



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 03:19 PM EDT

PDB ID : 4L0D / pdb_00004l0d
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)

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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

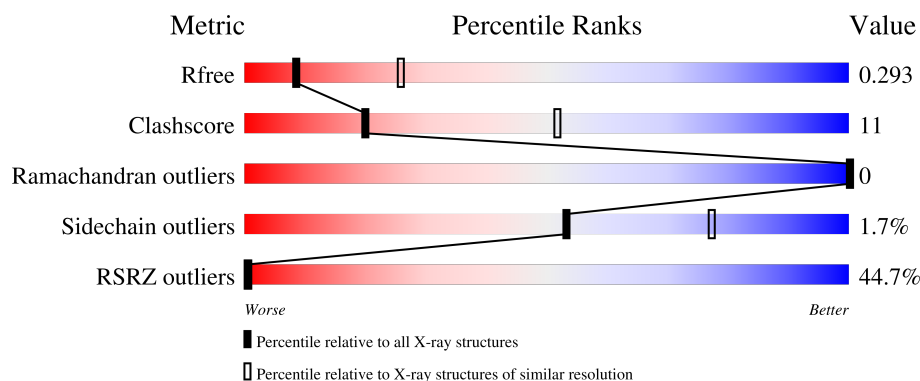
1 Overall quality at a glance

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}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (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 $\leq 5\%$. 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	549	42% 65% 25% 10%
1	B	549	39% 66% 24% 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	C	N	O	S	0	1	0
			3807	2413	667	705	22			
1	B	496	Total	C	N	O	S	0	1	0
			3805	2412	666	705	22			

There are 38 discrepancies between the modelled and reference sequences:

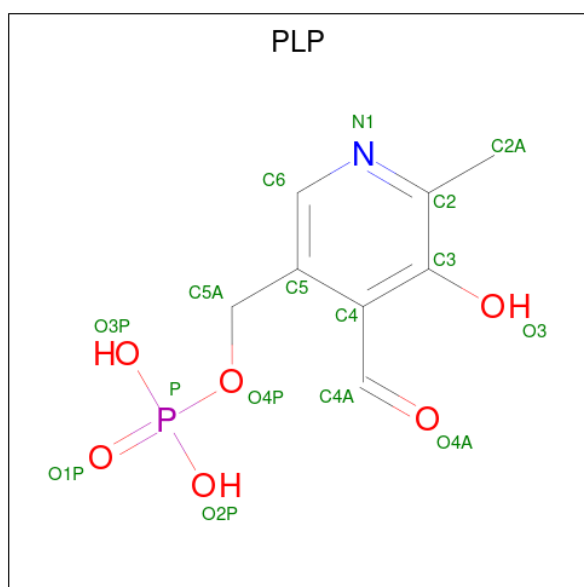
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	PRO	engineered mutation	UNP P35520
A	?	-	ILE	deletion	UNP P35520
A	?	-	GLN	deletion	UNP P35520
A	?	-	TYR	deletion	UNP P35520
A	?	-	HIS	deletion	UNP P35520
A	?	-	SER	deletion	UNP P35520
A	?	-	THR	deletion	UNP P35520
A	?	-	GLY	deletion	UNP P35520
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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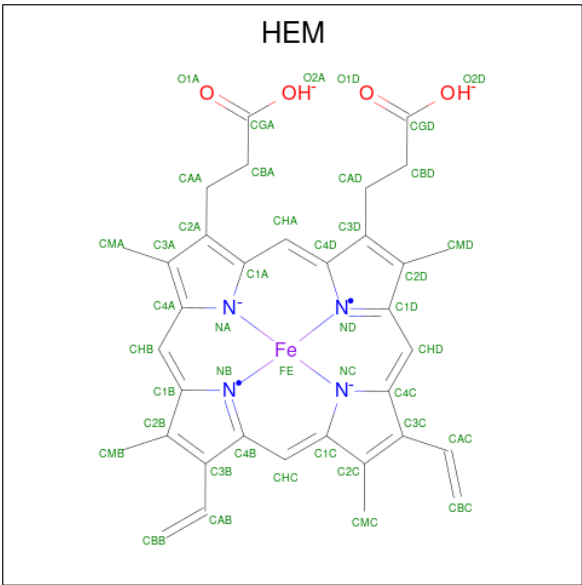
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP P35520
B	?	-	GLY	deletion	UNP P35520
B	?	-	LYS	deletion	UNP P35520
B	?	-	SER	deletion	UNP P35520
B	?	-	SER	deletion	UNP P35520
B	552	GLU	-	expression tag	UNP P35520
B	553	LEU	-	expression tag	UNP P35520
B	554	HIS	-	expression tag	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 (CCD ID: 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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

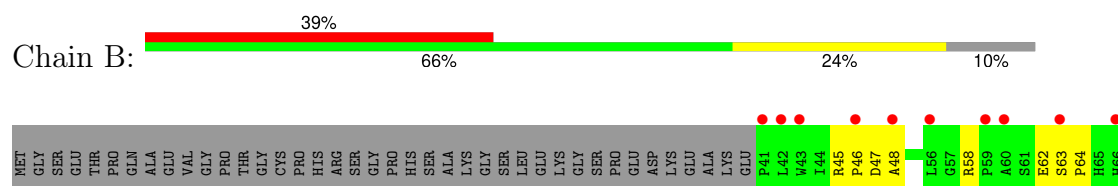
3 Residue-property plots

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: Cystathionine beta-synthase



• Molecule 1: Cystathionine beta-synthase





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 53.06 – 2.97	Depositor EDS
% Data completeness (in resolution range)	95.6 (53.06-2.97) 97.8 (53.06-2.97)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.240 , 0.284 0.248 , 0.293	Depositor DCC
R_{free} test set	1498 reflections (4.99%)	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)	0.34 , 77.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	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.*

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, 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	0.46	0/3878	0.92	7/5253 (0.1%)
1	B	0.47	0/3881	0.94	9/5261 (0.2%)
All	All	0.47	0/7759	0.93	16/10514 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	374	LEU	CA-C-N	7.67	127.21	118.85
1	B	374	LEU	C-N-CA	7.67	127.21	118.85
1	B	63	SER	CA-C-N	6.21	125.78	119.19
1	B	63	SER	C-N-CA	6.21	125.78	119.19
1	A	457	GLY	N-CA-C	6.18	118.20	110.29
1	A	512	VAL	N-CA-C	5.92	117.23	108.65
1	A	214	ILE	N-CA-C	5.79	114.33	107.73
1	A	374	LEU	CA-C-N	5.59	124.94	118.85
1	A	374	LEU	C-N-CA	5.59	124.94	118.85
1	B	93	ASN	N-CA-C	5.55	118.17	111.40
1	B	214	ILE	N-CA-C	5.45	113.83	107.89
1	B	505	MET	N-CA-C	5.31	119.91	113.38
1	B	451	GLU	N-CA-C	-5.27	105.65	111.71
1	A	63	SER	CA-C-N	5.13	124.62	119.19
1	A	63	SER	C-N-CA	5.13	124.62	119.19
1	B	94	LYS	N-CA-C	5.03	117.54	111.40

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	95	0
1	B	3805	0	3834	88	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	177	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 (177) 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:126:MET:HE2	1:B:220:LEU:HB3	1.69	0.72
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:A:126:MET:HE2	1:A:220:LEU:HB3	1.74	0.69
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:196:ARG:O	1:B:199:SER:OG	2.20	0.59
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLU:OE1	1:A:222:GLN:HG2	2.12	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:235:THR:OG1	1:A:236:THR:N	2.44	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:169:MET:HE2	1:A:173:MET:HB2	1.95	0.47
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
1:B:499:LEU:O	1:B:503:LEU:HG	2.13	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:147:SER:HA	1:B:173:MET:HE3	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:MET:HE2	1:A:386:LEU:HD13	1.99	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: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
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:505:MET:HE1	1:B:175:SER:HB3	2.01	0.42
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:126:MET:HE2	1:B:220:LEU:CB	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:232:HIS:CD2	1:B:260:THR:HA	2.54	0.42
1:B:250:MET:HE3	1:B:250:MET:HB2	1.91	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:A:126:MET:HE2	1:A:220:LEU:CB	2.48	0.41
1:A:169:MET:HE2	1:A:173:MET:CB	2.50	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
1:A:119:LYS:HD2	1:A:150:THR:OG1	2.21	0.40
1:A:431:CYS:SG	1:A:464:MET:HE1	2.61	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
1:B:349:SER:OG	2:B:601:PLP:N1	2.54	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%)	402 (99%)	5 (1%)	63	82
1	B	408/463 (88%)	399 (98%)	9 (2%)	45	73
All	All	815/926 (88%)	801 (98%)	14 (2%)	53	77

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	LEU
1	A	286	ILE
1	A	454	VAL
1	A	460	THR
1	A	534	VAL
1	B	299	THR
1	B	382	MET
1	B	435	ILE

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Mol	Chain	Res	Type
1	B	437	ILE
1	B	454	VAL
1	B	479	VAL
1	B	482	VAL
1	B	490	ILE
1	B	534	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	380	ASN
1	B	380	ASN
1	B	474	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	PLP	B	601	1	15,15,16	1.05	1 (6%)	21,22,23	1.24	3 (14%)
3	HEM	A	602	1	50,50,50	2.95	22 (44%)	67,82,82	3.43	28 (41%)
3	HEM	B	602	1	50,50,50	2.96	20 (40%)	67,82,82	3.40	26 (38%)
2	PLP	A	601	1	15,15,16	1.07	1 (6%)	21,22,23	1.23	2 (9%)

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	B	601	1	-	0/6/6/8	0/1/1/1
3	HEM	A	602	1	-	0/14/54/54	-
3	HEM	B	602	1	-	1/14/54/54	-
2	PLP	A	601	1	-	0/6/6/8	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	HEM	C3B-C2B	-9.32	1.18	1.37
3	B	602	HEM	C3B-C2B	-9.31	1.18	1.37
3	A	602	HEM	C3D-C2D	-9.05	1.17	1.36
3	B	602	HEM	C3D-C2D	-8.84	1.17	1.36
3	B	602	HEM	FE-NA	6.05	2.15	1.95
3	A	602	HEM	FE-NA	5.88	2.14	1.95
3	B	602	HEM	FE-NC	5.59	2.13	1.95
3	A	602	HEM	FE-NC	5.45	2.13	1.95
3	A	602	HEM	C1D-ND	4.54	1.47	1.38
3	B	602	HEM	C1D-ND	4.50	1.47	1.38
3	A	602	HEM	CBB-CAB	4.17	1.50	1.30
3	B	602	HEM	CBB-CAB	4.11	1.50	1.30
3	B	602	HEM	C1B-NB	3.95	1.47	1.40
3	B	602	HEM	C4D-ND	3.89	1.46	1.40
3	A	602	HEM	C4D-ND	3.86	1.46	1.40
3	A	602	HEM	C1B-NB	3.71	1.46	1.40
3	B	602	HEM	C4D-C3D	-3.69	1.38	1.45
3	A	602	HEM	C1C-C2C	-3.57	1.38	1.45
3	A	602	HEM	C4D-C3D	-3.48	1.39	1.45
3	B	602	HEM	C1C-C2C	-3.47	1.38	1.45
3	A	602	HEM	C3C-C4C	-3.37	1.40	1.46
3	B	602	HEM	CHB-C4A	3.11	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	HEM	C4B-NB	3.10	1.44	1.38
3	B	602	HEM	C3C-C4C	-3.07	1.40	1.46
3	B	602	HEM	C4B-NB	3.06	1.44	1.38
3	B	602	HEM	C3B-C4B	-3.04	1.39	1.44
3	B	602	HEM	CHC-C1C	2.98	1.44	1.38
3	A	602	HEM	C3C-C2C	2.90	1.43	1.37
3	B	602	HEM	C3C-C2C	2.75	1.42	1.37
3	A	602	HEM	CHC-C1C	2.71	1.43	1.38
3	A	602	HEM	C3B-C4B	-2.67	1.39	1.44
3	B	602	HEM	CHD-C4C	2.65	1.43	1.38
3	A	602	HEM	CHB-C4A	2.60	1.45	1.39
3	A	602	HEM	CHD-C4C	2.59	1.43	1.38
2	A	601	PLP	C2-N1	2.54	1.38	1.33
3	A	602	HEM	FE-ND	2.29	2.02	1.94
3	A	602	HEM	C1A-NA	-2.28	1.35	1.39
3	B	602	HEM	FE-ND	2.28	2.01	1.94
3	A	602	HEM	C1A-C2A	-2.24	1.40	1.44
3	B	602	HEM	C1A-C2A	-2.23	1.40	1.44
3	B	602	HEM	C1A-NA	-2.19	1.35	1.39
2	B	601	PLP	C2-N1	2.17	1.37	1.33
3	A	602	HEM	C1B-C2B	-2.12	1.40	1.44
3	A	602	HEM	CAB-C3B	2.11	1.53	1.47

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	HEM	C3B-C2B-C1B	11.23	114.84	106.41
3	B	602	HEM	C3B-C2B-C1B	10.97	114.65	106.41
3	A	602	HEM	C1D-C2D-C3D	8.45	115.87	106.98
3	B	602	HEM	C1D-C2D-C3D	8.28	115.69	106.98
3	B	602	HEM	C2D-C1D-ND	-8.12	100.51	109.90
3	A	602	HEM	C2D-C1D-ND	-8.12	100.52	109.90
3	A	602	HEM	C3B-C4B-NB	-7.93	103.77	109.47
3	B	602	HEM	C3B-C4B-NB	-7.76	103.89	109.47
3	A	602	HEM	C3D-C4D-ND	-7.48	101.97	110.17
3	B	602	HEM	C3D-C4D-ND	-7.32	102.14	110.17
3	A	602	HEM	CMB-C2B-C1B	-7.22	113.75	125.03
3	B	602	HEM	C4B-C3B-C2B	6.99	113.70	107.28
3	B	602	HEM	CMB-C2B-C1B	-6.94	114.19	125.03
3	B	602	HEM	C2B-C1B-NB	-6.84	101.98	109.84
3	A	602	HEM	C4B-C3B-C2B	6.60	113.35	107.28
3	A	602	HEM	C2B-C1B-NB	-6.56	102.30	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	HEM	C4D-C3D-C2D	5.39	114.73	106.89
3	B	602	HEM	C4D-C3D-C2D	5.38	114.72	106.89
3	B	602	HEM	CHD-C1D-C2D	5.17	133.20	125.03
3	A	602	HEM	CHD-C1D-C2D	5.00	132.93	125.03
3	A	602	HEM	CHC-C1C-NC	4.96	129.86	124.45
3	B	602	HEM	CMD-C2D-C1D	-4.73	117.64	125.03
3	A	602	HEM	CMD-C2D-C1D	-4.65	117.77	125.03
3	B	602	HEM	CHC-C1C-NC	4.60	129.46	124.45
3	B	602	HEM	CAD-C3D-C4D	-4.11	117.54	124.70
3	A	602	HEM	CHD-C4C-NC	3.90	128.71	124.45
3	B	602	HEM	CHD-C4C-NC	3.90	128.70	124.45
3	A	602	HEM	CAD-C3D-C4D	-3.53	118.55	124.70
3	B	602	HEM	CHA-C4D-ND	3.24	128.37	124.37
2	B	601	PLP	O4P-C5A-C5	3.16	115.27	109.36
3	A	602	HEM	CHA-C4D-ND	3.15	128.26	124.37
2	A	601	PLP	O4P-C5A-C5	3.15	115.26	109.36
3	A	602	HEM	C4C-NC-C1C	3.03	110.76	105.82
3	B	602	HEM	CAB-C3B-C4B	-3.02	111.03	124.39
3	B	602	HEM	C4C-NC-C1C	2.95	110.63	105.82
3	A	602	HEM	C4A-NA-C1A	2.89	110.53	105.82
2	B	601	PLP	C6-C5-C4	2.79	120.39	118.10
3	B	602	HEM	C4A-NA-C1A	2.79	110.37	105.82
3	A	602	HEM	CAB-C3B-C4B	-2.67	112.59	124.39
3	B	602	HEM	CHC-C4B-NB	2.57	127.19	124.42
3	A	602	HEM	C4C-C3C-C2C	2.47	108.96	106.81
3	B	602	HEM	C4C-C3C-C2C	2.46	108.95	106.81
3	A	602	HEM	CHA-C4D-C3D	2.46	129.76	125.23
3	A	602	HEM	CHB-C1B-NB	2.38	127.31	124.37
3	A	602	HEM	CHA-C1A-NA	2.36	128.13	123.86
3	A	602	HEM	CHC-C4B-C3B	2.33	129.72	125.07
3	B	602	HEM	CHA-C4D-C3D	2.31	129.49	125.23
3	A	602	HEM	C4C-CHD-C1D	-2.29	121.16	126.02
3	A	602	HEM	CHB-C4A-NA	2.27	127.97	123.86
3	B	602	HEM	CHA-C1A-NA	2.26	127.97	123.86
3	B	602	HEM	C4C-CHD-C1D	-2.22	121.29	126.02
2	B	601	PLP	C5-C6-N1	-2.22	120.22	123.83
2	A	601	PLP	C6-C5-C4	2.18	119.89	118.10
3	A	602	HEM	C2A-C1A-NA	-2.14	107.77	110.15
3	B	602	HEM	CAB-C3B-C2B	2.10	135.26	128.43
3	B	602	HEM	CHB-C1B-NB	2.10	126.97	124.37
3	A	602	HEM	CHC-C1C-C2C	-2.07	121.17	125.49
3	A	602	HEM	CAA-CBA-CGA	-2.06	108.19	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	HEM	CHB-C4A-NA	2.06	127.59	123.86

There are no chirality outliers.

All (1) torsion outliers are listed below:

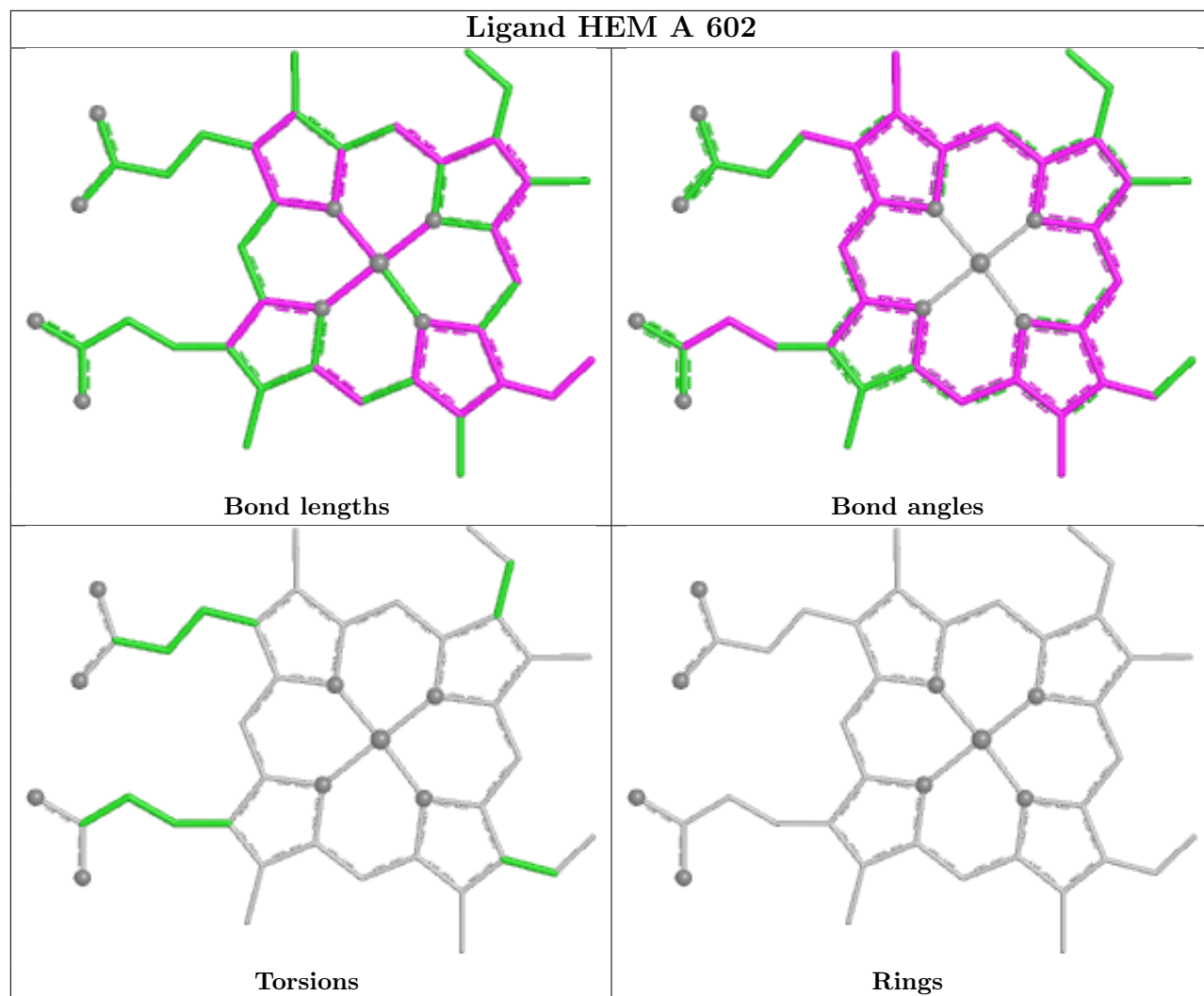
Mol	Chain	Res	Type	Atoms
3	B	602	HEM	C3D-CAD-CBD-CGD

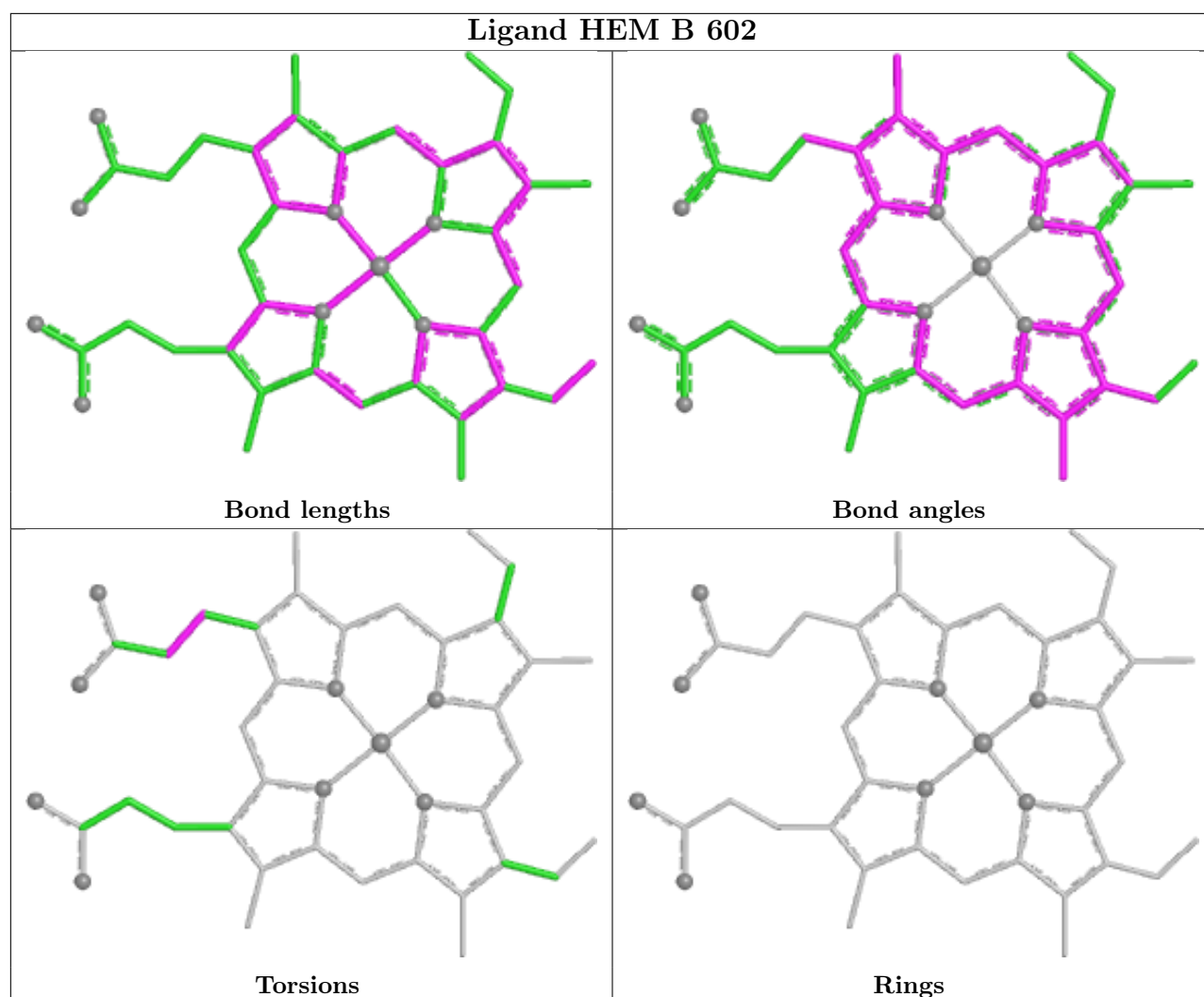
There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	PLP	3	0
3	A	602	HEM	5	0
3	B	602	HEM	6	0
2	A	601	PLP	3	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	496/549 (90%)	2.09	231 (46%)	0 0	41, 93, 150, 202	1 (0%)
1	B	496/549 (90%)	1.99	212 (42%)	0 1	46, 88, 142, 184	1 (0%)
All	All	992/1098 (90%)	2.04	443 (44%)	0 0	41, 90, 147, 202	2 (0%)

All (443) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	ASP	8.2
1	A	233	TYR	7.7
1	B	411	HIS	6.6
1	A	403	THR	6.6
1	B	252	VAL	5.9
1	A	254	SER	5.8
1	B	284	GLY	5.8
1	B	275	CYS	5.7
1	A	123	SER	5.7
1	B	76	ILE	5.6
1	A	280	VAL	5.5
1	A	508	PHE	5.5
1	A	532	GLY	5.5
1	B	248	LEU	5.4
1	A	90	VAL	5.3
1	A	271	LYS	5.3
1	B	348	GLY	5.3
1	A	246	GLY	5.3
1	A	480	GLY	5.3
1	B	194	ASN	5.3
1	A	142	ILE	5.2
1	A	194	ASN	5.2
1	A	540	LEU	5.1
1	B	533	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	77	LEU	5.0
1	B	403	THR	5.0
1	A	308	TYR	4.9
1	A	457	GLY	4.9
1	A	237	ALA	4.9
1	A	124	LEU	4.8
1	B	386	LEU	4.7
1	B	114	ALA	4.7
1	A	242	GLN	4.7
1	A	409	TRP	4.6
1	A	305	GLY	4.6
1	B	319	VAL	4.6
1	B	84	ILE	4.5
1	A	109	CYS	4.4
1	B	419	LEU	4.4
1	A	458	MET	4.4
1	A	122	ILE	4.4
1	B	222	GLN	4.4
1	B	81	LEU	4.4
1	B	74	PRO	4.3
1	B	42	LEU	4.3
1	A	311	ILE	4.2
1	A	71	ALA	4.2
1	B	371	VAL	4.2
1	B	48	ALA	4.2
1	B	401	ASP	4.2
1	A	530	VAL	4.2
1	A	539	LEU	4.2
1	A	513	HIS	4.1
1	A	386	LEU	4.1
1	A	198	ASP	4.1
1	A	481	LYS	4.1
1	A	53	THR	4.1
1	A	363	GLU	4.1
1	B	103	CYS	4.0
1	B	210	LEU	4.0
1	A	79	ASP	4.0
1	B	272	CYS	4.0
1	B	257	THR	3.9
1	A	366	GLU	3.9
1	B	359	LYS	3.9
1	A	407	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	245	ASP	3.9
1	A	514	GLU	3.9
1	A	160	VAL	3.9
1	B	264	ILE	3.9
1	A	42	LEU	3.9
1	B	251	LEU	3.9
1	B	402	LEU	3.9
1	A	482	VAL	3.9
1	B	356	VAL	3.9
1	A	188	ILE	3.9
1	B	473	VAL	3.8
1	B	262	THR	3.8
1	B	532	GLY	3.8
1	B	134	GLY	3.8
1	A	115	GLY	3.8
1	A	303	VAL	3.8
1	A	128	GLU	3.7
1	B	400	GLU	3.7
1	B	373	ILE	3.7
1	B	253	ALA	3.7
1	B	254	SER	3.6
1	A	120	ASP	3.6
1	B	233	TYR	3.6
1	A	272	CYS	3.6
1	A	238	ASP	3.6
1	B	95	ILE	3.6
1	A	165	CYS	3.6
1	A	126	MET	3.6
1	A	183	ALA	3.6
1	A	503	LEU	3.6
1	A	410	TRP	3.5
1	B	492	LEU	3.5
1	A	167	ILE	3.5
1	A	431	CYS	3.5
1	B	530	VAL	3.5
1	A	196	ARG	3.5
1	A	392	LEU	3.5
1	B	106	LEU	3.5
1	B	547	GLU	3.5
1	B	450	ASP	3.5
1	A	304	GLU	3.4
1	A	309	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	226	ALA	3.4
1	A	462	GLY	3.4
1	A	364	LEU	3.4
1	A	473	VAL	3.4
1	A	70	PRO	3.4
1	A	373	ILE	3.4
1	A	256	GLY	3.4
1	A	534	VAL	3.4
1	B	345	LEU	3.4
1	A	379	ARG	3.4
1	B	109	CYS	3.4
1	A	213	GLU	3.4
1	A	43	TRP	3.4
1	A	241	LEU	3.3
1	B	261	ILE	3.3
1	B	529	MET	3.3
1	B	73	SER	3.3
1	B	508	PHE	3.3
1	A	56	LEU	3.3
1	B	423	LEU	3.3
1	A	533	VAL	3.3
1	A	529	MET	3.3
1	B	56	LEU	3.3
1	A	223	TYR	3.3
1	A	186	ALA	3.3
1	B	67	HIS	3.3
1	B	472	LYS	3.3
1	A	505	MET	3.3
1	A	230	LEU	3.3
1	B	135	THR	3.3
1	A	349	SER	3.3
1	A	416	GLU	3.2
1	B	342	GLU	3.2
1	B	278	ILE	3.2
1	A	46	PRO	3.2
1	A	84	ILE	3.2
1	B	344	LEU	3.2
1	B	358	VAL	3.2
1	B	83	LYS	3.2
1	B	221	ASP	3.2
1	B	212	ASN	3.2
1	A	456	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	68	THR	3.2
1	B	104	GLU	3.2
1	A	163	TYR	3.2
1	B	349	SER	3.2
1	A	401	ASP	3.2
1	A	132	ARG	3.2
1	A	415	GLN	3.2
1	A	455	ILE	3.2
1	A	91	ARG	3.1
1	B	360	ALA	3.1
1	A	131	GLU	3.1
1	A	312	PRO	3.1
1	A	154	LEU	3.1
1	A	310	PHE	3.1
1	A	382	MET	3.1
1	B	462	GLY	3.1
1	B	392	LEU	3.1
1	B	406	LYS	3.1
1	B	258	GLY	3.1
1	B	307	GLY	3.1
1	A	81	LEU	3.1
1	B	46	PRO	3.1
1	B	449	VAL	3.1
1	B	339	ILE	3.1
1	A	344	LEU	3.1
1	B	330	GLU	3.1
1	A	444	ASP	3.0
1	B	120	ASP	3.0
1	B	198	ASP	3.0
1	B	357	ALA	3.0
1	A	127	ILE	3.0
1	A	317	ARG	3.0
1	A	488	LYS	3.0
1	B	369	ARG	3.0
1	A	448	VAL	3.0
1	B	224	ARG	3.0
1	A	268	LEU	3.0
1	A	66	HIS	3.0
1	A	220	LEU	3.0
1	B	549	ASP	3.0
1	B	260	THR	3.0
1	A	252	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	468	LEU	2.9
1	A	270	GLU	2.9
1	B	366	GLU	2.9
1	B	43	TRP	2.9
1	B	115	GLY	2.9
1	A	234	ASP	2.9
1	A	67	HIS	2.9
1	A	423	LEU	2.9
1	A	60	ALA	2.9
1	A	180	VAL	2.9
1	A	472	LYS	2.9
1	B	147	SER	2.9
1	A	68	THR	2.9
1	A	218	HIS	2.9
1	B	338	LEU	2.9
1	B	340	ALA	2.9
1	B	376	ASP	2.9
1	B	92	ILE	2.9
1	A	144	GLU	2.8
1	A	125	ARG	2.8
1	A	129	ASP	2.8
1	B	538	ASP	2.8
1	A	279	GLY	2.8
1	B	59	PRO	2.8
1	A	411	HIS	2.8
1	B	140	ASP	2.8
1	B	388	ASP	2.8
1	B	250	MET	2.8
1	B	399	GLU	2.8
1	B	454	VAL	2.8
1	B	469	LEU	2.8
1	B	540	LEU	2.8
1	A	235	THR	2.8
1	B	308	TYR	2.8
1	B	286	ILE	2.8
1	B	299	THR	2.8
1	A	197	PHE	2.7
1	B	60	ALA	2.7
1	A	156	LEU	2.7
1	A	137	LYS	2.7
1	A	250	MET	2.7
1	B	361	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	85	GLY	2.7
1	A	50	SER	2.7
1	A	378	VAL	2.7
1	A	454	VAL	2.7
1	A	179	ASP	2.7
1	B	375	PRO	2.7
1	A	104	GLU	2.7
1	B	420	SER	2.7
1	B	539	LEU	2.7
1	A	405	LYS	2.7
1	B	72	LYS	2.7
1	A	484	TYR	2.7
1	A	193	THR	2.7
1	B	300	THR	2.7
1	B	86	ASP	2.7
1	A	319	VAL	2.7
1	A	358	VAL	2.7
1	B	320	VAL	2.7
1	A	537	ILE	2.6
1	B	277	ILE	2.6
1	A	324	PHE	2.6
1	A	361	ALA	2.6
1	B	332	PHE	2.6
1	A	408	TRP	2.6
1	A	291	GLU	2.6
1	A	417	LEU	2.6
1	B	394	LYS	2.6
1	B	425	VAL	2.6
1	B	246	GLY	2.6
1	A	228	ASN	2.6
1	B	438	LEU	2.6
1	A	489	GLN	2.6
1	B	197	PHE	2.6
1	B	507	HIS	2.6
1	A	343	GLY	2.6
1	B	75	LYS	2.6
1	B	143	ILE	2.6
1	A	463	ASN	2.6
1	B	443	PHE	2.6
1	A	117	SER	2.6
1	A	92	ILE	2.6
1	A	130	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	421	ALA	2.6
1	A	269	LYS	2.5
1	B	382	MET	2.5
1	A	443	PHE	2.5
1	A	445	GLN	2.5
1	A	413	ARG	2.5
1	B	309	ASP	2.5
1	A	227	SER	2.5
1	B	480	GLY	2.5
1	A	112	PHE	2.5
1	A	260	THR	2.5
1	B	291	GLU	2.5
1	B	231	ALA	2.5
1	B	276	ARG	2.5
1	B	172	LYS	2.5
1	A	77	LEU	2.5
1	A	496	LEU	2.5
1	B	482	VAL	2.5
1	B	112	PHE	2.5
1	B	470	ALA	2.5
1	A	75	LYS	2.5
1	A	47	ASP	2.5
1	A	510	LEU	2.5
1	B	136	LEU	2.5
1	A	306	ILE	2.5
1	A	476	SER	2.5
1	B	223	TYR	2.5
1	A	121	ARG	2.5
1	A	507	HIS	2.5
1	A	103	CYS	2.5
1	A	181	LEU	2.4
1	A	261	ILE	2.4
1	B	63	SER	2.4
1	A	164	ARG	2.4
1	B	105	LEU	2.4
1	B	78	PRO	2.4
1	B	534	VAL	2.4
1	A	498	ARG	2.4
1	B	132	ARG	2.4
1	A	232	HIS	2.4
1	B	541	ASN	2.4
1	A	76	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	80	ILE	2.4
1	B	448	VAL	2.4
1	B	211	LYS	2.4
1	A	487	PHE	2.4
1	A	470	ALA	2.4
1	B	163	TYR	2.4
1	A	345	LEU	2.4
1	A	255	VAL	2.4
1	B	372	VAL	2.4
1	B	190	ARG	2.4
1	B	209[A]	ARG	2.4
1	B	316	ASP	2.4
1	A	492	LEU	2.4
1	A	152	ILE	2.4
1	B	282	PRO	2.4
1	A	398	LYS	2.3
1	A	116	GLY	2.3
1	A	99	PHE	2.3
1	A	538	ASP	2.3
1	B	249	ASP	2.3
1	A	114	ALA	2.3
1	A	547	GLU	2.3
1	B	404	GLU	2.3
1	B	298	GLN	2.3
1	B	528	GLN	2.3
1	B	337	MET	2.3
1	B	424	THR	2.3
1	B	429	ILE	2.3
1	B	422	PRO	2.3
1	B	463	ASN	2.3
1	A	176	GLU	2.3
1	B	128	GLU	2.3
1	B	265	ALA	2.3
1	B	331	ALA	2.3
1	B	505	MET	2.3
1	B	352	SER	2.3
1	B	66	HIS	2.3
1	B	290	PRO	2.3
1	B	451	GLU	2.3
1	A	316	ASP	2.3
1	B	281	ASP	2.3
1	A	199	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	441	LYS	2.3
1	B	318	THR	2.3
1	B	511	VAL	2.3
1	A	287	LEU	2.3
1	A	477	ASP	2.3
1	B	184	LEU	2.3
1	B	506	ASP	2.3
1	A	326	SER	2.3
1	B	543	VAL	2.3
1	A	461	LEU	2.2
1	B	499	LEU	2.2
1	A	298	GLN	2.2
1	A	506	ASP	2.2
1	A	54	TRP	2.2
1	A	41	PRO	2.2
1	A	118	VAL	2.2
1	A	371	VAL	2.2
1	A	171	GLU	2.2
1	A	248	LEU	2.2
1	B	144	GLU	2.2
1	B	113	ASN	2.2
1	B	240	ILE	2.2
1	B	445	GLN	2.2
1	B	444	ASP	2.2
1	A	535	THR	2.2
1	B	535	THR	2.2
1	A	89	MET	2.2
1	A	166	ILE	2.2
1	A	295	GLN	2.2
1	B	321	ASP	2.2
1	A	544	ALA	2.2
1	B	270	GLU	2.2
1	B	452	ALA	2.2
1	A	168	VAL	2.2
1	A	512	VAL	2.2
1	B	41	PRO	2.2
1	A	493	THR	2.2
1	B	102	LYS	2.2
1	B	139	GLY	2.2
1	B	208	TRP	2.2
1	B	409	TRP	2.2
1	B	370	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	184	LEU	2.2
1	B	496	LEU	2.2
1	A	340	ALA	2.2
1	A	548	ARG	2.1
1	B	415	GLN	2.1
1	B	479	VAL	2.1
1	A	257	THR	2.1
1	A	322	LYS	2.1
1	A	231	ALA	2.1
1	A	339	ILE	2.1
1	A	474	GLN	2.1
1	A	94	LYS	2.1
1	A	347	GLY	2.1
1	B	193	THR	2.1
1	B	493	THR	2.1
1	B	237	ALA	2.1
1	B	167	ILE	2.1
1	A	393	GLN	2.1
1	A	550	GLN	2.1
1	A	356	VAL	2.1
1	A	453	GLY	2.1
1	B	302	GLU	2.1
1	A	501	HIS	2.1
1	B	99	PHE	2.1
1	A	150	THR	2.1
1	B	161	ARG	2.1
1	A	264	ILE	2.1
1	A	502	ILE	2.1
1	B	297	GLU	2.1
1	A	247	LYS	2.0
1	A	136	LEU	2.0
1	B	79	ASP	2.0
1	B	166	ILE	2.0
1	A	192	PRO	2.0
1	A	397	LEU	2.0
1	B	426	LEU	2.0
1	B	548	ARG	2.0
1	B	487	PHE	2.0
1	A	236	THR	2.0
1	A	421	ALA	2.0
1	B	381	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](#)

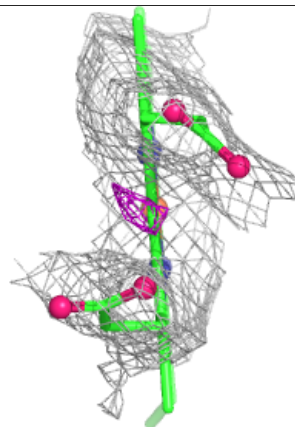
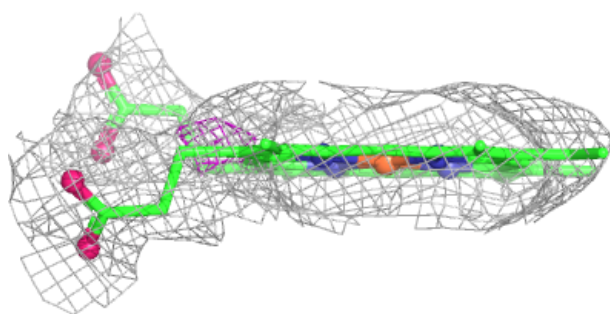
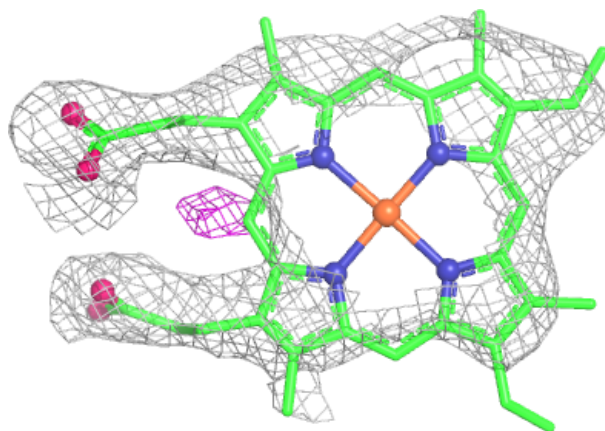
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	PLP	B	601	15/16	0.85	0.15	53,66,75,76	0
2	PLP	A	601	15/16	0.88	0.12	58,75,85,86	0
3	HEM	B	602	43/43	0.90	0.20	101,104,104,104	0
3	HEM	A	602	43/43	0.91	0.18	107,108,109,109	0

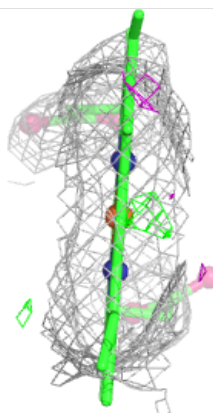
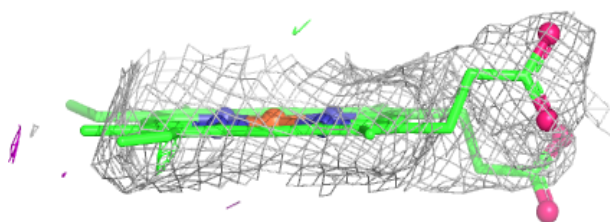
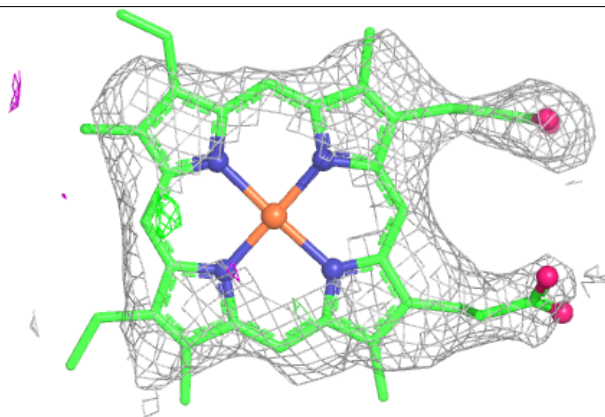
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

There are no such residues in this entry.