



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 02:27 PM UTC

PDB ID : 3G1Q / pdb_00003g1q
Title : Crystal structure of sterol 14-alpha demethylase (CYP51) from Trypanosoma brucei in ligand free state
Authors : Lepesheva, G.I.; Hargrove, T.Y.; Harp, J.; Wawrzak, Z.; Waterman, M.R.; Park, H.
Deposited on : 2009-01-30
Resolution : 1.89 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

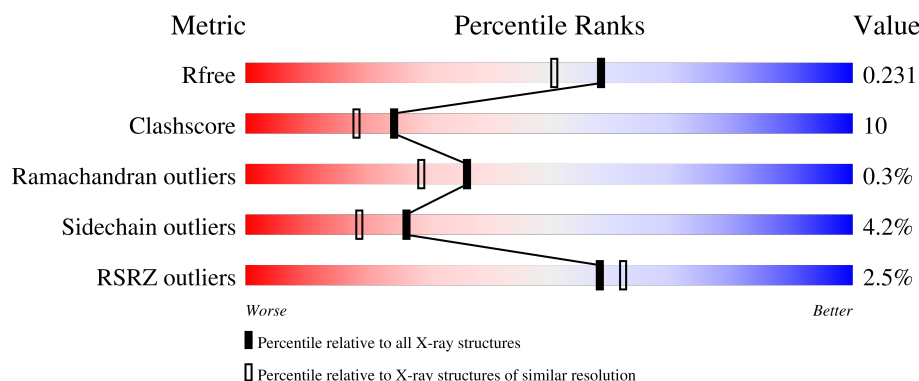
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	450	2% 80% 16% ..
1	B	450	2% 75% 22% ..
1	C	450	3% 81% 16% ...
1	D	450	4% 78% 19% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14858 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 Sterol 14-alpha-demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3557	2271	621	638	27			
1	B	444	Total	C	N	O	S	0	0	0
			3526	2254	615	630	27			
1	C	447	Total	C	N	O	S	0	0	0
			3552	2270	621	634	27			
1	D	448	Total	C	N	O	S	0	0	0
			3557	2271	621	638	27			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	SER	THR	engineered mutation	UNP Q385E8
A	28	LYS	ARG	engineered mutation	UNP Q385E8
A	29	GLY	PRO	engineered mutation	UNP Q385E8
A	30	LYS	THR	engineered mutation	UNP Q385E8
A	31	LEU	ASP	engineered mutation	UNP Q385E8
B	27	SER	THR	engineered mutation	UNP Q385E8
B	28	LYS	ARG	engineered mutation	UNP Q385E8
B	29	GLY	PRO	engineered mutation	UNP Q385E8
B	30	LYS	THR	engineered mutation	UNP Q385E8
B	31	LEU	ASP	engineered mutation	UNP Q385E8
C	27	SER	THR	engineered mutation	UNP Q385E8
C	28	LYS	ARG	engineered mutation	UNP Q385E8
C	29	GLY	PRO	engineered mutation	UNP Q385E8
C	30	LYS	THR	engineered mutation	UNP Q385E8
C	31	LEU	ASP	engineered mutation	UNP Q385E8
D	27	SER	THR	engineered mutation	UNP Q385E8
D	28	LYS	ARG	engineered mutation	UNP Q385E8
D	29	GLY	PRO	engineered mutation	UNP Q385E8
D	30	LYS	THR	engineered mutation	UNP Q385E8
D	31	LEU	ASP	engineered mutation	UNP Q385E8

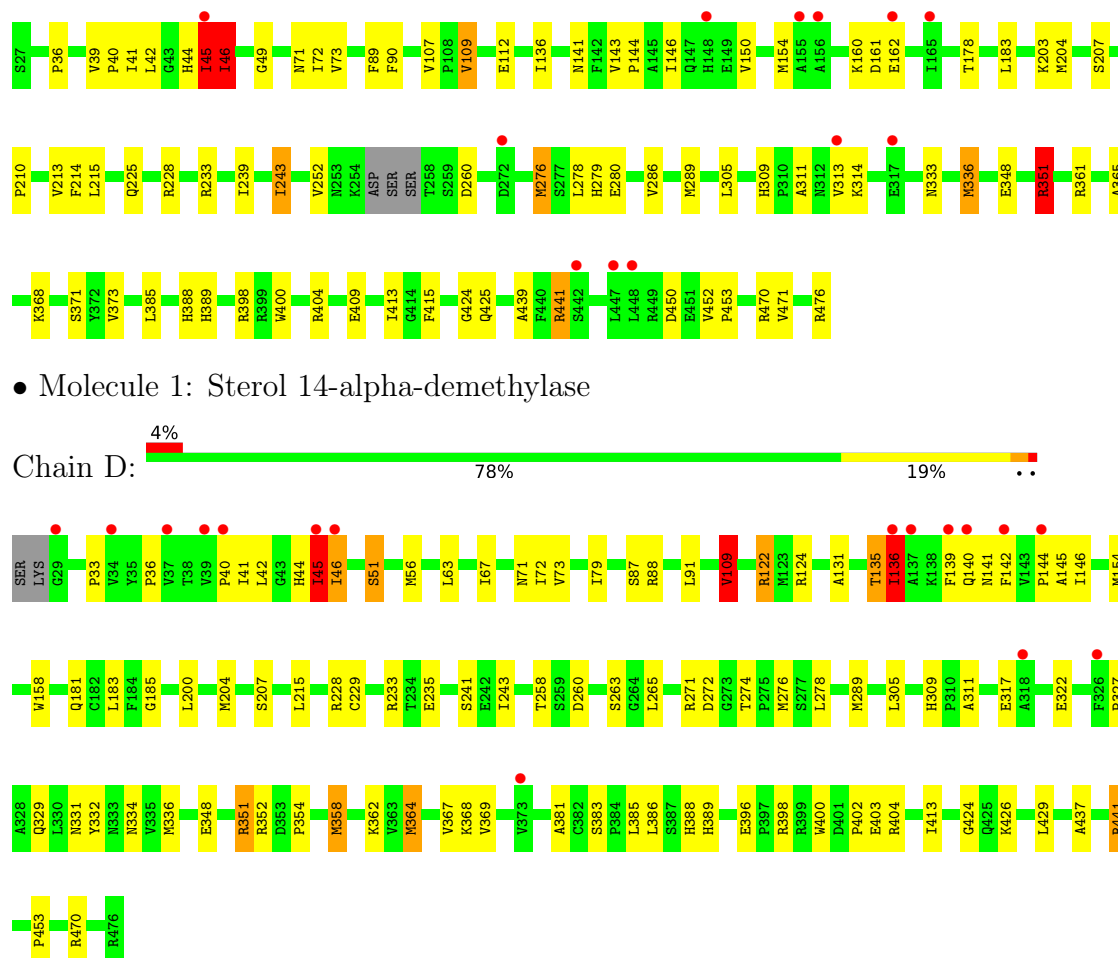
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	162	Total O 162 162	0	0
3	B	132	Total O 132 132	0	0
3	C	102	Total O 102 102	0	0
3	D	98	Total O 98 98	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.82Å 79.87Å 117.15Å 74.21° 81.56° 68.49°	Depositor
Resolution (Å)	28.62 – 1.89 28.62 – 1.89	Depositor EDS
% Data completeness (in resolution range)	97.5 (28.62-1.89) 97.4 (28.62-1.89)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.4.0061	Depositor
R, R_{free}	0.195 , 0.234 0.193 , 0.231	Depositor DCC
R_{free} test set	7519 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14858	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.55	18/3639 (0.5%)	1.22	12/4922 (0.2%)
1	B	1.56	19/3607 (0.5%)	1.23	12/4878 (0.2%)
1	C	1.35	10/3633 (0.3%)	1.16	6/4911 (0.1%)
1	D	1.32	6/3639 (0.2%)	1.20	12/4922 (0.2%)
All	All	1.45	53/14518 (0.4%)	1.20	42/19633 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	351	ARG	CD-NE	-8.99	1.33	1.46
1	B	396	GLU	CA-C	8.72	1.60	1.53
1	B	471	VAL	CA-CB	7.88	1.66	1.54
1	B	326	PHE	CA-C	-7.83	1.44	1.53
1	B	86	HIS	N-CA	7.35	1.55	1.46
1	A	107	VAL	CA-C	7.23	1.58	1.52
1	C	351	ARG	CD-NE	-6.99	1.36	1.46
1	C	46	ILE	CA-CB	6.93	1.63	1.54
1	B	202	ALA	CA-CB	6.45	1.63	1.53
1	D	424	GLY	C-O	-6.41	1.19	1.24
1	B	246	ALA	CA-CB	-6.24	1.43	1.53
1	C	313	VAL	CA-CB	6.22	1.62	1.54
1	A	352	ARG	N-CA	6.21	1.53	1.46
1	A	289	MET	N-CA	6.08	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	363	VAL	N-CA	6.08	1.53	1.46
1	B	187	ASP	N-CA	6.07	1.53	1.46
1	A	80	VAL	CA-C	-6.06	1.47	1.53
1	A	423	ILE	CG1-CD1	5.99	1.75	1.51
1	C	89	PHE	N-CA	5.95	1.53	1.46
1	D	109	VAL	CA-CB	5.93	1.61	1.55
1	D	354	PRO	CA-C	5.86	1.57	1.52
1	A	114	VAL	CA-CB	5.84	1.62	1.54
1	C	90	PHE	N-CA	5.77	1.53	1.46
1	A	29	GLY	N-CA	5.76	1.54	1.45
1	B	32	PRO	CA-C	5.75	1.57	1.52
1	A	59	CYS	N-CA	-5.69	1.39	1.46
1	A	33	PRO	CA-C	5.66	1.59	1.52
1	B	417	ALA	CA-CB	5.60	1.64	1.53
1	B	299	THR	CA-CB	5.58	1.62	1.53
1	D	396	GLU	CA-C	5.57	1.57	1.53
1	C	107	VAL	CA-C	5.55	1.58	1.52
1	B	313	VAL	CA-CB	5.49	1.63	1.54
1	B	145	ALA	N-CA	5.41	1.52	1.46
1	C	365	ALA	CA-CB	5.37	1.62	1.53
1	A	134	LEU	CA-C	5.32	1.59	1.52
1	A	399	ARG	CA-CB	5.31	1.60	1.53
1	C	361	ARG	CZ-NH1	5.30	1.40	1.32
1	A	297	SER	CA-C	5.28	1.59	1.52
1	C	373	VAL	CA-CB	-5.24	1.48	1.54
1	B	312	ASN	CA-CB	5.18	1.60	1.53
1	A	32	PRO	CA-C	5.15	1.56	1.52
1	B	286	VAL	CA-CB	5.14	1.60	1.54
1	B	119	PRO	N-CA	5.12	1.53	1.47
1	D	136	ILE	CA-CB	5.12	1.61	1.54
1	A	239	ILE	CA-CB	5.10	1.60	1.54
1	B	109	VAL	CA-CB	5.06	1.60	1.55
1	D	352	ARG	N-CA	5.06	1.52	1.46
1	B	454	ASP	C-O	-5.03	1.17	1.23
1	C	143	VAL	CA-C	5.03	1.57	1.52
1	A	309	HIS	N-CA	5.03	1.53	1.45
1	A	373	VAL	C-O	5.03	1.29	1.24
1	A	205	GLU	CA-C	5.02	1.59	1.52
1	B	424	GLY	C-O	-5.02	1.18	1.23

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	45	ILE	CB-CA-C	-9.76	98.96	112.14
1	A	351	ARG	NE-CZ-NH2	-9.20	110.92	119.20
1	A	313	VAL	CB-CA-C	-8.83	100.47	112.04
1	D	45	ILE	CB-CA-C	-8.39	101.14	111.88
1	D	136	ILE	N-CA-C	7.57	125.08	109.34
1	D	139	PHE	N-CA-C	7.15	119.94	111.71
1	D	136	ILE	CB-CA-C	-7.13	99.60	111.29
1	C	351	ARG	NE-CZ-NH2	-6.59	113.26	119.20
1	A	351	ARG	NE-CZ-NH1	6.42	127.92	121.50
1	A	351	ARG	CD-NE-CZ	6.40	133.36	124.40
1	A	207	SER	N-CA-C	6.32	120.99	113.28
1	B	39	VAL	CA-C-N	6.20	125.93	119.05
1	B	39	VAL	C-N-CA	6.20	125.93	119.05
1	D	429	LEU	N-CA-C	6.02	118.63	111.71
1	C	49	GLY	N-CA-C	6.00	120.14	112.83
1	C	404	ARG	NE-CZ-NH2	-5.94	113.86	119.20
1	B	115	ALA	CB-CA-C	-5.92	109.17	117.23
1	B	109	VAL	CA-CB-CG1	5.89	120.42	110.40
1	A	198	ALA	N-CA-C	5.74	118.00	111.11
1	D	46	ILE	N-CA-C	5.68	115.87	110.42
1	C	39	VAL	CA-C-N	5.66	126.92	119.84
1	C	39	VAL	C-N-CA	5.66	126.92	119.84
1	B	96	VAL	N-CA-C	-5.66	106.16	111.48
1	B	109	VAL	N-CA-CB	-5.65	102.71	110.68
1	A	39	VAL	N-CA-C	5.63	112.68	107.56
1	D	142	PHE	N-CA-C	5.59	118.91	111.75
1	D	51	SER	CA-C-N	5.59	125.05	119.24
1	D	51	SER	C-N-CA	5.59	125.05	119.24
1	D	45	ILE	N-CA-CB	5.58	116.70	110.51
1	A	231	GLU	CB-CA-C	-5.53	102.20	110.88
1	B	176	ILE	CB-CA-C	-5.53	104.90	111.97
1	B	251	GLU	N-CA-C	5.51	119.54	113.21
1	B	39	VAL	N-CA-C	5.37	112.87	107.55
1	B	319	LEU	N-CA-C	-5.37	105.51	111.36
1	B	335	VAL	N-CA-C	5.33	115.53	110.53
1	D	146	ILE	N-CA-C	5.28	115.48	110.42
1	A	471	VAL	CG1-CB-CG2	5.25	122.34	110.80
1	A	39	VAL	CA-C-N	5.22	126.37	119.84
1	A	39	VAL	C-N-CA	5.22	126.37	119.84
1	A	255	ASP	N-CA-C	-5.17	103.86	110.53
1	D	322	GLU	N-CA-C	5.16	116.71	111.14
1	B	109	VAL	CB-CA-C	5.02	117.73	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	135	THR	Peptide

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	3557	0	3594	71	0
1	B	3526	0	3565	78	0
1	C	3552	0	3597	60	0
1	D	3557	0	3594	75	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
2	C	43	0	30	4	0
2	D	43	0	30	1	0
3	A	162	0	0	7	0
3	B	132	0	0	22	0
3	C	102	0	0	9	0
3	D	98	0	0	14	0
All	All	14858	0	14470	284	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 10.

All (284) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ILE:CG1	1:A:423:ILE:CD1	1.75	1.64
1:B:336:MET:HE3	1:B:430:LEU:CD1	1.76	1.15
1:A:328:ALA:HA	1:A:441:ARG:HH22	1.08	1.12
1:B:336:MET:HE3	1:B:430:LEU:HD13	1.34	1.09
1:B:362:LYS:HG3	1:B:364:MET:HE3	1.35	1.07
1:D:135:THR:HB	1:D:136:ILE:HG13	1.37	1.06
1:D:336:MET:HE2	1:D:336:MET:HA	1.35	1.05
1:C:228:ARG:HD2	3:C:514:HOH:O	1.57	1.03
1:C:336:MET:HE2	1:C:336:MET:HA	1.44	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:GLU:OE1	1:A:351:ARG:HD3	1.61	0.99
1:D:336:MET:HE1	3:D:499:HOH:O	1.65	0.97
1:A:44:HIS:HD2	1:A:71:ASN:H	1.13	0.94
1:B:229:CYS:CB	3:B:603:HOH:O	2.14	0.94
1:A:328:ALA:HA	1:A:441:ARG:NH2	1.82	0.94
1:A:388:HIS:HE1	1:A:413:ILE:H	1.16	0.92
1:B:362:LYS:HG3	1:B:364:MET:CE	2.02	0.90
1:D:388:HIS:HE1	1:D:413:ILE:H	1.08	0.90
1:A:364:MET:HA	1:A:364:MET:CE	2.02	0.90
1:B:406:GLU:HG3	3:D:535:HOH:O	1.75	0.87
1:A:336:MET:HE1	1:A:430:LEU:HD13	1.58	0.86
1:B:388:HIS:HE1	1:B:413:ILE:H	1.19	0.86
1:C:388:HIS:HE1	1:C:413:ILE:H	1.20	0.85
1:B:336:MET:CE	1:B:430:LEU:CD1	2.55	0.85
1:A:336:MET:CE	1:A:430:LEU:HD13	2.05	0.85
1:B:44:HIS:HD2	1:B:71:ASN:H	1.23	0.85
1:A:409:GLU:OE2	1:C:368:LYS:HD2	1.75	0.85
1:B:229:CYS:HB3	3:B:603:HOH:O	1.71	0.84
1:B:336:MET:CE	1:B:430:LEU:HD13	2.08	0.83
1:C:210:PRO:O	1:C:213:VAL:HG12	1.78	0.83
1:B:252:VAL:HA	3:B:543:HOH:O	1.76	0.83
1:B:406:GLU:HB2	3:B:516:HOH:O	1.77	0.83
1:D:73:VAL:O	1:D:73:VAL:HG12	1.76	0.83
1:B:309:HIS:HD2	1:B:311:ALA:H	1.26	0.82
1:D:470:ARG:HD3	3:D:498:HOH:O	1.80	0.81
1:C:44:HIS:HD2	1:C:71:ASN:H	1.26	0.81
1:C:228:ARG:NH2	3:C:488:HOH:O	2.13	0.81
1:B:229:CYS:SG	3:B:603:HOH:O	2.39	0.80
1:D:388:HIS:CE1	1:D:413:ILE:H	1.97	0.80
1:A:309:HIS:HD2	1:A:311:ALA:H	1.29	0.80
1:C:389:HIS:HE1	1:C:398:ARG:HH11	1.28	0.79
1:D:207:SER:HB2	3:D:528:HOH:O	1.83	0.79
1:B:61:ARG:HD2	3:B:582:HOH:O	1.83	0.77
1:A:403:GLU:HG2	3:A:578:HOH:O	1.83	0.76
1:D:364:MET:HA	1:D:364:MET:HE2	1.67	0.75
1:A:191:ARG:HE	1:A:196:ARG:HH12	1.33	0.74
1:B:41:ILE:HG13	3:B:514:HOH:O	1.87	0.73
1:D:348:GLU:OE1	1:D:351:ARG:HD3	1.89	0.73
1:B:388:HIS:CE1	1:B:413:ILE:H	2.06	0.73
1:D:136:ILE:HA	3:D:547:HOH:O	1.88	0.72
1:B:336:MET:HE3	1:B:430:LEU:HD12	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:MET:HA	1:A:364:MET:HE3	1.70	0.72
1:A:389:HIS:HE1	1:A:398:ARG:HH11	1.35	0.72
1:D:389:HIS:HE1	1:D:398:ARG:HH11	1.37	0.71
1:D:229:CYS:SG	3:D:528:HOH:O	2.48	0.71
1:D:358:MET:HE1	1:D:381:ALA:HB1	1.71	0.71
1:D:44:HIS:HD2	1:D:71:ASN:H	1.39	0.71
1:C:45:ILE:HG23	1:C:72:ILE:HG23	1.70	0.71
1:A:423:ILE:CD1	1:A:423:ILE:CB	2.66	0.71
1:A:389:HIS:CE1	1:A:398:ARG:HH11	2.10	0.70
1:B:441:ARG:HG3	3:B:502:HOH:O	1.91	0.70
1:A:388:HIS:CE1	1:A:413:ILE:H	2.07	0.70
1:D:336:MET:HA	1:D:336:MET:CE	2.17	0.69
1:A:39:VAL:HG12	3:A:582:HOH:O	1.92	0.69
1:B:362:LYS:CG	1:B:364:MET:HE3	2.18	0.69
1:A:310:PRO:O	1:A:313:VAL:HG22	1.92	0.68
1:D:122:ARG:HD3	3:D:492:HOH:O	1.94	0.68
1:A:364:MET:HA	1:A:364:MET:HE2	1.75	0.68
1:B:364:MET:HE2	1:B:364:MET:HA	1.76	0.68
1:B:409:GLU:HB2	1:D:136:ILE:HG23	1.75	0.68
1:C:336:MET:HA	1:C:336:MET:CE	2.24	0.66
1:B:139:PHE:HA	1:B:142:PHE:HB2	1.78	0.66
1:D:331:ASN:H	1:D:334:ASN:HD22	1.42	0.66
1:B:133:GLU:HG3	1:B:261:LEU:HD12	1.77	0.65
1:B:385:LEU:O	1:B:389:HIS:HD2	1.79	0.65
1:D:437:ALA:O	1:D:441:ARG:HB2	1.96	0.65
1:A:309:HIS:CD2	1:A:311:ALA:H	2.12	0.65
1:C:389:HIS:CE1	1:C:398:ARG:HH11	2.11	0.65
1:D:229:CYS:HB2	3:D:528:HOH:O	1.97	0.65
1:D:332:TYR:CE1	1:D:336:MET:HG3	2.32	0.65
1:D:73:VAL:O	1:D:73:VAL:CG1	2.45	0.64
1:D:389:HIS:CE1	1:D:398:ARG:HH11	2.15	0.64
1:D:185:GLY:HA3	1:D:258:THR:HG21	1.79	0.64
1:B:336:MET:CE	1:B:430:LEU:HD12	2.25	0.64
1:B:310:PRO:O	1:B:313:VAL:HG23	1.98	0.63
1:A:328:ALA:CA	1:A:441:ARG:HH22	1.99	0.62
1:C:441:ARG:HD3	3:C:574:HOH:O	1.99	0.61
1:C:348:GLU:OE1	1:C:351:ARG:HD3	2.01	0.61
1:A:456:ASP:OD2	1:A:458:HIS:CE1	2.53	0.61
1:B:306:HIS:C	3:B:602:HOH:O	2.43	0.61
1:B:475:ARG:HD3	3:B:560:HOH:O	2.00	0.61
1:D:358:MET:CE	1:D:381:ALA:HB1	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:TRP:CZ3	3:B:602:HOH:O	2.52	0.60
1:B:154:MET:HE2	1:B:158:TRP:CZ3	2.37	0.60
1:A:184:PHE:HZ	1:A:289:MET:HE3	1.66	0.60
1:C:309:HIS:CD2	1:C:311:ALA:H	2.19	0.60
1:A:351:ARG:HD2	1:A:404:ARG:HD2	1.83	0.60
1:D:44:HIS:CD2	1:D:71:ASN:H	2.20	0.60
1:B:331:ASN:H	1:B:334:ASN:ND2	1.99	0.59
1:C:336:MET:HE1	3:C:505:HOH:O	2.01	0.59
1:B:279:HIS:HD2	3:B:519:HOH:O	1.86	0.59
1:A:256:SER:O	1:A:256:SER:OG	2.17	0.59
1:D:141:ASN:HB3	3:D:540:HOH:O	2.02	0.58
1:A:336:MET:HE2	1:A:430:LEU:HD13	1.84	0.58
1:A:348:GLU:OE1	1:A:351:ARG:CD	2.43	0.57
1:C:252:VAL:HG12	1:C:252:VAL:O	2.03	0.57
1:D:228:ARG:HD2	3:D:518:HOH:O	2.03	0.57
2:D:480:HEM:HMC1	2:D:480:HEM:HBC2	1.86	0.57
1:A:44:HIS:HD2	1:A:71:ASN:N	1.95	0.57
1:B:44:HIS:CD2	1:B:71:ASN:H	2.14	0.57
1:B:309:HIS:CD2	1:B:311:ALA:H	2.14	0.57
1:D:204:MET:HE3	1:D:233:ARG:HB2	1.85	0.57
1:C:309:HIS:HD2	1:C:311:ALA:H	1.52	0.56
1:C:441:ARG:O	1:C:476:ARG:HD3	2.04	0.56
1:B:389:HIS:HE1	1:B:398:ARG:HH11	1.52	0.56
1:B:191:ARG:HG3	3:B:556:HOH:O	2.05	0.56
1:B:44:HIS:HD2	1:B:71:ASN:N	1.99	0.56
2:C:480:HEM:HBC2	2:C:480:HEM:HMC2	1.86	0.56
1:C:388:HIS:CE1	1:C:413:ILE:H	2.12	0.56
1:A:44:HIS:CD2	1:A:71:ASN:H	2.06	0.56
1:B:331:ASN:H	1:B:334:ASN:HD22	1.54	0.56
1:C:160:LYS:HE2	3:C:556:HOH:O	2.06	0.56
1:C:44:HIS:CD2	1:C:71:ASN:H	2.16	0.55
1:A:265:LEU:O	1:A:276:MET:HE3	2.05	0.55
1:A:325:GLU:OE1	1:C:136:ILE:HG12	2.07	0.55
1:A:150:VAL:CG1	1:A:154:MET:HE3	2.37	0.55
1:A:331:ASN:H	1:A:334:ASN:ND2	2.04	0.55
1:D:145:ALA:HB1	1:D:181:GLN:HG3	1.88	0.55
1:A:336:MET:CG	1:C:409:GLU:HG3	2.37	0.55
1:D:358:MET:HE3	1:D:383:SER:HB2	1.90	0.54
1:D:229:CYS:CB	3:D:528:HOH:O	2.55	0.54
1:B:73:VAL:HG12	1:B:73:VAL:O	2.07	0.54
1:D:331:ASN:H	1:D:334:ASN:ND2	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:GLN:HG2	3:D:537:HOH:O	2.08	0.53
1:A:162:GLU:OE1	1:A:472:LYS:HE3	2.08	0.53
1:C:44:HIS:HD2	1:C:71:ASN:N	2.00	0.53
1:D:56:MET:HE3	1:D:79:ILE:HD13	1.90	0.53
1:A:191:ARG:NE	1:A:196:ARG:HH12	2.04	0.53
1:B:362:LYS:CG	1:B:364:MET:CE	2.82	0.53
1:A:385:LEU:O	1:A:389:HIS:HD2	1.92	0.53
1:B:332:TYR:CE1	1:B:336:MET:HG3	2.44	0.53
1:A:184:PHE:CZ	1:A:289:MET:HE3	2.42	0.52
1:C:73:VAL:HG12	1:C:73:VAL:O	2.10	0.52
1:D:265:LEU:O	1:D:276:MET:HE3	2.10	0.52
1:B:330:LEU:HA	1:B:334:ASN:HD22	1.75	0.52
1:A:41:ILE:HG22	1:A:41:ILE:O	2.09	0.52
1:A:424:GLY:HA3	2:A:480:HEM:C3C	2.45	0.52
2:B:480:HEM:HMC1	2:B:480:HEM:HBC2	1.93	0.51
1:A:364:MET:CE	1:A:364:MET:CA	2.82	0.51
1:B:105:PHE:HA	1:B:219:LEU:HD21	1.92	0.51
1:C:470:ARG:NE	3:C:571:HOH:O	2.39	0.51
1:B:309:HIS:HD2	1:B:311:ALA:N	2.02	0.51
1:D:87:SER:HB2	1:D:91:LEU:HD12	1.93	0.51
1:A:336:MET:HG3	1:C:409:GLU:HG3	1.93	0.51
1:C:42:LEU:HD13	1:C:46:ILE:HD13	1.92	0.51
1:B:348:GLU:OE1	1:B:404:ARG:HD3	2.11	0.50
1:C:109:VAL:HG22	1:C:204:MET:HB3	1.93	0.50
1:A:347:ARG:HD3	3:A:482:HOH:O	2.11	0.50
1:D:56:MET:HE2	1:D:386:LEU:HD22	1.93	0.50
1:A:109:VAL:HG13	1:A:286:VAL:HG11	1.92	0.50
1:C:425:GLN:NE2	3:C:518:HOH:O	2.17	0.50
1:D:400:TRP:CH2	1:D:402:PRO:HG3	2.47	0.50
1:B:351:ARG:HD3	1:B:394:PHE:CD2	2.46	0.50
1:C:213:VAL:HG13	1:C:214:PHE:CD1	2.48	0.49
1:C:42:LEU:HD22	1:C:45:ILE:HD11	1.94	0.49
1:C:228:ARG:CD	3:C:514:HOH:O	2.33	0.49
1:C:305:LEU:HD13	1:C:453:PRO:HD2	1.93	0.49
1:C:415:PHE:CE1	1:C:425:GLN:HG3	2.48	0.49
1:A:331:ASN:H	1:A:334:ASN:HD22	1.59	0.49
1:D:135:THR:HB	1:D:136:ILE:CG1	2.25	0.49
1:D:426:LYS:HD2	3:D:546:HOH:O	2.12	0.49
1:A:164:GLU:HG2	1:A:470:ARG:NH2	2.28	0.48
1:C:154:MET:HE1	1:C:439:ALA:HA	1.96	0.48
1:B:364:MET:HE2	3:B:599:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:ILE:HD12	1:B:441:ARG:HG2	1.96	0.48
1:C:160:LYS:HG3	1:C:162:GLU:O	2.13	0.48
1:B:389:HIS:CE1	1:B:398:ARG:HH11	2.30	0.48
1:B:109:VAL:HG23	3:B:603:HOH:O	2.13	0.47
1:B:424:GLY:HA3	2:B:480:HEM:C3C	2.48	0.47
2:C:480:HEM:HBC2	2:C:480:HEM:CMC	2.43	0.47
1:D:348:GLU:OE1	1:D:404:ARG:HD3	2.14	0.47
1:A:39:VAL:HA	1:A:40:PRO:HD2	1.70	0.47
1:A:271:ARG:C	1:A:273:GLY:H	2.20	0.47
1:A:422:CYS:HB3	1:A:425:GLN:HG3	1.95	0.47
1:C:146:ILE:HG23	1:C:178:THR:HG21	1.96	0.47
1:C:424:GLY:HA3	2:C:480:HEM:C3C	2.50	0.47
2:C:480:HEM:HBB2	2:C:480:HEM:HHC	1.97	0.47
1:D:154:MET:HE2	1:D:158:TRP:CZ3	2.50	0.47
1:B:279:HIS:CD2	3:B:519:HOH:O	2.65	0.47
1:B:364:MET:CE	3:B:599:HOH:O	2.63	0.47
1:D:305:LEU:HD13	1:D:453:PRO:HD2	1.97	0.47
1:A:339:MET:HE2	1:A:342:ALA:CB	2.46	0.46
1:B:58:GLU:OE1	1:B:61:ARG:NH1	2.49	0.46
1:B:161:ASP:HA	1:B:475:ARG:HB3	1.97	0.46
1:B:143:VAL:CG2	1:B:430:LEU:HD11	2.45	0.46
1:B:268:ALA:HB3	1:B:276:MET:HE3	1.98	0.46
1:A:268:ALA:HB3	1:A:276:MET:HE2	1.98	0.46
1:B:433:LYS:CE	3:B:538:HOH:O	2.64	0.46
1:C:183:LEU:O	1:C:260:ASP:HB2	2.15	0.46
1:A:41:ILE:N	3:A:582:HOH:O	2.48	0.46
2:A:480:HEM:HMC2	2:A:480:HEM:HBC2	1.98	0.46
1:C:183:LEU:HD12	1:C:289:MET:HE1	1.96	0.46
1:D:36:PRO:O	1:D:44:HIS:HE1	1.98	0.46
1:D:272:ASP:HB3	1:D:274:THR:H	1.81	0.46
1:D:88:ARG:HH21	1:D:368:LYS:HG3	1.82	0.45
1:B:339:MET:HE2	1:B:342:ALA:CB	2.45	0.45
1:D:145:ALA:HB1	1:D:181:GLN:CG	2.46	0.45
1:A:415:PHE:CD2	1:A:425:GLN:HG2	2.51	0.45
1:B:336:MET:CE	3:B:538:HOH:O	2.64	0.45
1:C:36:PRO:O	1:C:44:HIS:HE1	1.99	0.45
1:A:133:GLU:HG3	1:A:261:LEU:HD12	1.99	0.45
1:D:332:TYR:CZ	1:D:336:MET:HG3	2.52	0.45
1:D:362:LYS:CG	1:D:364:MET:HE3	2.47	0.45
1:B:389:HIS:HE1	1:B:398:ARG:HD2	1.82	0.45
1:C:213:VAL:HG11	3:C:522:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:MET:HE2	1:D:336:MET:CA	2.25	0.44
1:D:56:MET:HE1	1:D:383:SER:CB	2.47	0.44
1:D:271:ARG:NH2	3:D:491:HOH:O	2.50	0.44
1:B:29:GLY:N	3:B:590:HOH:O	2.50	0.44
1:C:112:GLU:O	1:C:279:HIS:HE1	2.01	0.44
1:B:41:ILE:HD12	1:B:42:LEU:HG	2.00	0.44
1:B:307:LEU:HA	3:B:602:HOH:O	2.17	0.44
1:C:204:MET:HE3	1:C:233:ARG:HB2	2.00	0.44
1:D:109:VAL:HG22	1:D:204:MET:HE2	2.00	0.44
1:D:131:ALA:O	1:D:135:THR:HG23	2.17	0.44
1:A:358:MET:HE3	1:A:358:MET:HB3	1.84	0.43
1:B:325:GLU:OE1	1:B:325:GLU:HA	2.17	0.43
1:D:45:ILE:H	1:D:45:ILE:HG13	1.63	0.43
1:B:354:PRO:HA	1:B:355:PRO:HD3	1.88	0.43
1:A:160:LYS:HG2	1:A:473:TYR:OH	2.19	0.43
1:A:313:VAL:HG22	3:A:558:HOH:O	2.18	0.43
1:B:368:LYS:HE2	1:B:370:GLY:O	2.18	0.43
1:A:313:VAL:CG2	3:A:558:HOH:O	2.66	0.43
1:B:409:GLU:HB2	1:D:136:ILE:CG2	2.47	0.43
1:D:73:VAL:HG11	1:D:215:LEU:HD21	2.01	0.43
1:C:141:ASN:O	1:C:144:PRO:HD2	2.18	0.42
1:C:150:VAL:CG1	1:C:154:MET:HE3	2.49	0.42
1:B:41:ILE:N	3:B:514:HOH:O	2.51	0.42
1:D:348:GLU:HG3	1:D:400:TRP:CD1	2.54	0.42
1:B:174:MET:O	1:B:178:THR:HG23	2.19	0.42
1:C:40:PRO:HB2	1:C:41:ILE:HG13	2.02	0.42
1:D:109:VAL:HG22	1:D:204:MET:HB3	2.02	0.42
1:A:470:ARG:HD2	3:A:598:HOH:O	2.20	0.42
1:D:45:ILE:HG23	1:D:72:ILE:HG23	1.99	0.42
1:A:109:VAL:HG13	1:A:286:VAL:CG1	2.49	0.42
1:C:348:GLU:HG3	1:C:400:TRP:CD1	2.54	0.42
1:D:336:MET:CE	1:D:336:MET:CA	2.93	0.42
1:D:309:HIS:CD2	1:D:311:ALA:H	2.38	0.42
1:A:36:PRO:O	1:A:44:HIS:HE1	2.02	0.42
1:A:437:ALA:O	1:A:441:ARG:HB2	2.20	0.42
1:C:207:SER:HA	1:C:225:GLN:HB3	2.02	0.42
1:C:276:MET:HG2	1:C:280:GLU:HB2	2.00	0.42
1:D:327:PRO:HG2	1:D:329:GLN:O	2.20	0.41
1:B:204:MET:CE	1:B:233:ARG:HA	2.50	0.41
1:D:51:SER:O	1:D:51:SER:OG	2.37	0.41
1:B:385:LEU:O	1:B:389:HIS:CD2	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:ILE:HD13	1:D:369:VAL:HG12	2.02	0.41
1:D:141:ASN:O	1:D:144:PRO:HD2	2.20	0.41
1:C:73:VAL:HG11	1:C:215:LEU:HG	2.01	0.41
1:D:33:PRO:HB2	1:D:63:LEU:HD22	2.02	0.41
1:B:101:GLU:H	1:B:101:GLU:CD	2.28	0.41
1:B:368:LYS:HA	1:B:368:LYS:HD2	1.96	0.41
1:C:415:PHE:CZ	1:C:425:GLN:HG3	2.55	0.41
1:D:260:ASP:H	1:D:263:SER:HG	1.67	0.41
1:D:385:LEU:O	1:D:389:HIS:HD2	2.04	0.41
1:C:252:VAL:O	1:C:252:VAL:CG1	2.67	0.41
1:A:208:LEU:HA	1:A:208:LEU:HD23	1.88	0.41
1:A:456:ASP:OD1	1:A:458:HIS:ND1	2.54	0.41
1:C:146:ILE:HG23	1:C:178:THR:CG2	2.51	0.41
1:C:203:LYS:HE2	1:C:228:ARG:HB3	2.03	0.41
1:C:239:ILE:O	1:C:243:ILE:HD12	2.20	0.41
1:C:385:LEU:O	1:C:389:HIS:HD2	2.04	0.41
1:A:458:HIS:CD2	1:A:458:HIS:C	2.99	0.40
1:B:148:HIS:O	1:B:152:LYS:HG3	2.21	0.40
1:C:109:VAL:HG13	1:C:286:VAL:CG1	2.52	0.40
1:A:404:ARG:HH11	1:A:404:ARG:HD3	1.79	0.40
1:A:94:ASN:HD21	1:A:123:MET:HE1	1.87	0.40
1:A:271:ARG:C	1:A:273:GLY:N	2.78	0.40
1:A:41:ILE:O	1:A:41:ILE:CG2	2.69	0.40
1:B:359:LEU:O	1:B:381:ALA:HA	2.21	0.40
1:D:183:LEU:HD12	1:D:289:MET:HE1	2.04	0.40
1:D:185:GLY:CA	1:D:258:THR:HG21	2.48	0.40
1:D:200:LEU:O	1:D:204:MET:HG3	2.21	0.40
1:C:309:HIS:HD2	1:C:311:ALA:HB3	1.85	0.40
1:D:42:LEU:HD13	1:D:46:ILE:HD12	2.02	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	446/450 (99%)	432 (97%)	11 (2%)	3 (1%)	18	10
1	B	440/450 (98%)	426 (97%)	13 (3%)	1 (0%)	43	36
1	C	443/450 (98%)	429 (97%)	14 (3%)	0	100	100
1	D	446/450 (99%)	424 (95%)	20 (4%)	2 (0%)	30	22
All	All	1775/1800 (99%)	1711 (96%)	58 (3%)	6 (0%)	36	29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	PRO
1	A	256	SER
1	B	272	ASP
1	D	136	ILE
1	A	272	ASP
1	D	40	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	390/392 (100%)	373 (96%)	17 (4%)	25	17
1	B	386/392 (98%)	371 (96%)	15 (4%)	28	21
1	C	389/392 (99%)	373 (96%)	16 (4%)	27	19
1	D	390/392 (100%)	373 (96%)	17 (4%)	25	17
All	All	1555/1568 (99%)	1490 (96%)	65 (4%)	26	19

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	SER
1	A	122	ARG
1	A	160	LYS
1	A	162	GLU
1	A	207	SER

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Mol	Chain	Res	Type
1	A	243	ILE
1	A	256	SER
1	A	276	MET
1	A	278	LEU
1	A	313	VAL
1	A	325	GLU
1	A	351	ARG
1	A	364	MET
1	A	371	SER
1	A	458	HIS
1	A	470	ARG
1	A	471	VAL
1	B	39	VAL
1	B	41	ILE
1	B	47	GLN
1	B	109	VAL
1	B	112	GLU
1	B	122	ARG
1	B	191	ARG
1	B	272	ASP
1	B	278	LEU
1	B	358	MET
1	B	405	ASP
1	B	447	LEU
1	B	452	VAL
1	B	471	VAL
1	B	476	ARG
1	C	45	ILE
1	C	46	ILE
1	C	109	VAL
1	C	161	ASP
1	C	243	ILE
1	C	276	MET
1	C	278	LEU
1	C	314	LYS
1	C	333	ASN
1	C	336	MET
1	C	351	ARG
1	C	371	SER
1	C	441	ARG
1	C	450	ASP
1	C	452	VAL

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Mol	Chain	Res	Type
1	C	471	VAL
1	D	41	ILE
1	D	45	ILE
1	D	109	VAL
1	D	122	ARG
1	D	124	ARG
1	D	136	ILE
1	D	235	GLU
1	D	241	SER
1	D	243	ILE
1	D	278	LEU
1	D	317	GLU
1	D	351	ARG
1	D	358	MET
1	D	364	MET
1	D	367	VAL
1	D	403	GLU
1	D	441	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	62	GLN
1	A	309	HIS
1	A	334	ASN
1	A	388	HIS
1	A	389	HIS
1	B	44	HIS
1	B	237	GLN
1	B	279	HIS
1	B	309	HIS
1	B	329	GLN
1	B	333	ASN
1	B	334	ASN
1	B	388	HIS
1	B	389	HIS
1	B	425	GLN
1	C	44	HIS
1	C	62	GLN
1	C	177	ASN
1	C	279	HIS

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Mol	Chain	Res	Type
1	C	309	HIS
1	C	333	ASN
1	C	334	ASN
1	C	388	HIS
1	C	389	HIS
1	D	44	HIS
1	D	279	HIS
1	D	309	HIS
1	D	334	ASN
1	D	388	HIS
1	D	389	HIS
1	D	425	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	A	480	1	50,50,50	2.07	13 (26%)	67,82,82	1.50	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	B	480	1	50,50,50	1.89	12 (24%)	67,82,82	1.22	5 (7%)
2	HEM	C	480	1	50,50,50	2.00	15 (30%)	67,82,82	1.41	12 (17%)
2	HEM	D	480	1	50,50,50	2.18	13 (26%)	67,82,82	1.47	11 (16%)

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	A	480	1	-	2/14/54/54	-
2	HEM	B	480	1	-	0/14/54/54	-
2	HEM	C	480	1	-	0/14/54/54	-
2	HEM	D	480	1	-	0/14/54/54	-

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	480	HEM	C3D-C2D	6.84	1.51	1.36
2	B	480	HEM	C3D-C2D	5.62	1.48	1.36
2	C	480	HEM	C3D-C2D	5.42	1.48	1.36
2	D	480	HEM	CMB-C2B	4.96	1.60	1.50
2	A	480	HEM	C3D-C2D	4.82	1.47	1.36
2	B	480	HEM	FE-NC	4.71	2.10	1.95
2	A	480	HEM	FE-NC	4.70	2.10	1.95
2	D	480	HEM	FE-NB	4.65	2.09	1.94
2	A	480	HEM	CMD-C2D	4.52	1.60	1.50
2	A	480	HEM	CAC-C3C	4.44	1.59	1.47
2	C	480	HEM	CMC-C2C	4.43	1.59	1.50
2	A	480	HEM	CMB-C2B	4.30	1.59	1.50
2	C	480	HEM	FE-NC	4.26	2.09	1.95
2	D	480	HEM	FE-NC	4.26	2.09	1.95
2	A	480	HEM	CMA-C3A	4.26	1.59	1.50
2	D	480	HEM	C3B-C2B	-4.15	1.28	1.37
2	D	480	HEM	FE-ND	4.13	2.07	1.94
2	A	480	HEM	FE-NB	3.76	2.06	1.94
2	B	480	HEM	FE-ND	3.75	2.06	1.94
2	B	480	HEM	CAB-C3B	3.72	1.57	1.47
2	C	480	HEM	CAB-C3B	3.67	1.57	1.47
2	C	480	HEM	CMB-C2B	3.64	1.58	1.50
2	B	480	HEM	CMD-C2D	3.56	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	480	HEM	CMD-C2D	3.53	1.58	1.50
2	A	480	HEM	FE-ND	3.53	2.05	1.94
2	D	480	HEM	CMD-C2D	3.39	1.57	1.50
2	C	480	HEM	CMA-C3A	3.33	1.57	1.50
2	D	480	HEM	CAB-C3B	3.30	1.56	1.47
2	B	480	HEM	CMB-C2B	3.25	1.57	1.50
2	C	480	HEM	FE-NB	3.19	2.04	1.94
2	D	480	HEM	CAA-C2A	2.99	1.59	1.51
2	C	480	HEM	CAA-C2A	2.86	1.58	1.51
2	C	480	HEM	FE-NA	2.77	2.04	1.95
2	A	480	HEM	C1D-C2D	-2.70	1.39	1.44
2	D	480	HEM	CMC-C2C	2.68	1.56	1.50
2	C	480	HEM	CAC-C3C	2.65	1.54	1.47
2	C	480	HEM	C3B-C2B	-2.65	1.31	1.37
2	B	480	HEM	CAA-C2A	2.63	1.58	1.51
2	B	480	HEM	FE-NB	2.58	2.02	1.94
2	B	480	HEM	CAC-C3C	2.56	1.54	1.47
2	A	480	HEM	FE-NA	2.50	2.03	1.95
2	D	480	HEM	O2D-CGD	-2.47	1.22	1.30
2	A	480	HEM	C4D-ND	-2.45	1.36	1.40
2	A	480	HEM	CAB-C3B	2.34	1.53	1.47
2	B	480	HEM	CMA-C3A	2.29	1.55	1.50
2	B	480	HEM	CMC-C2C	2.28	1.55	1.50
2	A	480	HEM	O2D-CGD	-2.25	1.23	1.30
2	C	480	HEM	FE-ND	2.20	2.01	1.94
2	B	480	HEM	FE-NA	2.19	2.02	1.95
2	C	480	HEM	C3C-C2C	-2.13	1.32	1.37
2	D	480	HEM	C1B-NB	-2.08	1.36	1.40
2	D	480	HEM	CBA-CGA	2.08	1.55	1.50
2	C	480	HEM	CAD-C3D	2.07	1.56	1.51

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	480	HEM	C4D-ND-C1D	5.36	111.56	105.21
2	A	480	HEM	CMD-C2D-C1D	4.26	131.69	125.03
2	A	480	HEM	C4D-ND-C1D	3.94	109.87	105.21
2	D	480	HEM	CAD-CBD-CGD	-3.35	104.78	113.67
2	B	480	HEM	C4D-ND-C1D	3.22	109.02	105.21
2	D	480	HEM	CHD-C1D-ND	2.98	127.63	124.42
2	C	480	HEM	O2D-CGD-CBD	2.91	123.18	114.00
2	A	480	HEM	CMC-C2C-C1C	-2.85	119.70	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	480	HEM	O2D-CGD-CBD	2.85	123.01	114.00
2	B	480	HEM	C3B-C2B-C1B	2.76	108.48	106.41
2	A	480	HEM	CHA-C4D-ND	2.76	127.78	124.37
2	C	480	HEM	C3B-C4B-NB	-2.71	107.52	109.47
2	C	480	HEM	CHD-C1D-ND	2.69	127.32	124.42
2	C	480	HEM	C4D-ND-C1D	2.62	108.31	105.21
2	D	480	HEM	C4C-C3C-C2C	2.62	109.08	106.81
2	D	480	HEM	O2A-CGA-CBA	2.56	122.10	114.00
2	A	480	HEM	C4A-C3A-C2A	2.53	109.71	106.82
2	B	480	HEM	O1D-CGD-CBD	-2.45	115.32	123.09
2	B	480	HEM	CMC-C2C-C1C	-2.44	120.44	124.73
2	A	480	HEM	C3B-C4B-NB	-2.39	107.75	109.47
2	A	480	HEM	CMD-C2D-C3D	-2.34	119.83	126.15
2	C	480	HEM	CHB-C4A-NA	2.32	128.08	123.86
2	D	480	HEM	O2D-CGD-CBD	2.32	121.32	114.00
2	D	480	HEM	CBD-CAD-C3D	-2.29	106.19	112.53
2	C	480	HEM	C3B-C2B-C1B	2.21	108.07	106.41
2	D	480	HEM	CAB-C3B-C2B	-2.20	121.28	128.43
2	C	480	HEM	CMD-C2D-C1D	2.20	128.47	125.03
2	A	480	HEM	C1A-CHA-C4D	-2.20	121.08	126.25
2	C	480	HEM	CAD-CBD-CGD	-2.18	107.88	113.67
2	A	480	HEM	CAC-C3C-C4C	-2.16	119.66	124.82
2	D	480	HEM	O1A-CGA-CBA	-2.16	116.24	123.09
2	C	480	HEM	O1D-CGD-CBD	-2.16	116.25	123.09
2	C	480	HEM	CHA-C4D-ND	2.15	127.03	124.37
2	A	480	HEM	CBC-CAC-C3C	-2.10	117.01	127.53
2	C	480	HEM	CAB-C3B-C2B	-2.09	121.65	128.43
2	D	480	HEM	C4B-C3B-C2B	2.08	109.19	107.28
2	D	480	HEM	C3B-C2B-C1B	2.06	107.96	106.41
2	C	480	HEM	CHD-C4C-NC	2.05	126.68	124.45

There are no chirality outliers.

All (2) torsion outliers are listed below:

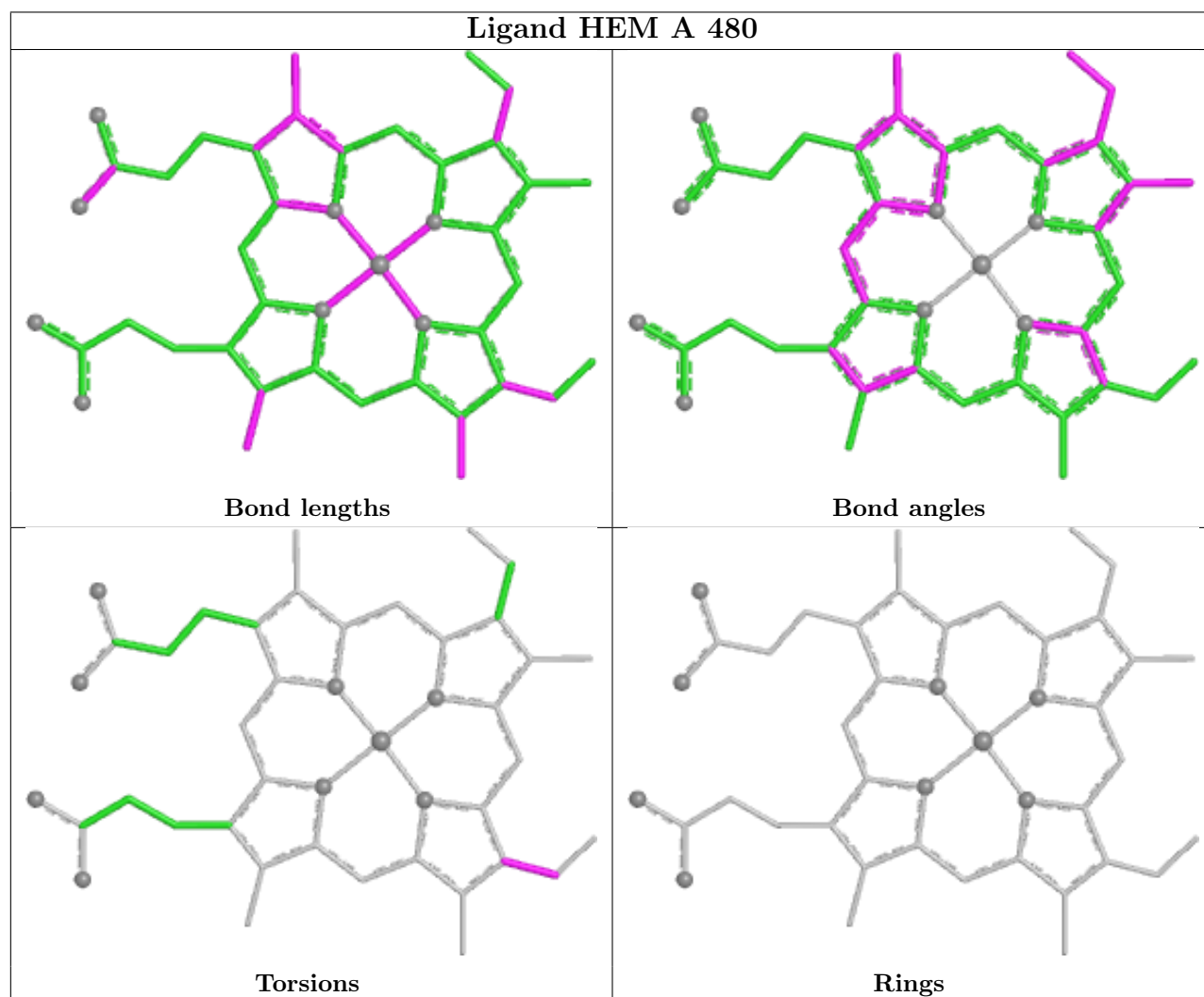
Mol	Chain	Res	Type	Atoms
2	A	480	HEM	C4B-C3B-CAB-CBB
2	A	480	HEM	C2B-C3B-CAB-CBB

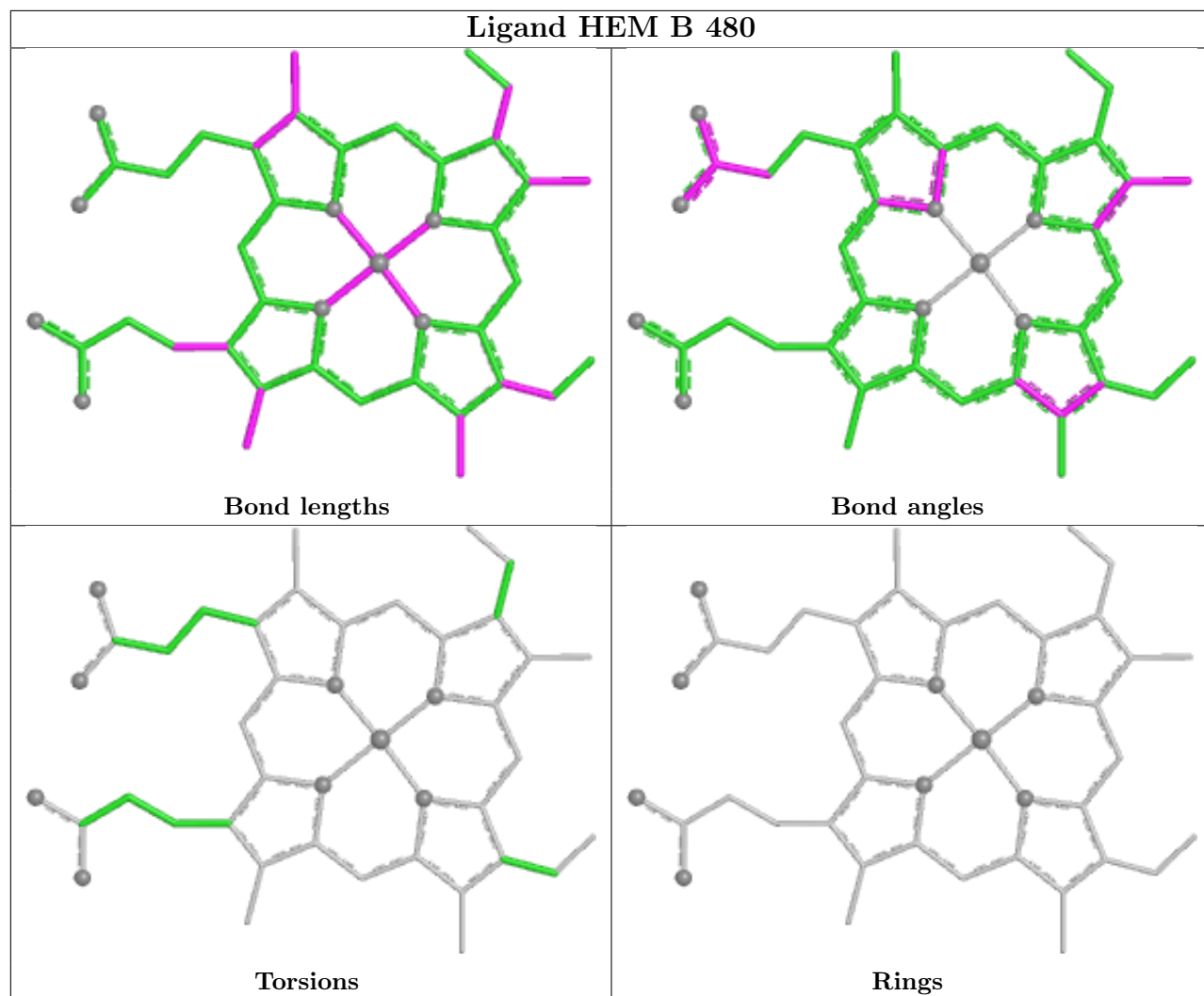
There are no ring outliers.

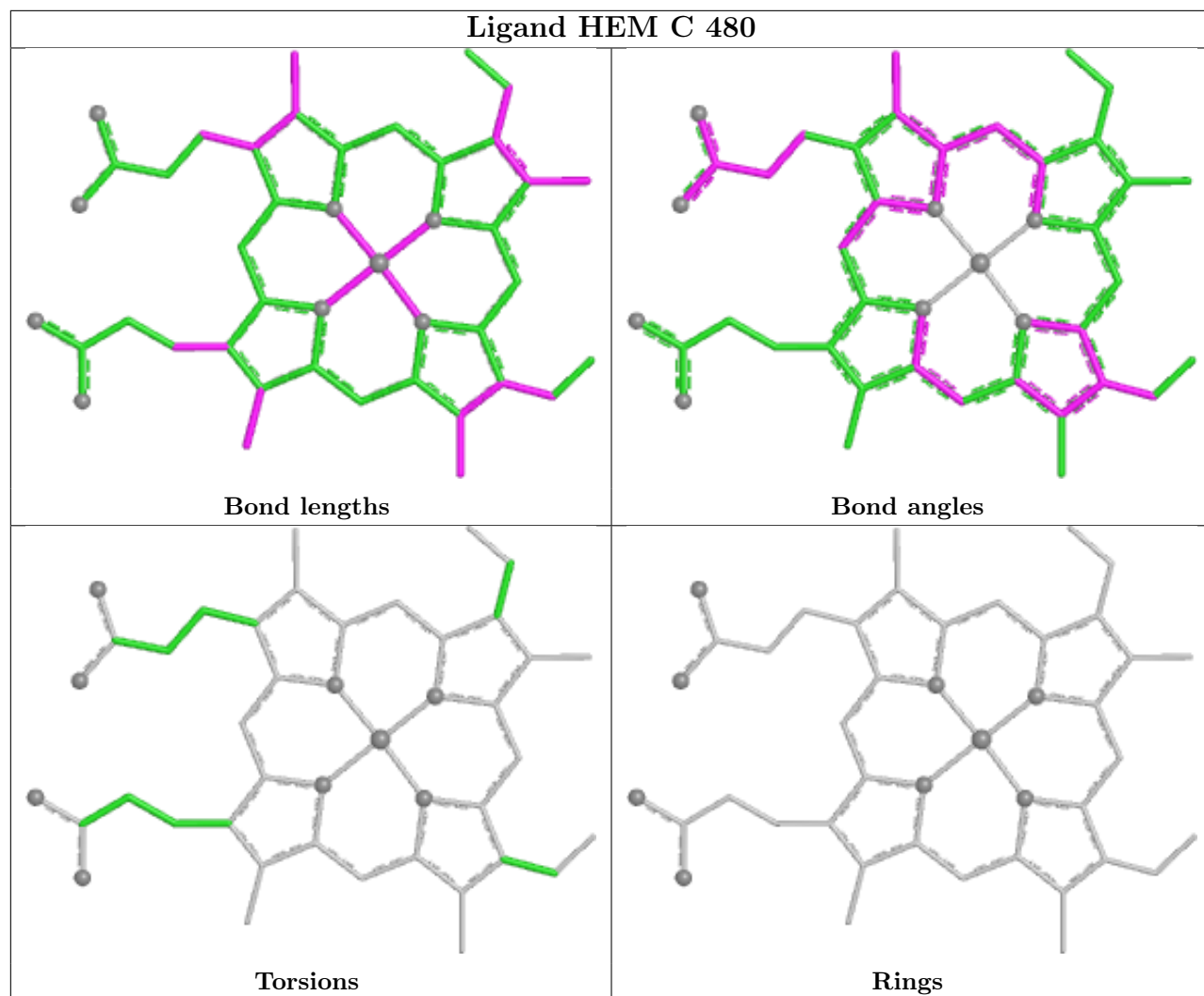
4 monomers are involved in 9 short contacts:

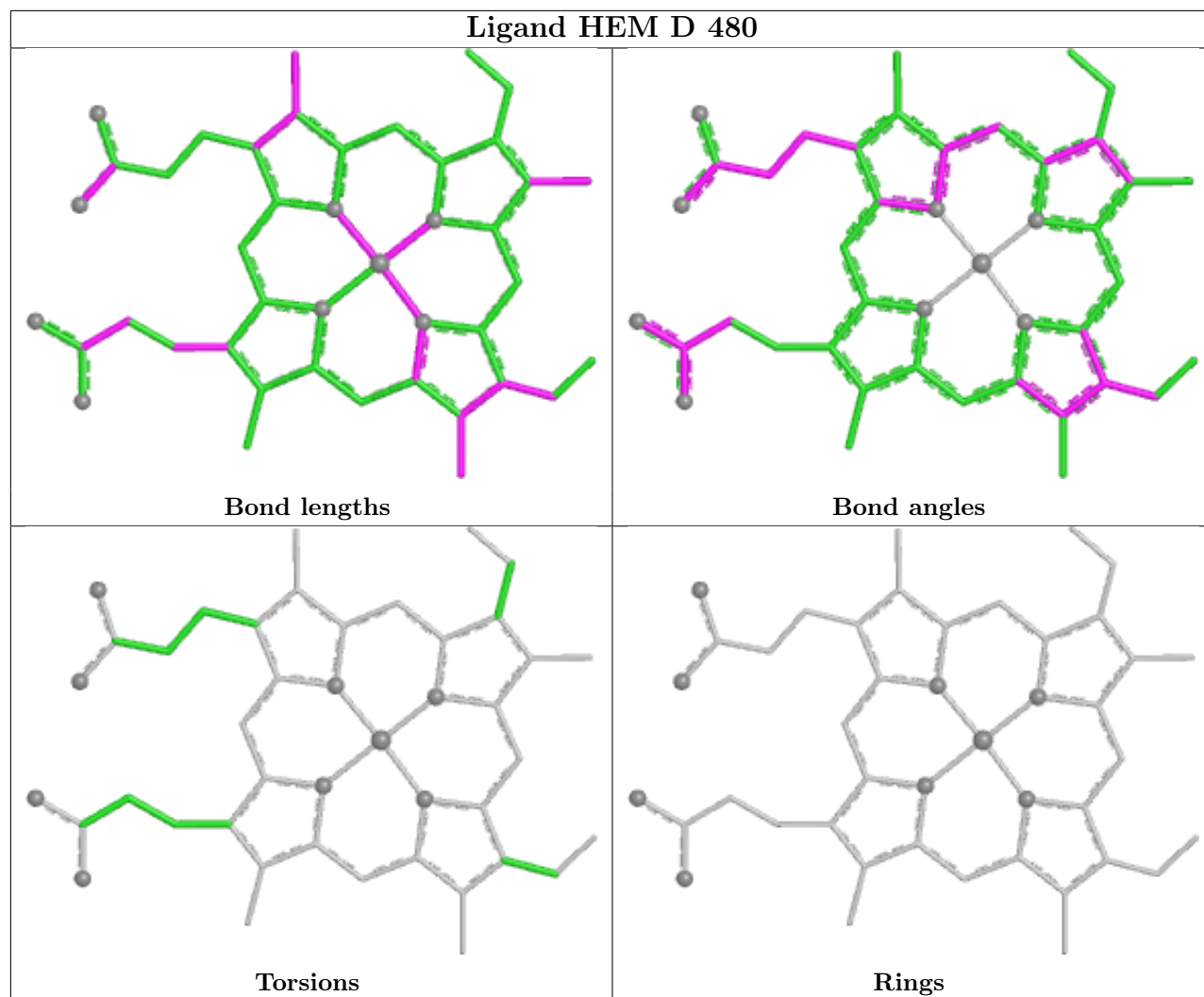
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	480	HEM	2	0
2	B	480	HEM	2	0
2	C	480	HEM	4	0
2	D	480	HEM	1	0

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









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	448/450 (99%)	-0.02	7 (1%) 70 74	16, 30, 47, 70	0
1	B	444/450 (98%)	0.18	10 (2%) 61 65	19, 33, 49, 61	0
1	C	447/450 (99%)	0.27	12 (2%) 56 60	21, 37, 58, 70	0
1	D	448/450 (99%)	0.35	16 (3%) 46 49	25, 39, 57, 69	0
All	All	1787/1800 (99%)	0.19	45 (2%) 58 62	16, 35, 55, 70	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	SER	4.3
1	A	257	SER	4.2
1	C	155	ALA	4.0
1	D	139	PHE	3.7
1	B	252	VAL	3.6
1	D	136	ILE	3.4
1	A	29	GLY	3.4
1	B	313	VAL	3.2
1	D	142	PHE	3.2
1	C	272	ASP	3.2
1	B	476	ARG	3.0
1	B	447	LEU	2.9
1	C	165	ILE	2.9
1	D	318	ALA	2.9
1	C	45	ILE	2.8
1	D	373	VAL	2.8
1	D	39	VAL	2.7
1	D	40	PRO	2.6
1	D	29	GLY	2.6
1	B	317	GLU	2.5
1	C	156	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	272	ASP	2.5
1	C	447	LEU	2.5
1	D	46	ILE	2.5
1	C	162	GLU	2.5
1	D	140	GLN	2.5
1	B	39	VAL	2.4
1	D	37	VAL	2.4
1	B	155	ALA	2.4
1	A	254	LYS	2.4
1	B	40	PRO	2.4
1	D	144	PRO	2.4
1	B	405	ASP	2.3
1	C	442	SER	2.3
1	A	253	ASN	2.3
1	D	34	VAL	2.2
1	A	458	HIS	2.2
1	D	326	PHE	2.1
1	C	313	VAL	2.1
1	D	137	ALA	2.1
1	C	317	GLU	2.1
1	C	448	LEU	2.1
1	D	45	ILE	2.0
1	C	148	HIS	2.0
1	B	318	ALA	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](#)

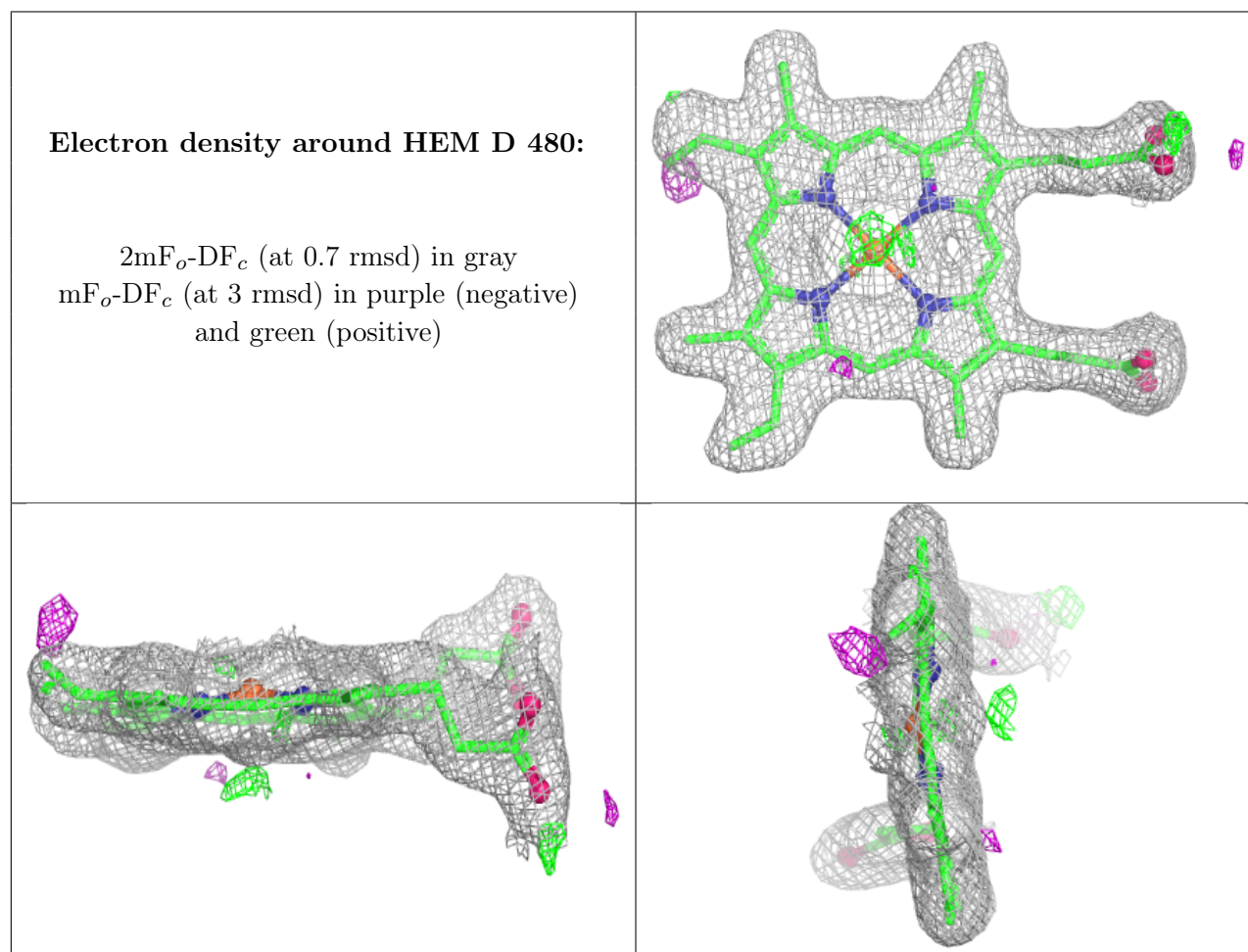
There are no oligosaccharides in this entry.

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.

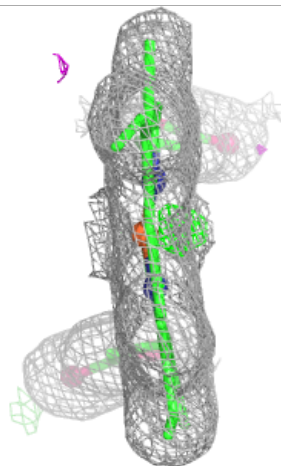
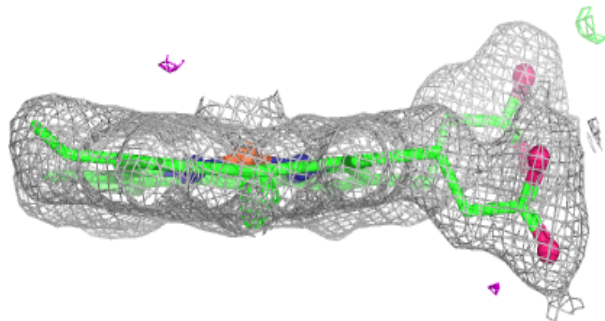
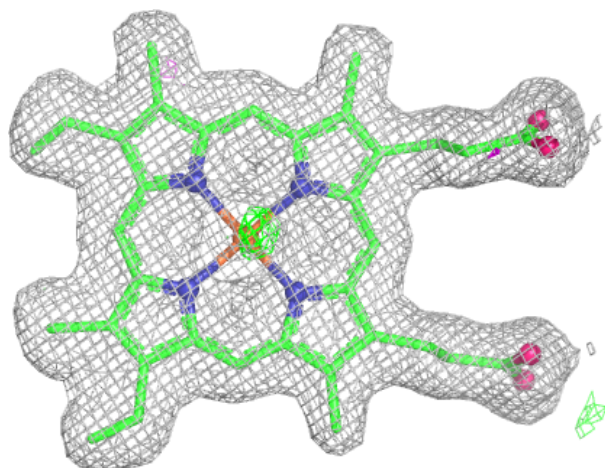
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	D	480	43/43	0.97	0.07	22,28,35,40	0
2	HEM	C	480	43/43	0.98	0.05	17,21,26,34	0
2	HEM	B	480	43/43	0.98	0.05	18,21,27,35	0
2	HEM	A	480	43/43	0.99	0.05	14,18,26,34	0

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.



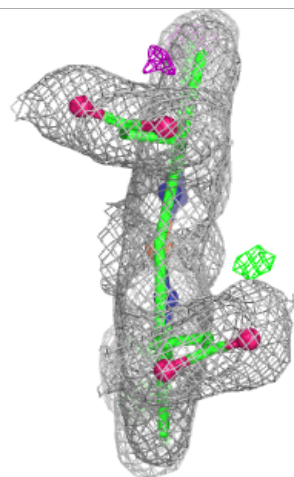
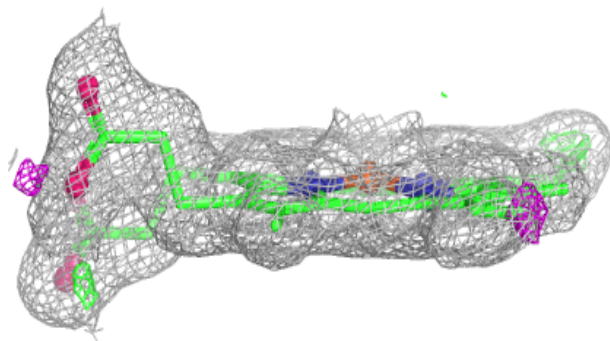
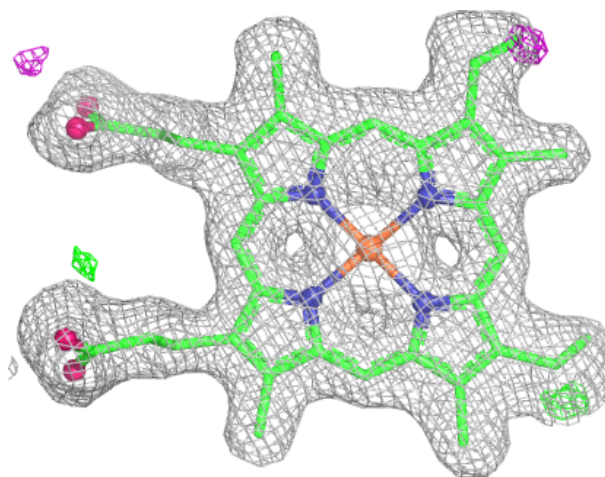
Electron density around HEM C 480:

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



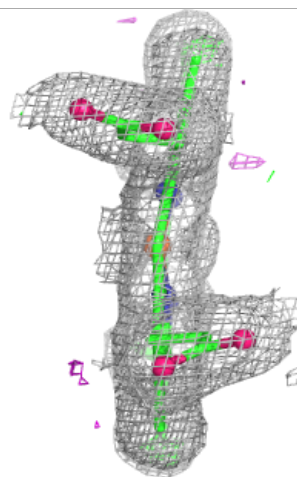
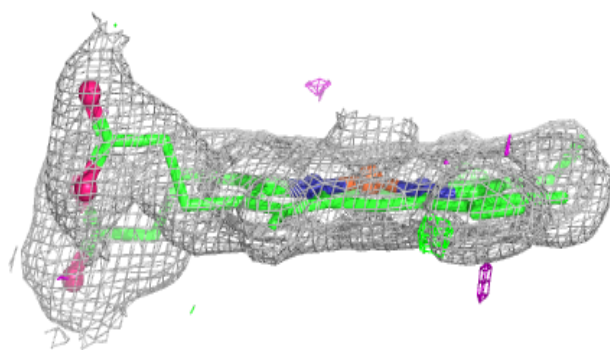
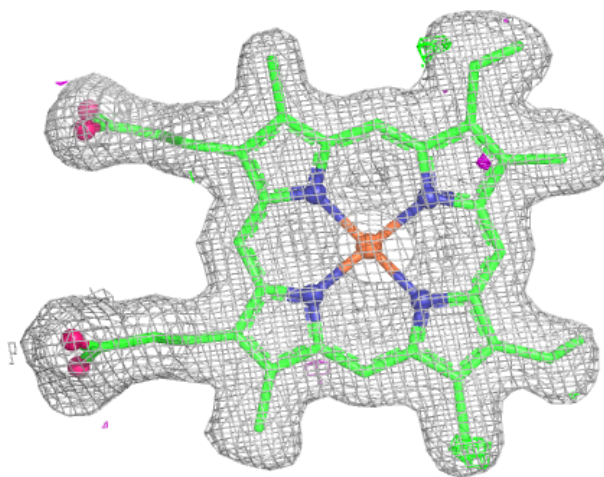
Electron density around HEM B 480:

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



Electron density around HEM A 480:

$2mF_o-DF_c$ (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.