WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 01:16 PM EDT

PDB ID	:	4L0D
Title	:	Crystal structure of delta516-525 human cystathionine beta-synthase containing C-terminal 6xHis-tag
Authors	:	Ereno, J.; Majtan, T.; Oyenarte, I.; Kraus, J.P.; Martinez-Cruz, L.A.
Deposited on	:	2013-05-31
Resolution	:	2.97 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.97 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.
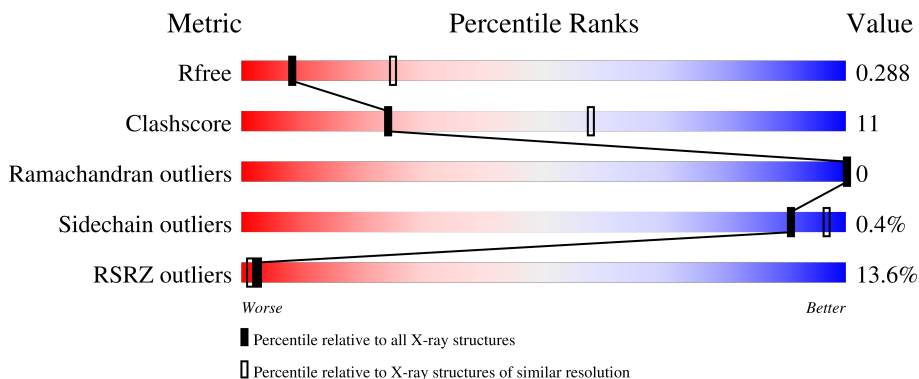
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 <=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	549	10% / 67% 23% 10%
1	B	549	14% / 68% 22% 10%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 7728 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 Cystathionine beta-synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total 3807	C 2413	N 667	O 705	S 22	0	1	0
1	B	496	Total 3805	C 2412	N 666	O 705	S 22	0	1	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	PRO	engineered mutation	UNP P35520
A	?	-	ILE	deletion	UNP P35520
A	?	-	GLN	deletion	UNP P35520
A	?	-	TYR	deletion	UNP P35520
A	?	-	HIS	deletion	UNP P35520
A	?	-	SER	deletion	UNP P35520
A	?	-	THR	deletion	UNP P35520
A	?	-	GLY	deletion	UNP P35520
A	?	-	LYS	deletion	UNP P35520
A	?	-	SER	deletion	UNP P35520
A	?	-	SER	deletion	UNP P35520
A	552	GLU	-	expression tag	UNP P35520
A	553	LEU	-	expression tag	UNP P35520
A	554	HIS	-	expression tag	UNP P35520
A	555	HIS	-	expression tag	UNP P35520
A	556	HIS	-	expression tag	UNP P35520
A	557	HIS	-	expression tag	UNP P35520
A	558	HIS	-	expression tag	UNP P35520
A	559	HIS	-	expression tag	UNP P35520
B	2	GLY	PRO	engineered mutation	UNP P35520
B	?	-	ILE	deletion	UNP P35520
B	?	-	GLN	deletion	UNP P35520
B	?	-	TYR	deletion	UNP P35520
B	?	-	HIS	deletion	UNP P35520
B	?	-	SER	deletion	UNP P35520

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP P35520
B	?	-	GLY	deletion	UNP P35520
B	?	-	LYS	deletion	UNP P35520
B	?	-	SER	deletion	UNP P35520
B	?	-	SER	deletion	UNP P35520
B	552	GLU	-	expression tag	UNP P35520
B	553	LEU	-	expression tag	UNP P35520
B	554	HIS	-	expression tag	UNP P35520
B	555	HIS	-	expression tag	UNP P35520
B	556	HIS	-	expression tag	UNP P35520
B	557	HIS	-	expression tag	UNP P35520
B	558	HIS	-	expression tag	UNP P35520
B	559	HIS	-	expression tag	UNP P35520

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).
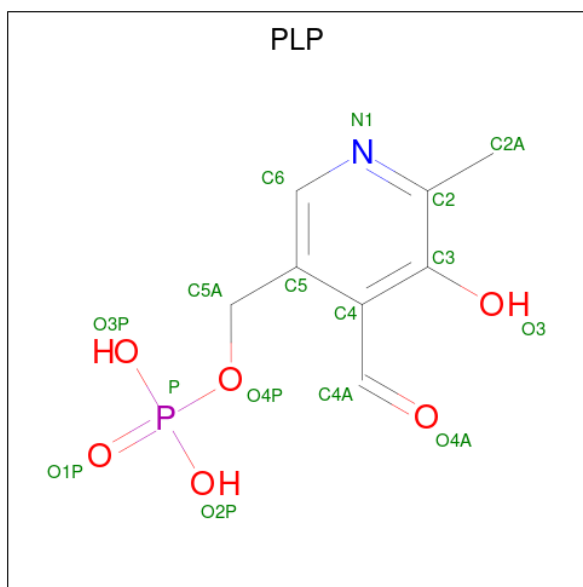
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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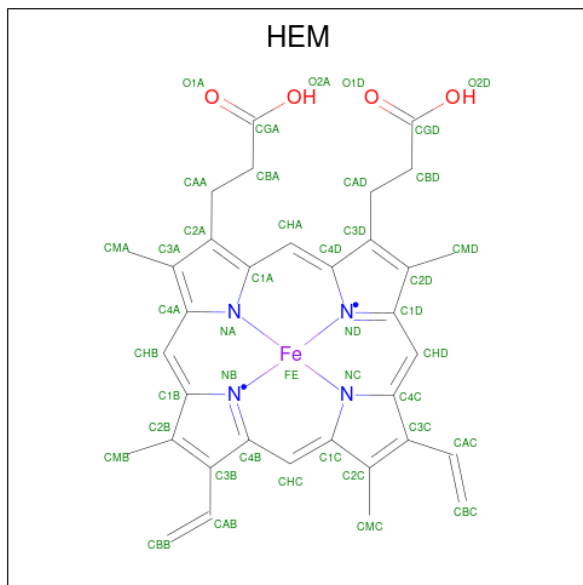
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HEM

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		

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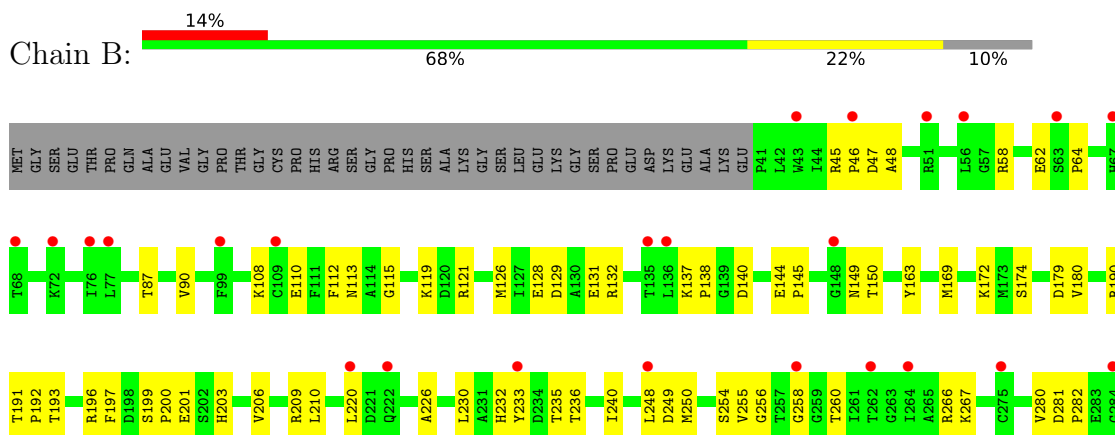, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cystathionine beta-synthase

Chain A:

• Molecule 1: Cystathionine beta-synthase

Chain B:
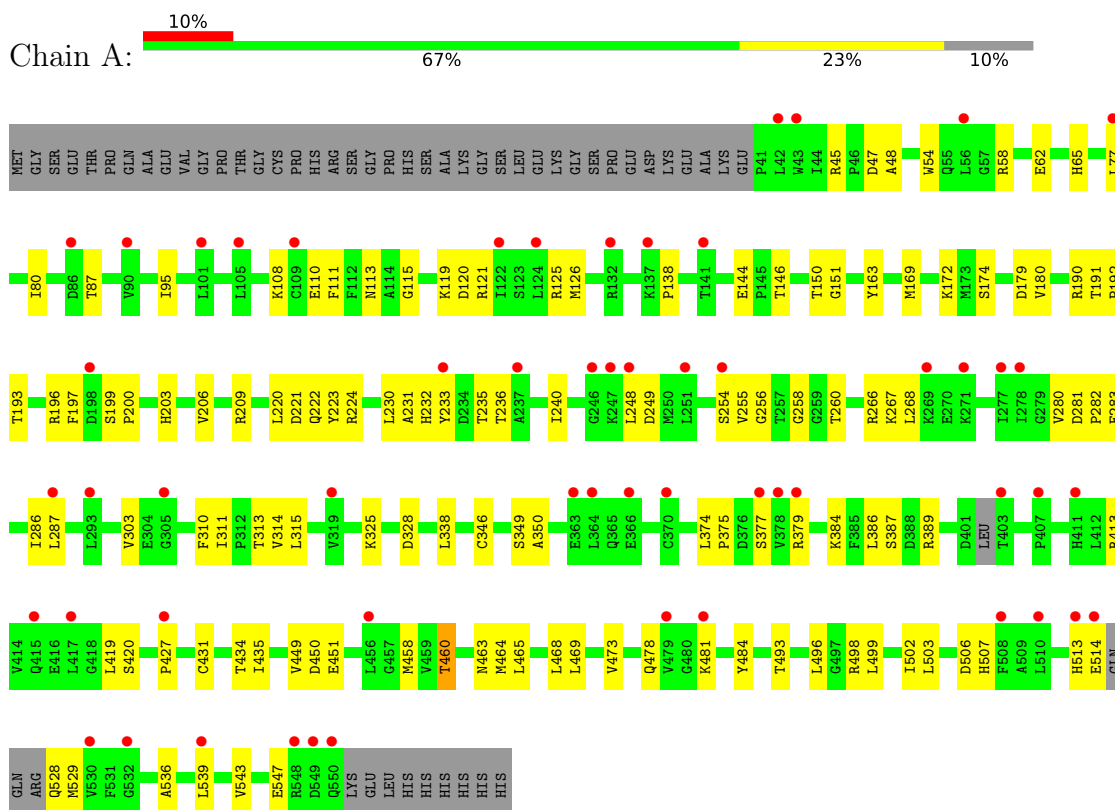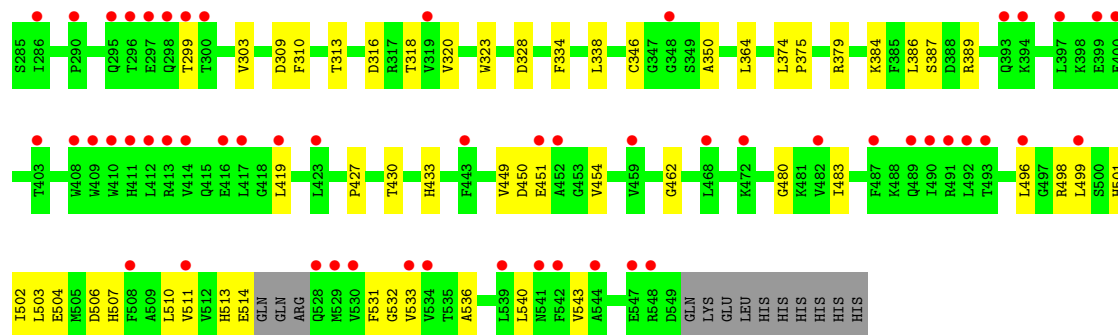
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	124.36Å 136.20Å 169.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.06 – 2.97 53.65 – 2.97	Depositor EDS
% Data completeness (in resolution range)	95.6 (53.06-2.97) 97.8 (53.65-2.97)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.07 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.240 , 0.284 0.245 , 0.288	Depositor DCC
R_{free} test set	1498 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	70.6	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 72.3	EDS
L-test for twinning[2]	$<|L|>$ = 0.46, $<L^2>$ = 0.28	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7728	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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, PLP

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	0.37	0/3878	0.56	0/5253
1	B	0.39	0/3881	0.57	0/5261
All	All	0.38	0/7759	0.57	0/10514

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3807	0	3832	90	0
1	B	3805	0	3834	84	0
2	A	15	0	7	3	0
2	B	15	0	7	3	0
3	A	43	0	30	5	0
3	B	43	0	30	6	0
All	All	7728	0	7740	170	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 11.

All (170) 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:413:ARG:NH1	1:A:493:THR:O	1.89	1.05
1:B:513:HIS:HB2	1:B:531:PHE:HE2	1.43	0.84
1:B:266:ARG:HD2	3:B:602:HEM:HBC2	1.63	0.81
1:B:110:GLU:OE2	1:B:121:ARG:NE	2.14	0.81
1:A:58:ARG:NE	1:A:62:GLU:OE1	2.16	0.78
1:B:513:HIS:HB2	1:B:531:PHE:CE2	2.26	0.71
1:A:191:THR:HG21	1:A:203:HIS:HA	1.73	0.70
1:B:180:VAL:HG21	1:B:379:ARG:NH1	2.07	0.68
1:B:303:VAL:HG23	1:B:328:ASP:OD2	1.93	0.68
1:B:350:ALA:HB1	1:B:374:LEU:HD22	1.76	0.65
1:A:303:VAL:HG23	1:A:328:ASP:OD2	1.97	0.65
1:A:110:GLU:OE2	1:A:121:ARG:NE	2.29	0.63
1:B:254:SER:HA	1:B:280:VAL:HB	1.80	0.62
1:B:191:THR:HG21	1:B:203:HIS:HA	1.81	0.62
1:A:255:VAL:HG13	1:A:258:GLY:HA2	1.82	0.61
1:A:179:ASP:HB3	1:B:386:LEU:HD22	1.80	0.61
1:A:180:VAL:HG21	1:A:379:ARG:NH1	2.15	0.61
1:B:58:ARG:NE	1:B:62:GLU:OE1	2.29	0.61
1:A:254:SER:HA	1:A:280:VAL:HB	1.82	0.61
1:A:281:ASP:OD2	1:A:282:PRO:HD2	2.00	0.61
1:B:255:VAL:HG13	1:B:258:GLY:HA2	1.82	0.61
1:B:129:ASP:OD2	1:B:132:ARG:NH1	2.33	0.61
1:B:172:LYS:HB2	1:B:193:THR:HG21	1.84	0.60
1:A:350:ALA:HB1	1:A:374:LEU:HD22	1.85	0.59
1:A:386:LEU:HD22	1:B:179:ASP:HB3	1.86	0.57
1:A:513:HIS:CG	1:A:514:GLU:N	2.72	0.57
1:B:200:PRO:HA	1:B:209[B]:ARG:HH12	1.69	0.57
1:B:232:HIS:CG	1:B:260:THR:HA	2.39	0.56
1:A:196:ARG:O	1:A:199:SER:OG	2.19	0.56
1:A:338:LEU:HD23	1:A:346:CYS:SG	2.46	0.56
1:B:235:THR:OG1	1:B:236:THR:N	2.37	0.56
1:A:200:PRO:O	1:A:209[B]:ARG:NH2	2.39	0.56
1:A:431:CYS:O	1:A:435:ILE:HD12	2.06	0.56
1:A:478:GLN:HB2	1:A:481:LYS:NZ	2.21	0.56
1:A:346:CYS:HA	1:A:377:SER:HA	1.88	0.55
1:B:540:LEU:HA	1:B:543:VAL:HG22	1.88	0.55
3:A:602:HEM:HMC2	3:A:602:HEM:HBC2	1.89	0.55
3:B:602:HEM:HMB1	3:B:602:HEM:HBB2	1.89	0.54
1:A:507:HIS:CG	1:B:192:PRO:HD3	2.42	0.54
1:B:513:HIS:CG	1:B:514:GLU:N	2.76	0.54
1:A:206:VAL:HG22	1:A:209[B]:ARG:HH21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:THR:O	1:B:240:ILE:HG13	2.08	0.54
1:B:119:LYS:HB3	1:B:150:THR:HA	1.89	0.53
1:B:138:PRO:HA	1:B:163:TYR:HE2	1.73	0.53
1:A:138:PRO:HA	1:A:163:TYR:HE2	1.74	0.53
1:A:111:PHE:HB2	1:A:377:SER:HB3	1.90	0.52
1:B:338:LEU:HD23	1:B:346:CYS:SG	2.49	0.52
1:A:258:GLY:HA3	1:A:315:LEU:HD13	1.92	0.52
1:B:196:ARG:O	1:B:199:SER:OG	2.20	0.52
1:B:256:GLY:H	2:B:601:PLP:H5A1	1.75	0.52
1:B:180:VAL:HG21	1:B:379:ARG:HH11	1.72	0.51
1:A:192:PRO:HD3	1:B:507:HIS:CG	2.44	0.51
1:A:119:LYS:HB3	1:A:150:THR:HA	1.92	0.50
1:B:316:ASP:OD2	1:B:318:THR:OG1	2.20	0.50
1:B:334:PHE:O	1:B:338:LEU:HB2	2.11	0.50
1:B:119:LYS:HG3	1:B:149:ASN:HB2	1.94	0.50
1:A:45:ARG:HD3	1:A:47:ASP:OD1	2.12	0.49
1:A:460:THR:HG23	1:A:463:ASN:HB3	1.94	0.49
1:A:110:GLU:HG3	1:A:113:ASN:ND2	2.27	0.49
1:A:200:PRO:HA	1:A:209[A]:ARG:NH1	2.28	0.49
1:A:144:GLU:OE1	1:A:222:GLN:HG2	2.12	0.49
1:A:235:THR:OG1	1:A:236:THR:N	2.44	0.49
1:A:287:LEU:HD23	1:A:311:ILE:HD13	1.94	0.49
1:A:503:LEU:HD13	1:A:536:ALA:HA	1.95	0.49
1:A:233:TYR:O	1:A:267:LYS:HD2	2.13	0.49
1:A:174:SER:HB3	1:A:384:LYS:HD2	1.95	0.49
1:A:465:LEU:O	1:A:469:LEU:HB2	2.13	0.49
1:A:266:ARG:NH1	3:A:602:HEM:C2C	2.81	0.48
1:A:115:GLY:N	1:A:120:ASP:OD2	2.46	0.48
1:A:528:GLN:HG3	1:A:529:MET:H	1.78	0.48
1:B:501:HIS:O	1:B:504:GLU:HB2	2.12	0.48
1:A:232:HIS:CG	1:A:260:THR:HA	2.49	0.48
1:A:87:THR:OG1	1:A:108:LYS:HE3	2.14	0.48
1:B:480:GLY:O	1:B:483:ILE:HG22	2.14	0.48
1:A:125:ARG:HG2	1:A:231:ALA:HB2	1.94	0.48
1:A:387:SER:OG	1:A:389:ARG:HG3	2.14	0.48
1:B:137:LYS:HE2	1:B:140:ASP:OD2	2.14	0.48
1:A:543:VAL:O	1:A:547:GLU:HG2	2.14	0.48
1:B:233:TYR:O	1:B:267:LYS:HD2	2.13	0.48
1:A:450:ASP:OD1	1:A:451:GLU:N	2.48	0.47
1:B:430:THR:HG23	1:B:433:HIS:H	1.79	0.47
1:A:169:MET:O	1:A:190:ARG:HA	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:LEU:O	1:B:503:LEU:HG	2.13	0.47
1:A:126:MET:HE3	1:A:222:GLN:HA	1.96	0.47
1:A:54:TRP:HB2	3:A:602:HEM:C4B	2.50	0.47
1:B:427:PRO:HD3	1:B:449:VAL:O	2.15	0.47
1:B:266:ARG:HD2	3:B:602:HEM:CBC	2.39	0.47
1:A:197:PHE:CE2	1:A:310:PHE:HB3	2.50	0.46
1:B:64:PRO:HD3	3:B:602:HEM:HMB2	1.96	0.46
1:A:266:ARG:NH1	3:A:602:HEM:C3C	2.83	0.46
1:B:200:PRO:HA	1:B:209[B]:ARG:NH1	2.31	0.46
1:B:510:LEU:HD22	1:B:533:VAL:HG22	1.98	0.46
1:B:46:PRO:HB2	1:B:310:PHE:CE1	2.51	0.46
1:B:502:ILE:O	1:B:506:ASP:N	2.48	0.46
1:B:174:SER:HB3	1:B:384:LYS:HD2	1.96	0.46
1:B:45:ARG:HD3	1:B:47:ASP:OD1	2.16	0.46
1:B:144:GLU:HG3	1:B:145:PRO:O	2.15	0.46
1:B:206:VAL:O	1:B:210:LEU:HG	2.16	0.46
1:A:138:PRO:HA	1:A:163:TYR:CE2	2.52	0.45
1:B:169:MET:O	1:B:190:ARG:HA	2.15	0.45
1:B:115:GLY:O	1:B:379:ARG:NH2	2.49	0.45
1:A:191:THR:HG22	1:A:206:VAL:HG21	1.98	0.45
1:A:484:TYR:HE2	1:B:201:GLU:HG2	1.82	0.45
1:A:496:LEU:O	1:A:499:LEU:HB3	2.16	0.45
1:B:110:GLU:OE2	1:B:121:ARG:NH2	2.50	0.45
1:B:387:SER:OG	1:B:389:ARG:HG3	2.16	0.45
1:A:283:GLU:HA	1:A:325:LYS:NZ	2.32	0.45
1:A:458:MET:HB2	1:A:484:TYR:HB2	1.98	0.45
1:B:126:MET:HE2	1:B:220:LEU:HB3	1.98	0.45
1:B:230:LEU:HD23	1:B:230:LEU:HA	1.80	0.45
1:A:77:LEU:HB2	1:B:90:VAL:HG22	1.98	0.45
1:B:87:THR:OG1	1:B:108:LYS:HE3	2.17	0.45
1:A:427:PRO:HD3	1:A:449:VAL:O	2.17	0.44
1:A:180:VAL:HG21	1:A:379:ARG:HH11	1.80	0.44
1:B:48:ALA:O	1:B:313:THR:HG22	2.17	0.44
1:B:256:GLY:H	2:B:601:PLP:C5A	2.30	0.44
1:B:226:ALA:HA	3:B:602:HEM:HMD2	2.00	0.44
1:A:502:ILE:O	1:A:506:ASP:N	2.51	0.44
1:B:419:LEU:HD13	1:B:532:GLY:HA3	1.99	0.44
1:B:496:LEU:O	1:B:499:LEU:HB3	2.18	0.44
1:B:450:ASP:OD1	1:B:451:GLU:N	2.51	0.44
1:B:87:THR:HG21	1:B:110:GLU:HA	2.00	0.43
1:B:511:VAL:O	1:B:531:PHE:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LYS:HB2	1:A:193:THR:HG21	2.00	0.43
1:B:248:LEU:HD12	1:B:249:ASP:H	1.82	0.43
1:A:47:ASP:HA	1:A:311:ILE:O	2.18	0.43
1:A:224:ARG:HA	1:A:313:THR:OG1	2.18	0.43
1:A:236:THR:O	1:A:240:ILE:HG13	2.19	0.43
1:B:197:PHE:HD2	1:B:309:ASP:OD2	2.01	0.43
1:A:431:CYS:O	1:A:434:THR:HB	2.19	0.43
1:A:468:LEU:HD23	1:A:473:VAL:O	2.19	0.43
1:A:65:HIS:HB3	1:A:230:LEU:HD11	2.01	0.42
1:A:349:SER:OG	2:A:601:PLP:N1	2.51	0.42
1:B:64:PRO:HD3	3:B:602:HEM:CMB	2.50	0.42
1:B:200:PRO:HB3	1:B:209[B]:ARG:NH2	2.34	0.42
1:A:256:GLY:H	2:A:601:PLP:H5A1	1.84	0.42
1:A:169:MET:HG3	1:A:190:ARG:NE	2.35	0.42
1:B:498:ARG:O	1:B:502:ILE:HG13	2.19	0.42
1:A:498:ARG:O	1:A:502:ILE:HG13	2.20	0.42
2:B:601:PLP:H2A1	2:B:601:PLP:HO3	1.71	0.42
1:B:110:GLU:HG3	1:B:113:ASN:ND2	2.35	0.42
1:A:221:ASP:OD1	1:A:224:ARG:NE	2.48	0.42
1:A:431:CYS:HA	1:A:464:MET:HE3	2.02	0.42
1:B:232:HIS:CD2	1:B:260:THR:HA	2.54	0.42
1:A:286:ILE:H	1:A:286:ILE:HG13	1.62	0.41
1:B:110:GLU:OE2	1:B:121:ARG:CZ	2.67	0.41
1:B:320:VAL:HG11	1:B:323:TRP:CE2	2.55	0.41
1:B:128:GLU:HA	1:B:131:GLU:OE2	2.19	0.41
1:B:250:MET:HE3	1:B:364:LEU:HD11	2.02	0.41
3:A:602:HEM:HMB1	3:A:602:HEM:HBB2	2.01	0.41
1:B:191:THR:HB	1:B:201:GLU:O	2.20	0.41
1:B:281:ASP:OD2	1:B:282:PRO:HD2	2.20	0.41
1:A:80:ILE:HD11	1:B:112:PHE:HZ	1.85	0.41
1:A:48:ALA:O	1:A:313:THR:HG22	2.20	0.41
1:A:95:ILE:HD12	1:A:338:LEU:HD12	2.03	0.41
1:B:503:LEU:HD13	1:B:536:ALA:HA	2.03	0.41
1:A:248:LEU:HD12	1:A:249:ASP:H	1.84	0.41
1:A:539:LEU:O	1:A:543:VAL:HG23	2.20	0.41
1:A:223:TYR:O	1:A:314:VAL:HG22	2.21	0.41
1:A:374:LEU:HA	1:A:375:PRO:HD3	1.82	0.41
1:A:419:LEU:HB3	1:A:420:SER:H	1.32	0.41
1:A:146:THR:HG21	1:A:151:GLY:HA3	2.02	0.40
1:A:200:PRO:HD2	1:B:462:GLY:HA3	2.01	0.40
1:A:256:GLY:H	2:A:601:PLP:C5A	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LYS:HD2	1:A:150:THR:OG1	2.21	0.40
1:B:374:LEU:HA	1:B:375:PRO:HD3	1.73	0.40
1:A:126:MET:HB3	1:A:220:LEU:HD13	2.03	0.40
1:A:499:LEU:O	1:A:503:LEU:HG	2.21	0.40
1:A:268:LEU:HD12	1:A:268:LEU:HA	1.85	0.40
1:B:126:MET:HB3	1:B:220:LEU:HD13	2.03	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	489/549 (89%)	474 (97%)	15 (3%)	0	100	100
1	B	493/549 (90%)	479 (97%)	14 (3%)	0	100	100
All	All	982/1098 (89%)	953 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	407/463 (88%)	406 (100%)	1 (0%)	93	98
1	B	408/463 (88%)	406 (100%)	2 (0%)	88	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	815/926 (88%)	812 (100%)	3 (0%)	91 97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	460	THR
1	B	299	THR
1	B	454	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	380	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	PLP	A	601	1	15,15,16	1.03	1 (6%)	20,22,23	1.23	2 (10%)
3	HEM	B	602	1	41,50,50	2.75	10 (24%)	45,82,82	3.86	21 (46%)
2	PLP	B	601	1	15,15,16	1.02	1 (6%)	20,22,23	1.25	3 (15%)
3	HEM	A	602	1	41,50,50	2.76	13 (31%)	45,82,82	3.87	20 (44%)

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	PLP	A	601	1	-	0/6/6/8	0/1/1/1
3	HEM	B	602	1	-	1/12/54/54	-
2	PLP	B	601	1	-	0/6/6/8	0/1/1/1
3	HEM	A	602	1	-	0/12/54/54	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	HEM	C3B-C2B	-9.41	1.18	1.37
3	B	602	HEM	C3B-C2B	-9.40	1.18	1.37
3	A	602	HEM	C3D-C2D	-9.11	1.17	1.36
3	B	602	HEM	C3D-C2D	-8.90	1.17	1.36
3	A	602	HEM	C1D-ND	4.34	1.47	1.38
3	B	602	HEM	C1D-ND	4.30	1.47	1.38
3	A	602	HEM	CBB-CAB	4.06	1.50	1.30
3	B	602	HEM	CBB-CAB	4.01	1.50	1.30
3	B	602	HEM	C1B-NB	3.90	1.47	1.40
3	B	602	HEM	C4D-ND	3.84	1.46	1.40
3	A	602	HEM	C4D-ND	3.82	1.46	1.40
3	A	602	HEM	C1B-NB	3.66	1.46	1.40
3	B	602	HEM	C4D-C3D	-3.64	1.38	1.45
3	A	602	HEM	C4D-C3D	-3.43	1.39	1.45
3	A	602	HEM	C4B-NB	2.97	1.44	1.38
3	B	602	HEM	C4B-NB	2.93	1.44	1.38
3	B	602	HEM	C3B-C4B	-2.91	1.39	1.44
3	A	602	HEM	C3B-C4B	-2.56	1.39	1.44
2	A	601	PLP	C2-N1	2.40	1.38	1.33
3	A	602	HEM	C1B-C2B	-2.25	1.40	1.44
3	B	602	HEM	CHB-C1B	2.08	1.40	1.35
3	A	602	HEM	C1D-C2D	-2.06	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	HEM	CAB-C3B	2.05	1.53	1.47
2	B	601	PLP	C2-N1	2.05	1.37	1.33
3	A	602	HEM	CAA-C2A	-2.03	1.49	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	HEM	C3B-C2B-C1B	11.27	114.84	106.49
3	B	602	HEM	C3B-C2B-C1B	11.00	114.65	106.49
3	A	602	HEM	C1D-C2D-C3D	8.48	115.87	106.96
3	B	602	HEM	C1D-C2D-C3D	8.31	115.69	106.96
3	B	602	HEM	C4B-C3B-C2B	8.30	113.70	107.11
3	A	602	HEM	C4B-C3B-C2B	7.85	113.35	107.11
3	B	602	HEM	C2D-C1D-ND	-7.82	100.51	109.88
3	A	602	HEM	C2D-C1D-ND	-7.82	100.52	109.88
3	A	602	HEM	CMB-C2B-C1B	-7.42	113.75	125.04
3	A	602	HEM	C3D-C4D-ND	-7.36	101.97	110.17
3	B	602	HEM	C3D-C4D-ND	-7.21	102.14	110.17
3	B	602	HEM	CMB-C2B-C1B	-7.12	114.19	125.04
3	B	602	HEM	C2B-C1B-NB	-6.63	101.98	109.84
3	A	602	HEM	C2B-C1B-NB	-6.36	102.30	109.84
3	A	602	HEM	C4D-C3D-C2D	5.38	114.73	106.90
3	B	602	HEM	C4D-C3D-C2D	5.37	114.72	106.90
3	B	602	HEM	CHD-C1D-C2D	5.26	133.20	124.98
3	A	602	HEM	CHD-C1D-C2D	5.09	132.93	124.98
3	B	602	HEM	CMD-C2D-C1D	-4.86	117.64	125.04
3	A	602	HEM	CMD-C2D-C1D	-4.78	117.77	125.04
3	B	602	HEM	CAD-C3D-C4D	-4.08	117.54	124.66
3	A	602	HEM	CAD-C3D-C4D	-3.50	118.55	124.66
3	A	602	HEM	CHC-C4B-C3B	3.36	129.72	124.57
3	B	602	HEM	CHA-C4D-ND	3.23	128.37	124.38
3	A	602	HEM	CHA-C4D-ND	3.14	128.26	124.38
2	B	601	PLP	O4P-C5A-C5	3.11	115.27	109.35
2	A	601	PLP	O4P-C5A-C5	3.10	115.26	109.35
3	A	602	HEM	CBA-CAA-C2A	-3.03	107.44	112.62
3	B	602	HEM	CBA-CAA-C2A	-3.00	107.50	112.62
3	A	602	HEM	C2C-C3C-C4C	2.95	108.96	106.90
3	B	602	HEM	C2C-C3C-C4C	2.93	108.95	106.90
3	B	602	HEM	CAB-C3B-C4B	-2.89	111.03	124.47
3	B	602	HEM	CHC-C4B-C3B	2.84	128.92	124.57
2	B	601	PLP	C6-C5-C4	2.83	120.39	118.16
3	A	602	HEM	C3C-C4C-NC	-2.63	105.98	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	HEM	C3C-C4C-NC	-2.62	106.00	110.94
3	A	602	HEM	CMC-C2C-C3C	2.60	129.54	124.68
3	A	602	HEM	CAB-C3B-C4B	-2.55	112.59	124.47
3	B	602	HEM	CHC-C4B-NB	2.53	127.19	124.43
3	A	602	HEM	CHB-C1B-NB	2.37	127.31	124.38
3	A	602	HEM	CHA-C4D-C3D	2.36	129.76	125.33
3	B	602	HEM	CHA-C4D-C3D	2.22	129.49	125.33
2	A	601	PLP	C6-C5-C4	2.19	119.89	118.16
2	B	601	PLP	C5-C6-N1	-2.16	120.22	123.82
3	B	602	HEM	CHB-C1B-NB	2.09	126.97	124.38
3	B	602	HEM	CAB-C3B-C2B	2.02	135.26	128.60

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	HEM	C3D-CAD-CBD-CGD

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	PLP	3	0
3	B	602	HEM	6	0
2	B	601	PLP	3	0
3	A	602	HEM	5	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HEM B 602

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 602
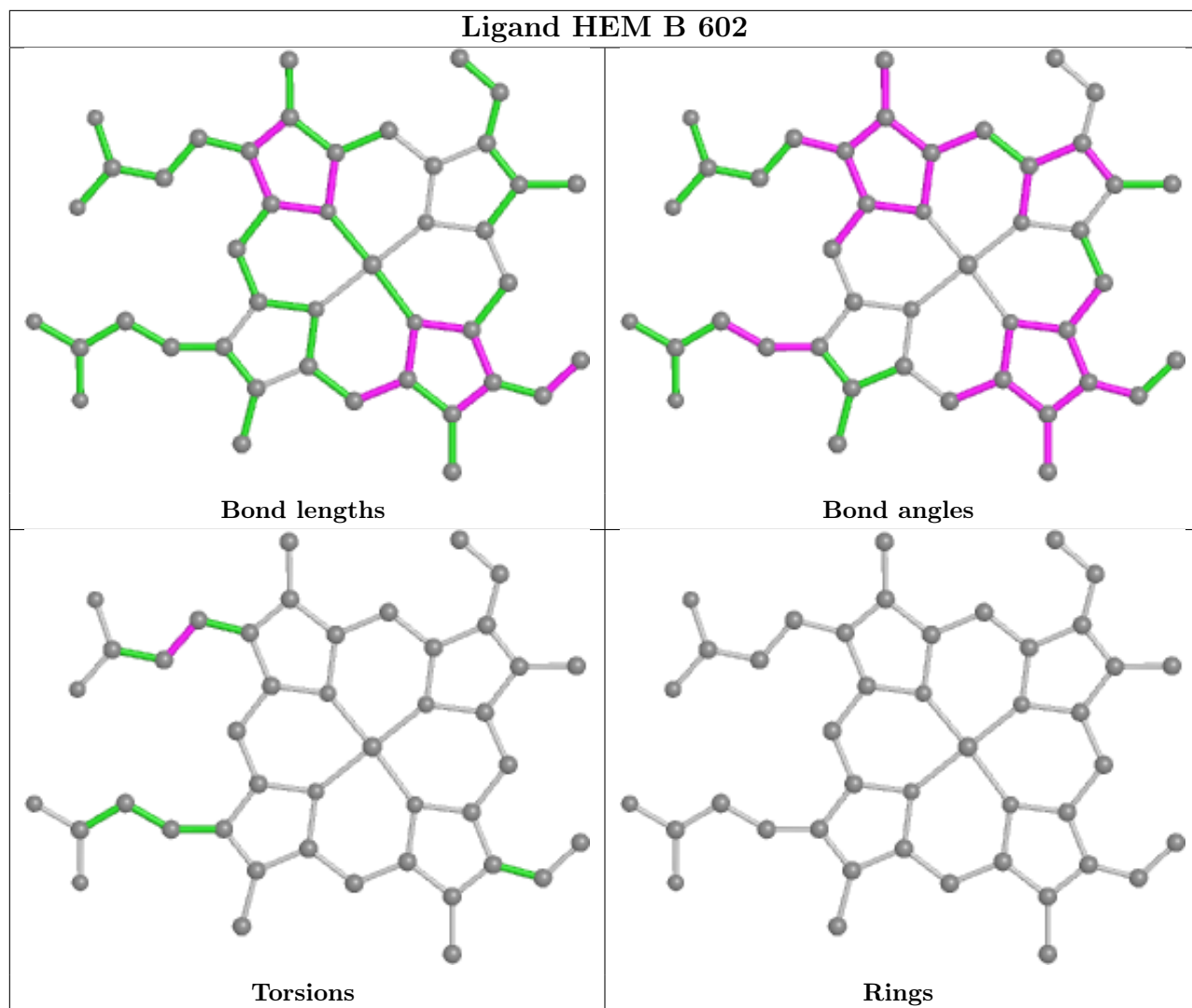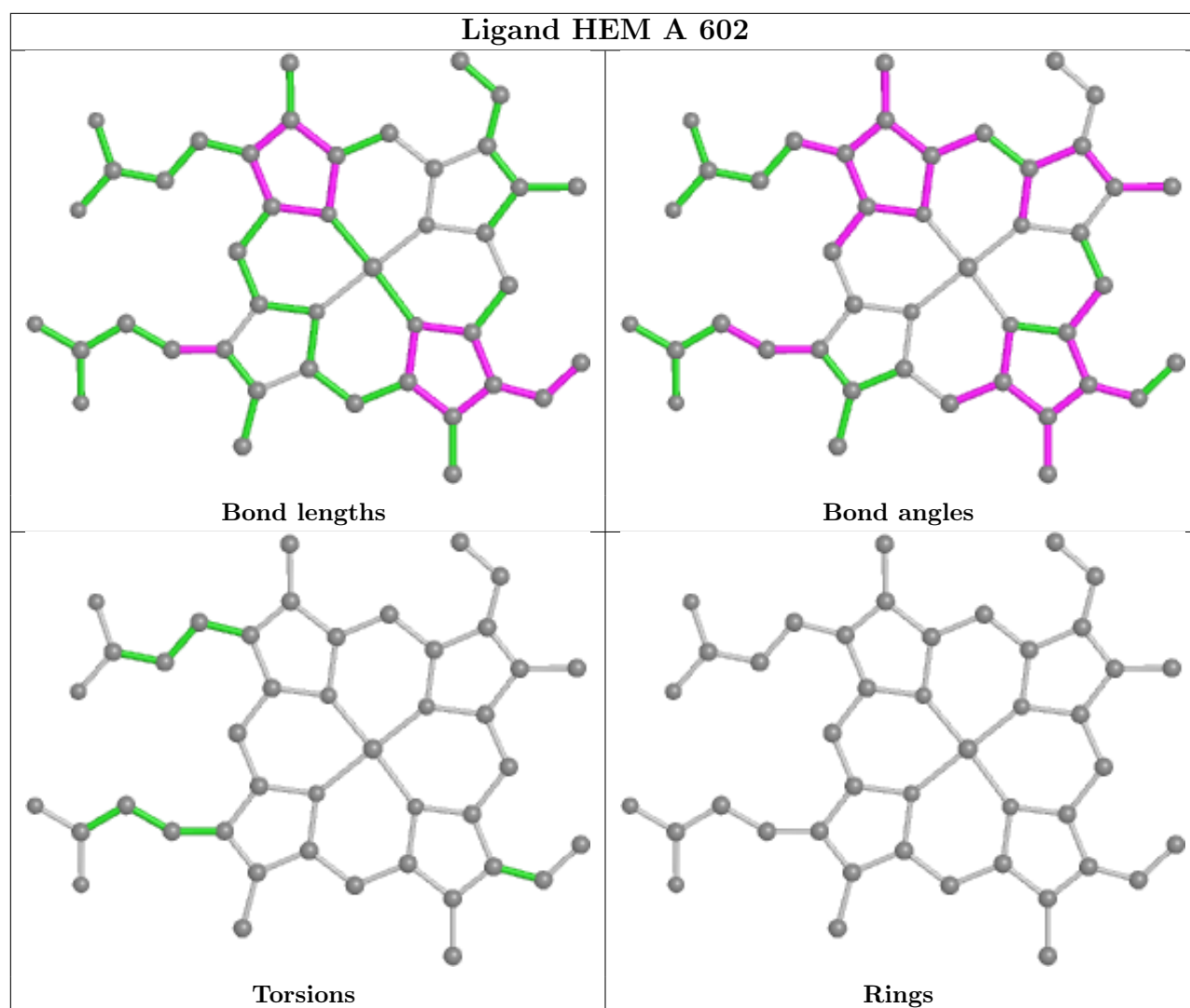
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	496/549 (90%)	0.98	56 (11%)	5	3	53, 93, 150, 202	0
1	B	496/549 (90%)	1.07	79 (15%)	1	1	46, 88, 142, 184	0
All	All	992/1098 (90%)	1.02	135 (13%)	3	1	46, 90, 147, 202	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	397	LEU	5.9
1	A	403	THR	5.6
1	B	403	THR	5.1
1	B	411	HIS	5.0
1	B	416	GLU	4.6
1	A	548	ARG	4.6
1	A	233	TYR	4.6
1	B	534	VAL	4.4
1	B	528	GLN	4.2
1	B	413	ARG	4.0
1	B	136	LEU	4.0
1	A	550	GLN	4.0
1	B	533	VAL	3.9
1	A	248	LEU	3.9
1	A	407	PRO	3.8
1	B	496	LEU	3.6
1	A	137	LYS	3.5
1	B	539	LEU	3.5
1	A	271	LYS	3.4
1	A	269	LYS	3.4
1	B	68	THR	3.3
1	A	417	LEU	3.3
1	A	56	LEU	3.3
1	A	549	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	262	THR	3.2
1	B	451	GLU	3.2
1	A	251	LEU	3.1
1	A	305	GLY	3.1
1	B	542	PHE	3.0
1	A	278	ILE	3.0
1	B	412	LEU	3.0
1	B	530	VAL	3.0
1	B	409	TRP	3.0
1	B	417	LEU	3.0
1	B	410	TRP	2.9
1	B	529	MET	2.9
1	A	246	GLY	2.9
1	A	122	ILE	2.9
1	A	530	VAL	2.9
1	A	532	GLY	2.9
1	B	492	LEU	2.9
1	A	105	LEU	2.9
1	B	452	ALA	2.9
1	A	277	ILE	2.8
1	A	42	LEU	2.7
1	B	135	THR	2.7
1	B	408	TRP	2.7
1	A	514	GLU	2.7
1	A	293	LEU	2.7
1	B	284	GLY	2.7
1	B	222	GLN	2.6
1	B	248	LEU	2.6
1	B	414	VAL	2.6
1	B	348	GLY	2.6
1	A	427	PRO	2.6
1	A	379	ARG	2.6
1	B	51	ARG	2.6
1	B	548	ARG	2.6
1	A	479	VAL	2.6
1	A	43	TRP	2.6
1	B	67	HIS	2.5
1	B	77	LEU	2.5
1	A	124	LEU	2.5
1	A	132	ARG	2.5
1	A	319	VAL	2.5
1	A	481	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	298	GLN	2.5
1	B	541	ASN	2.5
1	B	400	GLU	2.5
1	B	423	LEU	2.5
1	A	90	VAL	2.5
1	B	511	VAL	2.5
1	B	275	CYS	2.5
1	A	539	LEU	2.5
1	B	394	LYS	2.5
1	A	363	GLU	2.4
1	B	419	LEU	2.4
1	A	109	CYS	2.4
1	B	490	ILE	2.4
1	A	377	SER	2.4
1	A	364	LEU	2.4
1	B	46	PRO	2.4
1	B	297	GLU	2.3
1	A	254	SER	2.3
1	B	443	PHE	2.3
1	B	491	ARG	2.3
1	B	468	LEU	2.3
1	B	63	SER	2.3
1	A	287	LEU	2.3
1	A	247	LYS	2.3
1	A	513	HIS	2.3
1	B	43	TRP	2.3
1	A	411	HIS	2.3
1	A	237	ALA	2.3
1	B	56	LEU	2.3
1	B	295	GLN	2.3
1	B	547	GLU	2.3
1	B	109	CYS	2.3
1	A	415	GLN	2.3
1	B	72	LYS	2.3
1	B	508	PHE	2.2
1	B	220	LEU	2.2
1	B	233	TYR	2.2
1	B	300	THR	2.2
1	A	508	PHE	2.2
1	B	148	GLY	2.2
1	A	86	ASP	2.2
1	B	258	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	141	THR	2.2
1	B	290	PRO	2.2
1	B	299	THR	2.2
1	B	296	THR	2.1
1	B	487	PHE	2.1
1	B	393	GLN	2.1
1	B	286	ILE	2.1
1	B	99	PHE	2.1
1	A	198	ASP	2.1
1	A	366	GLU	2.1
1	A	77	LEU	2.1
1	B	493	THR	2.1
1	B	499	LEU	2.1
1	B	544	ALA	2.1
1	B	459	VAL	2.1
1	A	456	LEU	2.1
1	B	482	VAL	2.0
1	A	101	LEU	2.0
1	B	76	ILE	2.0
1	B	264	ILE	2.0
1	B	399	GLU	2.0
1	B	472	LYS	2.0
1	B	319	VAL	2.0
1	A	510	LEU	2.0
1	A	370	CYS	2.0
1	B	489	GLN	2.0
1	A	378	VAL	2.0

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

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

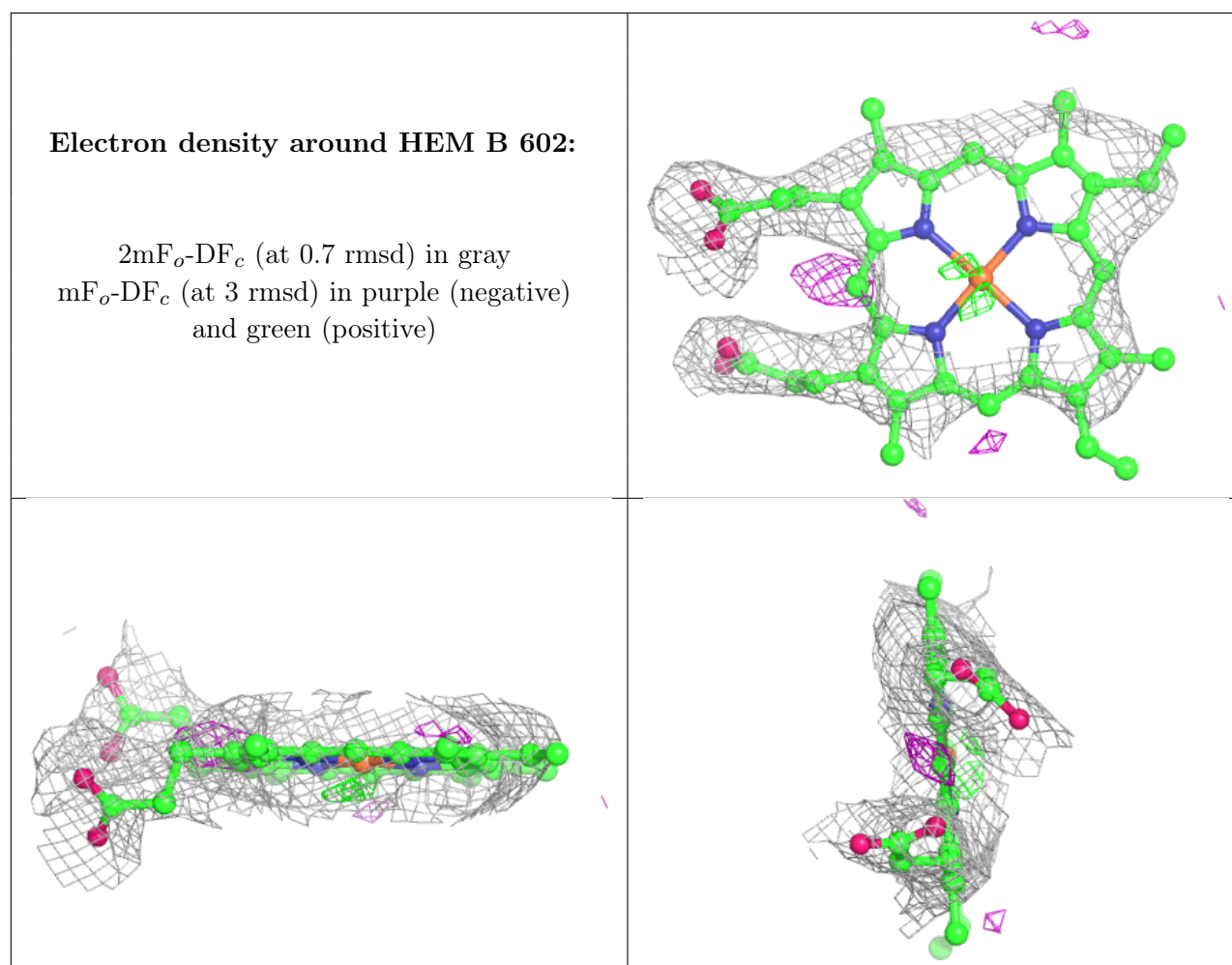## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.
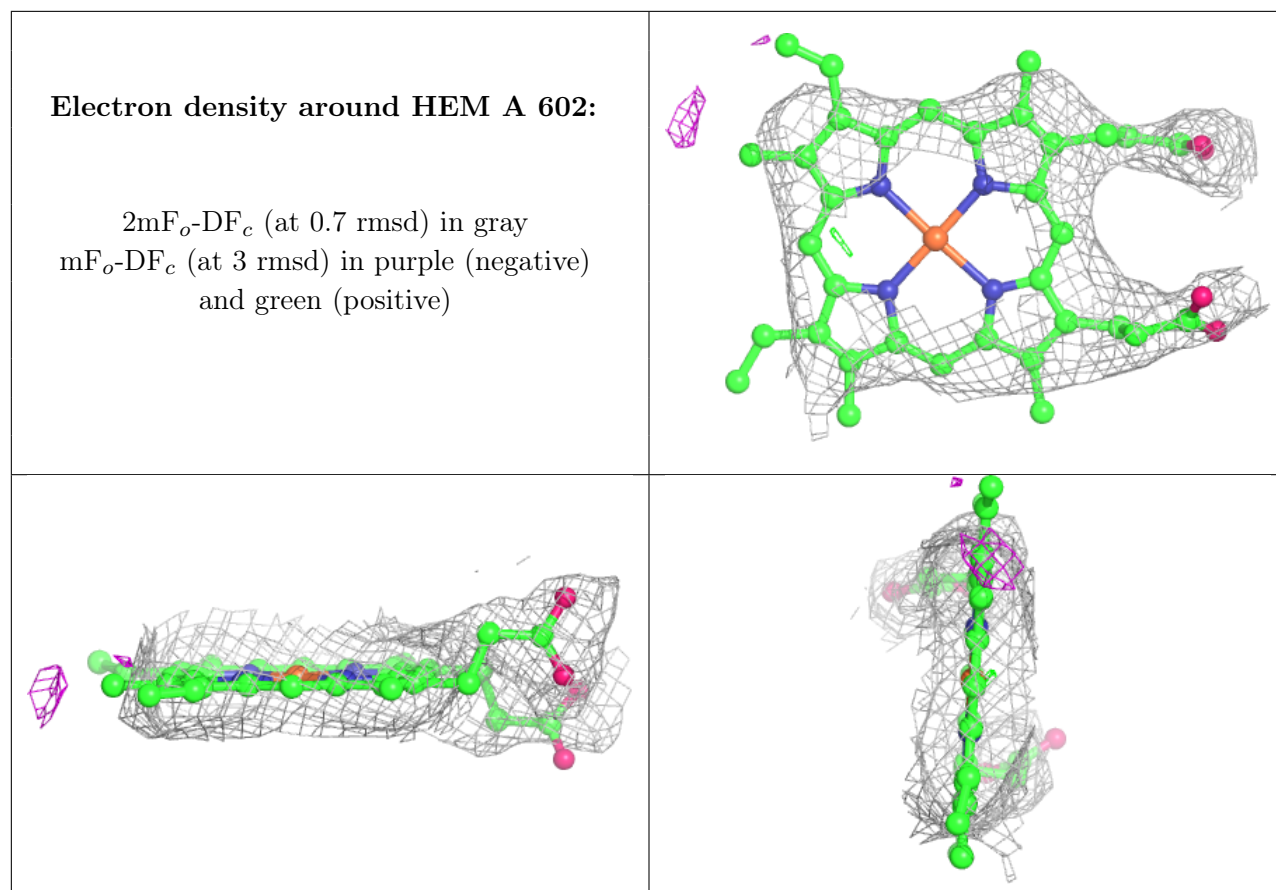
6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PLP	B	601	15/16	0.90	0.21	53,66,75,76	0
2	PLP	A	601	15/16	0.92	0.21	58,75,85,86	0
3	HEM	B	602	43/43	0.92	0.34	101,104,104,104	0
3	HEM	A	602	43/43	0.93	0.29	107,108,109,109	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 B 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 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)

6.5 Other polymers ⓘ

There are no such residues in this entry.