



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:46 PM GMT

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)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

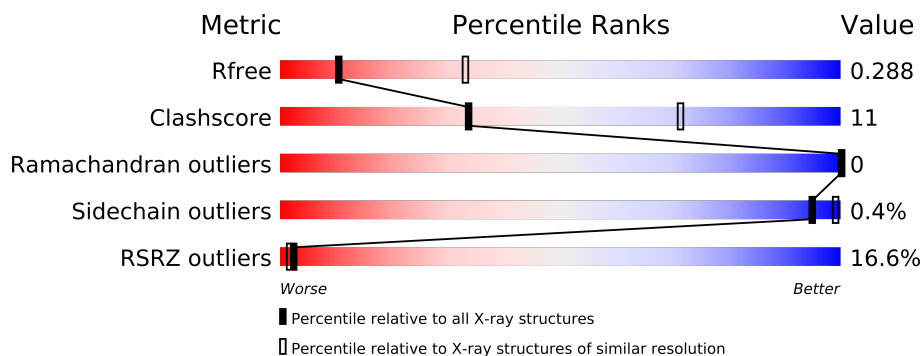
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1468 (3.00-2.96)
Clashscore	79885	1894 (3.00-2.96)
Ramachandran outliers	78287	1826 (3.00-2.96)
Sidechain outliers	78261	1829 (3.00-2.96)
RSRZ outliers	66119	1469 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	549	
1	B	549	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7728 atoms, of which 0 are hydrogen and 0 are deuterium.

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:

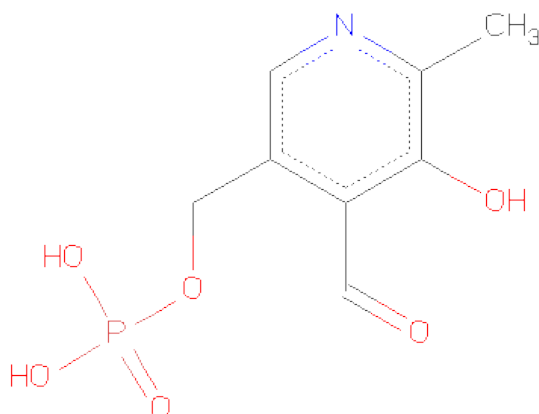
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	PRO	ENGINEERED MUTATION	UNP P35520
A	?	-	ILE	DELETION	UNP P35520
A	?	-	GLN	DELETION	UNP P35520
A	?	-	TYR	DELETION	UNP P35520
A	?	-	HIS	DELETION	UNP P35520
A	?	-	SER	DELETION	UNP P35520
A	?	-	THR	DELETION	UNP P35520
A	?	-	GLY	DELETION	UNP P35520
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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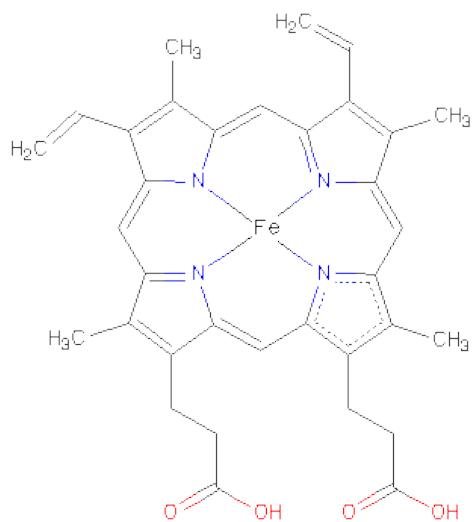
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	DELETION	UNP P35520
B	?	-	GLY	DELETION	UNP P35520
B	?	-	LYS	DELETION	UNP P35520
B	?	-	SER	DELETION	UNP P35520
B	?	-	SER	DELETION	UNP P35520
B	552	GLU	-	EXPRESSION TAG	UNP P35520
B	553	LEU	-	EXPRESSION TAG	UNP P35520
B	554	HIS	-	EXPRESSION TAG	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 (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: $C_{34}H_{32}FeN_4O_4$).

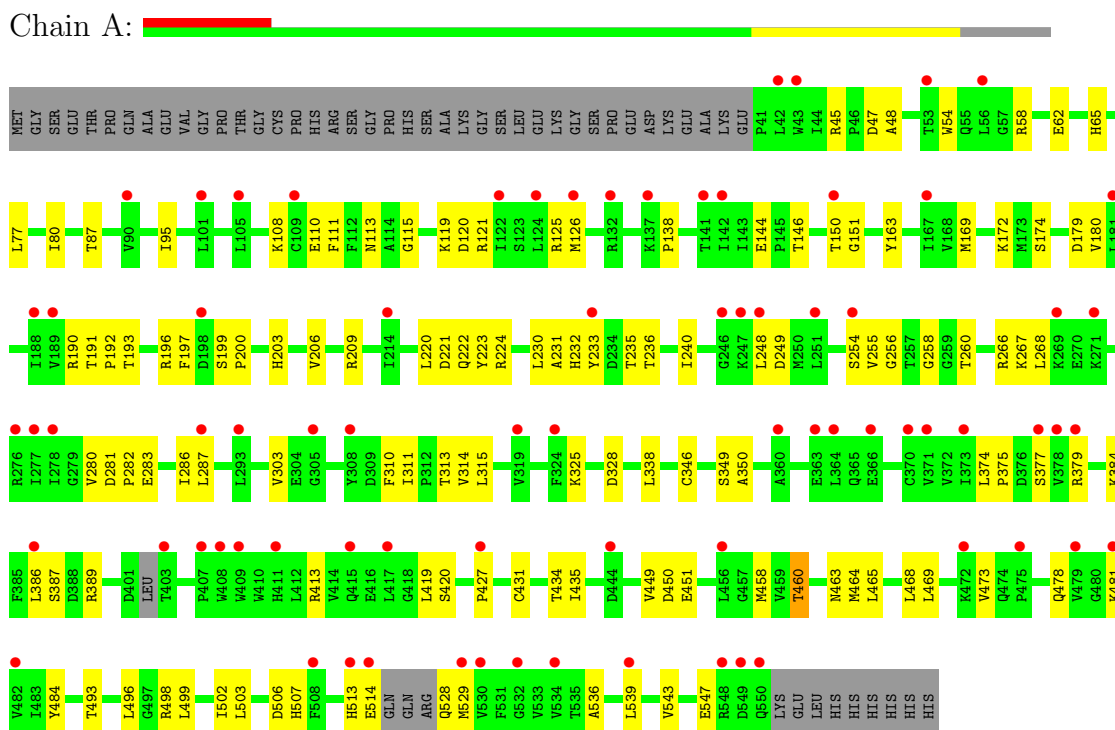


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

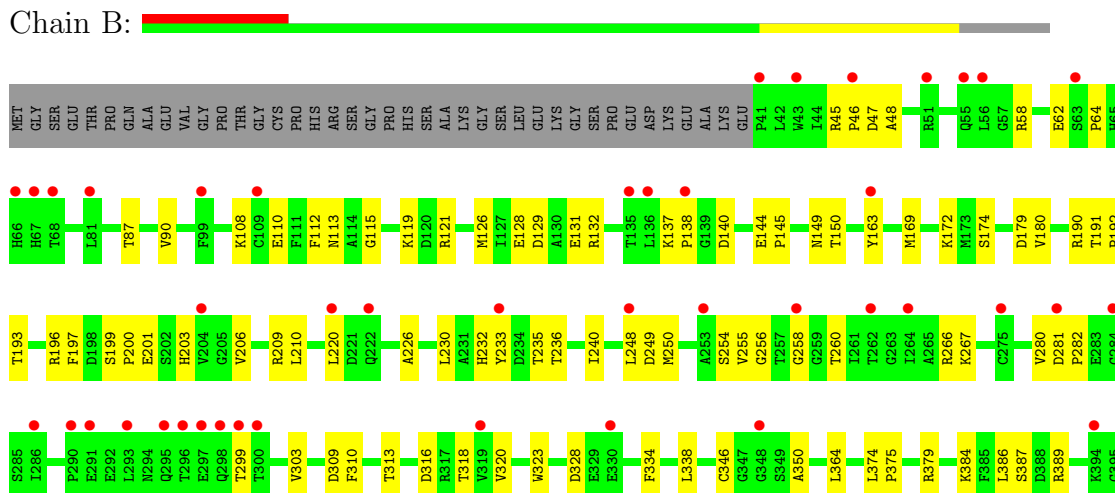
3 Residue-property plots

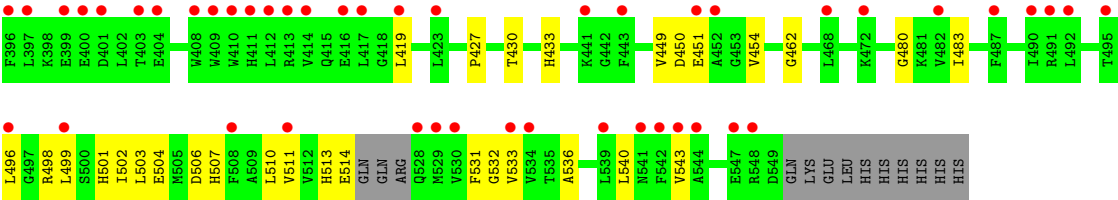
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 53.65 – 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
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.240 , 0.284 0.245 , 0.288	Depositor DCC
R_{free} test set	1495 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	70.6	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	3 of 29365 reflections (0.010%)	Xtriage
F_o, F_c correlation	0.91	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (170) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:B:58:ARG:NE	1:B:62:GLU:OE1	2.29	0.61
1:A:180:VAL:HG21	1:A:379:ARG:NH1	2.15	0.61
1:A:254:SER:HA	1:A:280:VAL:HB	1.82	0.61
1:B:255:VAL:HG13	1:B:258:GLY:HA2	1.82	0.61
1:A:281:ASP:OD2	1:A:282:PRO:HD2	2.00	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:B:235:THR:OG1	1:B:236:THR:N	2.37	0.56
1:A:338:LEU:HD23	1:A:346:CYS:SG	2.46	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:HBC2	3:A:602:HEM:HMC2	1.89	0.55
3:B:602:HEM:HBB2	3:B:602:HEM:HMB1	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:316:ASP:OD2	1:B:318:THR:OG1	2.20	0.50
1:A:119:LYS:HB3	1:A:150:THR:HA	1.92	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:287:LEU:HD23	1:A:311:ILE:HD13	1.94	0.49
1:A:235:THR:OG1	1:A:236:THR:N	2.44	0.49
1:A:144:GLU:OE1	1:A:222:GLN:HG2	2.12	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:465:LEU:O	1:A:469:LEU:HB2	2.13	0.49
1:A:174:SER:HB3	1:A:384:LYS:HD2	1.95	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:B:501:HIS:O	1:B:504:GLU:HB2	2.12	0.48
1:A:528:GLN:HG3	1:A:529:MET:H	1.78	0.48
1:A:232:HIS:CG	1:A:260:THR:HA	2.49	0.48
1:B:480:GLY:O	1:B:483:ILE:HG22	2.14	0.48
1:A:87:THR:OG1	1:A:108:LYS:HE3	2.14	0.48
1:A:125:ARG:HG2	1:A:231:ALA:HB2	1.94	0.48
1:B:137:LYS:HE2	1:B:140:ASP:OD2	2.14	0.48
1:A:387:SER:OG	1:A:389:ARG:HG3	2.14	0.48
1:B:233:TYR:O	1:B:267:LYS:HD2	2.13	0.48
1:A:543:VAL:O	1:A:547:GLU:HG2	2.14	0.48
1:B:430:THR:HG23	1:B:433:HIS:H	1.79	0.47
1:A:450:ASP:OD1	1:A:451:GLU:N	2.48	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:126:MET:HE3	1:A:222:GLN:HA	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:200:PRO:HA	1:B:209[B]:ARG:NH1	2.31	0.46
1:A:266:ARG:NH1	3:A:602:HEM:C3C	2.83	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: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:B:45:ARG:HD3	1:B:47:ASP:OD1	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:B:110:GLU:OE2	1:B:121:ARG:NH2	2.50	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:387:SER:OG	1:B:389:ARG:HG3	2.16	0.45
1:A:458:MET:HB2	1:A:484:TYR:HB2	1.98	0.45
1:B:230:LEU:HA	1:B:230:LEU:HD23	1.80	0.45
1:B:126:MET:HE2	1:B:220:LEU:HB3	1.98	0.45
1:A:283:GLU:HA	1:A:325:LYS:NZ	2.32	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:496:LEU:O	1:B:499:LEU:HB3	2.18	0.44
1:B:419:LEU:HD13	1:B:532:GLY:HA3	1.99	0.44
1:B:450:ASP:OD1	1:B:451:GLU:N	2.51	0.44
1:B:511:VAL:O	1:B:531:PHE:N	2.50	0.43
1:B:87:THR:HG21	1:B:110:GLU:HA	2.00	0.43
1:B:248:LEU:HD12	1:B:249:ASP:H	1.82	0.43
1:A:172:LYS:HB2	1:A:193:THR:HG21	2.00	0.43
1:A:47:ASP:HA	1:A:311:ILE:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:236:THR:O	1:A:240:ILE:HG13	2.19	0.43
1:A:224:ARG:HA	1:A:313:THR:OG1	2.18	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:349:SER:OG	2:A:601:PLP:N1	2.51	0.42
1:A:65:HIS:HB3	1:A:230:LEU:HD11	2.01	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
2:B:601:PLP:H2A1	2:B:601:PLP:HO3	1.71	0.42
1:A:498:ARG:O	1:A:502:ILE:HG13	2.20	0.42
1:B:110:GLU:HG3	1:B:113:ASN:ND2	2.35	0.42
1:B:232:HIS:CD2	1:B:260:THR:HA	2.54	0.42
1:A:431:CYS:HA	1:A:464:MET:HE3	2.02	0.42
1:A:221:ASP:OD1	1:A:224:ARG:NE	2.48	0.42
1:B:110:GLU:OE2	1:B:121:ARG:CZ	2.67	0.41
1:A:286:ILE:HG13	1:A:286:ILE:H	1.62	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
1:B:191:THR:HB	1:B:201:GLU:O	2.20	0.41
3:A:602:HEM:HMB1	3:A:602:HEM:HBB2	2.01	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: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:48:ALA:O	1:A:313:THR:HG22	2.20	0.41
1:A:539:LEU:O	1:A:543:VAL:HG23	2.20	0.41
1:A:248:LEU:HD12	1:A:249:ASP:H	1.84	0.41
1:A:374:LEU:HA	1:A:375:PRO:HD3	1.82	0.41
1:A:223:TYR:O	1:A:314:VAL:HG22	2.21	0.41
1:A:419:LEU:HB3	1:A:420:SER:H	1.32	0.41
1:A:200:PRO:HD2	1:B:462:GLY:HA3	2.01	0.40
1:A:146:THR:HG21	1:A:151:GLY:HA3	2.02	0.40
1:A:256:GLY:H	2:A:601:PLP:C5A	2.34	0.40
1:B:374:LEU:HA	1:B:375:PRO:HD3	1.73	0.40
1:A:119:LYS:HD2	1:A:150:THR:OG1	2.21	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:126:MET:HB3	1:B:220:LEU:HD13	2.03	0.40
1:A:268:LEU:HA	1:A:268:LEU:HD12	1.85	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%)	96	99
1	B	408/463 (88%)	406 (100%)	2 (0%)	94	99
All	All	815/926 (88%)	812 (100%)	3 (0%)	95	99

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

Some 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 chains 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 carbohydrates 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	14,15,16	1.00	1 (7%)	20,22,23	1.10	1 (5%)
3	HEM	A	602	1	49,50,50	5.88	19 (38%)	46,82,82	3.40	20 (43%)
2	PLP	B	601	1	14,15,16	1.03	2 (14%)	20,22,23	1.14	2 (10%)
3	HEM	B	602	1	49,50,50	5.80	20 (40%)	46,82,82	3.37	19 (41%)

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	A	602	1	-	0/14/114/114	0/0/8/8
2	PLP	B	601	1	-	0/6/6/8	0/1/1/1
3	HEM	B	602	1	-	0/14/114/114	0/0/8/8

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	HEM	C3D-C4D	-23.17	1.38	1.44
3	A	602	HEM	C3D-C4D	-21.73	1.39	1.44
3	A	602	HEM	C2B-C1B	-17.42	1.40	1.44
3	A	602	HEM	C2D-C1D	-15.94	1.40	1.44
3	A	602	HEM	C3D-C2D	-15.15	1.17	1.43
3	B	602	HEM	C2B-C1B	-15.11	1.40	1.44
3	B	602	HEM	C3D-C2D	-14.89	1.17	1.43
3	B	602	HEM	C2D-C1D	-14.67	1.40	1.44
3	A	602	HEM	C3B-C2B	-14.60	1.18	1.43
3	B	602	HEM	C3B-C2B	-14.59	1.18	1.43
3	B	602	HEM	FE-NA	5.27	2.15	1.92
3	A	602	HEM	FE-NA	5.14	2.14	1.92
3	B	602	HEM	C3B-C4B	-4.53	1.39	1.44
3	B	602	HEM	CHC-C1C	4.23	1.44	1.36
3	B	602	HEM	FE-NC	4.19	2.13	1.97
3	A	602	HEM	C1D-ND	4.10	1.47	1.37
3	A	602	HEM	FE-NC	4.06	2.13	1.97
3	B	602	HEM	C1D-ND	4.06	1.47	1.37
3	A	602	HEM	C3B-CAB	4.02	1.53	1.40
3	A	602	HEM	CHC-C1C	3.96	1.43	1.36
3	A	602	HEM	C3B-C4B	-3.94	1.39	1.44
3	B	602	HEM	C3B-CAB	3.92	1.52	1.40
3	B	602	HEM	CHD-C4C	3.89	1.43	1.36
3	A	602	HEM	CHD-C4C	3.83	1.43	1.36
3	A	602	HEM	CBB-CAB	3.71	1.50	1.28
3	B	602	HEM	CBB-CAB	3.66	1.50	1.28
3	B	602	HEM	C1B-NB	3.40	1.47	1.39
3	B	602	HEM	C4D-ND	3.36	1.46	1.39
3	A	602	HEM	C4D-ND	3.33	1.46	1.39
3	A	602	HEM	C1B-NB	3.21	1.46	1.39
3	B	602	HEM	CHB-C1B	3.12	1.40	1.35
3	B	602	HEM	C3C-CAC	2.94	1.49	1.40
3	A	602	HEM	C4B-NB	2.92	1.44	1.37
3	A	602	HEM	C3C-CAC	2.91	1.49	1.40
3	B	602	HEM	C4B-NB	2.89	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	HEM	CHB-C1B	2.74	1.39	1.35
2	A	601	PLP	C2-N1	2.44	1.38	1.33
3	B	602	HEM	C4A-CHB	2.38	1.46	1.39
2	B	601	PLP	C3-C2	-2.17	1.39	1.40
3	B	602	HEM	CHA-C4D	2.11	1.38	1.35
2	B	601	PLP	C2-N1	2.09	1.37	1.33
3	A	602	HEM	CHA-C4D	2.03	1.38	1.35

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	HEM	C3B-C4B-NB	-14.30	103.77	114.00
3	B	602	HEM	C3B-C4B-NB	-14.13	103.89	114.00
3	B	602	HEM	C2D-C1D-ND	-10.52	100.51	112.93
3	A	602	HEM	C2D-C1D-ND	-10.51	100.52	112.93
3	A	602	HEM	CHC-C1C-NC	5.90	129.86	124.73
3	B	602	HEM	CHC-C1C-NC	5.44	129.46	124.73
3	A	602	HEM	C4C-NC-C1C	5.02	110.76	105.53
3	B	602	HEM	C4C-NC-C1C	4.90	110.63	105.53
3	A	602	HEM	CHD-C4C-NC	4.57	128.71	124.73
3	B	602	HEM	CHD-C4C-NC	4.57	128.70	124.73
3	A	602	HEM	C4A-CHB-C1B	-3.90	122.34	127.47
3	B	602	HEM	CAD-C3D-C4D	-3.89	117.54	124.53
3	B	602	HEM	C4A-CHB-C1B	-3.76	122.52	127.47
3	A	602	HEM	CAD-C3D-C4D	-3.33	118.55	124.53
3	B	602	HEM	CHC-C4B-NB	3.13	127.19	124.58
3	A	602	HEM	CBA-CAA-C2A	-2.98	107.44	112.69
3	B	602	HEM	CHA-C4D-ND	2.96	128.37	124.31
2	B	601	PLP	O4P-C5A-C5	2.96	115.27	109.26
2	A	601	PLP	O4P-C5A-C5	2.95	115.26	109.26
3	B	602	HEM	CBA-CAA-C2A	-2.95	107.50	112.69
3	B	602	HEM	C3A-C4A-NA	-2.88	107.23	109.41
3	A	602	HEM	CHA-C4D-ND	2.88	128.26	124.31
3	A	602	HEM	C4A-NA-C1A	2.86	110.53	106.76
3	A	602	HEM	C1A-CHA-C4D	-2.82	123.76	127.47
3	B	602	HEM	C4A-NA-C1A	2.74	110.37	106.76
3	B	602	HEM	C1A-CHA-C4D	-2.55	124.11	127.47
3	A	602	HEM	CHD-C1D-ND	2.37	126.55	124.58
3	A	602	HEM	C3A-C4A-NA	-2.36	107.63	109.41
3	A	602	HEM	CHC-C4B-NB	2.32	126.51	124.58
3	A	602	HEM	CMB-C2B-C3B	2.23	131.41	126.16
3	A	602	HEM	CHB-C1B-NB	2.18	127.31	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	HEM	CHA-C1A-NA	2.13	128.13	124.58
3	B	602	HEM	CMB-C2B-C3B	2.12	131.16	126.16
3	B	602	HEM	CMA-C3A-C4A	-2.07	125.44	128.62
3	A	602	HEM	CMB-C2B-C1B	-2.06	113.75	126.30
3	A	602	HEM	C1D-CHD-C4C	-2.05	121.16	126.57
3	B	602	HEM	CHD-C1D-ND	2.05	126.29	124.58
3	A	602	HEM	CHB-C4A-NA	2.03	127.97	124.58
3	B	602	HEM	CHA-C1A-NA	2.03	127.97	124.58
3	B	602	HEM	CBD-CAD-C3D	-2.02	109.96	114.37
2	B	601	PLP	C5-C6-N1	-2.01	120.22	123.86
3	B	602	HEM	C1D-CHD-C4C	-2.00	121.29	126.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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%)	1.07	76 (15%) 3 2	53, 93, 150, 202	0
1	B	496/549 (90%)	1.15	89 (17%) 2 1	46, 88, 142, 184	0
All	All	992/1098 (90%)	1.11	165 (16%) 2 2	46, 90, 147, 202	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	397	LEU	6.1
1	B	403	THR	5.5
1	A	548	ARG	5.4
1	B	411	HIS	5.1
1	A	403	THR	5.1
1	B	416	GLU	5.0
1	A	550	GLN	5.0
1	B	534	VAL	4.8
1	B	413	ARG	4.6
1	A	248	LEU	4.5
1	B	533	VAL	4.5
1	B	136	LEU	4.4
1	A	233	TYR	4.3
1	A	549	ASP	4.3
1	B	528	GLN	4.2
1	A	56	LEU	4.0
1	A	271	LYS	4.0
1	A	269	LYS	3.9
1	A	407	PRO	3.8
1	A	417	LEU	3.8
1	B	262	THR	3.8
1	B	539	LEU	3.6
1	B	135	THR	3.6
1	B	68	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	496	LEU	3.4
1	A	278	ILE	3.4
1	A	251	LEU	3.4
1	A	530	VAL	3.3
1	A	246	GLY	3.3
1	A	42	LEU	3.3
1	B	299	THR	3.3
1	B	409	TRP	3.3
1	B	492	LEU	3.2
1	B	253	ALA	3.2
1	A	188	ILE	3.2
1	B	530	VAL	3.2
1	B	417	LEU	3.2
1	A	43	TRP	3.1
1	A	105	LEU	3.1
1	A	481	LYS	3.1
1	B	408	TRP	3.1
1	A	122	ILE	3.1
1	A	124	LEU	3.1
1	B	412	LEU	3.1
1	B	300	THR	3.0
1	B	46	PRO	3.0
1	B	348	GLY	3.0
1	A	379	ARG	3.0
1	A	277	ILE	3.0
1	B	410	TRP	3.0
1	B	414	VAL	3.0
1	B	542	PHE	3.0
1	B	43	TRP	2.9
1	A	319	VAL	2.9
1	B	286	ILE	2.9
1	B	394	LYS	2.9
1	A	364	LEU	2.9
1	A	479	VAL	2.9
1	B	330	GLU	2.8
1	B	298	GLN	2.8
1	A	539	LEU	2.8
1	A	137	LYS	2.8
1	B	284	GLY	2.8
1	B	490	ILE	2.8
1	A	427	PRO	2.8
1	B	99	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	532	GLY	2.7
1	B	296	THR	2.7
1	A	363	GLU	2.7
1	A	305	GLY	2.7
1	B	222	GLN	2.7
1	B	293	LEU	2.7
1	B	297	GLU	2.7
1	B	423	LEU	2.7
1	A	444	ASP	2.7
1	A	514	GLU	2.7
1	A	101	LEU	2.7
1	B	275	CYS	2.6
1	B	548	ARG	2.6
1	B	529	MET	2.6
1	B	468	LEU	2.6
1	A	482	VAL	2.6
1	B	396	PHE	2.6
1	B	482	VAL	2.6
1	B	233	TYR	2.6
1	B	290	PRO	2.6
1	B	541	ASN	2.6
1	B	443	PHE	2.6
1	B	452	ALA	2.6
1	A	247	LYS	2.6
1	A	109	CYS	2.5
1	B	67	HIS	2.5
1	B	400	GLU	2.5
1	B	295	GLN	2.5
1	B	472	LYS	2.5
1	B	419	LEU	2.5
1	B	264	ILE	2.5
1	B	220	LEU	2.5
1	A	373	ILE	2.4
1	B	451	GLU	2.4
1	A	411	HIS	2.4
1	B	109	CYS	2.4
1	B	544	ALA	2.4
1	A	214	ILE	2.4
1	A	287	LEU	2.4
1	A	141	THR	2.4
1	A	324	PHE	2.4
1	B	511	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	142	ILE	2.4
1	B	41	PRO	2.4
1	B	319	VAL	2.3
1	B	543	VAL	2.3
1	B	491	ARG	2.3
1	A	126	MET	2.3
1	B	248	LEU	2.3
1	A	377	SER	2.3
1	B	508	PHE	2.3
1	A	513	HIS	2.3
1	B	163	TYR	2.3
1	A	508	PHE	2.3
1	A	370	CYS	2.3
1	B	204	VAL	2.3
1	B	138	PRO	2.3
1	A	534	VAL	2.3
1	A	293	LEU	2.2
1	B	499	LEU	2.2
1	A	132	ARG	2.2
1	B	51	ARG	2.2
1	B	547	GLU	2.2
1	A	475	PRO	2.2
1	B	399	GLU	2.2
1	A	360	ALA	2.2
1	B	66	HIS	2.2
1	B	487	PHE	2.2
1	A	366	GLU	2.2
1	A	472	LYS	2.2
1	A	276	ARG	2.2
1	A	378	VAL	2.2
1	B	404	GLU	2.2
1	B	258	GLY	2.2
1	A	371	VAL	2.1
1	A	408	TRP	2.1
1	A	254	SER	2.1
1	B	55	GLN	2.1
1	A	456	LEU	2.1
1	B	81	LEU	2.1
1	A	53	THR	2.1
1	B	401	ASP	2.1
1	A	386	LEU	2.1
1	A	529	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	281	ASP	2.1
1	B	495	THR	2.1
1	A	415	GLN	2.1
1	B	441	LYS	2.1
1	A	150	THR	2.0
1	B	291	GLU	2.0
1	A	181	LEU	2.0
1	A	90	VAL	2.0
1	A	198	ASP	2.0
1	A	167	ILE	2.0
1	A	409	TRP	2.0
1	B	56	LEU	2.0
1	A	189	VAL	2.0
1	B	63	SER	2.0
1	A	308	TYR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	HEM	B	602	43/43	0.33	0.84	101,104,104,104	0
3	HEM	A	602	43/43	0.29	0.64	107,108,109,109	0
2	PLP	B	601	15/16	0.21	-0.85	53,66,75,76	0
2	PLP	A	601	15/16	0.19	-1.58	58,75,85,86	0

6.5 Other polymers ⓘ

There are no such residues in this entry.