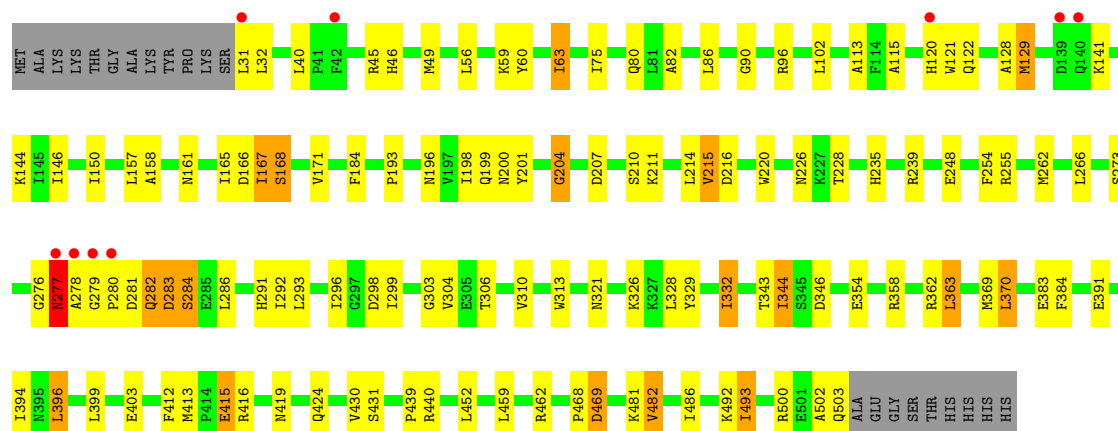


- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase





• Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.81Å 152.10Å 172.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.49 – 2.60 40.49 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.49-2.60) 100.0 (40.49-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.61Å)	Xtriage
Refinement program	REFMAC 6.1.13	Depositor
R, R_{free}	0.218 , 0.291 0.215 , 0.288	Depositor DCC
R_{free} test set	3531 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15332	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.85 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2224e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: AER, HEM

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	1.03	0/3796	1.16	5/5139 (0.1%)
1	B	1.01	3/3788 (0.1%)	1.20	12/5128 (0.2%)
1	C	0.96	1/3834 (0.0%)	1.14	11/5193 (0.2%)
1	D	1.00	3/3854 (0.1%)	1.16	6/5220 (0.1%)
All	All	1.00	7/15272 (0.0%)	1.17	34/20680 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	430	VAL	CA-CB	6.15	1.61	1.54
1	D	332	ILE	CA-CB	5.49	1.61	1.54
1	B	113	ALA	CA-CB	-5.40	1.44	1.53
1	B	70	THR	CA-CB	5.16	1.61	1.53
1	D	304	VAL	CA-CB	-5.07	1.47	1.54
1	B	480	PRO	C-O	-5.01	1.19	1.23
1	C	299	ILE	CA-CB	-5.01	1.48	1.54

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	223	ILE	CB-CA-C	-7.17	102.62	112.02
1	B	212	ASP	N-CA-C	-6.64	96.66	110.80
1	D	277	ASN	N-CA-C	6.51	118.56	109.31
1	B	482	VAL	N-CA-C	-6.41	104.08	110.62
1	B	137	ASP	N-CA-C	6.29	119.93	111.24
1	D	284	SER	N-CA-C	6.29	119.36	111.24
1	C	138	GLY	N-CA-C	-6.19	101.06	111.08
1	C	47	GLY	N-CA-C	6.00	119.58	111.72
1	C	367	ALA	CA-C-N	5.88	125.75	119.28
1	C	367	ALA	C-N-CA	5.88	125.75	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	79	HIS	N-CA-C	5.75	118.32	111.71
1	A	304	VAL	N-CA-C	5.62	116.27	110.82
1	A	109	ARG	N-CA-C	5.53	119.32	112.58
1	C	205	ILE	N-CA-C	5.48	115.62	110.30
1	D	384	PHE	N-CA-C	5.48	118.74	109.76
1	B	382	GLY	N-CA-C	-5.46	100.25	113.18
1	B	200	ASN	N-CA-C	5.38	117.56	111.11
1	A	132	PHE	N-CA-C	5.35	118.60	111.75
1	C	300	PHE	N-CA-C	5.33	116.89	111.14
1	C	57	GLN	N-CA-C	5.32	117.08	111.28
1	D	204	GLY	N-CA-C	5.29	118.64	112.50
1	D	276	GLY	N-CA-C	5.27	120.57	112.51
1	B	206	ILE	CA-C-N	5.21	127.26	120.28
1	B	206	ILE	C-N-CA	5.21	127.26	120.28
1	C	165	ILE	N-CA-C	5.19	117.22	108.81
1	B	453	PHE	N-CA-C	-5.17	105.64	111.28
1	A	147	CYS	N-CA-C	5.13	116.95	111.36
1	C	207	ASP	N-CA-C	5.10	117.74	111.82
1	B	467	VAL	CA-C-N	5.08	125.36	119.92
1	B	467	VAL	C-N-CA	5.08	125.36	119.92
1	C	183	CYS	N-CA-C	5.08	117.60	111.40
1	A	49	MET	N-CA-C	5.03	116.76	111.28
1	D	254	PHE	N-CA-C	5.03	117.59	110.10
1	B	132	PHE	N-CA-C	5.02	117.64	111.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3710	0	3784	67	0
1	B	3708	0	3779	46	0
1	C	3752	0	3814	69	0
1	D	3768	0	3829	85	0
2	A	43	0	30	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	5	0
3	A	26	0	31	4	0
3	B	26	0	31	1	0
3	C	26	0	31	0	0
3	D	26	0	31	2	0
4	A	43	0	0	1	0
4	B	22	0	0	0	0
4	C	23	0	0	1	0
4	D	30	0	0	0	0
All	All	15332	0	15450	265	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 9.

All (265) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:ASN:ND2	1:D:280:PRO:HG2	1.67	1.10
1:D:277:ASN:ND2	1:D:280:PRO:HB2	1.68	1.09
1:D:277:ASN:CG	1:D:280:PRO:HG2	1.78	1.08
1:D:277:ASN:HD21	1:D:280:PRO:HB2	1.25	1.02
1:D:277:ASN:HD22	1:D:277:ASN:H	1.09	0.99
1:D:277:ASN:ND2	1:D:280:PRO:CB	2.29	0.95
1:D:277:ASN:ND2	1:D:280:PRO:CG	2.30	0.94
1:D:277:ASN:ND2	1:D:277:ASN:H	1.52	0.94
1:C:169:PHE:O	1:C:173:VAL:HG23	1.73	0.89
1:A:479:ILE:HD11	1:A:487:ASP:OD1	1.74	0.88
1:D:306:THR:HB	2:D:600:HEM:HBB2	1.56	0.86
1:D:277:ASN:HD21	1:D:280:PRO:CB	1.90	0.85
1:C:120:HIS:CD2	1:C:286:LEU:HD22	2.13	0.83
1:A:125:ARG:O	1:A:129:MET:HG3	1.80	0.82
1:C:275:ASN:O	1:C:277:ASN:N	2.13	0.81
1:D:266:LEU:HD13	1:D:292:ILE:HG23	1.63	0.79
1:D:413:MET:O	1:D:416:ARG:HG2	1.82	0.78
1:A:306:THR:O	1:A:310:VAL:HG23	1.84	0.78
1:A:40:LEU:HD21	1:A:68:MET:HE1	1.68	0.76
1:B:419:ASN:HD21	1:B:421:ALA:HB3	1.51	0.76
1:C:226:ASN:OD1	1:C:228:THR:HG23	1.85	0.75
1:C:354:GLU:O	1:C:358:ARG:HG3	1.84	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:GLY:N	1:D:280:PRO:HD2	2.02	0.75
1:C:470:ASP:HA	4:C:14:HOH:O	1.85	0.75
1:A:407:HIS:O	1:A:408:GLN:HB2	1.85	0.75
1:D:502:ALA:O	1:D:503:GLN:HG2	1.87	0.75
1:D:370:LEU:HD21	1:D:396:LEU:HG	1.69	0.74
1:D:158:ALA:O	1:D:161:ASN:HB2	1.88	0.74
1:D:115:ALA:O	1:D:440:ARG:NH2	2.20	0.73
1:D:277:ASN:O	1:D:281:ASP:HB2	1.89	0.72
1:D:167:ILE:HD12	1:D:171:VAL:HG21	1.71	0.71
2:C:600:HEM:HHD	2:C:600:HEM:HBC2	1.74	0.70
1:D:419:ASN:ND2	1:D:424:GLN:HG2	2.07	0.70
1:A:141:LYS:HB3	1:A:144:LYS:HG3	1.75	0.69
1:A:167:ILE:HD11	1:A:315:LEU:HD12	1.74	0.68
1:D:167:ILE:HD12	1:D:171:VAL:CG2	2.23	0.68
1:C:315:LEU:O	1:C:319:LEU:HD13	1.94	0.67
1:B:209:LEU:HD23	1:B:482:VAL:HG21	1.75	0.67
1:A:445:GLU:O	1:A:449:ARG:HG3	1.94	0.67
1:D:277:ASN:ND2	1:D:277:ASN:N	2.29	0.66
1:A:500:ARG:C	1:A:502:ALA:H	2.03	0.65
1:A:461:GLN:O	1:A:496:ARG:HD3	1.96	0.65
1:A:40:LEU:CD2	1:A:68:MET:HE1	2.25	0.65
1:D:277:ASN:HD22	1:D:277:ASN:N	1.81	0.65
1:D:281:ASP:O	1:D:283:ASP:N	2.30	0.65
1:D:157:LEU:HD22	1:D:493:ILE:HD13	1.78	0.65
1:D:279:GLY:H	1:D:280:PRO:HD2	1.61	0.64
1:D:362:ARG:NH2	1:D:363:LEU:HG	2.11	0.64
1:D:440:ARG:NH1	2:D:600:HEM:O2D	2.31	0.64
1:D:226:ASN:OD1	1:D:228:THR:HG23	1.97	0.64
1:A:319:LEU:HD21	1:A:491:VAL:HG12	1.81	0.63
1:A:370:LEU:HD21	1:A:396:LEU:HG	1.80	0.62
1:C:455:ILE:O	1:C:459:LEU:HD13	2.00	0.62
1:C:277:ASN:O	1:C:279:GLY:N	2.29	0.61
1:C:120:HIS:CD2	1:C:286:LEU:CD2	2.84	0.61
1:D:196:ASN:O	1:D:200:ASN:HB2	2.01	0.61
1:A:201:TYR:CE1	1:A:239:ARG:HG2	2.36	0.61
1:C:277:ASN:C	1:C:279:GLY:H	2.07	0.61
1:D:279:GLY:N	1:D:280:PRO:CD	2.64	0.60
1:A:462:ARG:O	1:A:496:ARG:HG3	2.01	0.60
1:A:366:VAL:HG21	2:A:600:HEM:HMB2	1.84	0.60
2:A:600:HEM:C1D	3:A:601:AER:H21	2.37	0.60
1:C:136:LYS:O	1:C:137:ASP:HB3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:ASP:OD2	1:B:472:GLN:HB2	2.03	0.58
1:A:442:CYS:SG	2:A:600:HEM:NC	2.76	0.58
1:D:310:VAL:HG11	1:D:452:LEU:HD13	1.85	0.58
1:B:497:GLN:OE1	1:B:497:GLN:HA	2.04	0.58
2:A:600:HEM:HBB2	2:A:600:HEM:CMB	2.34	0.58
1:C:167:ILE:HD11	1:C:315:LEU:HD12	1.86	0.58
1:C:53:PHE:O	1:C:64:TYR:OH	2.22	0.57
1:B:38:GLY:HA3	1:D:40:LEU:HD23	1.87	0.57
1:B:362:ARG:HA	1:B:400:HIS:HD1	1.69	0.57
1:C:201:TYR:CE1	1:C:239:ARG:HG2	2.39	0.57
1:D:328:LEU:O	1:D:332:ILE:HG22	2.04	0.57
1:C:167:ILE:O	1:C:171:VAL:HG23	2.05	0.57
1:A:442:CYS:SG	2:A:600:HEM:NB	2.78	0.56
1:B:332:ILE:HA	1:B:350:LEU:HD21	1.88	0.56
1:A:366:VAL:CG2	2:A:600:HEM:HMB2	2.36	0.56
1:A:169:PHE:O	1:A:173:VAL:HG23	2.06	0.56
1:A:175:VAL:HG23	1:A:304:VAL:HA	1.87	0.56
1:C:214:LEU:O	1:C:215:VAL:HG22	2.05	0.56
1:A:133:ALA:C	1:A:135:PHE:H	2.15	0.55
1:A:67:ARG:HH21	1:C:41:PRO:HA	1.71	0.55
1:D:96:ARG:CZ	1:D:440:ARG:HD3	2.37	0.55
1:D:419:ASN:HD22	1:D:424:GLN:HG2	1.72	0.55
1:B:362:ARG:NH2	1:B:363:LEU:HG	2.22	0.54
1:D:214:LEU:O	1:D:215:VAL:HG22	2.07	0.54
1:B:40:LEU:HD21	1:B:68:MET:HE1	1.89	0.54
1:A:442:CYS:SG	2:A:600:HEM:NA	2.80	0.54
1:D:113:ALA:HA	2:D:600:HEM:HAD1	1.88	0.54
1:D:128:ALA:HA	1:D:262:MET:HE2	1.90	0.54
1:D:303:GLY:HA2	2:D:600:HEM:HMC3	1.89	0.54
1:B:362:ARG:HA	1:B:400:HIS:ND1	2.23	0.54
1:A:220:TRP:HB3	1:C:223:ILE:CG2	2.38	0.54
1:A:165:ILE:HD12	1:A:167:ILE:HG22	1.90	0.53
3:A:601:AER:H25	3:A:601:AER:H18B	1.89	0.53
1:A:212:ASP:HB3	4:A:550:HOH:O	2.07	0.53
1:C:413:MET:O	1:C:416:ARG:HD2	2.09	0.53
1:B:419:ASN:ND2	1:B:421:ALA:H	2.07	0.53
1:D:468:PRO:HA	1:D:492:LYS:HB2	1.90	0.53
2:A:600:HEM:HMB2	2:A:600:HEM:HBB2	1.90	0.53
1:A:266:LEU:HB3	1:A:292:ILE:HG12	1.90	0.53
1:A:35:PRO:HG2	1:C:63:ILE:O	2.09	0.53
1:D:146:ILE:HG22	1:D:150:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:ASP:OD1	1:B:496:ARG:HG2	2.10	0.52
1:D:120[A]:HIS:CD2	1:D:286:LEU:HD22	2.44	0.52
1:D:165:ILE:HD12	1:D:167:ILE:HG22	1.91	0.52
1:C:201:TYR:CE1	1:C:239:ARG:CG	2.92	0.52
1:C:496:ARG:HB2	1:C:499:TRP:HB2	1.90	0.52
1:B:203:GLU:O	1:B:207:ASP:HB2	2.10	0.52
1:C:121:TRP:HZ2	1:C:439:PRO:O	1.91	0.52
1:D:141:LYS:HB3	1:D:144:LYS:HG3	1.90	0.52
1:C:206:ILE:HD11	1:C:305:GLU:HG3	1.92	0.52
1:B:49:MET:HE1	1:B:217:LEU:HG	1.91	0.51
1:C:65:SER:HA	1:C:73:THR:O	2.10	0.51
1:C:81:LEU:O	1:C:85:VAL:HG23	2.10	0.51
1:D:370:LEU:CD2	1:D:396:LEU:HG	2.40	0.51
1:A:67:ARG:NH2	1:C:41:PRO:HB3	2.25	0.51
1:C:163:GLN:O	1:C:492:LYS:HA	2.11	0.50
1:C:328:LEU:HD22	1:C:353:LEU:HD13	1.93	0.50
1:D:354:GLU:O	1:D:358:ARG:HG3	2.11	0.50
1:A:369:MET:O	1:A:370:LEU:C	2.55	0.50
1:C:169:PHE:HB3	1:C:170:PRO:HD3	1.93	0.50
1:A:370:LEU:CD2	1:A:396:LEU:HG	2.42	0.50
1:D:120[B]:HIS:CE1	1:D:291:HIS:ND1	2.80	0.50
1:D:198:ILE:HA	1:D:201:TYR:CE2	2.47	0.50
1:A:500:ARG:O	1:A:502:ALA:N	2.44	0.50
1:B:440:ARG:NH1	2:B:600:HEM:O2D	2.36	0.50
1:D:121:TRP:O	1:D:122:GLN:C	2.55	0.49
1:B:239:ARG:C	1:B:239:ARG:HD2	2.37	0.49
1:A:66:VAL:CG1	1:A:68:MET:HE3	2.42	0.49
1:D:166:ASP:OD1	1:D:168:SER:OG	2.31	0.49
1:A:407:HIS:O	1:A:407:HIS:CG	2.66	0.49
1:C:362:ARG:NH2	1:C:363:LEU:HG	2.27	0.49
1:D:63:ILE:HA	1:D:75:ILE:O	2.12	0.49
1:C:255:ARG:NH2	1:C:257:ASP:OD1	2.45	0.49
1:A:59:LYS:HD3	1:A:60:TYR:CZ	2.48	0.48
1:C:407:HIS:O	1:C:416:ARG:NH2	2.46	0.48
1:D:45:ARG:O	1:D:46:HIS:HB2	2.13	0.48
1:A:66:VAL:HG11	1:A:217:LEU:HD11	1.94	0.48
1:D:211:LYS:HB2	1:D:220:TRP:HZ3	1.78	0.48
1:B:328:LEU:O	1:B:332:ILE:HG22	2.13	0.48
1:C:341:THR:HB	1:C:458:TRP:CZ2	2.48	0.48
1:B:167:ILE:HD11	1:B:315:LEU:HD12	1.95	0.48
1:C:461:GLN:O	1:C:461:GLN:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LEU:O	1:A:364:ARG:HD3	2.12	0.48
1:B:81:LEU:O	1:B:85:VAL:HG23	2.13	0.48
1:C:201:TYR:CZ	1:C:239:ARG:HG2	2.49	0.48
1:C:371:ILE:HD12	2:C:600:HEM:HAA1	1.95	0.48
1:A:89:LYS:HG2	1:A:92:ASP:OD2	2.13	0.48
1:A:500:ARG:C	1:A:502:ALA:N	2.72	0.48
1:C:379:SER:OG	1:C:380:SER:N	2.43	0.48
1:A:444:GLY:HA3	2:A:600:HEM:C3C	2.49	0.47
1:B:396:LEU:HD21	1:B:433:LEU:HB2	1.96	0.47
1:D:282:GLN:C	1:D:284:SER:H	2.22	0.47
1:C:165:ILE:HD12	1:C:167:ILE:HG22	1.95	0.47
1:A:408:GLN:HE22	1:D:193:PRO:HD3	1.79	0.47
1:C:329:TYR:OH	1:C:464:ASP:HA	2.14	0.47
1:D:226:ASN:CG	1:D:228:THR:HG23	2.40	0.47
1:A:110:LYS:HD3	1:A:291:HIS:CD2	2.50	0.47
1:A:167:ILE:HD11	1:A:315:LEU:CD1	2.43	0.47
1:B:496:ARG:O	1:B:497:GLN:C	2.58	0.47
1:C:131:THR:HG22	1:C:131:THR:O	2.14	0.47
1:D:216:ASP:HB3	1:D:391:GLU:OE1	2.14	0.47
1:B:143:GLU:OE2	1:B:343:THR:HB	2.14	0.47
1:C:179:ILE:HD12	1:C:179:ILE:HA	1.74	0.47
1:D:210:SER:O	1:D:481:LYS:NZ	2.44	0.46
1:C:58:LYS:HE3	1:C:58:LYS:HB2	1.74	0.46
1:C:272:ASN:O	1:C:277:ASN:CB	2.63	0.46
1:D:201:TYR:CE1	1:D:239:ARG:HG2	2.51	0.46
1:A:407:HIS:O	1:A:408:GLN:CB	2.59	0.46
1:C:331:GLU:O	1:C:335:ASN:HB2	2.16	0.46
1:D:399:LEU:O	1:D:431:SER:OG	2.32	0.46
1:A:462:ARG:C	1:A:496:ARG:HG3	2.41	0.46
1:D:502:ALA:C	1:D:503:GLN:HG2	2.40	0.46
1:A:175:VAL:CG2	1:A:304:VAL:HA	2.46	0.46
1:C:319:LEU:HD21	1:C:491:VAL:HG12	1.97	0.46
1:A:270:LYS:HD3	1:A:287:LEU:HB2	1.98	0.45
1:A:37:VAL:HG22	1:C:65:SER:O	2.16	0.45
1:D:313:TRP:CE3	1:D:486:ILE:HD12	2.51	0.45
1:D:415:GLU:H	1:D:415:GLU:CD	2.25	0.45
1:A:191:GLY:HA3	1:B:191:GLY:CA	2.47	0.45
1:B:463:PHE:C	1:B:496:ARG:HG3	2.41	0.45
1:B:329:TYR:CD1	1:B:496:ARG:NH1	2.85	0.45
1:C:172:PHE:CD2	1:C:172:PHE:C	2.95	0.45
1:C:124:HIS:ND1	1:C:295:THR:OG1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:462:ARG:C	1:C:496:ARG:HG3	2.42	0.44
1:A:66:VAL:CG1	1:A:68:MET:CE	2.96	0.44
1:B:107:ASN:O	1:B:110:LYS:HG3	2.17	0.44
1:B:464:ASP:CG	1:B:496:ARG:HG2	2.43	0.44
1:D:262:MET:SD	1:D:299:ILE:HG13	2.57	0.44
1:C:321:ASN:ND2	1:C:412:PHE:CD2	2.85	0.44
1:D:343:THR:O	1:D:346:ASP:HB2	2.17	0.44
1:B:448:ALA:HB2	2:B:600:HEM:HMC2	1.98	0.44
1:B:133:ALA:C	1:B:135:PHE:H	2.26	0.44
1:A:298:ASP:HA	3:A:601:AER:H7	2.00	0.43
1:B:131:THR:HG21	1:B:262:MET:HB2	2.00	0.43
1:C:500:ARG:C	1:C:501:GLU:OE1	2.60	0.43
1:D:90:GLY:C	1:D:439:PRO:HG2	2.43	0.43
1:C:182:ILE:O	1:C:261:ASN:HB2	2.18	0.43
1:D:129:MET:HE2	1:D:129:MET:HA	2.00	0.43
1:A:66:VAL:HG11	1:A:68:MET:HE3	2.00	0.43
1:D:363:LEU:HD11	1:D:412:PHE:HA	2.01	0.43
1:C:127:LEU:HD22	1:C:265:THR:HG22	1.99	0.43
1:C:307:THR:HG21	1:C:451:GLU:OE1	2.19	0.43
1:D:326:LYS:HA	1:D:329:TYR:HD2	1.82	0.43
1:A:407:HIS:O	1:A:407:HIS:CD2	2.71	0.43
1:D:56:LEU:HD22	1:D:60:TYR:HD2	1.82	0.42
1:D:214:LEU:HD11	1:D:482:VAL:HG12	2.00	0.42
1:A:313:TRP:CZ3	1:A:364:ARG:HG3	2.54	0.42
1:A:448:ALA:O	1:A:452:LEU:HG	2.18	0.42
1:A:343:THR:O	1:A:346:ASP:HB2	2.19	0.42
1:C:142:LEU:HD11	1:C:447:LEU:HD13	2.00	0.42
1:B:301:GLY:HA3	3:B:601:AER:H7	2.01	0.42
1:D:298:ASP:HA	3:D:601:AER:H7	2.02	0.42
1:B:89:LYS:O	1:B:90:GLY:C	2.63	0.42
1:B:219:PRO:HB2	1:B:222:LYS:HD3	2.00	0.42
1:D:201:TYR:CE1	1:D:239:ARG:CG	3.02	0.42
1:C:346:ASP:O	1:C:350:LEU:HB2	2.19	0.42
2:A:600:HEM:ND	3:A:601:AER:H21	2.32	0.42
1:D:129:MET:HA	1:D:129:MET:CE	2.50	0.42
1:A:83:LYS:HG2	1:A:87:ILE:HD12	2.02	0.42
1:A:220:TRP:CG	1:C:223:ILE:HG23	2.55	0.42
1:A:391:GLU:HG2	1:A:393:ILE:HD12	2.01	0.41
1:B:156:MET:SD	1:B:190:ASN:ND2	2.93	0.41
1:B:462:ARG:HD2	1:B:499:TRP:CE2	2.55	0.41
1:C:275:ASN:C	1:C:277:ASN:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:ALA:HB2	1:C:489:PHE:CZ	2.55	0.41
1:C:213:SER:HB2	1:C:369:MET:HE3	2.02	0.41
1:C:462:ARG:O	1:C:462:ARG:HG2	2.20	0.41
1:B:369:MET:O	1:B:370:LEU:C	2.63	0.41
1:C:281:ASP:OD2	1:C:281:ASP:C	2.63	0.41
1:D:500:ARG:O	1:D:502:ALA:O	2.38	0.41
1:B:416:ARG:O	1:B:428:PRO:HG3	2.19	0.41
1:A:42:PHE:CD2	1:A:52:ASN:HB3	2.56	0.41
1:A:329:TYR:O	1:A:332:ILE:HG22	2.20	0.41
1:B:464:ASP:HB2	1:B:494:LYS:HB2	2.03	0.41
1:C:344:ILE:HD12	1:C:450:GLN:HG2	2.03	0.41
1:D:273:SER:HB2	1:D:281:ASP:O	2.20	0.41
1:D:86:LEU:HD21	1:D:394:ILE:HG13	2.01	0.41
1:D:299:ILE:HG23	2:D:600:HEM:HBC1	2.02	0.41
1:A:344:ILE:HD13	1:A:344:ILE:HA	1.98	0.41
1:C:57:GLN:HG2	1:C:61:GLY:O	2.20	0.41
1:B:336:VAL:HG13	1:B:340:ARG:NH1	2.35	0.41
1:D:204:GLY:HA3	1:D:235:HIS:CD2	2.56	0.41
1:B:73:THR:CG2	1:B:393:ILE:HD12	2.50	0.41
1:B:106:SER:O	1:B:294:THR:HG21	2.21	0.41
1:B:382:GLY:O	1:B:383:GLU:HG2	2.20	0.41
1:D:344:ILE:HD13	1:D:344:ILE:HA	1.94	0.41
1:D:462:ARG:O	1:D:462:ARG:HG3	2.16	0.41
1:A:131:THR:HG21	1:A:262:MET:HB2	2.02	0.40
1:B:211:LYS:C	1:B:211:LYS:HD3	2.47	0.40
1:B:315:LEU:HD23	1:B:315:LEU:HA	1.93	0.40
1:C:351:LEU:H	1:C:351:LEU:HG	1.73	0.40
1:D:167:ILE:HD12	1:D:171:VAL:HG23	2.03	0.40
1:A:363:LEU:HD22	1:A:364:ARG:NH1	2.35	0.40
1:B:229:LEU:HD12	1:B:229:LEU:HA	1.95	0.40
1:D:82:ALA:O	1:D:86:LEU:HG	2.22	0.40
1:D:281:ASP:O	1:D:282:GLN:C	2.63	0.40
1:B:175:VAL:HG23	1:B:304:VAL:HA	2.02	0.40
1:C:271:MET:HE2	1:C:271:MET:HB3	1.83	0.40
1:C:272:ASN:O	1:C:277:ASN:HB3	2.21	0.40
3:D:601:AER:H25	3:D:601:AER:H18B	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	462/494 (94%)	424 (92%)	32 (7%)	6 (1%)	9	21
1	B	461/494 (93%)	432 (94%)	26 (6%)	3 (1%)	18	38
1	C	470/494 (95%)	423 (90%)	40 (8%)	7 (2%)	8	18
1	D	472/494 (96%)	436 (92%)	31 (7%)	5 (1%)	11	25
All	All	1865/1976 (94%)	1715 (92%)	129 (7%)	21 (1%)	11	25

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	GLU
1	C	276	GLY
1	C	278	ALA
1	C	280	PRO
1	D	282	GLN
1	A	134	LEU
1	A	370	LEU
1	A	471	GLY
1	C	284	SER
1	C	415	GLU
1	D	469	ASP
1	C	137	ASP
1	C	288	SER
1	D	278	ALA
1	D	283	ASP
1	D	370	LEU
1	B	370	LEU
1	B	497	GLN
1	B	90	GLY
1	A	90	GLY
1	A	215	VAL

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	416/436 (95%)	388 (93%)	28 (7%)	15	33
1	B	415/436 (95%)	381 (92%)	34 (8%)	10	24
1	C	419/436 (96%)	380 (91%)	39 (9%)	8	18
1	D	421/436 (97%)	390 (93%)	31 (7%)	13	29
All	All	1671/1744 (96%)	1539 (92%)	132 (8%)	11	26

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	49	MET
1	A	70	THR
1	A	71	LYS
1	A	88	LYS
1	A	98	GLN
1	A	137[A]	ASP
1	A	137[B]	ASP
1	A	165	ILE
1	A	175	VAL
1	A	199	GLN
1	A	221	LEU
1	A	222	LYS
1	A	248	GLU
1	A	252	GLU
1	A	290	ASN
1	A	292	ILE
1	A	319	LEU
1	A	334	GLN
1	A	343	THR
1	A	345	SER
1	A	349	ARG
1	A	363	LEU
1	A	393	ILE

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Mol	Chain	Res	Type
1	A	396	LEU
1	A	410	ASP
1	A	467	VAL
1	A	482	VAL
1	B	31	LEU
1	B	36	LEU
1	B	43	LEU
1	B	92	ASP
1	B	101	THR
1	B	129	MET
1	B	140	GLN
1	B	167	ILE
1	B	175	VAL
1	B	179	ILE
1	B	199	GLN
1	B	200	ASN
1	B	207	ASP
1	B	211	LYS
1	B	228	THR
1	B	229	LEU
1	B	270	LYS
1	B	293	LEU
1	B	343	THR
1	B	344	ILE
1	B	347	ARG
1	B	349	ARG
1	B	379	SER
1	B	388	LYS
1	B	396	LEU
1	B	403	GLU
1	B	415	GLU
1	B	424	GLN
1	B	459	LEU
1	B	470	ASP
1	B	482	VAL
1	B	491	VAL
1	B	493	ILE
1	B	501	GLU
1	C	31	LEU
1	C	32	LEU
1	C	33	SER
1	C	34	LEU

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Mol	Chain	Res	Type
1	C	45	ARG
1	C	70	THR
1	C	102	LEU
1	C	109	ARG
1	C	129	MET
1	C	134	LEU
1	C	136	LYS
1	C	151	SER
1	C	165	ILE
1	C	179	ILE
1	C	199	GLN
1	C	207	ASP
1	C	213	SER
1	C	215	VAL
1	C	217	LEU
1	C	221	LEU
1	C	222	LYS
1	C	247	LEU
1	C	251	LYS
1	C	256	SER
1	C	281	ASP
1	C	282	GLN
1	C	350	LEU
1	C	351	LEU
1	C	363	LEU
1	C	388	LYS
1	C	396	LEU
1	C	423	THR
1	C	427	SER
1	C	431	SER
1	C	464	ASP
1	C	469	ASP
1	C	470	ASP
1	C	482	VAL
1	C	493	ILE
1	D	31	LEU
1	D	32	LEU
1	D	49	MET
1	D	59	LYS
1	D	63	ILE
1	D	80	GLN
1	D	102	LEU

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Mol	Chain	Res	Type
1	D	129	MET
1	D	167	ILE
1	D	168	SER
1	D	184	PHE
1	D	199	GLN
1	D	207	ASP
1	D	215	VAL
1	D	248	GLU
1	D	255	ARG
1	D	277	ASN
1	D	293	LEU
1	D	296	ILE
1	D	321	ASN
1	D	344	ILE
1	D	363	LEU
1	D	369	MET
1	D	383	GLU
1	D	396	LEU
1	D	403	GLU
1	D	415	GLU
1	D	459	LEU
1	D	469	ASP
1	D	482	VAL
1	D	493	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	120	HIS
1	A	407	HIS
1	A	408	GLN
1	B	46	HIS
1	B	78	HIS
1	B	98	GLN
1	B	472	GLN
1	C	107	ASN
1	C	208	ASN
1	C	240	ASN
1	C	249	ASN
1	D	57	GLN
1	D	200	ASN

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Mol	Chain	Res	Type
1	D	235	HIS
1	D	277	ASN
1	D	401	HIS
1	D	497	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 ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	D	600	1,3	50,50,50	1.97	9 (18%)	67,82,82	1.47	11 (16%)
2	HEM	A	600	1,3	50,50,50	2.10	9 (18%)	67,82,82	1.65	14 (20%)
3	AER	C	601	2	30,30,30	2.14	2 (6%)	47,47,47	2.46	13 (27%)
3	AER	B	601	2	30,30,30	2.20	3 (10%)	47,47,47	2.20	13 (27%)
3	AER	A	601	2	30,30,30	2.37	3 (10%)	47,47,47	2.48	15 (31%)
3	AER	D	601	2	30,30,30	2.45	5 (16%)	47,47,47	2.28	12 (25%)
2	HEM	C	600	1,3	50,50,50	2.11	9 (18%)	67,82,82	1.62	12 (17%)
2	HEM	B	600	1,3	50,50,50	2.35	11 (22%)	67,82,82	2.11	19 (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	HEM	D	600	1,3	-	4/14/54/54	-
2	HEM	A	600	1,3	-	2/14/54/54	-
3	AER	C	601	2	-	0/4/62/62	0/5/5/5
3	AER	B	601	2	-	0/4/62/62	0/5/5/5
3	AER	A	601	2	-	0/4/62/62	0/5/5/5
3	AER	D	601	2	-	0/4/62/62	0/5/5/5
2	HEM	C	600	1,3	-	4/14/54/54	-
2	HEM	B	600	1,3	-	0/14/54/54	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	AER	C16-C17	11.30	1.52	1.33
3	D	601	AER	C16-C17	11.23	1.52	1.33
3	C	601	AER	C16-C17	10.67	1.51	1.33
3	B	601	AER	C16-C17	10.54	1.51	1.33
2	B	600	HEM	FE-ND	9.00	2.22	1.94
2	C	600	HEM	C3D-C2D	7.56	1.53	1.36
2	A	600	HEM	C3D-C2D	7.54	1.53	1.36
2	C	600	HEM	FE-NB	7.44	2.17	1.94
2	D	600	HEM	C3D-C2D	7.43	1.52	1.36
2	B	600	HEM	C3D-C2D	7.39	1.52	1.36
2	A	600	HEM	FE-ND	7.16	2.16	1.94
2	B	600	HEM	FE-NB	6.42	2.14	1.94
2	C	600	HEM	FE-ND	5.59	2.12	1.94
2	D	600	HEM	FE-NB	5.34	2.11	1.94
2	D	600	HEM	FE-ND	4.63	2.09	1.94
3	A	601	AER	C13-C17	-4.59	1.49	1.53
2	A	600	HEM	FE-NB	3.99	2.07	1.94
3	D	601	AER	C10-C9	-3.69	1.50	1.56
3	D	601	AER	C20-C17	3.58	1.53	1.48
3	B	601	AER	C13-C17	-3.47	1.50	1.53
2	B	600	HEM	CMC-C2C	3.40	1.57	1.50
2	A	600	HEM	CMB-C2B	3.35	1.57	1.50
2	A	600	HEM	CMC-C2C	3.35	1.57	1.50
2	D	600	HEM	FE-NC	3.32	2.06	1.95
2	D	600	HEM	CAC-C3C	3.15	1.55	1.47
2	B	600	HEM	FE-NA	3.12	2.05	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	HEM	CMB-C2B	3.11	1.57	1.50
2	B	600	HEM	CMA-C3A	2.98	1.56	1.50
2	C	600	HEM	CAC-C3C	2.97	1.55	1.47
2	B	600	HEM	CAB-C3B	2.93	1.55	1.47
2	D	600	HEM	CAB-C3B	2.87	1.55	1.47
2	A	600	HEM	CAC-C3C	2.76	1.54	1.47
3	B	601	AER	C20-C17	2.76	1.52	1.48
2	B	600	HEM	CAC-C3C	2.64	1.54	1.47
2	A	600	HEM	CAB-C3B	2.61	1.54	1.47
2	A	600	HEM	FE-NC	2.61	2.03	1.95
2	D	600	HEM	CMA-C3A	2.59	1.56	1.50
2	B	600	HEM	CAD-C3D	2.58	1.58	1.51
2	C	600	HEM	CMC-C2C	2.56	1.56	1.50
2	B	600	HEM	CMB-C2B	2.53	1.56	1.50
2	C	600	HEM	CAB-C3B	2.53	1.54	1.47
2	B	600	HEM	FE-NC	2.45	2.03	1.95
2	A	600	HEM	CMA-C3A	2.41	1.55	1.50
2	C	600	HEM	CMB-C2B	2.40	1.55	1.50
3	A	601	AER	C20-C17	2.36	1.51	1.48
2	D	600	HEM	CMC-C2C	2.28	1.55	1.50
3	D	601	AER	C15-C16	2.18	1.53	1.50
2	C	600	HEM	CMA-C3A	2.17	1.55	1.50
3	D	601	AER	C13-C17	-2.10	1.51	1.53
2	C	600	HEM	C1B-NB	-2.03	1.36	1.40
3	C	601	AER	C13-C17	-2.00	1.52	1.53

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	AER	C15-C16-C17	-11.31	102.75	112.56
3	B	601	AER	C15-C16-C17	-10.27	103.65	112.56
3	C	601	AER	C15-C16-C17	-9.17	104.60	112.56
3	C	601	AER	C15-C14-C13	8.65	110.10	104.05
3	D	601	AER	C15-C14-C13	8.13	109.74	104.05
3	D	601	AER	C15-C16-C17	-7.56	106.00	112.56
2	B	600	HEM	C4D-ND-C1D	7.13	113.65	105.21
2	C	600	HEM	C4D-ND-C1D	6.32	112.69	105.21
2	A	600	HEM	C4D-ND-C1D	5.79	112.06	105.21
2	B	600	HEM	C3B-C4B-NB	-5.28	105.67	109.47
2	B	600	HEM	CHC-C1C-NC	4.88	129.76	124.45
2	B	600	HEM	C1B-NB-C4B	4.46	110.49	105.21
2	D	600	HEM	C4D-ND-C1D	4.40	110.42	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	HEM	C1B-NB-C4B	4.37	110.38	105.21
3	D	601	AER	C18-C13-C14	4.33	119.20	112.99
3	A	601	AER	C4-C5-C10	4.26	121.88	116.42
3	C	601	AER	C14-C8-C9	-4.25	103.54	109.09
2	D	600	HEM	C3B-C4B-NB	-4.24	106.42	109.47
3	C	601	AER	C1-C2-C3	4.16	115.99	110.48
3	A	601	AER	C4-C5-C6	-4.14	114.95	120.57
2	B	600	HEM	CAA-CBA-CGA	-4.07	102.86	113.67
3	A	601	AER	C15-C14-C13	3.86	106.75	104.05
2	D	600	HEM	CAA-CBA-CGA	-3.81	103.56	113.67
3	B	601	AER	C4-C5-C10	3.65	121.10	116.42
3	A	601	AER	C12-C13-C14	-3.58	103.32	108.88
3	D	601	AER	C7-C8-C9	3.47	113.73	109.72
3	D	601	AER	C11-C9-C10	-3.43	108.86	113.08
3	C	601	AER	C13-C17-C16	3.41	112.69	109.66
2	C	600	HEM	C3B-C4B-NB	-3.40	107.03	109.47
2	D	600	HEM	C1B-NB-C4B	3.40	109.23	105.21
2	C	600	HEM	C1B-NB-C4B	3.36	109.18	105.21
2	C	600	HEM	CHC-C1C-NC	3.35	128.10	124.45
3	A	601	AER	C14-C15-C16	3.34	106.39	101.25
3	A	601	AER	C18-C13-C14	3.34	117.79	112.99
3	B	601	AER	C7-C6-C5	-3.32	119.41	125.02
2	A	600	HEM	C2A-C1A-NA	-3.10	106.71	110.15
2	B	600	HEM	C2D-C1D-ND	-3.09	106.33	109.90
2	C	600	HEM	CHB-C4A-NA	3.07	129.42	123.86
3	A	601	AER	C13-C17-C16	3.03	112.36	109.66
2	A	600	HEM	C2B-C1B-NB	-3.01	106.38	109.84
2	B	600	HEM	CMD-C2D-C1D	2.98	129.69	125.03
2	A	600	HEM	CBA-CAA-C2A	2.97	120.75	112.53
2	D	600	HEM	CHD-C4C-NC	2.95	127.67	124.45
3	D	601	AER	C11-C9-C8	2.89	115.82	111.78
2	B	600	HEM	C4C-C3C-C2C	2.88	109.31	106.81
2	B	600	HEM	CHD-C1D-C2D	2.87	129.55	125.03
3	A	601	AER	C15-C14-C8	-2.85	118.61	121.63
2	A	600	HEM	C3B-C4B-NB	-2.84	107.43	109.47
3	D	601	AER	C18-C13-C12	-2.79	107.92	111.10
3	B	601	AER	C14-C15-C16	2.77	105.51	101.25
3	C	601	AER	C19-C10-C9	2.75	114.75	111.66
3	A	601	AER	C20-C21-N22	-2.74	119.43	123.50
3	B	601	AER	C4-C5-C6	-2.73	116.87	120.57
3	A	601	AER	C23-N22-C21	2.73	121.64	116.85
2	B	600	HEM	C2A-C1A-NA	-2.70	107.15	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	AER	C18-C13-C12	2.66	114.14	111.10
2	A	600	HEM	CHA-C1A-NA	2.63	128.63	123.86
3	A	601	AER	C14-C8-C9	-2.61	105.67	109.09
3	C	601	AER	C3-C4-C5	-2.61	107.90	112.05
2	B	600	HEM	CHA-C1A-NA	2.59	128.56	123.86
2	D	600	HEM	O1A-CGA-CBA	-2.59	114.89	123.09
3	C	601	AER	C7-C8-C9	2.58	112.70	109.72
3	A	601	AER	C19-C10-C5	2.54	112.26	108.38
3	D	601	AER	C19-C10-C5	2.54	112.26	108.38
2	B	600	HEM	C1A-CHA-C4D	2.52	132.17	126.25
2	B	600	HEM	C2B-C1B-NB	-2.51	106.95	109.84
3	B	601	AER	C18-C13-C17	-2.48	103.91	107.81
2	B	600	HEM	CHC-C4B-C3B	2.48	130.01	125.07
2	B	600	HEM	C4C-NC-C1C	2.46	109.83	105.82
2	A	600	HEM	CHC-C4B-NB	2.45	127.06	124.42
3	B	601	AER	C15-C14-C8	-2.43	119.06	121.63
3	C	601	AER	C12-C13-C17	-2.42	116.50	119.30
2	A	600	HEM	CHD-C4C-NC	2.40	127.07	124.45
2	C	600	HEM	CHC-C4B-C3B	2.39	129.84	125.07
3	A	601	AER	C19-C10-C1	-2.38	105.81	109.43
2	C	600	HEM	CAD-CBD-CGD	-2.36	107.41	113.67
2	B	600	HEM	C3B-C2B-C1B	2.31	108.15	106.41
3	B	601	AER	C15-C14-C13	2.31	105.66	104.05
2	B	600	HEM	CAD-C3D-C4D	2.29	128.69	124.70
2	C	600	HEM	CAC-C3C-C4C	2.29	130.29	124.82
2	D	600	HEM	C4B-C3B-C2B	2.27	109.36	107.28
2	A	600	HEM	CBB-CAB-C3B	-2.25	116.29	127.53
2	A	600	HEM	C1D-C2D-C3D	-2.24	104.62	106.98
2	B	600	HEM	CAC-C3C-C2C	-2.23	121.19	128.43
3	D	601	AER	C23-N22-C21	2.22	120.74	116.85
3	C	601	AER	C1-C10-C9	-2.19	105.84	108.74
2	D	600	HEM	C1D-C2D-C3D	-2.15	104.72	106.98
2	C	600	HEM	CHB-C4A-C3A	-2.14	121.22	127.43
2	A	600	HEM	CHD-C1D-ND	2.14	126.72	124.42
2	D	600	HEM	CHC-C4B-C3B	2.13	129.31	125.07
2	A	600	HEM	C4A-NA-C1A	2.10	109.25	105.82
2	C	600	HEM	C1D-C2D-C3D	-2.10	104.77	106.98
3	B	601	AER	C20-C17-C16	-2.10	122.37	125.08
3	B	601	AER	C19-C10-C5	-2.10	105.18	108.38
3	D	601	AER	C4-C5-C10	2.09	119.09	116.42
3	C	601	AER	C23-N22-C21	2.08	120.49	116.85
2	D	600	HEM	O2A-CGA-CBA	2.07	120.55	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	AER	C12-C11-C9	2.07	116.65	113.14
2	C	600	HEM	CMD-C2D-C1D	2.06	128.25	125.03
3	B	601	AER	C1-C2-C3	-2.05	107.76	110.48
2	A	600	HEM	CMD-C2D-C3D	2.04	131.67	126.15
3	D	601	AER	C1-C10-C9	-2.03	106.05	108.74
2	B	600	HEM	C2C-C1C-NC	-2.03	105.88	109.64
2	D	600	HEM	CAC-C3C-C4C	-2.03	119.98	124.82
3	C	601	AER	C12-C13-C14	-2.02	105.75	108.88
2	C	600	HEM	CAC-C3C-C2C	-2.02	121.87	128.43
3	A	601	AER	C18-C13-C17	-2.02	104.64	107.81
3	D	601	AER	C3-C4-C5	-2.01	108.85	112.05
3	C	601	AER	C7-C6-C5	-2.01	121.63	125.02

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	600	HEM	C2B-C3B-CAB-CBB
2	C	600	HEM	C4C-C3C-CAC-CBC
2	D	600	HEM	C4B-C3B-CAB-CBB
2	D	600	HEM	CAA-CBA-CGA-O1A
2	D	600	HEM	CAA-CBA-CGA-O2A
2	A	600	HEM	CAD-CBD-CGD-O2D
2	C	600	HEM	CAD-CBD-CGD-O2D
2	C	600	HEM	CAA-CBA-CGA-O2A
2	A	600	HEM	CAA-CBA-CGA-O2A
2	C	600	HEM	CAD-CBD-CGD-O1D

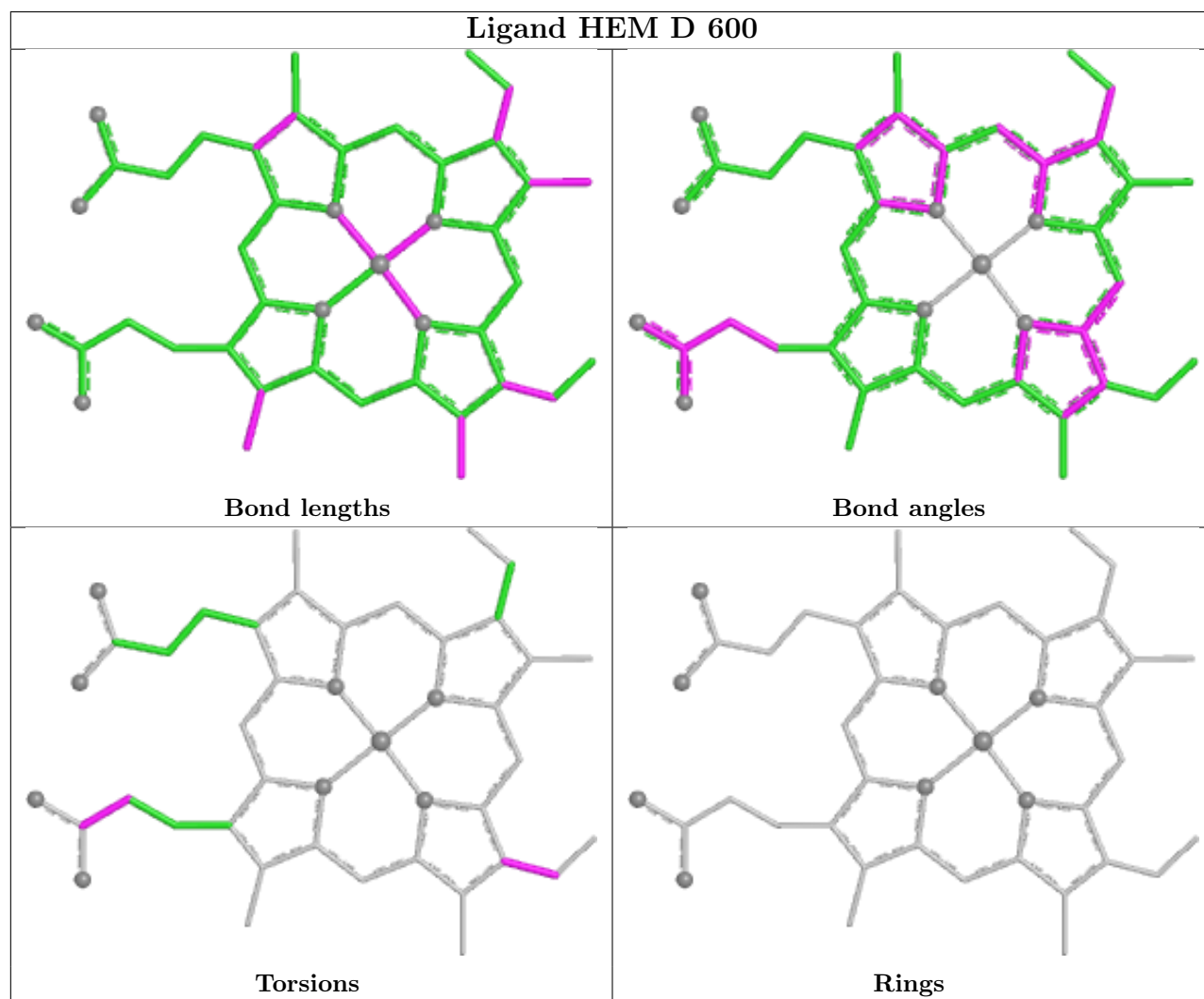
There are no ring outliers.

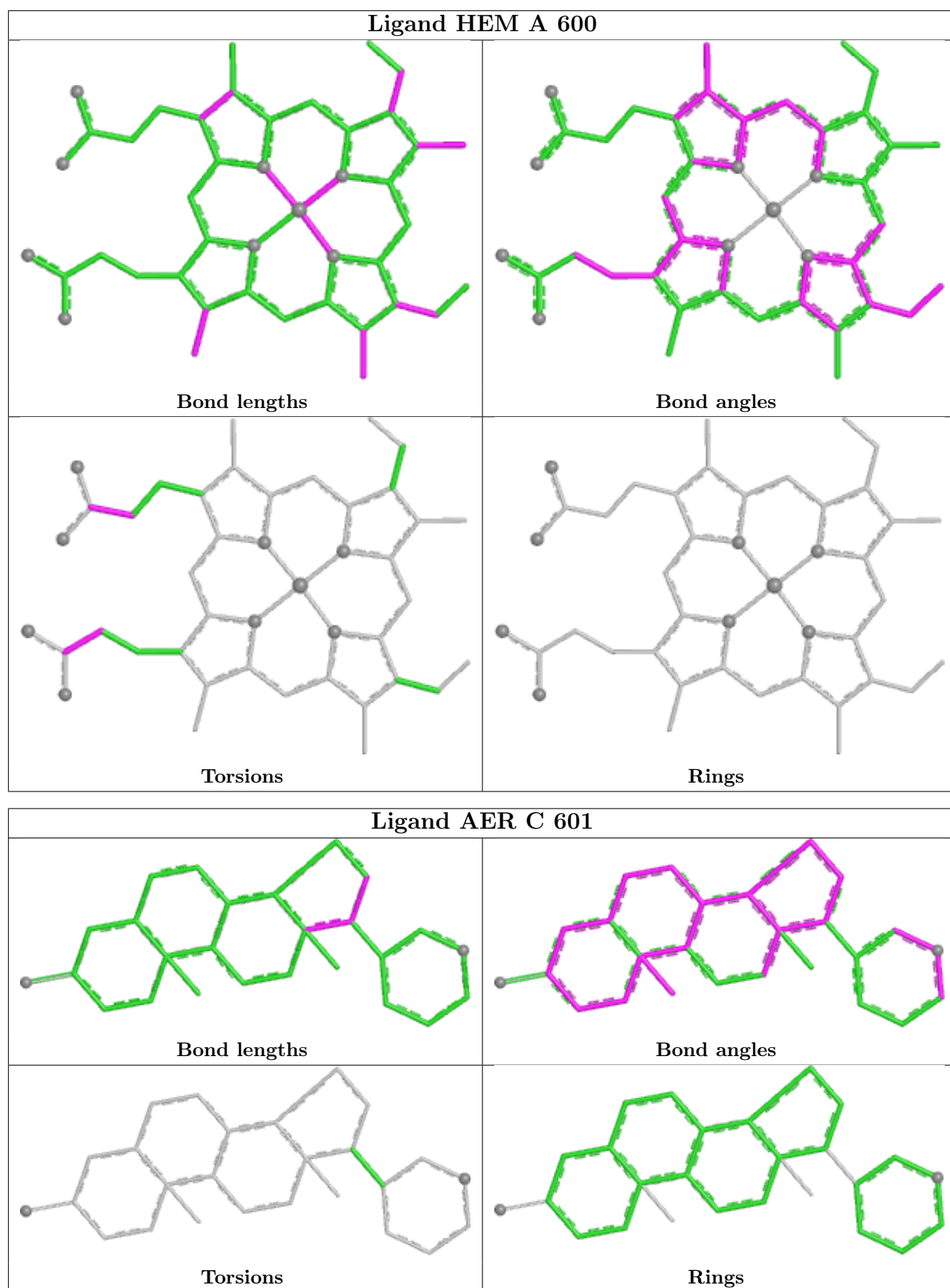
7 monomers are involved in 24 short contacts:

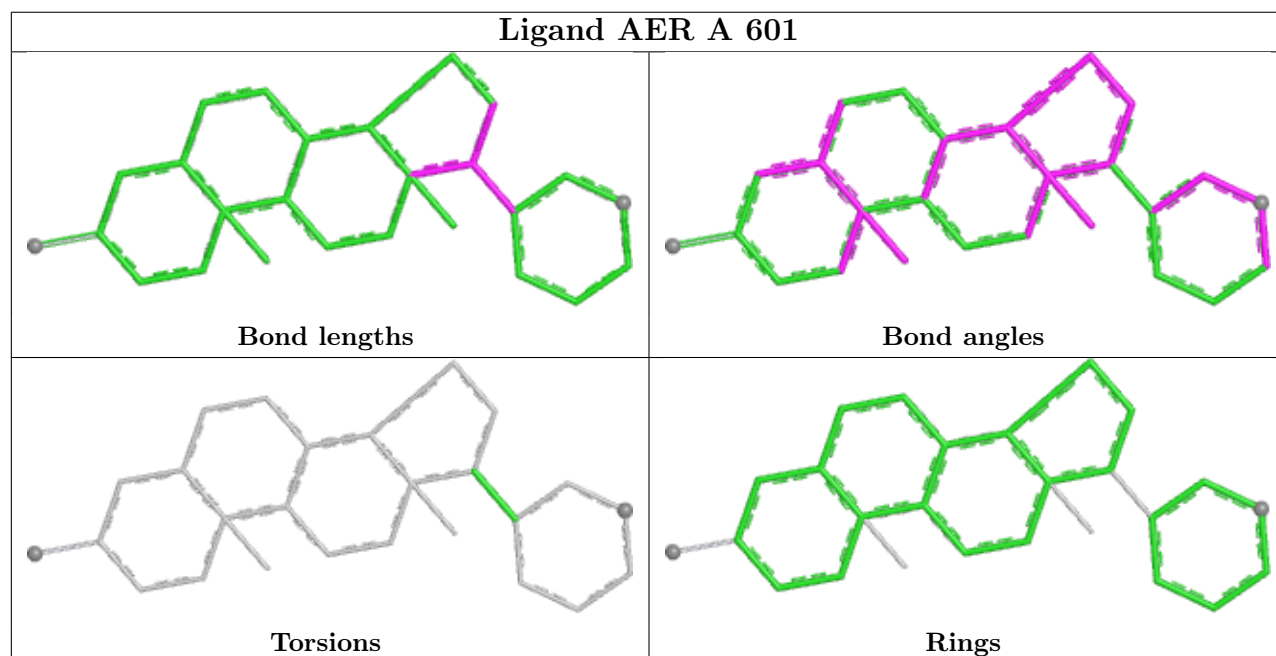
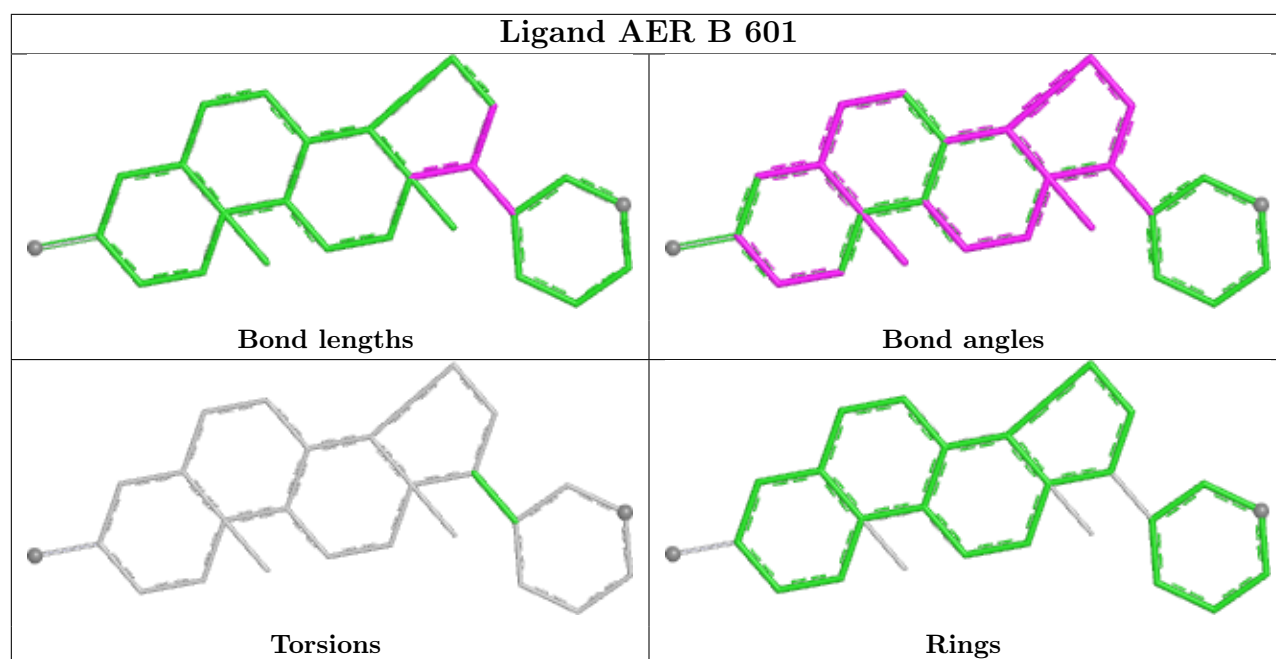
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	600	HEM	5	0
2	A	600	HEM	10	0
3	B	601	AER	1	0
3	A	601	AER	4	0
3	D	601	AER	2	0
2	C	600	HEM	2	0
2	B	600	HEM	2	0

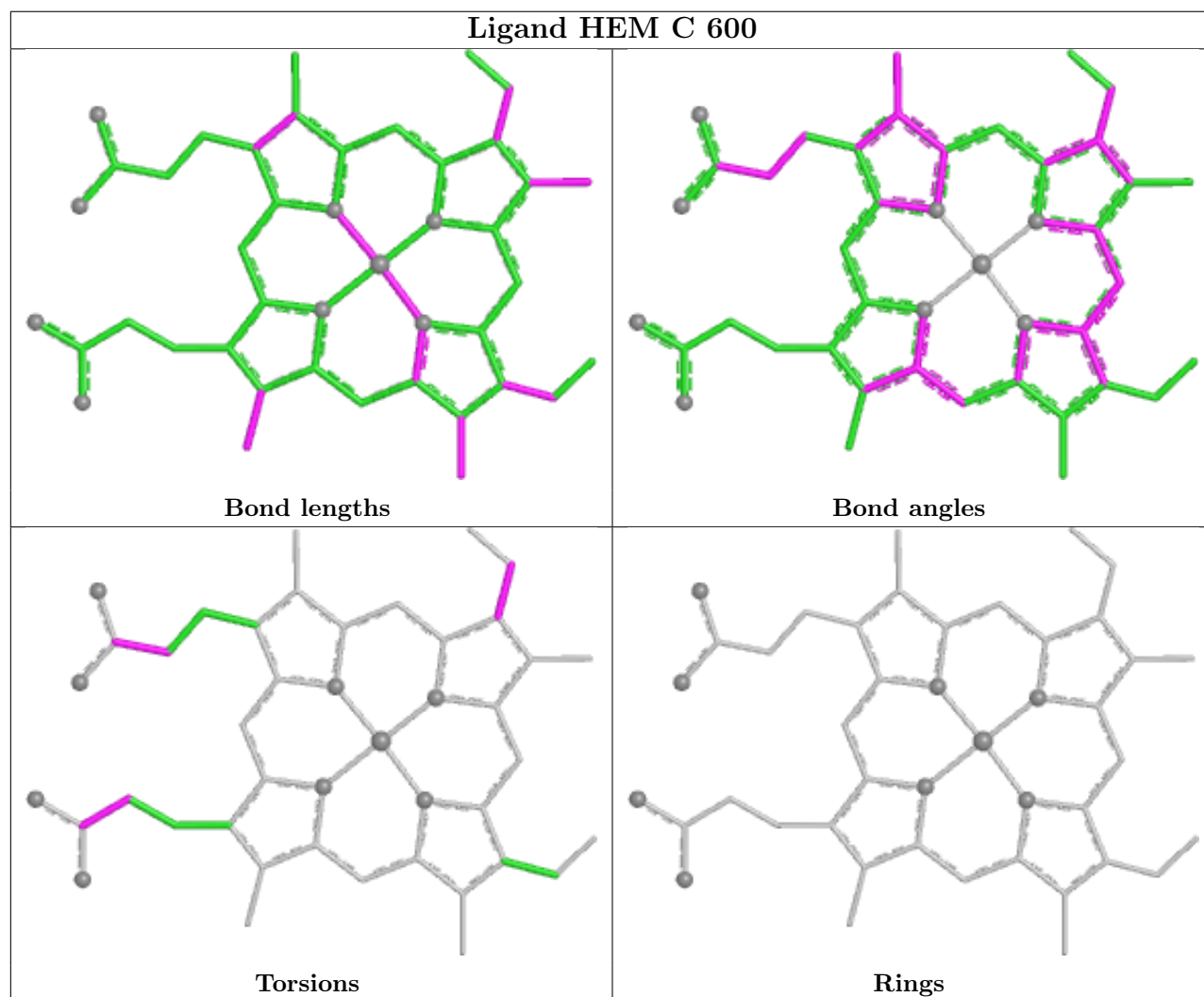
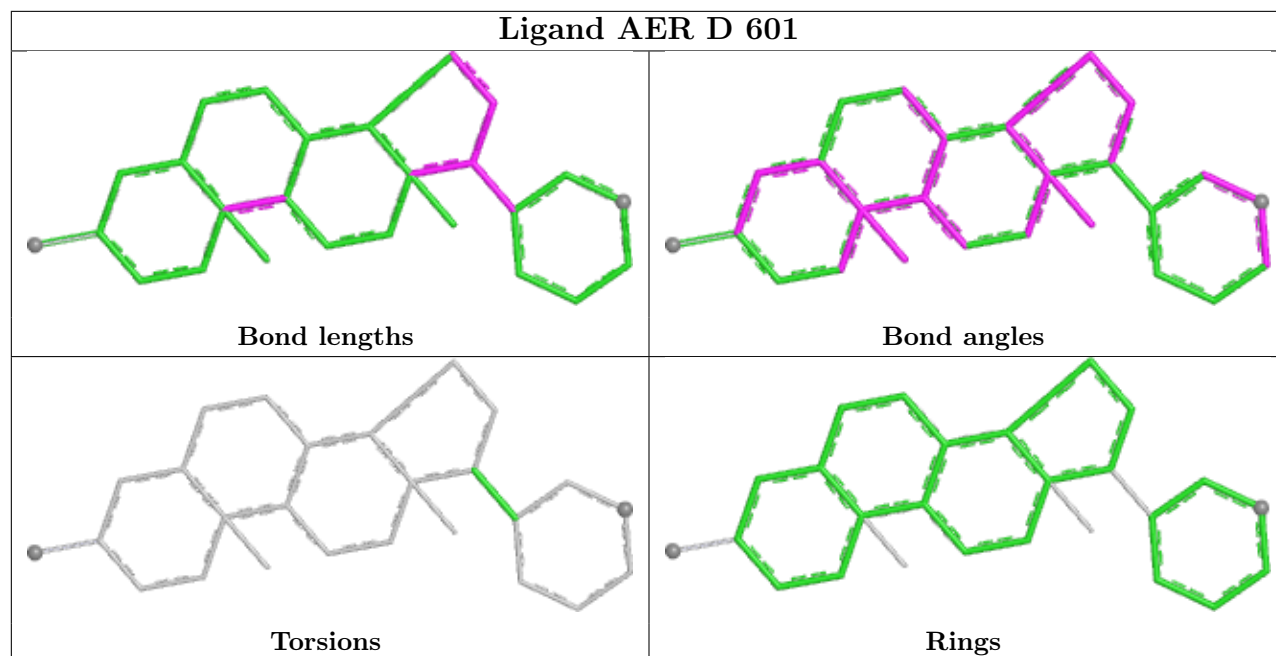
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

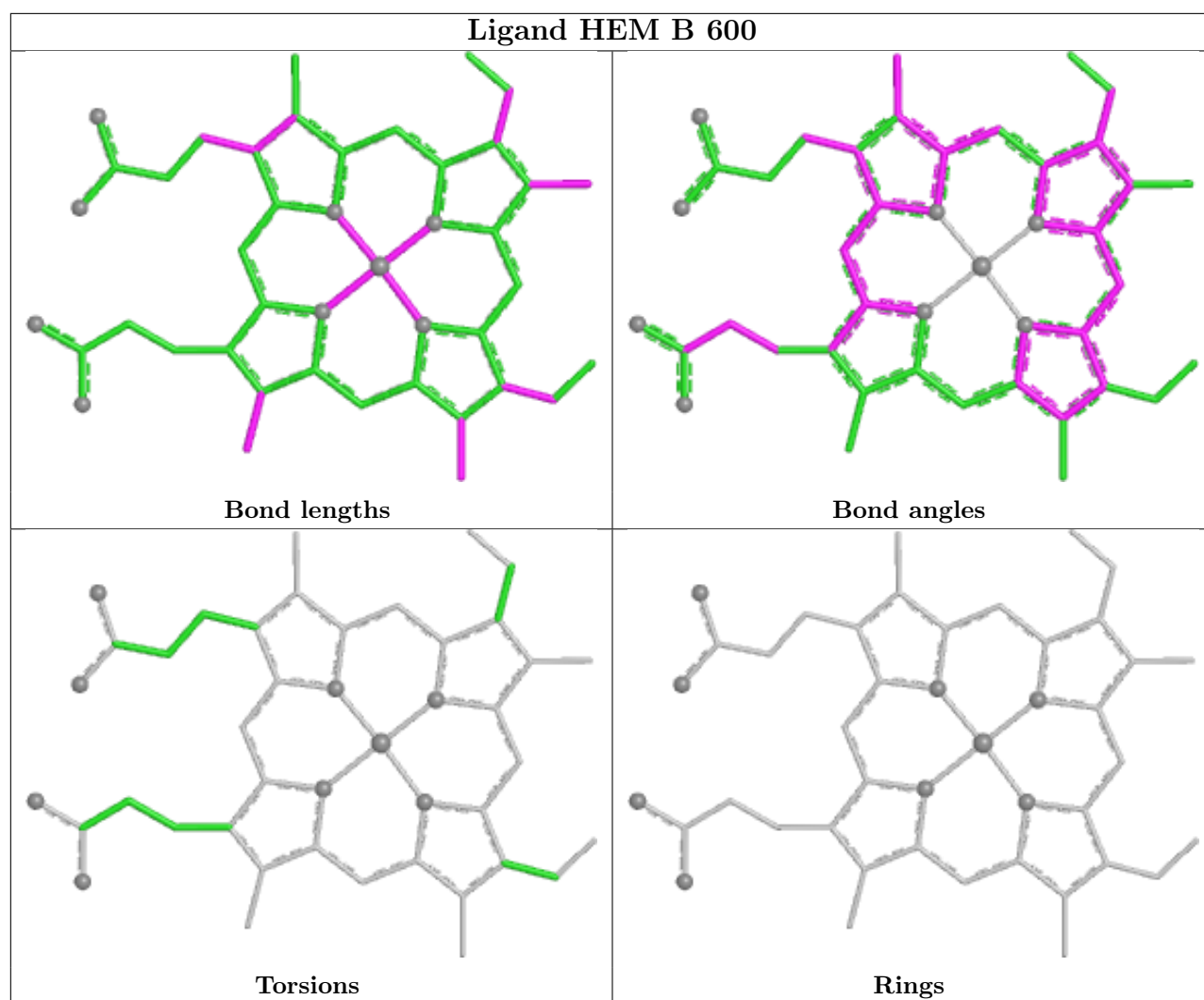
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.











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	464/494 (93%)	-0.17	6 (1%) 75 71	19, 38, 62, 72	2 (0%)
1	B	465/494 (94%)	-0.21	5 (1%) 78 74	20, 38, 60, 73	0
1	C	472/494 (95%)	0.05	9 (1%) 66 61	26, 44, 72, 82	0
1	D	473/494 (95%)	-0.06	9 (1%) 66 61	20, 42, 65, 78	1 (0%)
All	All	1874/1976 (94%)	-0.09	29 (1%) 72 68	19, 40, 67, 82	3 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	277	ASN	5.3
1	D	278	ALA	5.1
1	C	278	ALA	5.0
1	D	279	GLY	4.6
1	D	280	PRO	4.5
1	D	42	PHE	4.1
1	C	277	ASN	3.9
1	C	42	PHE	3.6
1	C	502	ALA	3.4
1	C	279	GLY	3.1
1	C	161	ASN	3.1
1	C	280	PRO	2.8
1	D	140	GLN	2.6
1	A	31	LEU	2.6
1	B	139	ASP	2.5
1	A	139	ASP	2.5
1	D	120[A]	HIS	2.4
1	B	217	LEU	2.3
1	A	137[A]	ASP	2.3
1	B	140	GLN	2.3
1	D	31	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	212	ASP	2.2
1	C	281	ASP	2.2
1	A	273	SER	2.2
1	C	473	LEU	2.2
1	A	407	HIS	2.2
1	D	139	ASP	2.1
1	B	284	SER	2.1
1	A	225	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

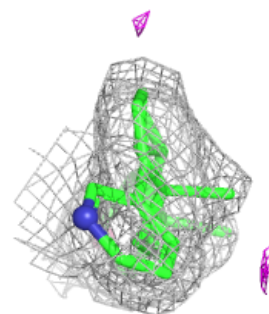
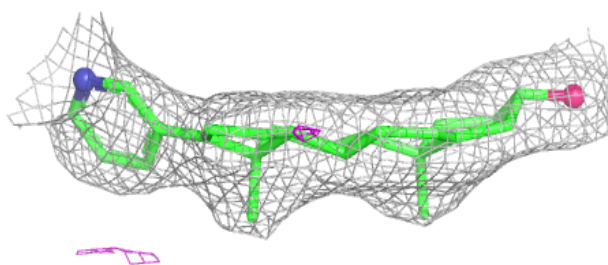
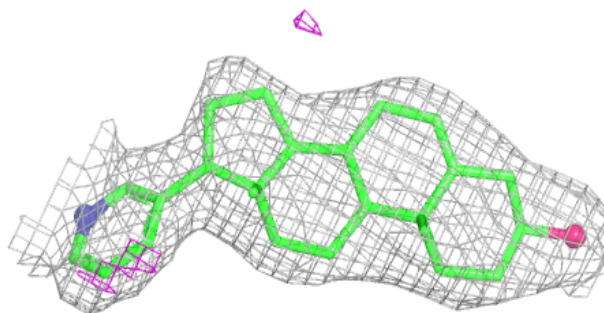
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AER	A	601	26/26	0.96	0.08	27,31,34,34	0
3	AER	B	601	26/26	0.96	0.07	26,30,31,32	0
3	AER	C	601	26/26	0.96	0.08	26,30,31,32	0
3	AER	D	601	26/26	0.96	0.07	21,27,29,30	0
2	HEM	A	600	43/43	0.98	0.06	18,27,31,36	0
2	HEM	B	600	43/43	0.98	0.06	19,24,28,31	0
2	HEM	C	600	43/43	0.98	0.07	21,30,35,38	0
2	HEM	D	600	43/43	0.98	0.06	21,27,33,41	0

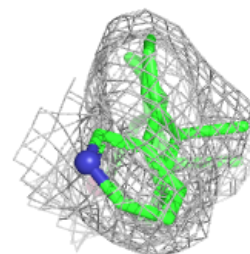
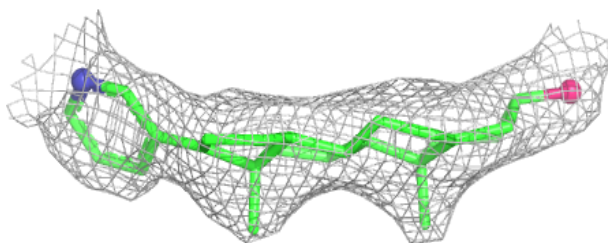
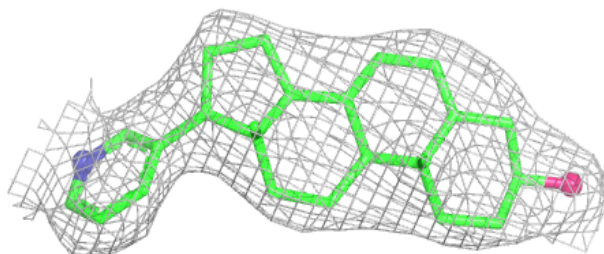
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AER A 601:

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

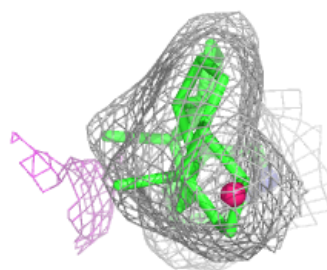
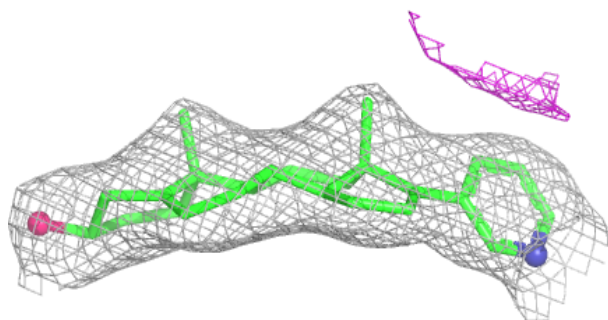
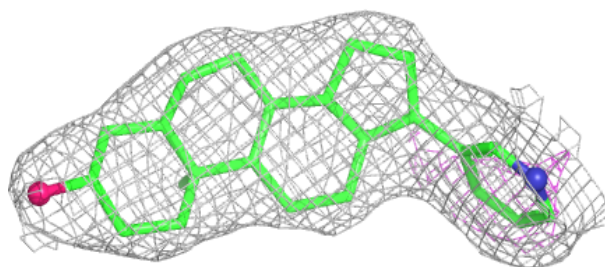
**Electron density around AER B 601:**

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

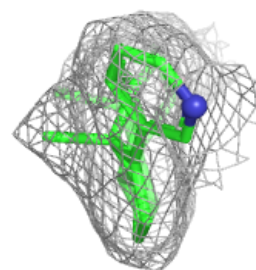
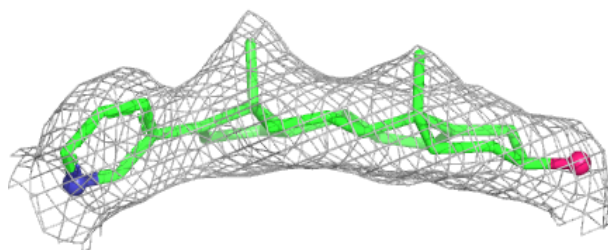
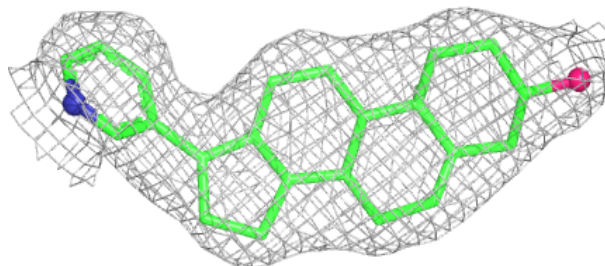


Electron density around AER C 601:

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

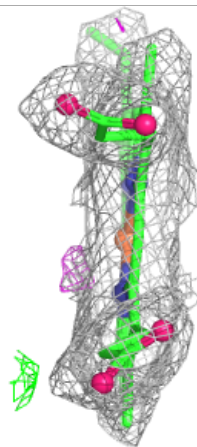
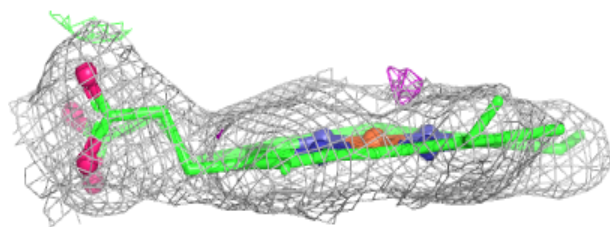
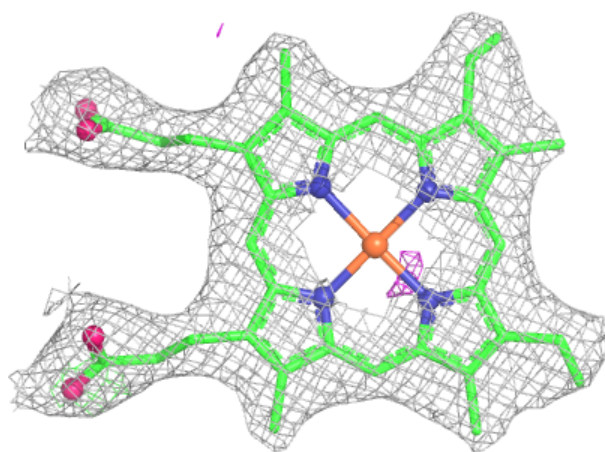
**Electron density around AER D 601:**

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



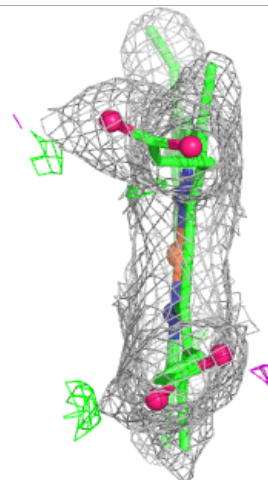
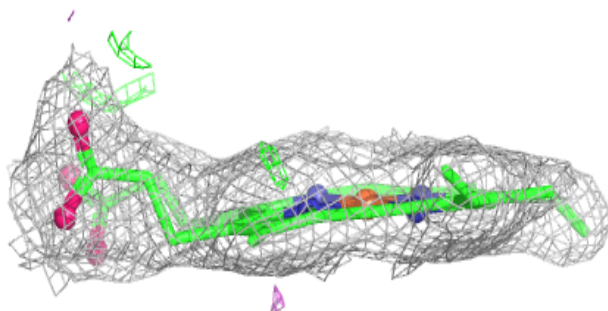
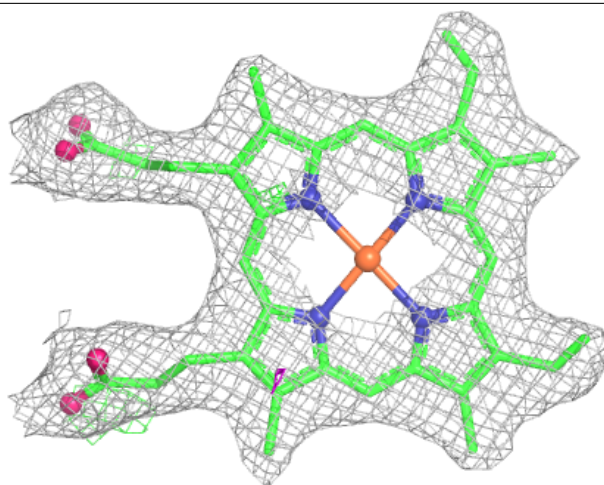
Electron density around HEM A 600:

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



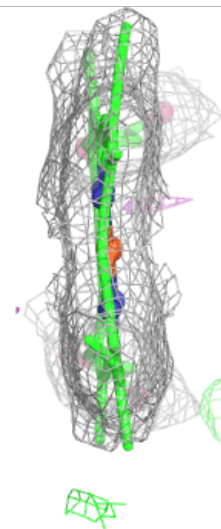
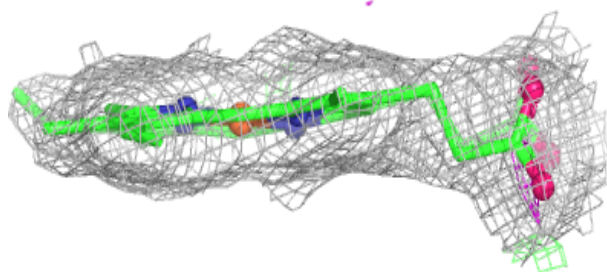
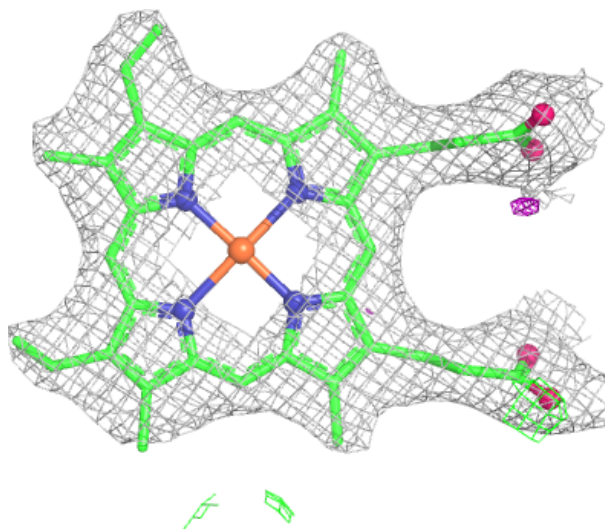
Electron density around HEM B 600:

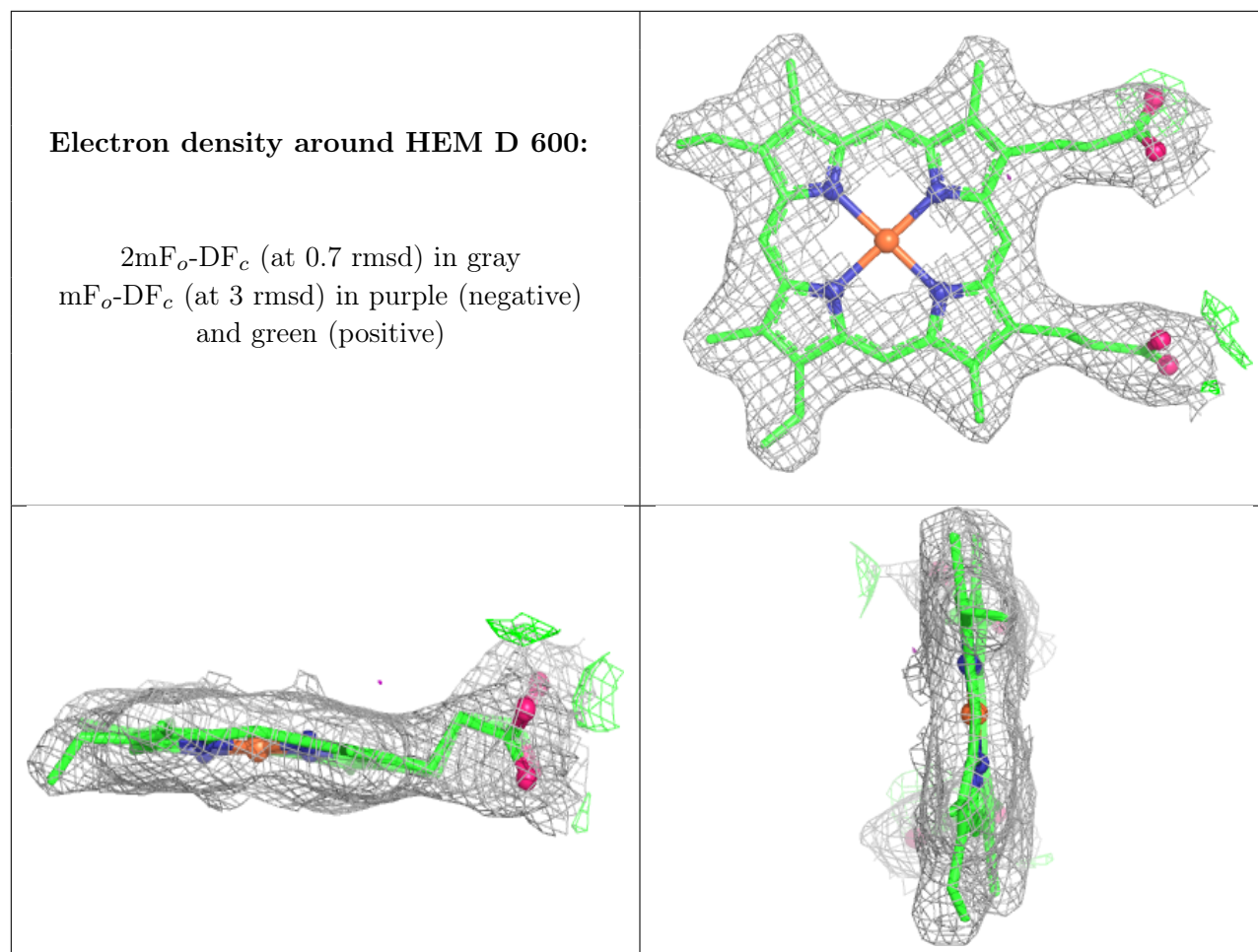
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 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.