



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2025 – 05:01 PM EDT

PDB ID : 4L28  
Title : Crystal structure of delta516-525 human cystathionine beta-synthase D444N mutant containing C-terminal 6xHis tag  
Authors : Ereno, J.; Majtan, T.; Oyenarte, I.; Kraus, J.P.; Martinez, L.A.  
Deposited on : 2013-06-04  
Resolution : 2.63 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

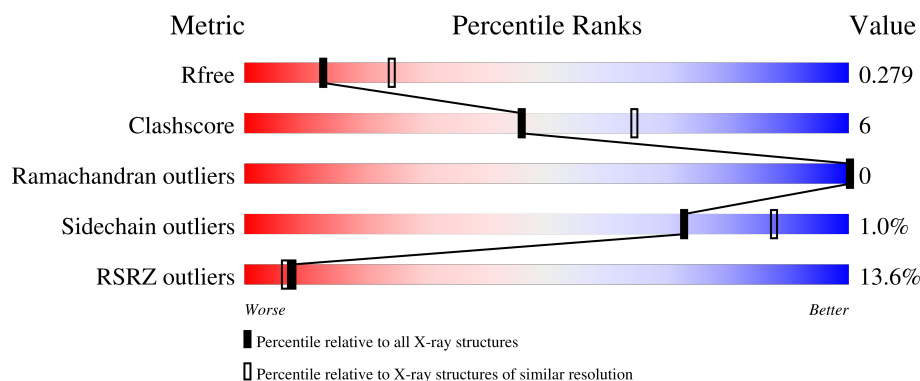
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



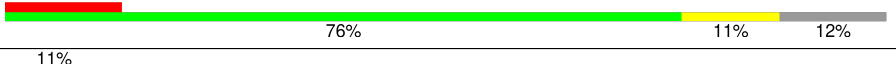

The reported resolution of this entry is 2.63 Å.

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))
$R_{free}$	164625	4623 (2.64-2.60)
Clashscore	180529	5071 (2.64-2.60)
Ramachandran outliers	177936	5006 (2.64-2.60)
Sidechain outliers	177891	5006 (2.64-2.60)
RSRZ outliers	164620	4622 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	558	
1	B	558	
1	C	558	
1	D	558	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15455 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	493	Total	C	N	O	S	0	0	0
			3803	2410	665	706	22			
1	B	494	Total	C	N	O	S	0	0	0
			3813	2414	669	708	22			
1	C	491	Total	C	N	O	S	0	0	0
			3791	2403	666	700	22			
1	D	493	Total	C	N	O	S	0	0	0
			3816	2416	668	710	22			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	444	ASN	ASP	engineered mutation	UNP P35520
A	552	LEU	-	expression tag	UNP P35520
A	553	GLU	-	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	444	ASN	ASP	engineered mutation	UNP P35520
B	552	LEU	-	expression tag	UNP P35520
B	553	GLU	-	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
C	444	ASN	ASP	engineered mutation	UNP P35520
C	552	LEU	-	expression tag	UNP P35520
C	553	GLU	-	expression tag	UNP P35520

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Chain	Residue	Modelled	Actual	Comment	Reference
C	554	HIS	-	expression tag	UNP P35520
C	555	HIS	-	expression tag	UNP P35520
C	556	HIS	-	expression tag	UNP P35520
C	557	HIS	-	expression tag	UNP P35520
C	558	HIS	-	expression tag	UNP P35520
C	559	HIS	-	expression tag	UNP P35520
D	444	ASN	ASP	engineered mutation	UNP P35520
D	552	LEU	-	expression tag	UNP P35520
D	553	GLU	-	expression tag	UNP P35520
D	554	HIS	-	expression tag	UNP P35520
D	555	HIS	-	expression tag	UNP P35520
D	556	HIS	-	expression tag	UNP P35520
D	557	HIS	-	expression tag	UNP P35520
D	558	HIS	-	expression tag	UNP P35520
D	559	HIS	-	expression tag	UNP P35520

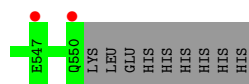
- PLP
- 
- The diagram illustrates the chemical structure of PLP (Pyridoxal Phosphate). It features a central pyridine ring with a nitrogen atom (N1) at the top. The ring is substituted with a phosphate group at the 3-position (C3) and an aldehyde group at the 4-position (C4). The phosphate group is shown as a phosphorus atom (P) bonded to four oxygen atoms: one double-bonded (O1P), one single-bonded (O2P), and two others (O3P, O4P) that are part of the phosphate chain. The aldehyde group consists of a carbonyl carbon (C4A) double-bonded to an oxygen atom (O4A) and single-bonded to a hydrogen atom (H4A). The pyridine ring carbons are labeled C2, C3, C4, C5, and C6. The phosphate group is labeled C5A. The aldehyde group is labeled C4A. The nitrogen atom is labeled N1. The oxygen atoms are labeled O1P, O2P, O3P, O4P, O4A, and O3. The carbon atoms are labeled C2, C3, C4, C5, C6, C5A, and C4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 15	C 8	N 1	O 5	P 1	0	0
2	B	1	Total 15	C 8	N 1	O 5	P 1	0	0
2	C	1	Total 15	C 8	N 1	O 5	P 1	0	0
2	D	1	Total 15	C 8	N 1	O 5	P 1	0	0

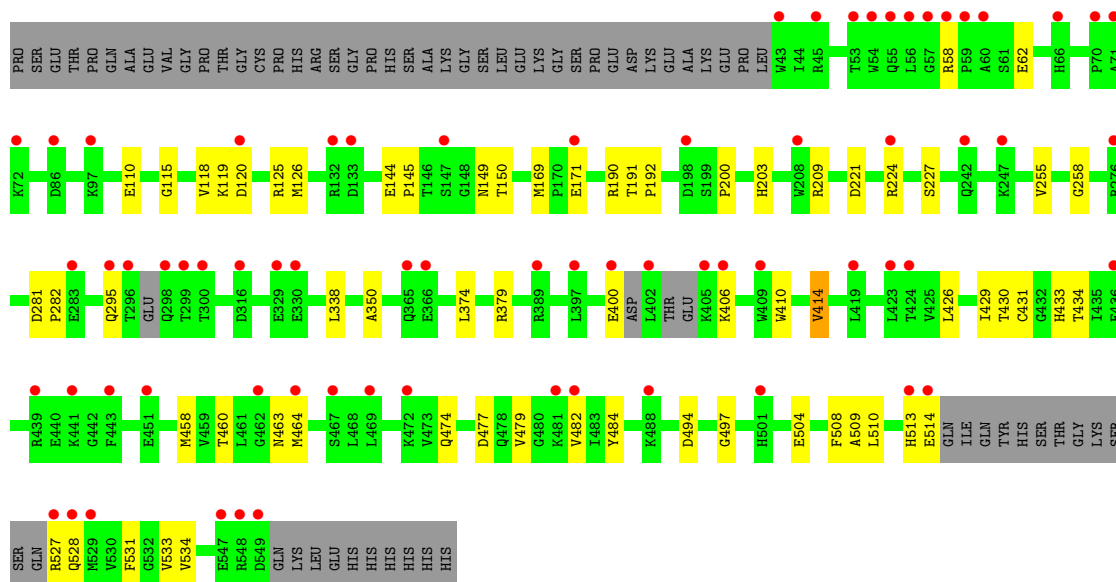
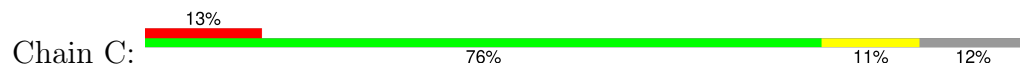
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- The diagram illustrates the chemical structure of Heme (HEM). It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The ring is substituted with various side chains, including vinyl groups (C3A, C3B, C3C, C3D), methyl groups (C2A, C2B, C2C, C2D), and a long phytol chain (C1A, C1B, C1C, C1D). The central iron atom is also coordinated by a proximal histidine residue (NA) and a distal water molecule (ND). The overall structure is shown in a 2D representation with green lines for the carbon skeleton and blue lines for the nitrogen and iron atoms.

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

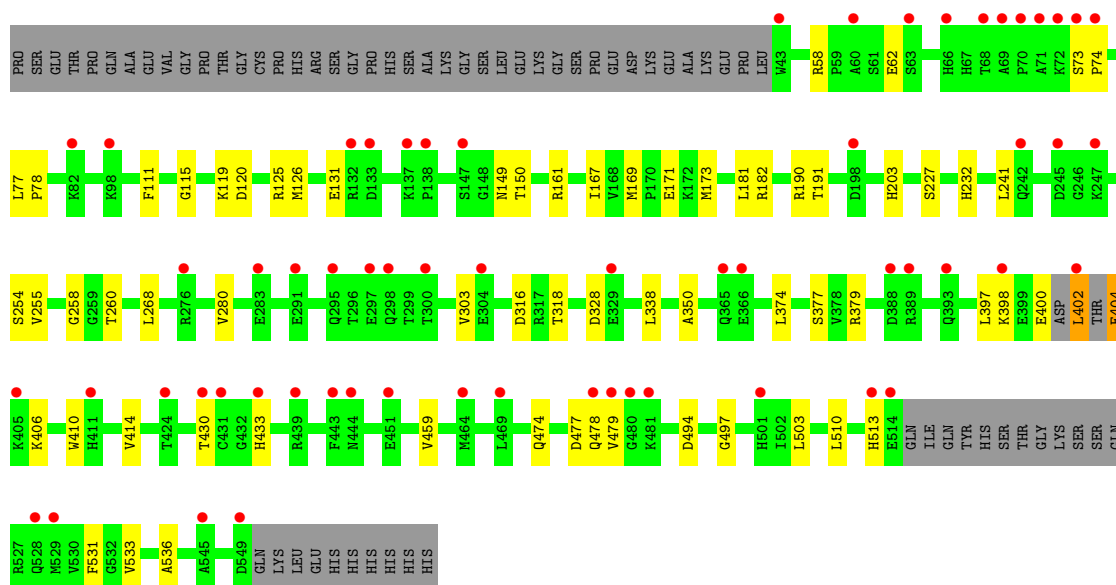
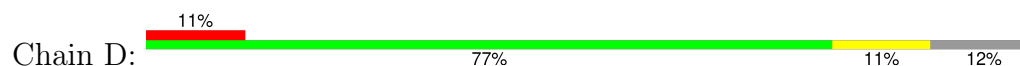




• Molecule 1: Cystathionine beta-synthase



• Molecule 1: Cystathionine beta-synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.48Å 131.07Å 207.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.39 – 2.63 48.39 – 2.63	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.39-2.63) 98.3 (48.39-2.63)	Depositor EDS
$R_{merge}$	0.36	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.256 , 0.281 0.256 , 0.279	Depositor DCC
$R_{free}$ test set	4472 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.8	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 56.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15455	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.2651e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.60	0/3874	0.52	0/5245
1	B	0.60	0/3882	0.52	0/5253
1	C	0.60	0/3860	0.52	0/5222
1	D	0.62	0/3886	0.53	0/5258
All	All	0.61	0/15502	0.52	0/20978

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3803	0	3855	41	0
1	B	3813	0	3859	42	0
1	C	3791	0	3852	49	0
1	D	3816	0	3871	43	0
2	A	15	0	6	2	0
2	B	15	0	6	2	0
2	C	15	0	6	2	0
2	D	15	0	6	2	0
3	A	43	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	43	0	30	1	0
3	C	43	0	30	2	0
3	D	43	0	30	2	0
All	All	15455	0	15581	176	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 6.

All (176) 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:B:48:ALA:HB3	1:B:224:ARG:HH12	1.19	1.07
1:A:403:THR:HA	1:A:406:LYS:HD2	1.43	0.99
1:D:513:HIS:HB2	1:D:531:PHE:HE2	1.45	0.80
1:B:431:CYS:HB3	1:B:464:MET:HE1	1.63	0.79
1:B:514:GLU:O	1:B:527:ARG:NH2	2.17	0.78
1:A:406:LYS:HD3	1:A:410:TRP:CE2	2.19	0.77
1:A:513:HIS:HB2	1:A:531:PHE:HE2	1.53	0.72
1:B:504:GLU:OE1	1:D:182:ARG:NH1	2.23	0.72
1:C:464:MET:SD	1:C:482:VAL:HG21	2.30	0.71
1:B:419:LEU:HD13	1:B:511:VAL:HG11	1.72	0.71
1:A:66:HIS:CE1	1:A:132:ARG:NH1	2.60	0.69
1:C:513:HIS:HB2	1:C:531:PHE:HE2	1.56	0.69
1:B:458:MET:HE1	1:B:510:LEU:HD21	1.75	0.69
1:B:48:ALA:HB3	1:B:224:ARG:NH1	2.01	0.68
1:A:66:HIS:CE1	1:A:132:ARG:HH12	2.12	0.68
1:D:350:ALA:HB1	1:D:374:LEU:HD22	1.77	0.66
1:A:182:ARG:NH1	1:C:504:GLU:OE1	2.29	0.65
1:C:513:HIS:HB2	1:C:531:PHE:CE2	2.34	0.63
1:B:48:ALA:CB	1:B:224:ARG:HH12	2.05	0.63
1:B:149:ASN:ND2	2:B:601:PLP:H2A1	2.15	0.62
1:D:149:ASN:ND2	2:D:601:PLP:H2A1	2.14	0.62
1:A:149:ASN:ND2	2:A:601:PLP:H2A1	2.14	0.61
3:B:602:HEM:HMB1	3:B:602:HEM:HBB2	1.82	0.61
1:B:439:ARG:HH21	1:B:465:LEU:HD21	1.65	0.61
1:D:430:THR:HG23	1:D:433:HIS:HB2	1.83	0.60
1:B:200:PRO:O	1:B:209:ARG:NH2	2.35	0.60
1:B:398:LYS:NZ	1:C:400:GLU:OE1	2.33	0.60
3:A:602:HEM:HMB1	3:A:602:HEM:HBB2	1.83	0.59
1:A:350:ALA:HB1	1:A:374:LEU:HD22	1.85	0.59
1:B:350:ALA:HB1	1:B:374:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ALA:HB1	1:C:374:LEU:HD22	1.85	0.59
1:A:191:THR:HG21	1:A:203:HIS:HA	1.85	0.58
1:B:464:MET:SD	1:B:482:VAL:HG11	2.44	0.58
1:D:406:LYS:HD3	1:D:410:TRP:CE2	2.39	0.58
1:B:191:THR:HG21	1:B:203:HIS:HA	1.86	0.57
1:C:115:GLY:O	1:C:379:ARG:NH2	2.37	0.57
1:C:200:PRO:O	1:C:209:ARG:NH2	2.37	0.57
1:C:429:ILE:HD13	1:C:434:THR:HG22	1.86	0.57
3:D:602:HEM:HMB1	3:D:602:HEM:HBB2	1.85	0.57
1:A:254:SER:HA	1:A:280:VAL:HB	1.87	0.57
1:C:281:ASP:OD2	1:C:282:PRO:HD2	2.04	0.56
1:D:513:HIS:HB2	1:D:531:PHE:CE2	2.35	0.56
1:B:45:ARG:O	1:B:224:ARG:NH1	2.39	0.55
1:B:413:ARG:NH1	1:B:493:THR:HB	2.22	0.55
1:B:379:ARG:HG2	1:B:379:ARG:HH11	1.72	0.55
1:C:430:THR:HG23	1:C:433:HIS:HB2	1.88	0.55
1:C:406:LYS:HD3	1:C:410:TRP:CE2	2.41	0.55
1:B:431:CYS:CB	1:B:464:MET:HE1	2.36	0.54
1:C:58:ARG:NE	1:C:62:GLU:OE1	2.38	0.54
1:C:379:ARG:HG2	1:C:379:ARG:HH11	1.72	0.54
1:D:406:LYS:HD3	1:D:410:TRP:NE1	2.22	0.54
1:B:429:ILE:HG23	1:B:479:VAL:HG21	1.90	0.54
1:D:254:SER:HA	1:D:280:VAL:HB	1.90	0.54
1:A:119:LYS:HB3	1:A:150:THR:HA	1.90	0.54
1:C:149:ASN:ND2	2:C:601:PLP:H2A1	2.21	0.54
1:D:191:THR:HG21	1:D:203:HIS:HA	1.90	0.54
1:D:510:LEU:HD22	1:D:533:VAL:HG12	1.90	0.54
1:B:281:ASP:OD2	1:B:282:PRO:HD2	2.09	0.53
1:A:430:THR:HG23	1:A:433:HIS:HB2	1.91	0.53
1:C:527:ARG:HG3	1:C:528:GLN:H	1.74	0.52
1:C:430:THR:O	1:C:434:THR:HG23	2.09	0.52
1:C:509:ALA:HB3	1:C:534:VAL:HG13	1.92	0.52
1:D:379:ARG:HH11	1:D:379:ARG:HG2	1.75	0.52
1:C:119:LYS:HB3	1:C:150:THR:HA	1.92	0.52
1:A:458:MET:HE1	1:A:510:LEU:HD21	1.90	0.51
1:A:435:ILE:HG23	1:A:439:ARG:HD2	1.91	0.51
1:B:119:LYS:HB3	1:B:150:THR:HA	1.92	0.51
1:D:404:GLU:N	1:D:404:GLU:OE2	2.42	0.51
1:C:125:ARG:HG3	1:C:227:SER:HB3	1.92	0.51
1:D:115:GLY:N	1:D:120:ASP:OD2	2.43	0.51
1:B:413:ARG:NH1	1:B:493:THR:CB	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:ASN:HD22	2:D:601:PLP:H2A1	1.74	0.50
1:A:149:ASN:HD22	2:A:601:PLP:H2A1	1.75	0.50
3:C:602:HEM:HBB2	3:C:602:HEM:HMB1	1.93	0.50
3:C:602:HEM:HMC1	3:C:602:HEM:HBC2	1.94	0.50
1:C:458:MET:HE1	1:C:533:VAL:HG21	1.93	0.50
1:A:414:VAL:HG23	1:A:494:ASP:O	2.12	0.49
1:D:126:MET:HG3	1:D:227:SER:HB2	1.94	0.49
1:D:303:VAL:HG23	1:D:328:ASP:OD2	2.12	0.49
1:A:58:ARG:NE	1:A:62:GLU:OE1	2.44	0.49
1:D:414:VAL:HG23	1:D:494:ASP:O	2.13	0.49
1:C:510:LEU:HD22	1:C:533:VAL:HG22	1.94	0.49
1:B:126:MET:HG3	1:B:227:SER:HB2	1.95	0.49
1:C:295:GLN:HG3	1:D:478:GLN:OE1	2.13	0.49
1:D:111:PHE:HB2	1:D:377:SER:HB3	1.95	0.48
1:A:379:ARG:HH11	1:A:379:ARG:HG2	1.78	0.48
1:B:149:ASN:HD22	2:B:601:PLP:H2A1	1.77	0.48
1:C:458:MET:HE2	1:C:533:VAL:HG11	1.94	0.48
1:A:406:LYS:HD3	1:A:410:TRP:NE1	2.28	0.48
1:B:414:VAL:HG23	1:B:417:LEU:HD12	1.94	0.48
3:D:602:HEM:HBC2	3:D:602:HEM:HMC1	1.96	0.48
1:A:115:GLY:N	1:A:120:ASP:OD2	2.46	0.47
1:D:58:ARG:NE	1:D:62:GLU:OE1	2.46	0.47
1:C:115:GLY:N	1:C:120:ASP:OD2	2.47	0.47
1:D:119:LYS:HB3	1:D:150:THR:HA	1.97	0.47
1:B:111:PHE:HB2	1:B:377:SER:HB3	1.97	0.47
1:C:149:ASN:HD22	2:C:601:PLP:H2A1	1.80	0.47
1:D:459:VAL:HG21	1:D:479:VAL:CG1	2.45	0.47
1:D:131:GLU:OE2	1:D:161:ARG:NH1	2.48	0.46
1:A:192:PRO:HG2	1:A:195:ALA:HB2	1.97	0.46
1:C:464:MET:HB3	1:C:464:MET:HE3	1.44	0.46
1:A:171:GLU:CD	1:A:192:PRO:HA	2.36	0.46
1:B:398:LYS:NZ	1:C:400:GLU:CD	2.69	0.46
1:C:406:LYS:HD3	1:C:410:TRP:NE1	2.31	0.46
1:A:303:VAL:HG23	1:A:328:ASP:OD2	2.15	0.46
1:D:255:VAL:HG13	1:D:258:GLY:HA2	1.98	0.46
1:A:51:ARG:HB3	3:A:602:HEM:HBA1	1.98	0.45
1:C:126:MET:HG3	1:C:227:SER:HB2	1.98	0.45
1:D:232:HIS:CD2	1:D:260:THR:HA	2.51	0.45
1:C:119:LYS:HD2	1:C:150:THR:OG1	2.16	0.45
1:A:400:GLU:H	1:A:400:GLU:HG2	1.57	0.45
1:C:171:GLU:CD	1:C:192:PRO:HA	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:VAL:HG13	1:C:258:GLY:HA2	1.98	0.45
1:B:430:THR:O	1:B:434:THR:HG23	2.16	0.45
1:A:255:VAL:HG13	1:A:258:GLY:HA2	1.99	0.45
1:A:169:MET:O	1:A:190:ARG:HA	2.16	0.45
1:C:169:MET:O	1:C:190:ARG:HA	2.17	0.45
1:A:111:PHE:HB2	1:A:377:SER:HB3	1.99	0.44
1:D:169:MET:HE2	1:D:173:MET:HB2	1.99	0.44
1:D:169:MET:O	1:D:190:ARG:HA	2.16	0.44
1:B:125:ARG:HG3	1:B:227:SER:HB3	1.99	0.44
1:C:410:TRP:CE2	1:C:497:GLY:HA3	2.52	0.44
1:C:426:LEU:O	1:C:429:ILE:HG22	2.18	0.44
1:D:459:VAL:HG21	1:D:479:VAL:HG13	2.00	0.44
1:A:426:LEU:O	1:A:429:ILE:HG22	2.16	0.44
1:D:397:LEU:HD13	1:D:402:LEU:HD12	2.00	0.44
1:B:206:VAL:HG22	1:B:209:ARG:HH21	1.82	0.44
1:B:459:VAL:HG11	1:B:479:VAL:HG13	1.99	0.44
1:B:379:ARG:HG2	1:B:379:ARG:NH1	2.33	0.44
1:B:439:ARG:NH2	1:B:465:LEU:HD21	2.31	0.43
1:B:422:PRO:HD2	1:B:530:VAL:O	2.18	0.43
1:C:191:THR:HG21	1:C:203:HIS:HA	2.00	0.43
1:C:414:VAL:HG12	1:C:494:ASP:O	2.18	0.43
1:C:379:ARG:HG2	1:C:379:ARG:NH1	2.34	0.43
1:A:398:LYS:HB3	1:A:400:GLU:HG2	2.00	0.43
1:C:221:ASP:OD1	1:C:224:ARG:HD3	2.19	0.43
1:D:316:ASP:OD2	1:D:318:THR:OG1	2.27	0.43
1:D:410:TRP:CE2	1:D:497:GLY:HA3	2.54	0.43
1:D:167:ILE:HG13	1:D:181:LEU:HD22	2.01	0.43
1:A:459:VAL:HG21	1:A:479:VAL:HG13	2.00	0.42
1:D:406:LYS:HD3	1:D:410:TRP:CD1	2.54	0.42
1:D:474:GLN:O	1:D:477:ASP:HB2	2.19	0.42
1:A:424:THR:HG22	1:A:447:PRO:HG2	2.01	0.42
1:A:474:GLN:O	1:A:477:ASP:HB2	2.20	0.42
1:D:77:LEU:HA	1:D:78:PRO:HD2	1.89	0.42
1:B:115:GLY:N	1:B:120:ASP:OD2	2.53	0.42
1:B:254:SER:HA	1:B:280:VAL:HB	2.01	0.42
1:C:474:GLN:O	1:C:477:ASP:HB2	2.20	0.42
1:A:125:ARG:HG3	1:A:227:SER:HB3	2.02	0.41
1:C:513:HIS:CG	1:C:514:GLU:N	2.87	0.41
1:A:282:PRO:HD3	1:A:306:ILE:HD12	2.02	0.41
1:C:431:CYS:HB3	1:C:464:MET:CE	2.51	0.41
1:D:379:ARG:HG2	1:D:379:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:460:THR:HG22	1:C:463:ASN:H	1.85	0.41
1:D:503:LEU:HD13	1:D:536:ALA:HA	2.01	0.41
1:B:255:VAL:HG13	1:B:258:GLY:HA2	2.01	0.41
1:D:73:SER:HA	1:D:74:PRO:HD2	1.91	0.41
1:B:490:ILE:O	1:B:511:VAL:HA	2.21	0.41
1:B:499:LEU:O	1:B:503:LEU:HG	2.21	0.41
1:C:484:TYR:CD2	1:C:508:PHE:HE2	2.39	0.41
1:B:463:ASN:ND2	1:B:482:VAL:HG22	2.35	0.41
1:A:77:LEU:HA	1:A:78:PRO:HD2	1.91	0.41
1:A:379:ARG:HG2	1:A:379:ARG:NH1	2.35	0.41
1:C:431:CYS:HB3	1:C:464:MET:HE2	2.03	0.41
1:D:125:ARG:HG3	1:D:227:SER:HB3	2.03	0.41
1:A:480:GLY:O	1:A:483:ILE:HG22	2.22	0.40
1:B:527:ARG:HG3	1:B:528:GLN:H	1.86	0.40
1:D:171:GLU:HA	1:D:190:ARG:NH2	2.35	0.40
1:A:144:GLU:HA	1:A:145:PRO:HD2	1.98	0.40
1:A:169:MET:HA	1:A:170:PRO:HD3	1.94	0.40
1:A:400:GLU:O	1:A:404:GLU:HG2	2.22	0.40
1:C:110:GLU:HG2	1:C:118:VAL:HB	2.03	0.40
1:C:144:GLU:HA	1:C:145:PRO:HD2	1.93	0.40
1:C:434:THR:HG21	1:C:479:VAL:HG21	2.03	0.40
1:D:119:LYS:HD2	1:D:150:THR:OG1	2.22	0.40
1:D:241:LEU:HA	1:D:241:LEU:HD23	1.91	0.40

There are no symmetry-related clashes.

## 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	487/558 (87%)	480 (99%)	7 (1%)	0	100	100
1	B	485/558 (87%)	476 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	482/558 (86%)	475 (98%)	7 (2%)	0	100	100
1	D	486/558 (87%)	480 (99%)	6 (1%)	0	100	100
All	All	1940/2232 (87%)	1911 (98%)	29 (2%)	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	412/472 (87%)	407 (99%)	5 (1%)	67	84
1	B	413/472 (88%)	410 (99%)	3 (1%)	81	92
1	C	411/472 (87%)	409 (100%)	2 (0%)	86	95
1	D	415/472 (88%)	409 (99%)	6 (1%)	62	81
All	All	1651/1888 (87%)	1635 (99%)	16 (1%)	73	87

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	LEU
1	A	338	LEU
1	A	399	GLU
1	A	400	GLU
1	A	405	LYS
1	B	268	LEU
1	B	338	LEU
1	B	399	GLU
1	C	338	LEU
1	C	414	VAL
1	D	268	LEU
1	D	338	LEU
1	D	398	LYS
1	D	400	GLU

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Mol	Chain	Res	Type
1	D	402	LEU
1	D	404	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	D	528	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	HEM	A	602	1	42,50,50	1.83	4 (9%)	46,82,82	1.29	6 (13%)
2	PLP	C	601	1	15,15,16	3.40	8 (53%)	21,22,23	2.11	7 (33%)
2	PLP	A	601	1	15,15,16	3.31	7 (46%)	21,22,23	2.03	5 (23%)
3	HEM	D	602	1	42,50,50	1.85	5 (11%)	46,82,82	1.28	6 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PLP	D	601	1	15,15,16	3.42	7 (46%)	21,22,23	1.99	5 (23%)
3	HEM	C	602	1	42,50,50	1.87	5 (11%)	46,82,82	1.23	6 (13%)
3	HEM	B	602	1	42,50,50	1.87	4 (9%)	46,82,82	1.24	6 (13%)
2	PLP	B	601	1	15,15,16	3.44	7 (46%)	21,22,23	2.18	7 (33%)

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

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	PLP	C2A-C2	-8.26	1.37	1.50
2	B	601	PLP	C2A-C2	-8.23	1.37	1.50
2	C	601	PLP	C2A-C2	-8.20	1.37	1.50
2	A	601	PLP	C2A-C2	-8.19	1.37	1.50
2	B	601	PLP	C4A-C4	-7.58	1.36	1.51
2	D	601	PLP	C4A-C4	-7.38	1.36	1.51
2	C	601	PLP	C4A-C4	-7.37	1.36	1.51
3	B	602	HEM	C3D-C2D	7.28	1.52	1.36
2	A	601	PLP	C4A-C4	-7.14	1.37	1.51
3	C	602	HEM	C3D-C2D	7.09	1.52	1.36
3	D	602	HEM	C3D-C2D	6.95	1.51	1.36
3	A	602	HEM	C3D-C2D	6.75	1.51	1.36
3	A	602	HEM	C3C-C2C	-5.46	1.33	1.40
3	B	602	HEM	C3C-C2C	-5.36	1.33	1.40
3	D	602	HEM	C3C-C2C	-5.28	1.33	1.40
3	C	602	HEM	C3C-C2C	-5.14	1.33	1.40
2	D	601	PLP	C5A-C5	-3.55	1.41	1.50
3	D	602	HEM	C3C-CAC	3.51	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	PLP	C5A-C5	-3.51	1.41	1.50
2	D	601	PLP	C3-C2	-3.47	1.37	1.41
3	C	602	HEM	C3C-CAC	3.36	1.55	1.47
2	C	601	PLP	C5A-C5	-3.34	1.42	1.50
2	A	601	PLP	C5A-C5	-3.32	1.42	1.50
3	A	602	HEM	C3C-CAC	3.27	1.55	1.47
3	B	602	HEM	C3C-CAC	3.17	1.54	1.47
2	C	601	PLP	C3-C2	-3.00	1.37	1.41
2	B	601	PLP	C3-C2	-2.99	1.37	1.41
2	A	601	PLP	P-O3P	-2.96	1.43	1.54
3	B	602	HEM	CAB-C3B	2.87	1.55	1.47
3	C	602	HEM	CAB-C3B	2.84	1.55	1.47
2	B	601	PLP	P-O3P	-2.83	1.44	1.54
2	D	601	PLP	P-O3P	-2.83	1.44	1.54
2	C	601	PLP	P-O3P	-2.83	1.44	1.54
3	D	602	HEM	CAB-C3B	2.82	1.54	1.47
3	A	602	HEM	CAB-C3B	2.80	1.54	1.47
2	C	601	PLP	P-O2P	-2.72	1.44	1.54
2	B	601	PLP	P-O2P	-2.68	1.44	1.54
2	A	601	PLP	P-O2P	-2.68	1.44	1.54
2	A	601	PLP	C3-C2	-2.63	1.38	1.41
2	C	601	PLP	C6-N1	2.60	1.39	1.34
2	D	601	PLP	P-O2P	-2.57	1.45	1.54
2	B	601	PLP	C6-N1	2.56	1.39	1.34
3	C	602	HEM	C3C-C4C	2.39	1.44	1.41
2	A	601	PLP	C6-N1	2.29	1.39	1.34
2	D	601	PLP	C6-N1	2.28	1.39	1.34
3	D	602	HEM	C3C-C4C	2.27	1.44	1.41
2	C	601	PLP	P-O1P	-2.09	1.44	1.50

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	PLP	O4P-C5A-C5	5.81	120.24	109.36
2	C	601	PLP	O4P-C5A-C5	5.57	119.80	109.36
2	D	601	PLP	O4P-C5A-C5	5.01	118.75	109.36
2	A	601	PLP	O4P-C5A-C5	4.63	118.04	109.36
2	A	601	PLP	O3P-P-O4P	-4.42	95.13	106.67
2	B	601	PLP	O3P-P-O4P	-3.75	96.90	106.67
2	C	601	PLP	O3P-P-O4P	-3.75	96.90	106.67
2	D	601	PLP	O3P-P-O4P	-3.71	97.00	106.67
3	B	602	HEM	C4D-ND-C1D	3.53	109.38	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	PLP	O4P-P-O1P	-3.51	96.96	106.44
3	D	602	HEM	C4D-ND-C1D	3.35	109.17	105.21
2	A	601	PLP	O4P-P-O1P	-3.34	97.41	106.44
2	C	601	PLP	O4P-P-O1P	-3.24	97.68	106.44
3	C	602	HEM	C4D-ND-C1D	3.20	108.99	105.21
2	B	601	PLP	O4P-P-O1P	-3.16	97.91	106.44
2	C	601	PLP	O3P-P-O2P	2.81	118.35	107.80
2	B	601	PLP	O3P-P-O2P	2.81	118.34	107.80
3	D	602	HEM	CAA-CBA-CGA	-2.74	106.44	113.83
2	D	601	PLP	O3P-P-O2P	2.70	117.91	107.80
2	A	601	PLP	O3P-P-O2P	2.66	117.79	107.80
3	A	602	HEM	C4D-ND-C1D	2.66	108.35	105.21
2	B	601	PLP	O2P-P-O4P	-2.61	99.86	106.67
3	A	602	HEM	CMA-C3A-C4A	-2.55	124.73	128.46
3	C	602	HEM	CMC-C2C-C3C	2.43	129.54	124.68
3	A	602	HEM	C4C-CHD-C1D	2.39	125.71	122.56
3	B	602	HEM	CMA-C3A-C4A	-2.33	125.05	128.46
3	B	602	HEM	C4B-CHC-C1C	2.30	125.60	122.56
2	B	601	PLP	C6-C5-C4	-2.26	116.25	118.10
3	C	602	HEM	C4B-CHC-C1C	2.25	125.53	122.56
2	C	601	PLP	O2P-P-O4P	-2.24	100.84	106.67
3	A	602	HEM	CMD-C2D-C1D	2.23	128.51	125.03
3	D	602	HEM	C4C-CHD-C1D	2.22	125.49	122.56
3	B	602	HEM	CAD-C3D-C4D	2.21	128.56	124.70
3	D	602	HEM	C4B-CHC-C1C	2.20	125.47	122.56
2	B	601	PLP	C3-C2-N1	-2.20	118.18	120.96
3	C	602	HEM	C4C-CHD-C1D	2.20	125.46	122.56
3	C	602	HEM	CAD-C3D-C4D	2.18	128.50	124.70
2	D	601	PLP	O2P-P-O4P	-2.17	101.00	106.67
3	A	602	HEM	CMC-C2C-C3C	2.14	128.97	124.68
2	C	601	PLP	C6-C5-C4	-2.14	116.34	118.10
3	B	602	HEM	C4C-CHD-C1D	2.10	125.34	122.56
2	C	601	PLP	C3-C2-N1	-2.10	118.31	120.96
3	D	602	HEM	CBA-CAA-C2A	2.10	116.06	112.54
2	A	601	PLP	O3P-P-O1P	2.07	118.91	110.83
3	C	602	HEM	CMA-C3A-C4A	-2.04	125.47	128.46
3	A	602	HEM	C4D-C3D-C2D	-2.03	103.94	106.89
3	B	602	HEM	CMC-C2C-C3C	2.02	128.72	124.68
3	D	602	HEM	CMA-C3A-C4A	-2.02	125.50	128.46

There are no chirality outliers.

All (6) torsion outliers are listed below:

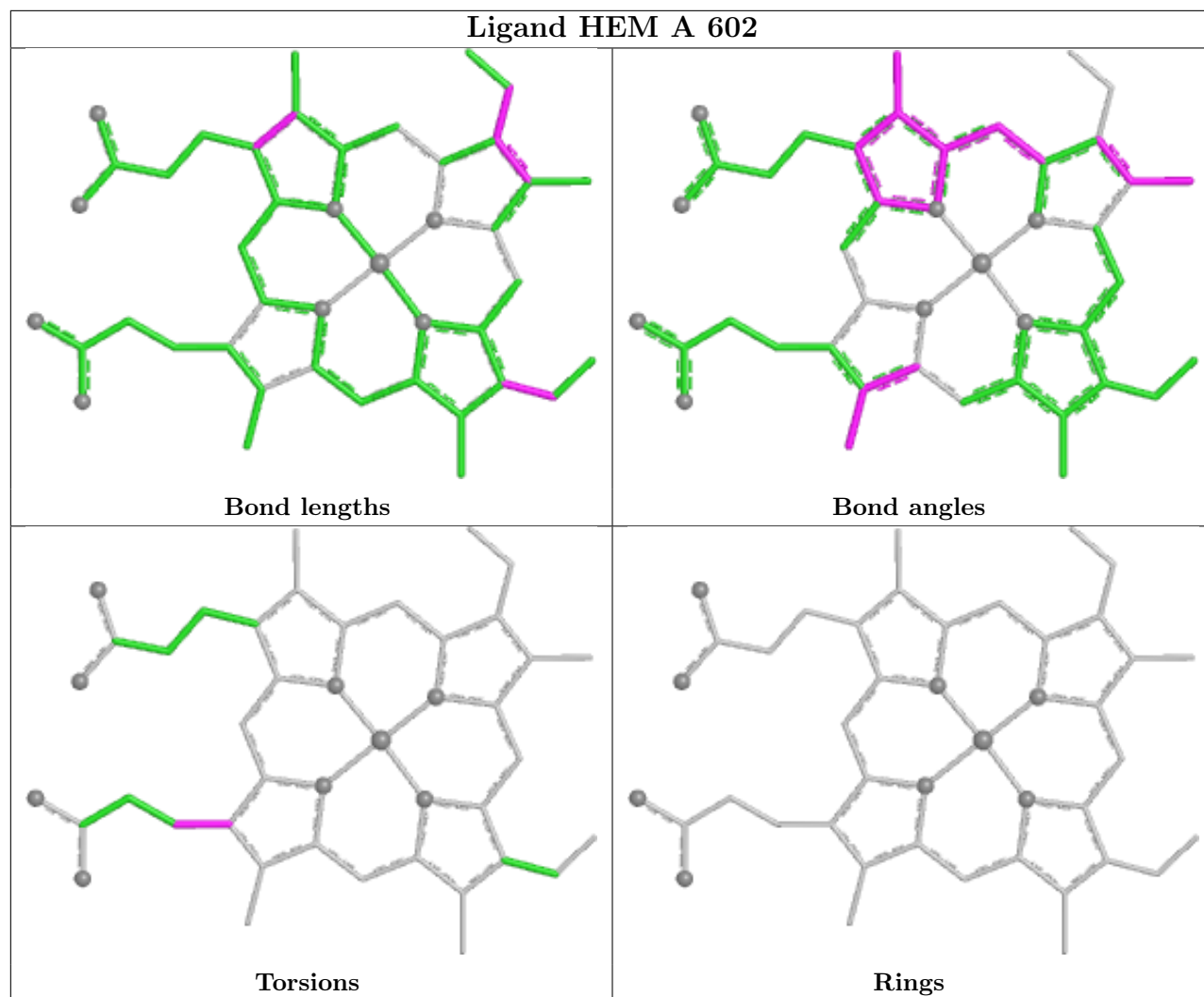
Mol	Chain	Res	Type	Atoms
3	B	602	HEM	C1A-C2A-CAA-CBA
3	D	602	HEM	CAA-CBA-CGA-O2A
3	A	602	HEM	C1A-C2A-CAA-CBA
3	D	602	HEM	CAA-CBA-CGA-O1A
3	B	602	HEM	CAA-CBA-CGA-O2A
3	B	602	HEM	CAA-CBA-CGA-O1A

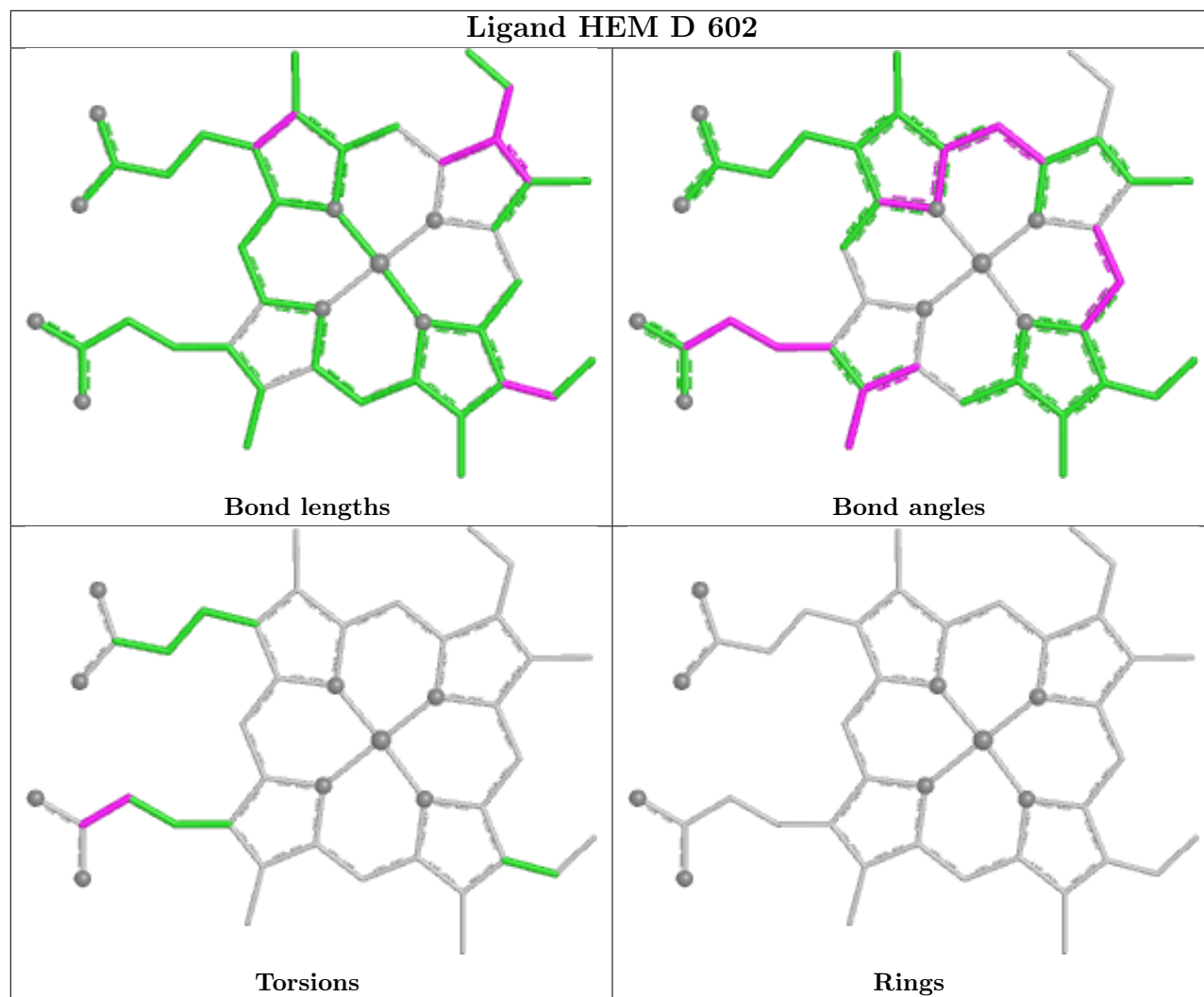
There are no ring outliers.

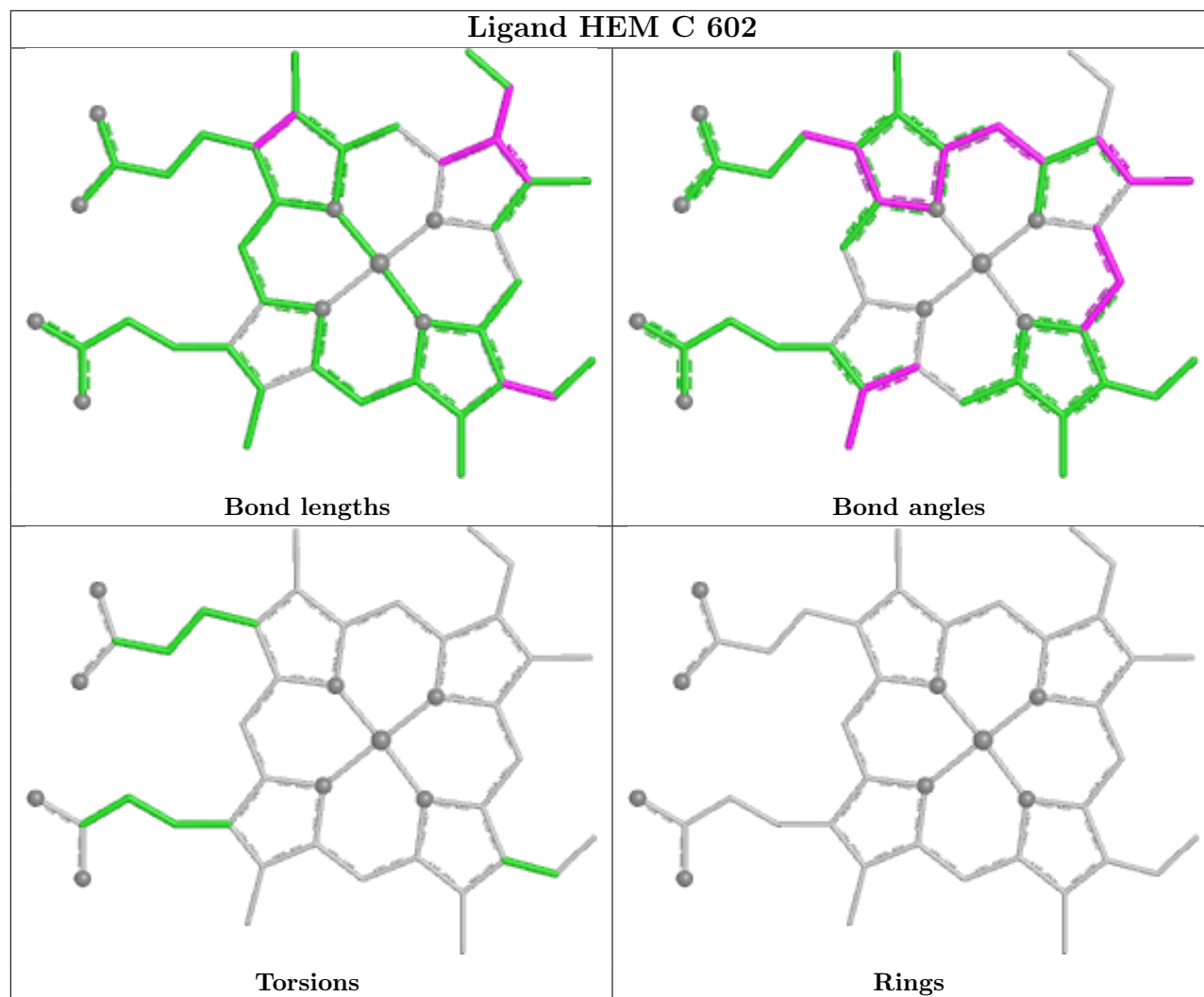
8 monomers are involved in 15 short contacts:

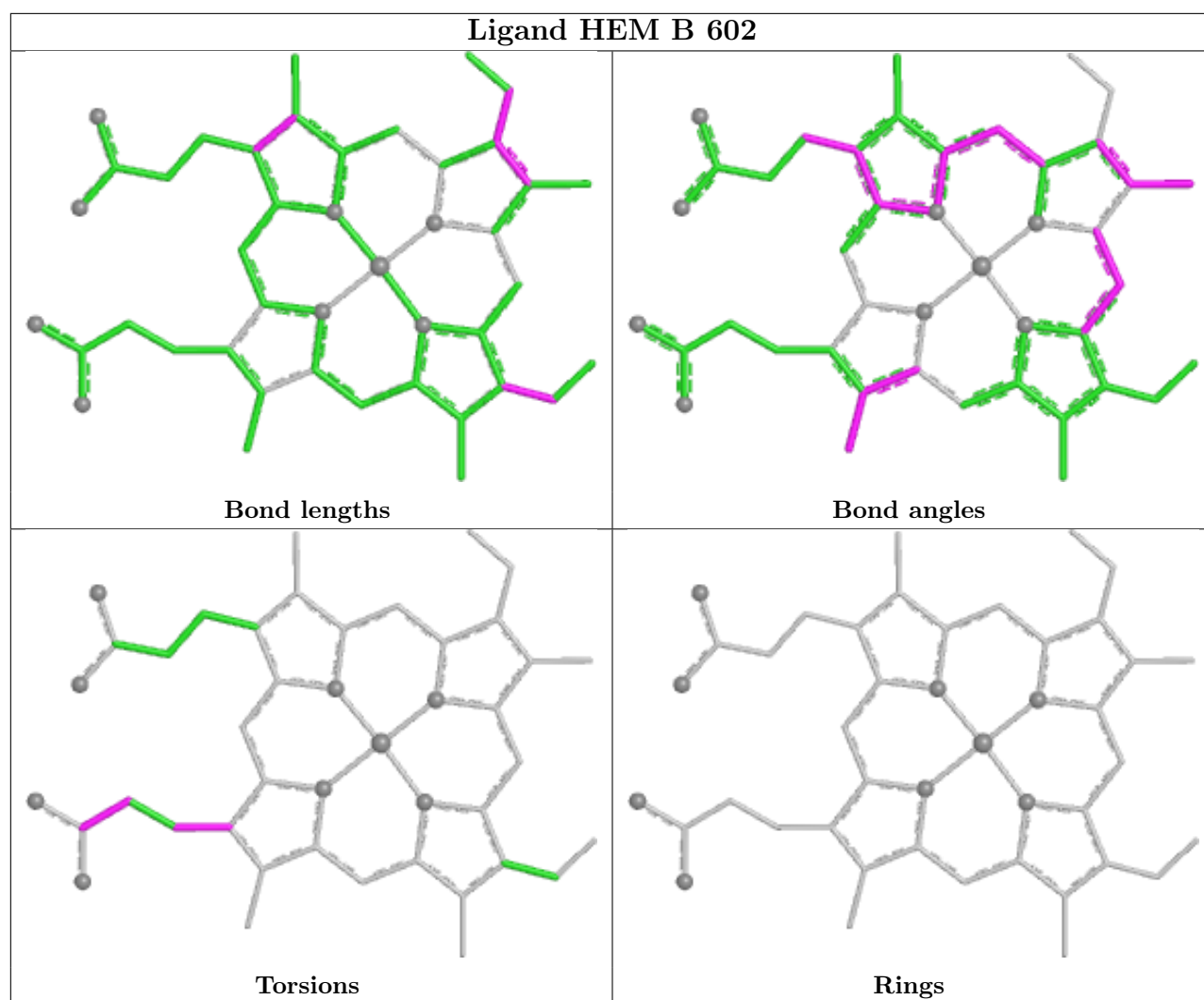
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	HEM	2	0
2	C	601	PLP	2	0
2	A	601	PLP	2	0
3	D	602	HEM	2	0
2	D	601	PLP	2	0
3	C	602	HEM	2	0
3	B	602	HEM	1	0
2	B	601	PLP	2	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	493/558 (88%)	1.06	68 (13%) 8 6	58, 82, 128, 160	0
1	B	494/558 (88%)	1.03	70 (14%) 7 6	60, 85, 130, 158	0
1	C	491/558 (87%)	0.97	70 (14%) 7 6	58, 83, 127, 162	0
1	D	493/558 (88%)	0.97	61 (12%) 9 8	55, 80, 127, 159	0
All	All	1971/2232 (88%)	1.01	269 (13%) 8 7	55, 83, 128, 162	0

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	LEU	8.2
1	B	42	LEU	8.0
1	A	401	ASP	8.0
1	C	402	LEU	7.5
1	A	514	GLU	6.0
1	C	549	ASP	6.0
1	B	402	LEU	5.5
1	D	402	LEU	5.0
1	C	58	ARG	5.0
1	D	69	ALA	4.8
1	C	66	HIS	4.8
1	B	397	LEU	4.8
1	A	69	ALA	4.7
1	C	527	ARG	4.6
1	A	171	GLU	4.5
1	A	132	ARG	4.4
1	A	68	THR	4.4
1	B	527	ARG	4.3
1	A	366	GLU	4.1
1	A	71	ALA	4.0
1	C	299	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	70	PRO	3.9
1	C	514	GLU	3.9
1	D	529	MET	3.9
1	B	66	HIS	3.9
1	C	43	TRP	3.8
1	B	400	GLU	3.8
1	C	300	THR	3.7
1	D	549	ASP	3.7
1	A	66	HIS	3.7
1	D	68	THR	3.7
1	D	132	ARG	3.7
1	A	431	CYS	3.7
1	B	132	ARG	3.6
1	D	514	GLU	3.6
1	B	224	ARG	3.6
1	B	508	PHE	3.6
1	A	529	MET	3.6
1	C	389	ARG	3.6
1	B	309	ASP	3.6
1	B	514	GLU	3.5
1	C	296	THR	3.5
1	B	60	ALA	3.5
1	C	70	PRO	3.5
1	C	71	ALA	3.5
1	C	397	LEU	3.5
1	B	296	THR	3.4
1	D	389	ARG	3.4
1	C	224	ARG	3.4
1	B	424	THR	3.4
1	A	297	GLU	3.4
1	A	43	TRP	3.4
1	B	120	ASP	3.4
1	D	71	ALA	3.4
1	D	433	HIS	3.4
1	C	481	LYS	3.4
1	A	403	THR	3.3
1	D	411	HIS	3.3
1	A	513	HIS	3.3
1	B	69	ALA	3.3
1	D	43	TRP	3.3
1	C	501	HIS	3.3
1	A	481	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	72	LYS	3.3
1	A	137	LYS	3.2
1	B	398	LYS	3.2
1	D	528	GLN	3.2
1	B	366	GLU	3.2
1	C	529	MET	3.2
1	D	451	GLU	3.2
1	A	423	LEU	3.2
1	C	451	GLU	3.1
1	C	298	GLN	3.1
1	B	389	ARG	3.1
1	A	398	LYS	3.1
1	D	444	ASN	3.1
1	C	295	GLN	3.1
1	D	443	PHE	3.1
1	B	481	LYS	3.0
1	B	291	GLU	3.0
1	D	479	VAL	3.0
1	B	298	GLN	3.0
1	D	291	GLU	3.0
1	D	133	ASP	3.0
1	D	247	LYS	3.0
1	D	501	HIS	3.0
1	C	55	GLN	3.0
1	C	120	ASP	2.9
1	A	304	GLU	2.9
1	D	545	ALA	2.9
1	D	300	THR	2.9
1	B	70	PRO	2.9
1	D	431	CYS	2.9
1	D	82	LYS	2.9
1	D	298	GLN	2.9
1	D	70	PRO	2.9
1	C	405	LYS	2.8
1	A	72	LYS	2.8
1	B	404	GLU	2.8
1	B	405	LYS	2.8
1	D	405	LYS	2.8
1	D	63	SER	2.8
1	A	501	HIS	2.8
1	C	132	ARG	2.8
1	B	61	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	247	LYS	2.8
1	B	198	ASP	2.8
1	B	501	HIS	2.8
1	D	60	ALA	2.7
1	B	423	LEU	2.7
1	C	198	ASP	2.7
1	A	55	GLN	2.7
1	B	299	THR	2.7
1	A	433	HIS	2.7
1	D	439	ARG	2.7
1	B	464	MET	2.7
1	A	448	VAL	2.7
1	A	512	VAL	2.7
1	A	426	LEU	2.7
1	A	508	PHE	2.7
1	C	329	GLU	2.7
1	A	478	GLN	2.7
1	B	51	ARG	2.7
1	C	462	GLY	2.7
1	A	547	GLU	2.6
1	B	171	GLU	2.6
1	C	366	GLU	2.6
1	C	547	GLU	2.6
1	B	194	ASN	2.6
1	B	444	ASN	2.6
1	B	529	MET	2.6
1	B	72	LYS	2.6
1	D	137	LYS	2.6
1	A	242	GLN	2.6
1	C	53	THR	2.6
1	D	424	THR	2.6
1	A	411	HIS	2.6
1	D	66	HIS	2.6
1	C	400	GLU	2.6
1	C	464	MET	2.6
1	A	365	GLN	2.6
1	B	47	ASP	2.6
1	B	86	ASP	2.6
1	D	480	GLY	2.6
1	B	43	TRP	2.6
1	C	72	LYS	2.6
1	C	528	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	63	SER	2.5
1	A	74	PRO	2.5
1	A	198	ASP	2.5
1	A	548	ARG	2.5
1	A	528	GLN	2.5
1	A	48	ALA	2.5
1	A	329	GLU	2.5
1	C	54	TRP	2.5
1	B	147	SER	2.5
1	A	51	ARG	2.5
1	A	283	GLU	2.5
1	A	292	GLU	2.5
1	C	171	GLU	2.5
1	A	147	SER	2.5
1	C	439	ARG	2.5
1	D	276	ARG	2.5
1	B	53	THR	2.5
1	D	147	SER	2.4
1	C	365	GLN	2.4
1	C	86	ASP	2.4
1	B	209	ARG	2.4
1	C	59	PRO	2.4
1	C	60	ALA	2.4
1	D	366	GLU	2.4
1	C	423	LEU	2.4
1	C	469	LEU	2.4
1	A	405	LYS	2.4
1	B	490	ILE	2.4
1	C	443	PHE	2.4
1	D	365	GLN	2.4
1	B	71	ALA	2.4
1	B	316	ASP	2.4
1	C	424	THR	2.3
1	C	436	GLU	2.3
1	A	425	VAL	2.3
1	C	242	GLN	2.3
1	D	198	ASP	2.3
1	A	424	THR	2.3
1	B	56	LEU	2.3
1	B	315	LEU	2.3
1	B	283	GLU	2.3
1	D	98	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	310	PHE	2.3
1	A	437	ILE	2.3
1	A	291	GLU	2.3
1	D	464	MET	2.3
1	B	550	GLN	2.3
1	D	478	GLN	2.3
1	C	467	SER	2.3
1	D	73	SER	2.3
1	A	82	LYS	2.3
1	C	441	LYS	2.3
1	A	209	ARG	2.3
1	A	450	ASP	2.3
1	C	316	ASP	2.3
1	D	297	GLU	2.3
1	D	295	GLN	2.3
1	B	496	LEU	2.3
1	C	147	SER	2.3
1	C	419	LEU	2.3
1	C	276	ARG	2.2
1	B	495	THR	2.2
1	A	309	ASP	2.2
1	D	388	ASP	2.2
1	A	247	LYS	2.2
1	B	451	GLU	2.2
1	D	283	GLU	2.2
1	C	513	HIS	2.2
1	A	482	VAL	2.2
1	B	55	GLN	2.2
1	C	45	ARG	2.2
1	C	133	ASP	2.2
1	C	97	LYS	2.2
1	C	406	LYS	2.2
1	A	169	MET	2.2
1	A	392	LEU	2.2
1	C	57	GLY	2.2
1	D	138	PRO	2.2
1	B	133	ASP	2.2
1	D	245	ASP	2.2
1	A	473	VAL	2.2
1	B	445	GLN	2.2
1	D	393	GLN	2.2
1	C	472	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	256	GLY	2.2
1	C	548	ARG	2.2
1	B	409	TRP	2.1
1	A	451	GLU	2.1
1	A	73	SER	2.1
1	C	56	LEU	2.1
1	B	58	ARG	2.1
1	C	208	TRP	2.1
1	A	440	GLU	2.1
1	B	489	GLN	2.1
1	D	242	GLN	2.1
1	B	50	SER	2.1
1	A	216	ASN	2.1
1	A	298	GLN	2.1
1	B	44	ILE	2.1
1	A	444	ASN	2.1
1	B	220	LEU	2.1
1	C	283	GLU	2.1
1	C	409	TRP	2.1
1	D	513	HIS	2.1
1	C	488	LYS	2.1
1	A	262	THR	2.1
1	D	430	THR	2.1
1	B	295	GLN	2.1
1	B	547	GLU	2.0
1	D	304	GLU	2.0
1	B	300	THR	2.0
1	D	74	PRO	2.0
1	C	330	GLU	2.0
1	D	329	GLU	2.0
1	D	398	LYS	2.0
1	D	481	LYS	2.0
1	B	410	TRP	2.0
1	A	445	GLN	2.0
1	B	248	LEU	2.0
1	B	528	GLN	2.0
1	C	482	VAL	2.0
1	D	469	LEU	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, 95<sup>th</sup> 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.

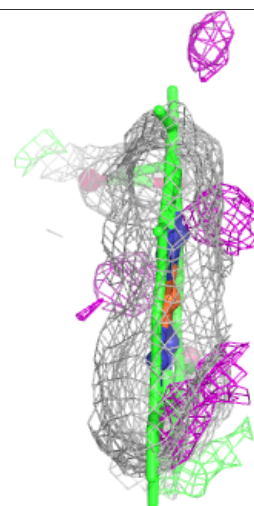
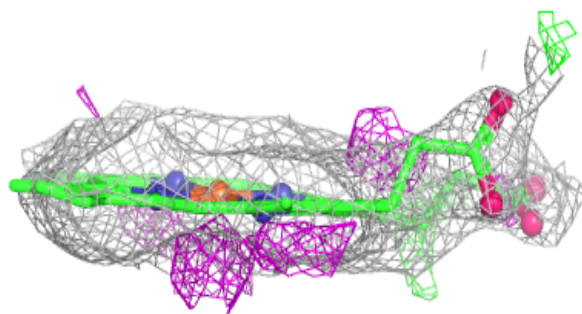
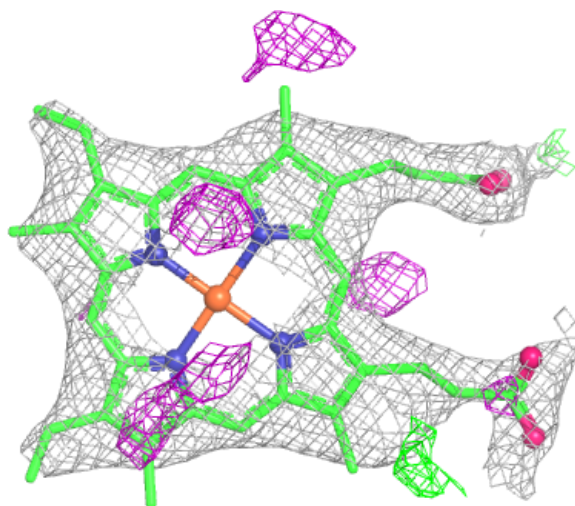
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	PLP	C	601	15/16	0.92	0.12	60,72,75,78	0
2	PLP	D	601	15/16	0.92	0.12	63,69,78,79	0
3	HEM	B	602	43/43	0.92	0.17	102,102,103,103	0
2	PLP	B	601	15/16	0.93	0.12	61,74,84,85	0
2	PLP	A	601	15/16	0.94	0.11	53,69,79,80	0
3	HEM	C	602	43/43	0.94	0.15	90,91,91,92	0
3	HEM	A	602	43/43	0.95	0.13	71,72,72,72	0
3	HEM	D	602	43/43	0.95	0.13	74,74,75,75	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.



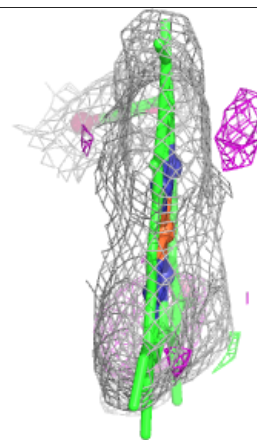
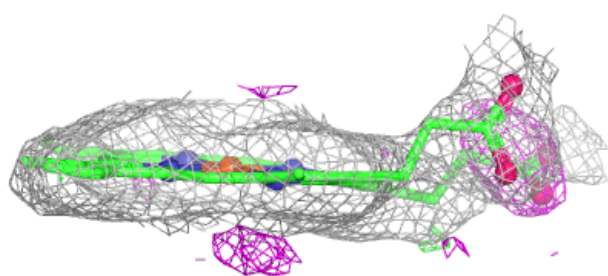
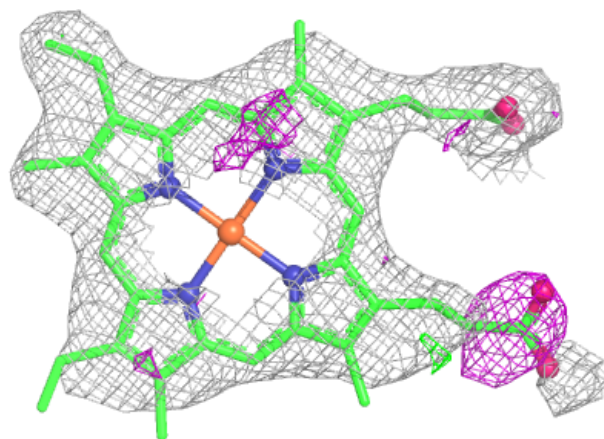
**Electron density around HEM B 602:**

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



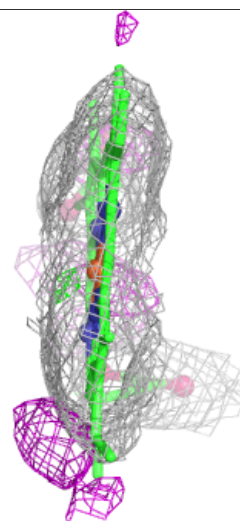
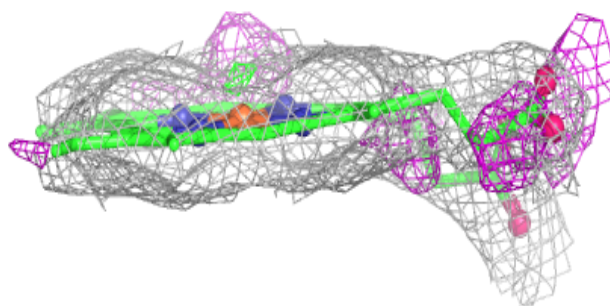
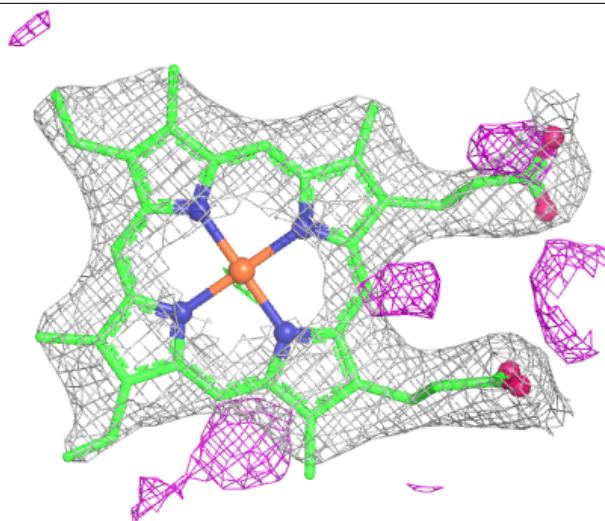
**Electron density around HEM C 602:**

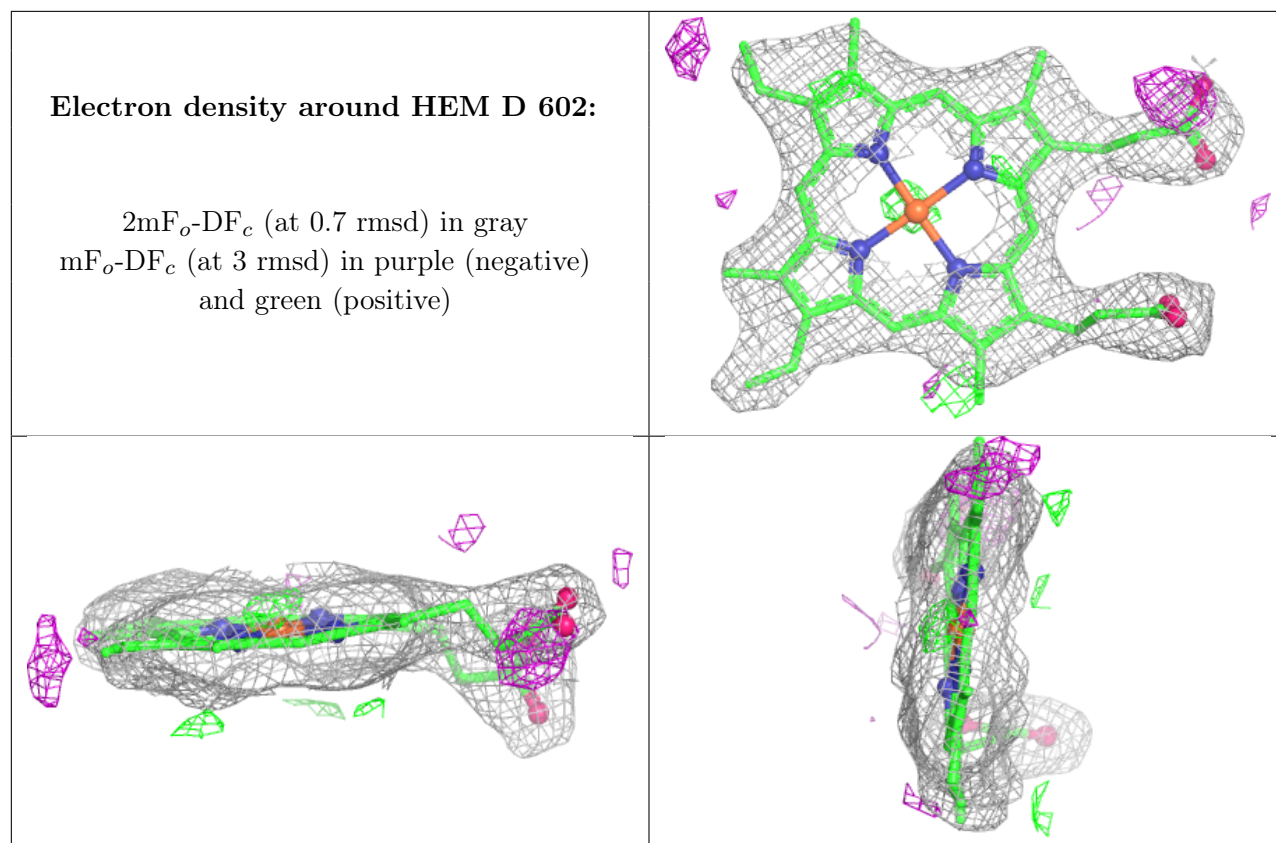
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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.