



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:25 AM UTC

PDB ID : 1N97 / pdb_00001n97
Title : Crystal Structure of CYP175A1 from *Thermus thermophilus* strain HB27
Authors : Yano, J.K.; Blasco, F.; Li, H.; Schmid, R.D.; Henne, A.; Poulos, T.L.
Deposited on : 2002-11-22
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	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

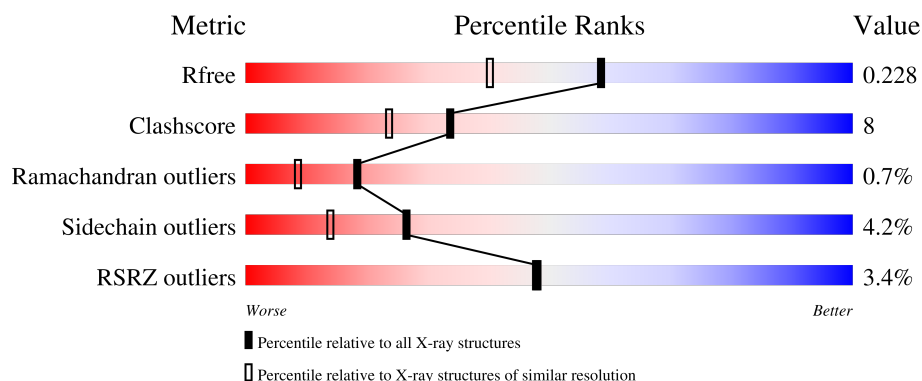
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	389	4% 79% 17% ...
1	B	389	3% 78% 19% ...

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	SRT	A	601	X	X	-	-
2	SRT	B	602	X	-	-	-

2 Entry composition [i](#)

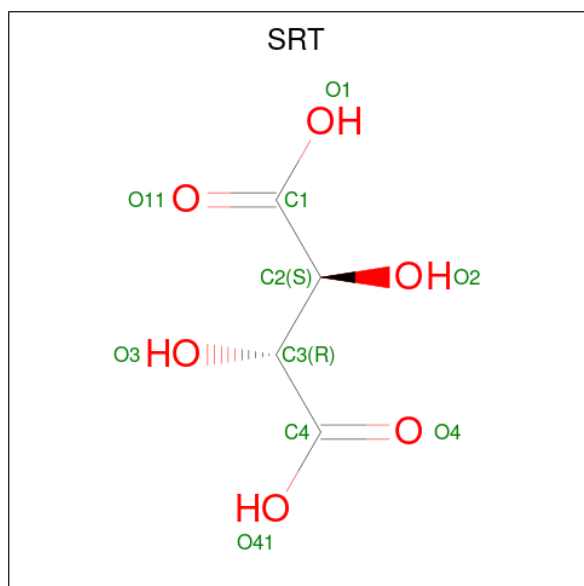
There are 5 unique types of molecules in this entry. The entry contains 6832 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CYP175A1.

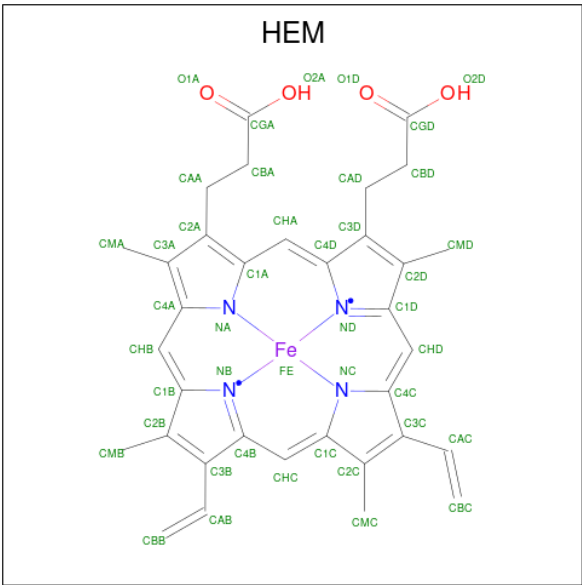
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			3052	1972	557	518	5			
1	B	385	Total	C	N	O	S	27	0	0
			3074	1985	560	524	5			

- Molecule 2 is S,R MESO-TARTARIC ACID (CCD ID: SRT) (formula: $C_4H_6O_6$).



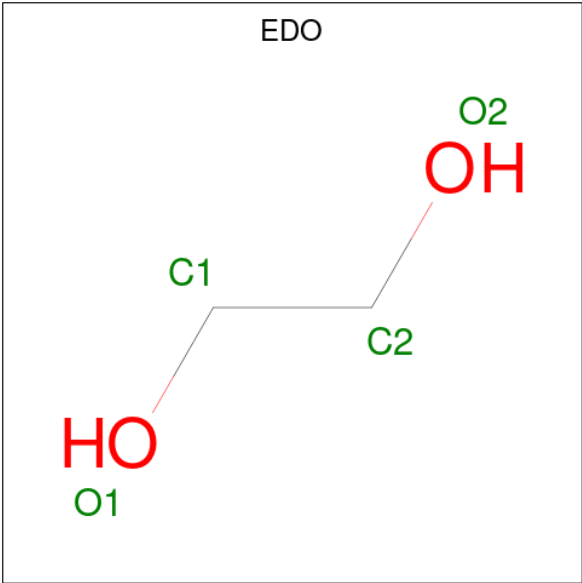
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		
2	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

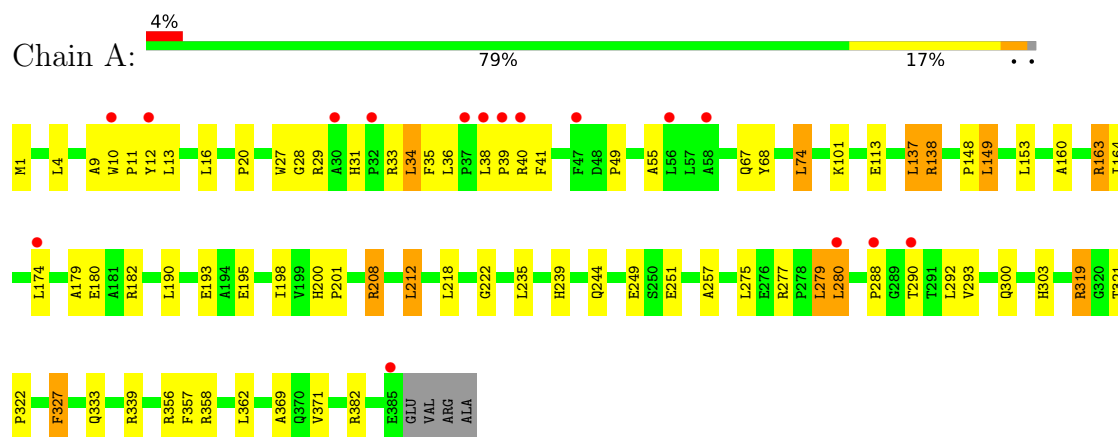
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	206	Total O 206 206	0	0
5	B	322	Total O 322 322	0	0

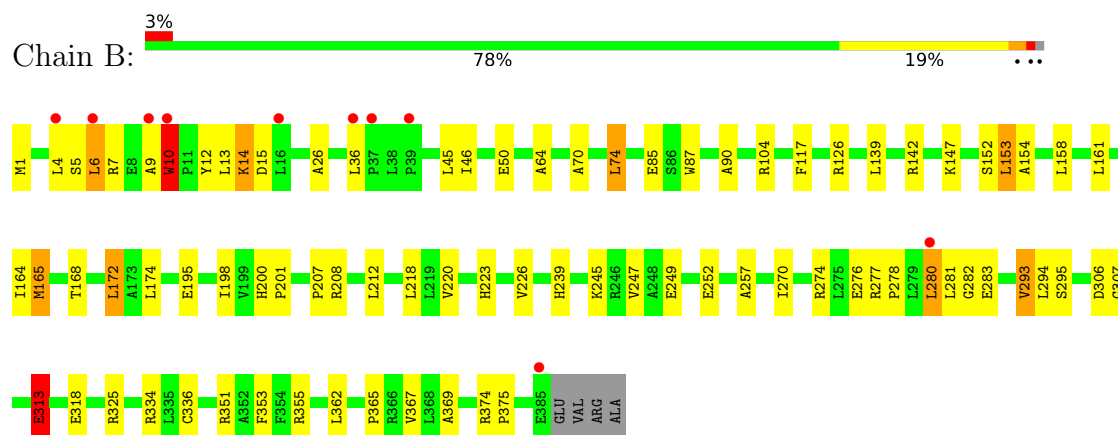
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: CYP175A1



• Molecule 1: CYP175A1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.54Å 90.70Å 74.52Å 90.00° 99.68° 90.00°	Depositor
Resolution (Å)	19.99 – 1.80 19.99 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.0 (19.99-1.80) 92.0 (19.99-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.92 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.182 , 0.222 0.190 , 0.228	Depositor DCC
R_{free} test set	3764 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6832	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 5.57% 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, SRT, EDO

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	1.40	10/3136 (0.3%)	1.17	4/4263 (0.1%)
1	B	1.75	31/3158 (1.0%)	1.33	15/4288 (0.3%)
All	All	1.58	41/6294 (0.7%)	1.25	19/8551 (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	B	0	1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	10	TRP	C-N	-20.18	1.09	1.34
1	B	13	LEU	C-N	17.75	1.58	1.33
1	B	1	MET	SD-CE	-9.75	1.55	1.79
1	B	90	ALA	C-O	-7.90	1.14	1.24
1	A	257	ALA	CA-CB	7.26	1.64	1.53
1	B	223	HIS	C-O	7.08	1.29	1.23
1	B	165	MET	SD-CE	-6.89	1.62	1.79
1	A	160	ALA	CA-CB	-6.66	1.43	1.53
1	B	50	GLU	C-O	-6.60	1.16	1.24
1	B	198	ILE	CA-CB	-6.20	1.45	1.54
1	B	313	GLU	CD-OE1	6.12	1.36	1.25
1	A	322	PRO	CA-C	5.98	1.59	1.52
1	A	293	VAL	CA-CB	-5.97	1.46	1.54
1	B	313	GLU	CD-OE2	-5.89	1.14	1.25
1	B	26	ALA	C-O	-5.87	1.17	1.24
1	B	295	SER	C-O	5.66	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	GLN	CA-C	-5.65	1.45	1.52
1	B	293	VAL	CA-CB	-5.51	1.47	1.54
1	B	257	ALA	CA-CB	5.44	1.61	1.53
1	B	325	ARG	CB-CG	-5.43	1.36	1.52
1	B	369	ALA	CA-CB	-5.39	1.45	1.52
1	B	147	LYS	C-O	-5.35	1.18	1.24
1	A	319	ARG	CG-CD	5.34	1.68	1.52
1	A	369	ALA	CA-CB	-5.33	1.45	1.52
1	B	104	ARG	C-O	-5.31	1.17	1.24
1	B	154	ALA	CA-CB	5.30	1.61	1.53
1	B	26	ALA	CA-CB	-5.30	1.45	1.53
1	B	307	GLY	C-O	5.30	1.30	1.24
1	A	327	PHE	CA-CB	5.29	1.61	1.53
1	B	334	ARG	CA-C	5.27	1.60	1.52
1	B	152	SER	CA-C	5.27	1.59	1.52
1	B	374	ARG	C-N	-5.26	1.28	1.33
1	B	226	VAL	CA-CB	5.24	1.61	1.54
1	A	321	THR	CB-CG2	-5.19	1.35	1.52
1	B	64	ALA	CA-CB	5.18	1.59	1.52
1	B	353	PHE	CA-CB	5.13	1.61	1.53
1	B	375	PRO	CA-CB	-5.12	1.47	1.53
1	B	367	VAL	N-CA	5.11	1.52	1.46
1	A	20	PRO	CA-C	5.09	1.59	1.52
1	B	87	TRP	N-CA	5.07	1.52	1.46
1	B	212	LEU	CA-C	5.01	1.59	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	TRP	O-C-N	-10.90	108.79	121.32
1	B	201	PRO	CA-C-O	-8.76	113.81	120.73
1	A	201	PRO	CA-C-O	-8.31	114.17	120.73
1	B	10	TRP	CA-C-N	7.81	127.36	118.85
1	B	10	TRP	C-N-CA	7.81	127.36	118.85
1	B	201	PRO	O-C-N	7.38	124.62	121.15
1	B	139	LEU	N-CA-C	6.58	118.11	111.07
1	B	153	LEU	N-CA-C	-6.39	104.40	111.36
1	B	90	ALA	N-CA-C	-6.24	104.56	111.36
1	B	13	LEU	CA-C-N	-6.07	109.95	121.54
1	B	13	LEU	C-N-CA	-6.07	109.95	121.54
1	B	85	GLU	N-CA-C	5.42	117.27	111.36
1	B	306	ASP	N-CA-C	-5.31	104.08	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	HIS	CA-C-N	5.30	123.48	119.66
1	A	200	HIS	C-N-CA	5.30	123.48	119.66
1	B	70	ALA	N-CA-C	-5.15	105.58	111.14
1	A	251	GLU	N-CA-C	-5.08	105.75	111.28
1	B	200	HIS	CA-C-N	5.05	123.29	119.66
1	B	200	HIS	C-N-CA	5.05	123.29	119.66

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	10	TRP	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3052	0	3082	62	0
1	B	3074	0	3119	34	1
2	A	10	0	5	1	0
2	B	10	0	4	0	0
3	A	43	0	30	2	0
3	B	43	0	30	1	0
4	A	28	0	42	3	0
4	B	44	0	66	9	0
5	A	206	0	0	3	1
5	B	322	0	0	6	1
All	All	6832	0	6378	97	2

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 8.

All (97) 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:218:LEU:HD21	5:A:734:HOH:O	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HB2	1:A:164:ILE:CD1	2.17	0.74
1:A:280:LEU:H	1:A:280:LEU:HD23	1.52	0.74
1:B:74:LEU:HD12	1:B:161:LEU:HG	1.70	0.73
1:A:292:LEU:HD12	1:A:292:LEU:N	2.05	0.72
1:A:300:GLN:HE21	1:A:327:PHE:H	1.37	0.72
1:A:138:ARG:HH11	1:A:138:ARG:HB3	1.55	0.71
1:B:195:GLU:OE2	1:B:208:ARG:NH2	2.24	0.70
1:A:249:GLU:OE1	5:A:764:HOH:O	2.11	0.67
1:A:163:ARG:HD3	1:A:180:GLU:OE2	1.95	0.66
1:A:280:LEU:H	1:A:280:LEU:CD2	2.08	0.66
4:B:709:EDO:H21	5:B:980:HOH:O	1.97	0.64
1:A:113:GLU:OE2	1:A:138:ARG:NH1	2.30	0.64
1:B:280:LEU:H	1:B:280:LEU:HD23	1.63	0.62
1:A:10:TRP:HZ2	1:A:39:PRO:HG2	1.63	0.62
1:B:351:ARG:NH2	1:B:355:ARG:HH21	1.96	0.62
1:A:113:GLU:OE2	1:A:138:ARG:CZ	2.48	0.61
1:A:74:LEU:HB2	1:A:164:ILE:HD12	1.81	0.60
1:A:275:LEU:HD13	1:A:292:LEU:HD11	1.84	0.60
1:A:13:LEU:C	1:A:13:LEU:HD13	2.26	0.59
1:A:198:ILE:HD13	1:A:212:LEU:HD13	1.84	0.59
1:A:292:LEU:N	1:A:292:LEU:CD1	2.66	0.58
1:A:138:ARG:HH11	1:A:138:ARG:CB	2.15	0.58
1:A:358:ARG:HH11	1:A:358:ARG:HG2	1.68	0.58
1:A:1:MET:HE2	1:A:34:LEU:C	2.29	0.58
1:B:9:ALA:O	1:B:14:LYS:HB2	2.05	0.57
1:A:10:TRP:CZ2	1:A:39:PRO:HG2	2.39	0.57
1:A:382:ARG:NE	5:A:898:HOH:O	2.37	0.57
1:A:67:GLN:HE21	4:A:715:EDO:H21	1.69	0.57
1:A:49:PRO:HD3	1:A:303:HIS:CD2	2.39	0.57
1:A:239:HIS:HE1	1:A:362:LEU:O	1.88	0.57
1:A:163:ARG:HA	1:A:163:ARG:HE	1.69	0.56
1:A:275:LEU:HD13	1:A:292:LEU:CD1	2.35	0.56
1:A:358:ARG:HG2	1:A:358:ARG:NH1	2.20	0.56
1:A:40:ARG:O	1:A:41:PHE:CD1	2.58	0.56
1:A:300:GLN:NE2	1:A:327:PHE:H	2.01	0.56
1:A:10:TRP:HB2	1:A:11:PRO:HD3	1.87	0.56
1:A:356:ARG:NH1	1:A:357:PHE:CZ	2.75	0.55
1:B:351:ARG:HG3	5:B:879:HOH:O	2.07	0.55
1:B:46:ILE:HD13	1:B:281:LEU:HD21	1.89	0.54
1:A:275:LEU:HD11	1:A:279:LEU:HD12	1.89	0.54
1:B:355:ARG:NH1	5:B:903:HOH:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LEU:HD12	1:A:190:LEU:HD12	1.89	0.54
1:B:5:SER:C	1:B:7:ARG:H	2.18	0.51
1:B:10:TRP:CD1	1:B:10:TRP:N	2.78	0.51
1:B:239:HIS:HE1	1:B:362:LEU:O	1.94	0.51
1:B:164:ILE:O	1:B:168:THR:HG23	2.10	0.51
1:A:275:LEU:HD22	1:A:290:THR:HB	1.93	0.51
1:B:252:GLU:CD	5:B:970:HOH:O	2.55	0.49
1:B:172:LEU:N	1:B:172:LEU:HD12	2.28	0.49
1:B:142:ARG:HG2	5:B:982:HOH:O	2.12	0.48
1:B:351:ARG:HH21	1:B:355:ARG:HH21	1.60	0.48
1:A:138:ARG:HH11	1:A:138:ARG:CG	2.25	0.48
1:B:207:PRO:HA	4:B:703:EDO:H11	1.94	0.48
1:A:222:GLY:HA3	3:A:602:HEM:HBC2	1.96	0.48
1:B:45:LEU:HD23	1:B:293:VAL:HB	1.97	0.47
1:A:1:MET:HB2	1:A:33:ARG:CB	2.45	0.47
1:A:29:ARG:HH11	1:A:29:ARG:HG2	1.79	0.47
1:B:270:ILE:HD13	1:B:294:LEU:O	2.15	0.46
1:B:4:LEU:HD12	1:B:36:LEU:HG	1.97	0.46
1:B:220:VAL:HA	4:B:710:EDO:H12	1.97	0.46
1:B:158:LEU:CD2	4:B:710:EDO:H22	2.46	0.46
1:B:158:LEU:HG	4:B:710:EDO:H22	1.98	0.46
1:A:163:ARG:NH1	1:A:180:GLU:OE2	2.35	0.46
1:B:117:PHE:CD1	4:B:707:EDO:H21	2.51	0.46
1:B:277:ARG:HB2	1:B:278:PRO:CD	2.46	0.45
1:A:239:HIS:CE1	1:A:362:LEU:O	2.70	0.45
1:A:28:GLY:HA2	1:A:31:HIS:O	2.17	0.44
1:A:138:ARG:HA	1:A:148:PRO:HB3	1.98	0.44
1:A:137:LEU:HD22	1:A:149:LEU:HB2	1.98	0.44
1:A:333:GLN:HE22	4:A:714:EDO:H21	1.82	0.44
1:A:36:LEU:HB3	1:A:38:LEU:CD2	2.47	0.44
1:A:29:ARG:HG2	1:A:29:ARG:NH1	2.32	0.43
1:B:313:GLU:H	1:B:313:GLU:CD	2.27	0.43
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.83	0.43
1:A:1:MET:HE2	1:A:35:PHE:HB2	2.00	0.43
1:A:68:TYR:OH	3:A:602:HEM:O2A	2.37	0.43
1:A:174:LEU:O	1:A:174:LEU:HG	2.19	0.43
1:A:195:GLU:CD	1:A:208:ARG:HH21	2.27	0.43
1:B:126:ARG:HH22	4:B:708:EDO:H21	1.84	0.43
1:B:117:PHE:CG	4:B:707:EDO:H21	2.54	0.43
1:B:247:VAL:O	1:B:351:ARG:HD2	2.18	0.43
1:A:55:ALA:HB1	1:A:292:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ALA:HA	1:A:182:ARG:HH11	1.85	0.42
1:A:4:LEU:HD13	1:A:12:TYR:HD1	1.83	0.42
1:A:101:LYS:HG3	4:A:717:EDO:H11	2.01	0.42
1:B:245:LYS:NZ	1:B:249:GLU:OE1	2.53	0.42
1:B:142:ARG:HD3	5:B:934:HOH:O	2.20	0.42
1:A:16:LEU:HD21	1:A:27:TRP:CZ3	2.55	0.41
1:A:153:LEU:HA	1:A:193:GLU:OE2	2.19	0.41
1:B:336:CYS:HA	3:B:603:HEM:CHA	2.50	0.41
1:B:117:PHE:CE1	4:B:707:EDO:H12	2.56	0.41
1:A:9:ALA:HB1	1:A:38:LEU:HD22	2.02	0.41
1:A:339:ARG:HH22	2:A:601:SRT:C4	2.34	0.41
1:A:138:ARG:NH1	1:A:138:ARG:CG	2.83	0.41
1:A:277:ARG:HA	1:A:288:PRO:HB3	2.02	0.41
1:B:274:ARG:HG2	1:B:274:ARG:HH11	1.87	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:748:HOH:O	5:B:1016:HOH:O[2_645]	1.70	0.50
1:B:252:GLU:OE1	5:A:867:HOH:O[2_656]	2.10	0.10

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	383/389 (98%)	375 (98%)	7 (2%)	1 (0%)	36	25
1	B	383/389 (98%)	368 (96%)	11 (3%)	4 (1%)	12	4
All	All	766/778 (98%)	743 (97%)	18 (2%)	5 (1%)	18	8

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	14	LYS
1	A	208	ARG
1	B	6	LEU
1	B	12	TYR
1	B	282	GLY

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	305/319 (96%)	293 (96%)	12 (4%)	28	16
1	B	310/319 (97%)	296 (96%)	14 (4%)	24	12
All	All	615/638 (96%)	589 (96%)	26 (4%)	26	14

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	74	LEU
1	A	137	LEU
1	A	138	ARG
1	A	149	LEU
1	A	163	ARG
1	A	212	LEU
1	A	235	LEU
1	A	279	LEU
1	A	280	LEU
1	A	319	ARG
1	A	371	VAL
1	B	6	LEU
1	B	15	ASP
1	B	74	LEU
1	B	153	LEU
1	B	165	MET
1	B	172	LEU
1	B	174	LEU

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Mol	Chain	Res	Type
1	B	218	LEU
1	B	276	GLU
1	B	280	LEU
1	B	283	GLU
1	B	313	GLU
1	B	318	GLU
1	B	365	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	67	GLN
1	A	156	HIS
1	A	200	HIS
1	A	259	GLN
1	A	300	GLN
1	A	333	GLN
1	A	370	GLN
1	B	31	HIS
1	B	200	HIS
1	B	239	HIS
1	B	259	GLN
1	B	333	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

22 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
4	EDO	A	705	-	3,3,3	0.54	0	2,2,2	0.44	0
4	EDO	B	704	-	3,3,3	0.61	0	2,2,2	0.03	0
4	EDO	A	717	-	3,3,3	0.46	0	2,2,2	0.30	0
4	EDO	A	715	-	3,3,3	0.50	0	2,2,2	0.29	0
4	EDO	B	710	-	3,3,3	0.43	0	2,2,2	0.26	0
3	HEM	B	603	1	50,50,50	1.79	8 (16%)	67,82,82	2.02	19 (28%)
4	EDO	B	701	-	3,3,3	0.76	0	2,2,2	0.16	0
4	EDO	A	718	-	3,3,3	0.46	0	2,2,2	0.54	0
3	HEM	A	602	1	50,50,50	2.14	17 (34%)	67,82,82	2.31	21 (31%)
4	EDO	B	709	-	3,3,3	0.48	0	2,2,2	0.29	0
4	EDO	B	708	-	3,3,3	0.52	0	2,2,2	0.42	0
4	EDO	B	707	-	3,3,3	0.76	0	2,2,2	0.44	0
4	EDO	B	711	-	3,3,3	0.61	0	2,2,2	0.85	0
4	EDO	B	703	-	3,3,3	0.29	0	2,2,2	0.55	0
4	EDO	B	706	-	3,3,3	0.40	0	2,2,2	0.29	0
2	SRT	B	602	-	9,9,9	1.18	1 (11%)	12,12,12	3.09	3 (25%)
4	EDO	A	714	-	3,3,3	0.33	0	2,2,2	0.42	0
2	SRT	A	601	-	9,9,9	1.20	1 (11%)	12,12,12	2.29	4 (33%)
4	EDO	B	702	-	3,3,3	0.82	0	2,2,2	0.29	0
4	EDO	A	719	-	3,3,3	0.37	0	2,2,2	0.70	0
4	EDO	A	713	-	3,3,3	0.38	0	2,2,2	0.40	0
4	EDO	B	712	-	3,3,3	0.58	0	2,2,2	0.17	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
4	EDO	A	705	-	-	1/1/1/1	-
4	EDO	B	704	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	717	-	-	0/1/1/1	-
4	EDO	A	715	-	-	1/1/1/1	-
4	EDO	B	710	-	-	1/1/1/1	-
3	HEM	B	603	1	-	4/14/54/54	-
4	EDO	B	701	-	-	1/1/1/1	-
4	EDO	A	718	-	-	0/1/1/1	-
3	HEM	A	602	1	-	2/14/54/54	-
4	EDO	B	709	-	-	0/1/1/1	-
4	EDO	B	708	-	-	1/1/1/1	-
4	EDO	B	707	-	-	1/1/1/1	-
4	EDO	B	711	-	-	0/1/1/1	-
4	EDO	B	703	-	-	0/1/1/1	-
4	EDO	B	706	-	-	0/1/1/1	-
2	SRT	B	602	-	2/2/4/4	8/12/12/12	-
4	EDO	A	714	-	-	1/1/1/1	-
2	SRT	A	601	-	2/2/4/4	10/12/12/12	-
4	EDO	B	702	-	-	0/1/1/1	-
4	EDO	A	719	-	-	1/1/1/1	-
4	EDO	A	713	-	-	0/1/1/1	-
4	EDO	B	712	-	-	1/1/1/1	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	HEM	FE-NC	-4.84	1.79	1.95
3	B	603	HEM	C3D-C2D	4.65	1.46	1.36
3	A	602	HEM	CMC-C2C	4.60	1.60	1.50
3	A	602	HEM	C3C-C4C	-4.57	1.38	1.46
3	B	603	HEM	FE-ND	4.43	2.08	1.94
3	A	602	HEM	FE-ND	4.24	2.08	1.94
3	A	602	HEM	FE-NB	4.03	2.07	1.94
3	B	603	HEM	C4D-ND	-4.00	1.33	1.40
3	A	602	HEM	C3D-C2D	3.95	1.45	1.36
3	A	602	HEM	C1C-NC	3.87	1.46	1.39
3	B	603	HEM	CMD-C2D	3.77	1.58	1.50
3	B	603	HEM	FE-NB	3.73	2.06	1.94
3	B	603	HEM	CBD-CGD	3.06	1.57	1.50
3	A	602	HEM	C3C-C2C	-2.78	1.31	1.37
3	A	602	HEM	C4C-NC	2.77	1.44	1.39
2	B	602	SRT	C3-C4	-2.74	1.48	1.52
2	A	601	SRT	O1-C1	2.69	1.39	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	HEM	C4D-ND	-2.65	1.35	1.40
3	A	602	HEM	C1A-C2A	-2.64	1.39	1.44
3	B	603	HEM	O2A-CGA	-2.57	1.22	1.30
3	A	602	HEM	C2A-C3A	-2.46	1.32	1.38
3	A	602	HEM	C1B-NB	-2.34	1.36	1.40
3	B	603	HEM	CBA-CGA	2.13	1.55	1.50
3	A	602	HEM	CHB-C1B	-2.05	1.34	1.38
3	A	602	HEM	C4B-NB	-2.04	1.34	1.38
3	A	602	HEM	CHD-C1D	-2.04	1.34	1.39
3	A	602	HEM	CAA-C2A	2.02	1.56	1.51

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	SRT	O2-C2-C3	-9.35	91.14	110.17
3	B	603	HEM	C4D-ND-C1D	6.82	113.28	105.21
3	A	602	HEM	C4C-NC-C1C	-6.72	94.87	105.82
3	A	602	HEM	C4C-C3C-C2C	6.56	112.50	106.81
3	A	602	HEM	C4D-ND-C1D	6.10	112.42	105.21
2	A	601	SRT	O2-C2-C3	-5.39	99.20	110.17
3	A	602	HEM	C3C-C2C-C1C	-5.30	102.03	107.05
3	B	603	HEM	C4C-C3C-C2C	5.04	111.18	106.81
3	B	603	HEM	CHD-C1D-ND	4.38	129.14	124.42
3	A	602	HEM	C1B-NB-C4B	4.37	110.38	105.21
3	B	603	HEM	C3B-C4B-NB	-4.29	106.38	109.47
3	A	602	HEM	C3B-C4B-NB	-4.29	106.39	109.47
3	B	603	HEM	CHC-C4B-NB	4.28	129.03	124.42
3	A	602	HEM	CHD-C1D-ND	3.88	128.60	124.42
3	B	603	HEM	C2D-C1D-ND	-3.82	105.49	109.90
3	A	602	HEM	C2C-C1C-NC	3.72	116.51	109.64
3	A	602	HEM	CHD-C4C-NC	-3.70	120.42	124.45
3	A	602	HEM	CHC-C1C-C2C	-3.59	118.03	125.49
2	B	602	SRT	C2-C3-C4	3.52	117.63	109.82
2	A	601	SRT	O3-C3-C4	3.37	117.89	110.69
3	B	603	HEM	C1B-NB-C4B	3.33	109.15	105.21
3	B	603	HEM	C3C-C2C-C1C	-3.22	104.00	107.05
3	A	602	HEM	C3D-C4D-ND	-3.19	106.68	110.17
3	A	602	HEM	CAD-CBD-CGD	-2.96	105.81	113.67
3	B	603	HEM	CHA-C4D-ND	2.72	127.73	124.37
2	A	601	SRT	O1-C1-C2	2.60	120.55	113.31
3	A	602	HEM	CHC-C4B-NB	2.59	127.21	124.42
3	B	603	HEM	CBD-CAD-C3D	-2.56	105.46	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	HEM	C2A-C1A-NA	2.54	112.97	110.15
3	A	602	HEM	CHA-C4D-ND	2.50	127.46	124.37
3	A	602	HEM	C2D-C1D-ND	-2.43	107.10	109.90
3	B	603	HEM	C4A-NA-C1A	-2.37	101.97	105.82
3	B	603	HEM	CAC-C3C-C2C	-2.31	120.92	128.43
3	B	603	HEM	C4B-C3B-C2B	2.29	109.38	107.28
2	B	602	SRT	O3-C3-C2	2.28	114.81	110.17
3	B	603	HEM	O1D-CGD-CBD	-2.27	115.90	123.09
3	A	602	HEM	CBD-CAD-C3D	-2.26	106.29	112.53
3	B	603	HEM	CAD-CBD-CGD	-2.21	107.81	113.67
3	B	603	HEM	C4C-NC-C1C	-2.18	102.26	105.82
2	A	601	SRT	O11-C1-C2	-2.18	115.80	121.62
3	A	602	HEM	O1D-CGD-CBD	-2.16	116.26	123.09
3	A	602	HEM	C1C-CHC-C4B	-2.13	121.48	126.02
3	A	602	HEM	CHB-C4A-NA	2.10	127.67	123.86
3	A	602	HEM	C4A-NA-C1A	-2.10	102.40	105.82
3	B	603	HEM	CBA-CAA-C2A	2.04	118.16	112.53
3	B	603	HEM	CHD-C4C-NC	-2.03	122.24	124.45
3	A	602	HEM	CMC-C2C-C1C	2.02	128.29	124.73

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	SRT	C2
2	A	601	SRT	C3
2	B	602	SRT	C2
2	B	602	SRT	C3

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	SRT	O2-C2-C3-O3
2	A	601	SRT	O3-C3-C4-O41
2	B	602	SRT	O2-C2-C3-O3
2	A	601	SRT	O2-C2-C3-C4
2	B	602	SRT	O2-C2-C3-C4
2	A	601	SRT	O3-C3-C4-O4
2	A	601	SRT	C2-C3-C4-O4
2	A	601	SRT	C2-C3-C4-O41
2	B	602	SRT	C2-C3-C4-O4
2	B	602	SRT	C2-C3-C4-O41
2	A	601	SRT	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	B	602	SRT	C1-C2-C3-O3
2	B	602	SRT	O3-C3-C4-O41
2	B	602	SRT	O3-C3-C4-O4
4	B	707	EDO	O1-C1-C2-O2
3	B	603	HEM	C2C-C3C-CAC-CBC
4	A	714	EDO	O1-C1-C2-O2
4	A	715	EDO	O1-C1-C2-O2
4	A	719	EDO	O1-C1-C2-O2
4	B	704	EDO	O1-C1-C2-O2
4	B	710	EDO	O1-C1-C2-O2
2	B	602	SRT	C1-C2-C3-C4
2	A	601	SRT	C1-C2-C3-C4
3	B	603	HEM	C4C-C3C-CAC-CBC
4	A	705	EDO	O1-C1-C2-O2
3	A	602	HEM	CAD-CBD-CGD-O1D
3	B	603	HEM	CAD-CBD-CGD-O1D
3	A	602	HEM	CAD-CBD-CGD-O2D
3	B	603	HEM	CAD-CBD-CGD-O2D
4	B	712	EDO	O1-C1-C2-O2
2	A	601	SRT	O11-C1-C2-O2
4	B	701	EDO	O1-C1-C2-O2
4	B	708	EDO	O1-C1-C2-O2
2	A	601	SRT	O1-C1-C2-O2

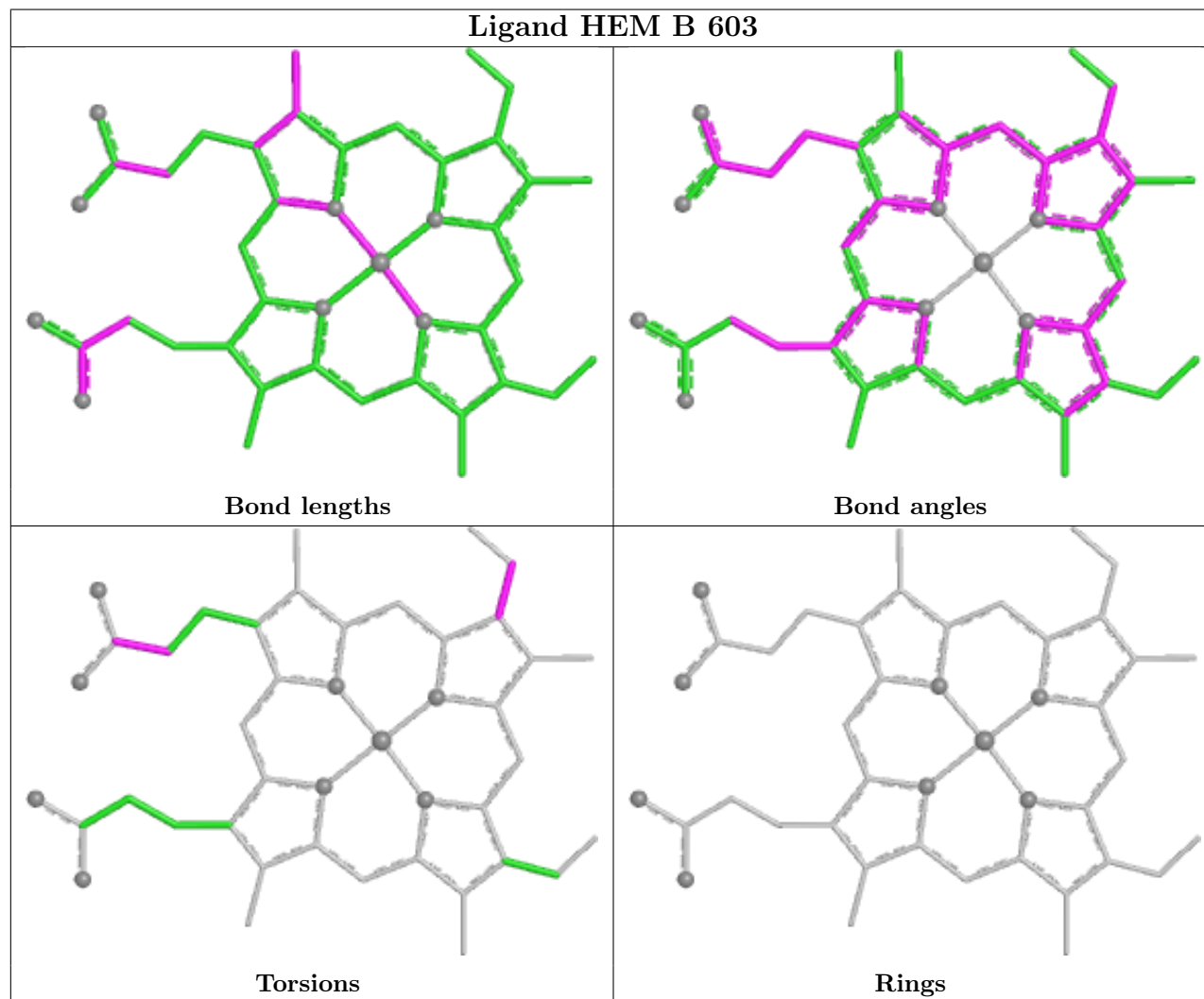
There are no ring outliers.

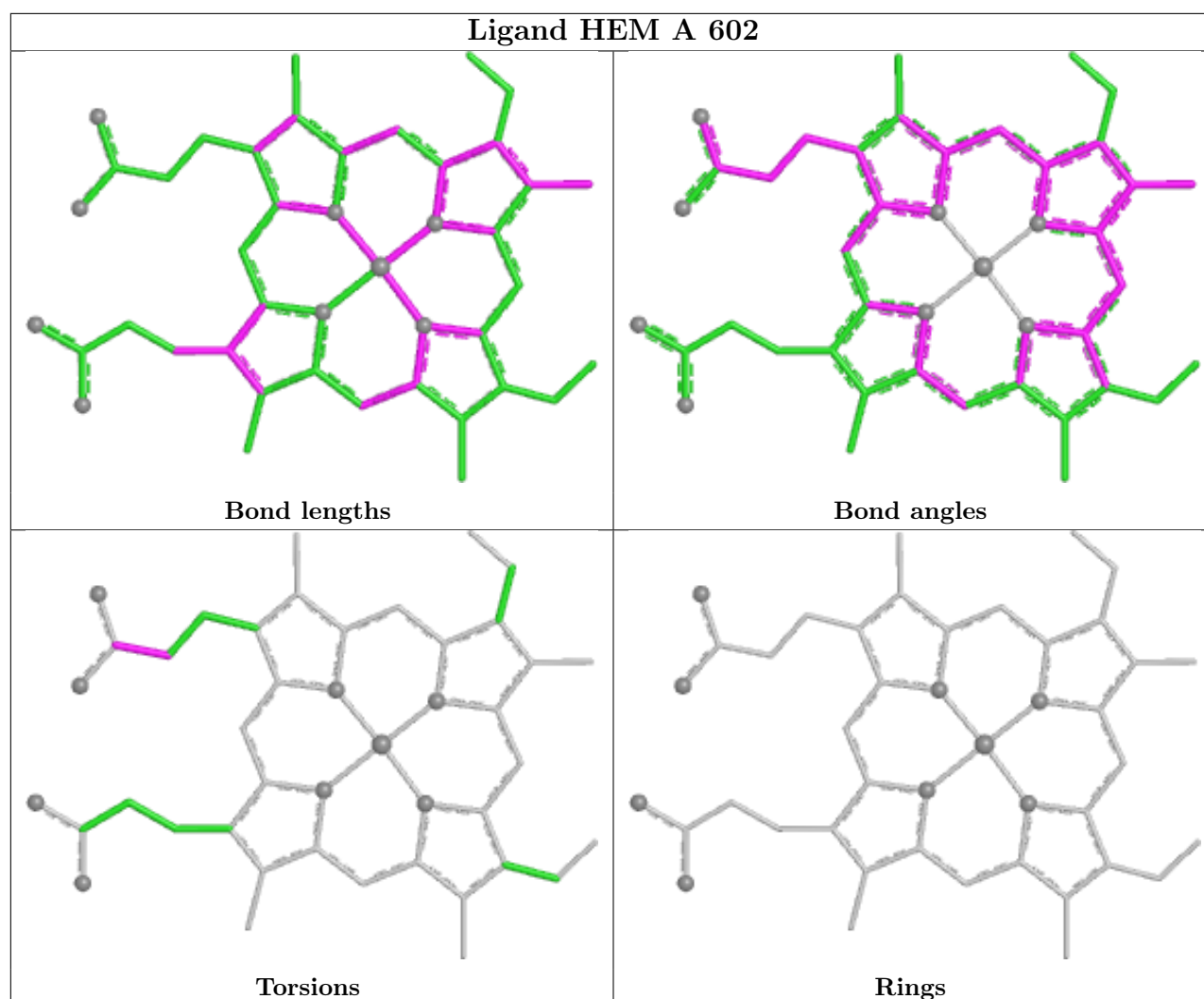
11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	717	EDO	1	0
4	A	715	EDO	1	0
4	B	710	EDO	3	0
3	B	603	HEM	1	0
3	A	602	HEM	2	0
4	B	709	EDO	1	0
4	B	708	EDO	1	0
4	B	707	EDO	3	0
4	B	703	EDO	1	0
4	A	714	EDO	1	0
2	A	601	SRT	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	10:TRP	C	11:PRO	N	1.09

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	385/389 (98%)	0.36	16 (4%)	40 40	20, 39, 59, 69	25 (6%)
1	B	382/389 (98%)	-0.12	10 (2%)	57 57	14, 26, 54, 82	54 (14%)
All	All	767/778 (98%)	0.12	26 (3%)	48 48	14, 32, 58, 82	79 (10%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	37	PRO	7.5
1	B	39	PRO	6.9
1	A	38	LEU	5.2
1	B	10	TRP	3.8
1	A	37	PRO	3.7
1	B	6	LEU	3.5
1	B	280	LEU	3.5
1	A	10	TRP	3.3
1	A	40	ARG	3.1
1	A	39	PRO	3.1
1	A	280	LEU	2.9
1	A	174	LEU	2.7
1	B	385	GLU	2.7
1	A	32	PRO	2.5
1	B	16	LEU	2.4
1	B	36	LEU	2.4
1	B	9	ALA	2.3
1	A	385	GLU	2.3
1	B	4	LEU	2.3
1	A	288	PRO	2.2
1	A	58	ALA	2.1
1	A	30	ALA	2.1
1	A	290	THR	2.0
1	A	56	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	47	PHE	2.0
1	A	12	TYR	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
4	EDO	B	708	4/4	0.67	0.14	60,63,68,68	0
4	EDO	A	714	4/4	0.68	0.11	69,70,70,71	0
4	EDO	A	719	4/4	0.73	0.12	58,66,66,71	0
4	EDO	A	715	4/4	0.74	0.12	67,70,70,72	0
4	EDO	B	704	4/4	0.78	0.16	58,64,67,70	0
4	EDO	A	717	4/4	0.79	0.13	62,68,68,69	0
4	EDO	A	713	4/4	0.79	0.12	69,69,69,69	0
4	EDO	B	709	4/4	0.82	0.14	55,64,69,71	0
2	SRT	A	601	10/10	0.83	0.10	41,49,55,56	0
4	EDO	A	705	4/4	0.84	0.13	50,51,54,59	0
4	EDO	B	712	4/4	0.86	0.09	60,62,62,63	0
4	EDO	B	707	4/4	0.88	0.21	40,44,50,50	0
4	EDO	A	718	4/4	0.88	0.11	45,48,50,54	0
4	EDO	B	703	4/4	0.89	0.10	45,47,50,53	0
4	EDO	B	706	4/4	0.89	0.14	39,48,49,55	0
4	EDO	B	711	4/4	0.90	0.12	33,40,43,45	0
4	EDO	B	710	4/4	0.90	0.14	38,45,46,53	0
4	EDO	B	702	4/4	0.91	0.09	33,38,39,42	0
2	SRT	B	602	10/10	0.91	0.08	32,36,41,41	0
4	EDO	B	701	4/4	0.94	0.08	33,37,39,41	0
3	HEM	A	602	43/43	0.98	0.05	18,24,32,37	0

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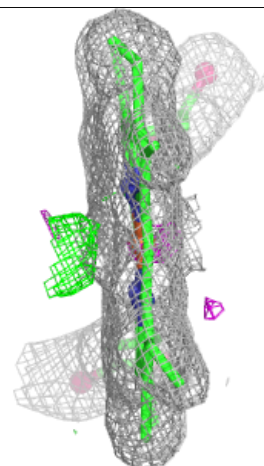
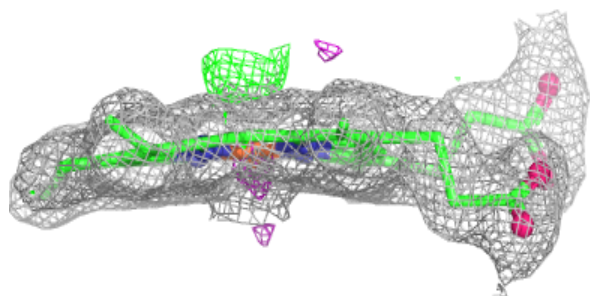
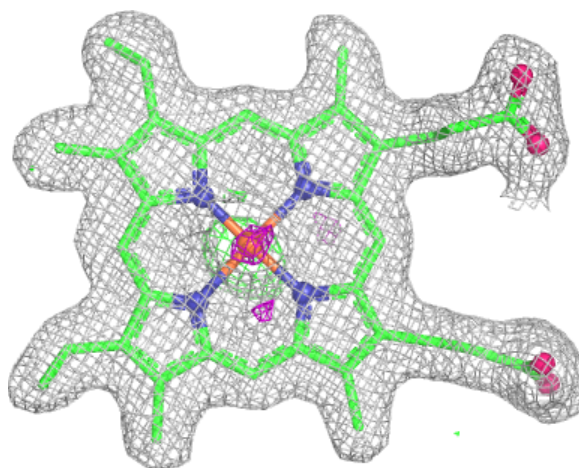
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEM	B	603	43/43	0.99	0.04	11,15,24,30	0

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.

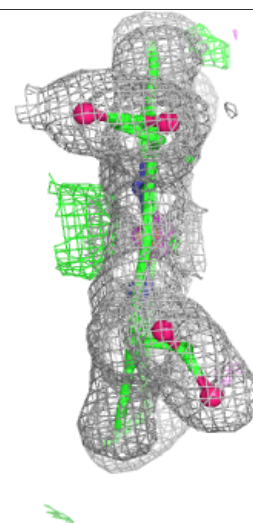
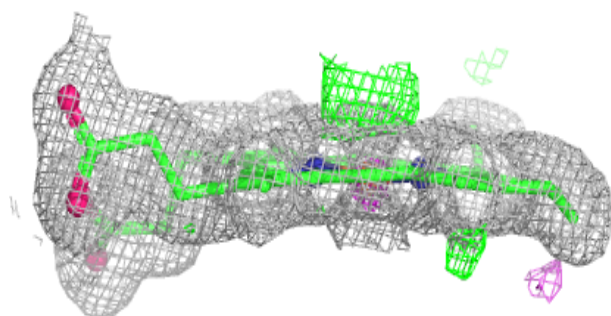
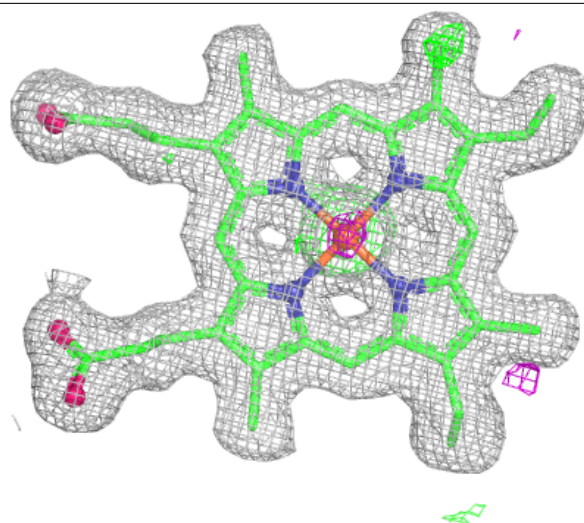
Electron density around HEM A 602:

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 603:

$2mF_o-DF_c$ (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.