



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:20 am GMT

PDB ID : 4L27
Title : Crystal structure of delta1-39 and 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 : 3.39 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

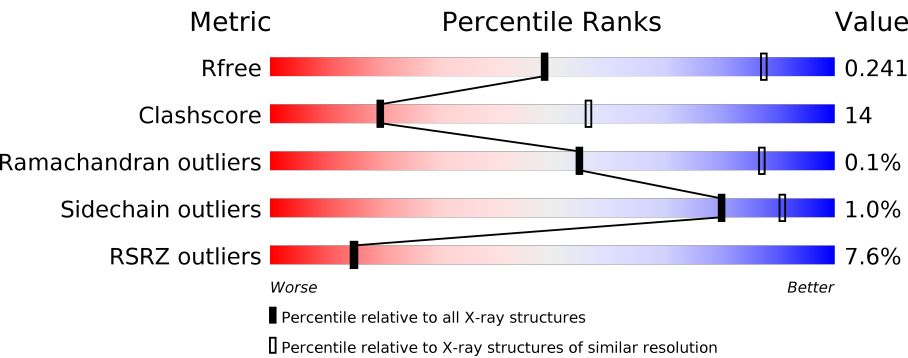
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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}	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

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. 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	548	<div><div>13%</div><div><div>65%</div><div>23%</div><div>•</div><div>11%</div></div></div>
1	B	548	<div><div>4%</div><div><div>69%</div><div>20%</div><div>•</div><div>11%</div></div></div>
1	C	548	<div><div>3%</div><div><div>66%</div><div>24%</div><div>10%</div></div></div>
1	D	548	<div><div>7%</div><div><div>69%</div><div>20%</div><div>•</div><div>10%</div></div></div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HEM	C	602	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15361 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	B	490	Total	C	N	O	S	0	0	0
			3791	2402	661	706	22			
1	D	491	Total	C	N	O	S	0	0	0
			3788	2398	662	706	22			
1	A	485	Total	C	N	O	S	0	0	0
			3757	2381	656	698	22			
1	C	491	Total	C	N	O	S	0	0	0
			3793	2403	665	703	22			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	444	ASN	ASP	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
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	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
D	444	ASN	ASP	ENGINEERED MUTATION	UNP P35520
D	?	-	ILE	DELETION	UNP P35520

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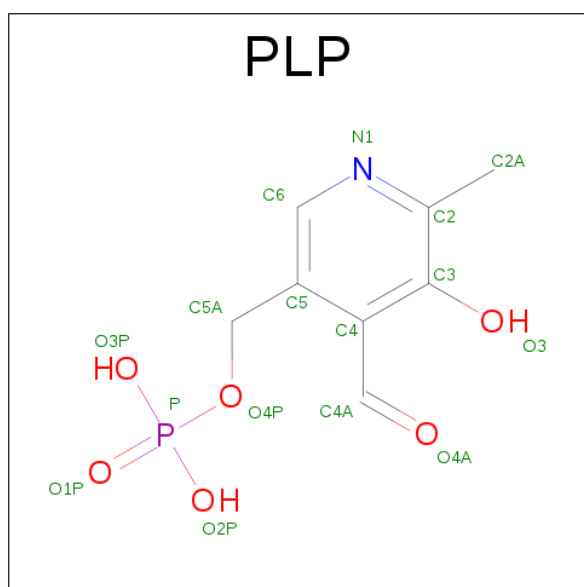
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLN	DELETION	UNP P35520
D	?	-	TYR	DELETION	UNP P35520
D	?	-	HIS	DELETION	UNP P35520
D	?	-	SER	DELETION	UNP P35520
D	?	-	THR	DELETION	UNP P35520
D	?	-	GLY	DELETION	UNP P35520
D	?	-	LYS	DELETION	UNP P35520
D	?	-	SER	DELETION	UNP P35520
D	?	-	SER	DELETION	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
A	444	ASN	ASP	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	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
C	444	ASN	ASP	ENGINEERED MUTATION	UNP P35520
C	?	-	ILE	DELETION	UNP P35520
C	?	-	GLN	DELETION	UNP P35520
C	?	-	TYR	DELETION	UNP P35520
C	?	-	HIS	DELETION	UNP P35520
C	?	-	SER	DELETION	UNP P35520

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	THR	DELETION	UNP P35520
C	?	-	GLY	DELETION	UNP P35520
C	?	-	LYS	DELETION	UNP P35520
C	?	-	SER	DELETION	UNP P35520
C	?	-	SER	DELETION	UNP P35520
C	552	LEU	-	EXPRESSION TAG	UNP P35520
C	553	GLU	-	EXPRESSION TAG	UNP P35520
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

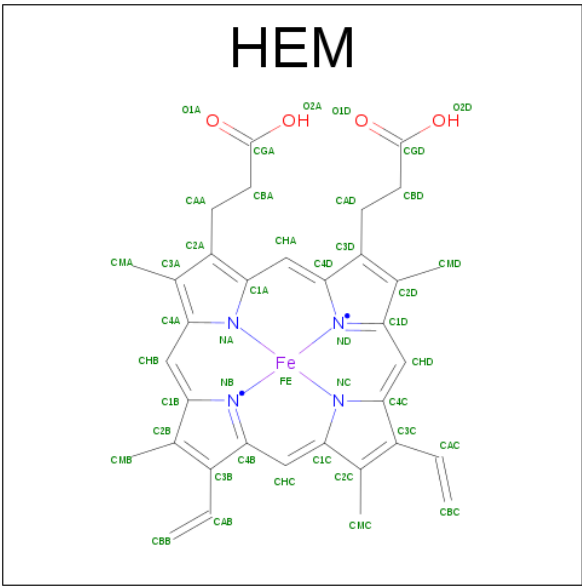
- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C₃₄H₃₂FeN₄O₄).

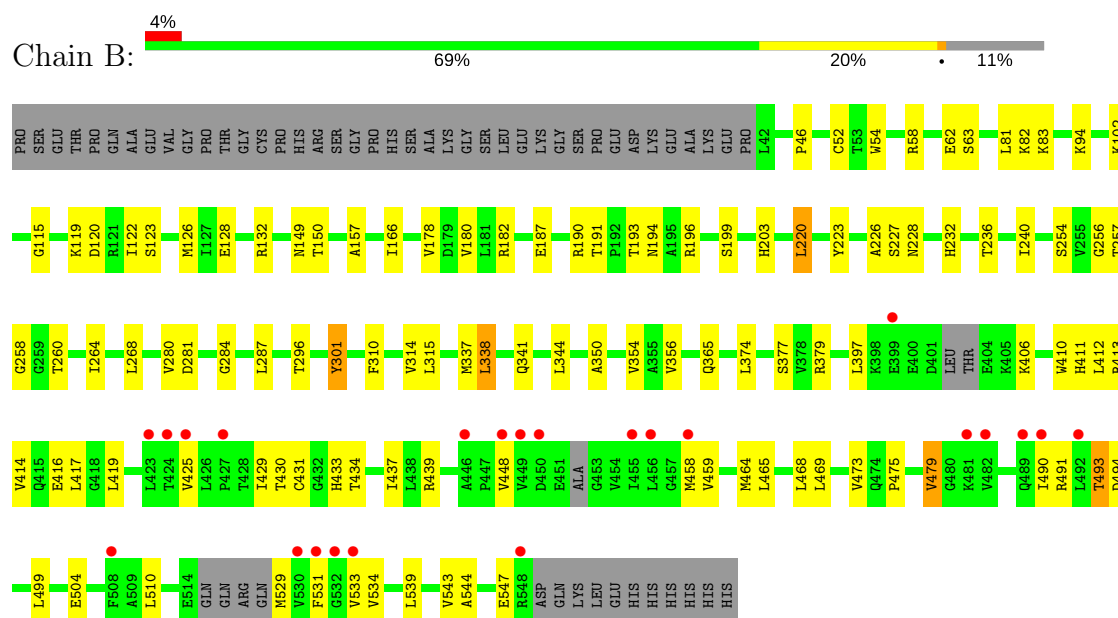


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

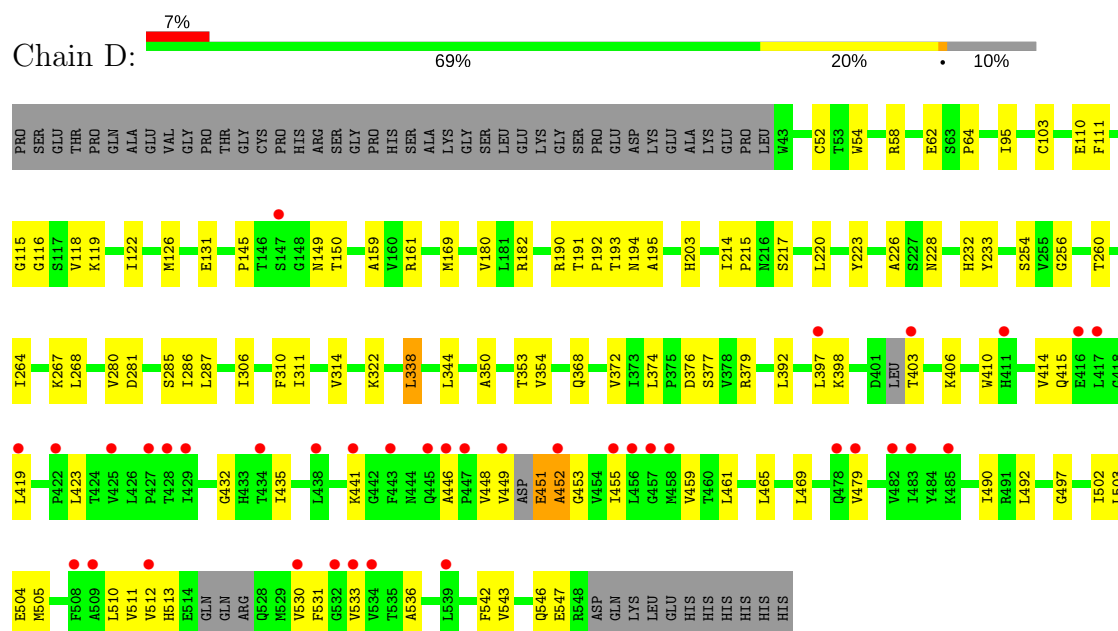
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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

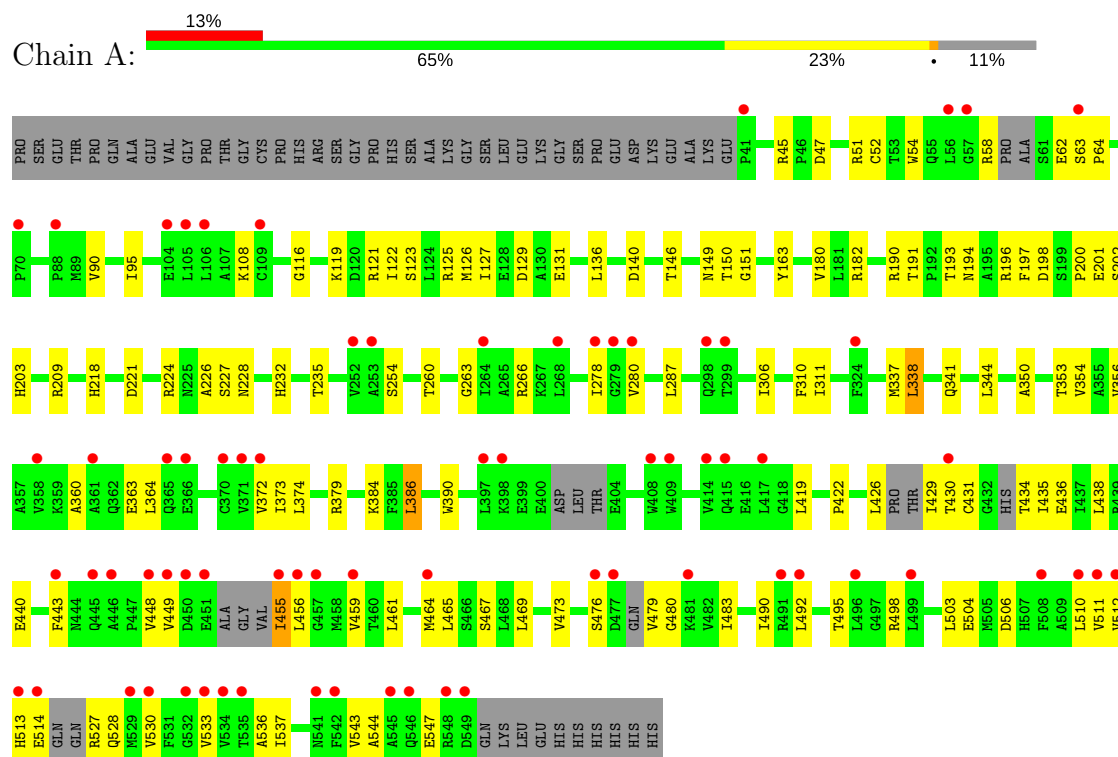


• Molecule 1: Cystathionine beta-synthase



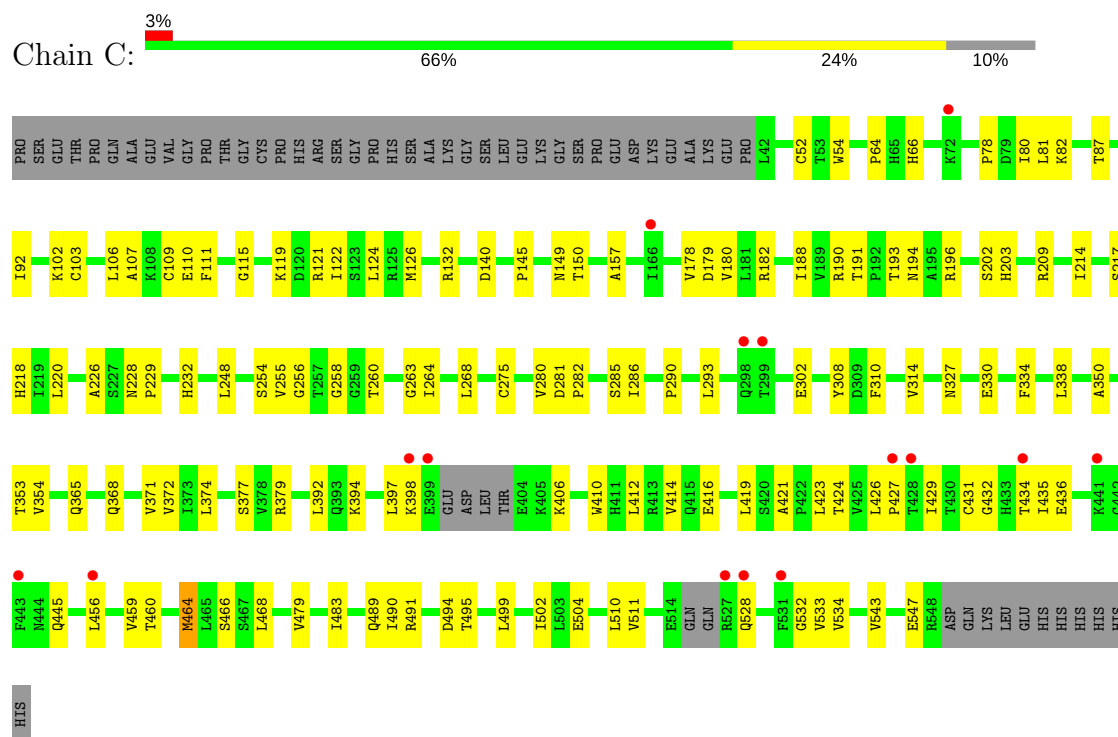
● Molecule 1: Cystathionine beta-synthase

Chain A:



● Molecule 1: Cystathionine beta-synthase

Chain C:



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	190.45Å 190.45Å 140.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.62 – 3.39 57.01 – 3.39	Depositor EDS
% Data completeness (in resolution range)	99.7 (56.62-3.39) 99.7 (57.01-3.39)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.206 , 0.244 0.200 , 0.241	Depositor DCC
R_{free} test set	2002 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	120.5	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.079 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15361	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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	0.30	0/3820	0.58	4/5157 (0.1%)
1	B	0.28	0/3861	0.52	1/5225 (0.0%)
1	C	0.29	0/3864	0.55	1/5230 (0.0%)
1	D	0.28	0/3858	0.53	1/5220 (0.0%)
All	All	0.29	0/15403	0.55	7/20832 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	GLY	O-C-N	-8.89	108.48	122.70
1	A	123	SER	O-C-N	-7.32	110.99	122.70
1	A	116	GLY	C-N-CA	6.36	137.61	121.70
1	D	116	GLY	O-C-N	-6.34	112.56	122.70
1	C	124	LEU	O-C-N	-6.30	112.62	122.70
1	B	123	SER	O-C-N	-5.85	113.34	122.70
1	A	116	GLY	CA-C-N	5.78	129.92	117.20

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	3757	0	3811	141	1
1	B	3791	0	3845	97	0
1	C	3793	0	3849	112	1
1	D	3788	0	3831	94	0
2	A	15	0	7	4	0
2	B	15	0	7	3	0
2	C	15	0	7	2	0
2	D	15	0	7	3	0
3	A	43	0	30	15	0
3	B	43	0	30	12	0
3	C	43	0	30	14	0
3	D	43	0	30	9	0
All	All	15361	0	15484	443	1

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 14.

All (443) 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:178:VAL:CG2	1:B:190:ARG:HH21	1.36	1.39
1:B:178:VAL:HG21	1:B:190:ARG:NH2	1.29	1.38
1:A:431:CYS:SG	1:A:464:MET:HE1	1.68	1.32
1:B:178:VAL:CG2	1:B:190:ARG:NH2	1.94	1.24
1:A:431:CYS:SG	1:A:464:MET:CE	2.32	1.18
1:A:480:GLY:HA2	1:A:483:ILE:CD1	1.73	1.17
1:B:439:ARG:NH2	1:B:465:LEU:HD21	1.61	1.16
1:A:492:LEU:HD23	1:A:511:VAL:HG21	1.15	1.08
1:A:479:VAL:O	1:A:483:ILE:HG13	1.54	1.07
1:A:58:ARG:NE	1:A:62:GLU:OE2	1.86	1.07
1:A:480:GLY:HA2	1:A:483:ILE:HD12	1.01	1.01
1:B:178:VAL:HG22	1:B:190:ARG:HH21	1.26	0.98
1:A:480:GLY:CA	1:A:483:ILE:HD12	1.93	0.98
1:D:264:ILE:O	1:D:268:LEU:HD13	1.63	0.96
1:B:439:ARG:HH21	1:B:465:LEU:HD21	1.20	0.95
1:D:451:GLU:O	1:D:453:GLY:N	2.00	0.95
3:A:602:HEM:HHA	3:A:602:HEM:HBD1	1.45	0.95
1:B:178:VAL:HG21	1:B:190:ARG:HH22	1.23	0.94
1:C:264:ILE:O	1:C:268:LEU:HD13	1.66	0.93
1:A:232:HIS:HD2	1:A:260:THR:HA	1.32	0.92
1:A:429:ILE:HD11	1:A:434:THR:CG2	2.01	0.90
1:D:419:LEU:HD12	1:D:511:VAL:HG11	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:CYS:SG	1:C:435:ILE:HD11	2.12	0.90
1:A:465:LEU:O	1:A:469:LEU:HD13	1.71	0.89
1:A:492:LEU:HD23	1:A:511:VAL:CG2	2.02	0.89
1:B:264:ILE:O	1:B:268:LEU:HD13	1.74	0.88
1:B:54:TRP:HD1	3:B:602:HEM:CBB	1.87	0.88
1:A:492:LEU:CD2	1:A:511:VAL:HG21	2.01	0.87
1:C:431:CYS:O	1:C:435:ILE:HG13	1.74	0.86
1:B:63:SER:HB2	3:B:602:HEM:HAB	1.59	0.84
1:D:419:LEU:CD1	1:D:511:VAL:HG11	2.07	0.84
3:A:602:HEM:CBD	3:A:602:HEM:HHA	2.06	0.83
1:A:467:SER:C	1:A:473:VAL:HG12	1.99	0.83
1:A:429:ILE:CD1	1:A:434:THR:CG2	2.57	0.82
1:A:260:THR:OG1	2:A:601:PLP:O1P	1.98	0.82
1:A:429:ILE:HD11	1:A:434:THR:HG22	1.61	0.80
1:A:232:HIS:CD2	1:A:260:THR:HA	2.16	0.80
1:C:334:PHE:O	1:C:338:LEU:HD23	1.82	0.79
1:D:392:LEU:CD2	1:D:397:LEU:HD12	2.12	0.79
3:B:602:HEM:HBD1	3:B:602:HEM:HHA	1.65	0.79
1:A:149:ASN:ND2	2:A:601:PLP:H2A1	1.98	0.78
1:B:54:TRP:CD1	3:B:602:HEM:HBB2	2.17	0.78
1:C:397:LEU:HD13	1:C:397:LEU:C	2.04	0.78
1:B:193:THR:O	1:B:194:ASN:OD1	2.02	0.77
1:D:392:LEU:HD21	1:D:397:LEU:HD12	1.66	0.77
1:A:449:VAL:HG22	1:A:455:ILE:HG12	1.64	0.77
1:C:334:PHE:O	1:C:338:LEU:CD2	2.33	0.77
1:B:149:ASN:ND2	2:B:601:PLP:H2A1	2.01	0.76
1:A:350:ALA:HB1	1:A:374:LEU:HD22	1.69	0.74
1:C:397:LEU:HD13	1:C:398:LYS:O	1.88	0.73
1:D:397:LEU:HD13	1:D:397:LEU:C	2.09	0.73
1:D:490:ILE:HD12	1:D:502:ILE:HD12	1.71	0.72
1:C:464:MET:O	1:C:468:LEU:HD13	1.89	0.72
3:B:602:HEM:CBD	3:B:602:HEM:HHA	2.21	0.71
1:A:58:ARG:HH11	1:A:62:GLU:CD	1.93	0.70
1:A:429:ILE:CD1	1:A:434:THR:HG22	2.18	0.70
1:C:256:GLY:HA3	2:C:601:PLP:H5A1	1.74	0.70
1:B:54:TRP:CD1	3:B:602:HEM:CBB	2.72	0.70
1:A:430:THR:OG1	1:A:476:SER:O	2.10	0.69
1:A:512:VAL:HG12	1:A:513:HIS:N	2.06	0.69
1:A:467:SER:HB3	1:A:473:VAL:CG1	2.22	0.69
1:A:426:LEU:HD13	1:A:426:LEU:C	2.13	0.69
1:B:58:ARG:NE	1:B:62:GLU:OE1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:HIS:CD2	1:C:260:THR:HA	2.29	0.68
1:D:122:ILE:O	1:D:126:MET:HG3	1.94	0.68
1:C:543:VAL:O	1:C:547:GLU:HG3	1.93	0.68
1:A:419:LEU:CD1	1:A:511:VAL:HG11	2.23	0.67
1:A:431:CYS:HG	1:A:464:MET:CE	2.08	0.67
1:C:423:LEU:HD12	1:C:424:THR:H	1.59	0.67
1:A:434:THR:HG21	1:A:479:VAL:HG21	1.77	0.67
1:D:350:ALA:HB1	1:D:374:LEU:HD22	1.76	0.67
1:C:412:LEU:HB3	1:C:416:GLU:OE1	1.95	0.67
1:C:431:CYS:O	1:C:435:ILE:CG1	2.42	0.66
1:D:191:THR:HG21	1:D:203:HIS:HA	1.78	0.66
3:D:602:HEM:HBB2	3:D:602:HEM:HMB1	1.77	0.66
1:B:193:THR:O	1:B:194:ASN:CG	2.35	0.65
1:D:451:GLU:OE2	1:D:451:GLU:N	2.30	0.65
1:B:232:HIS:CD2	1:B:260:THR:HA	2.31	0.65
1:D:119:LYS:HD2	1:D:150:THR:OG1	1.96	0.65
1:D:149:ASN:HD22	2:D:601:PLP:H2A1	1.62	0.64
1:A:182:ARG:NH1	1:C:504:GLU:OE1	2.30	0.64
1:A:459:VAL:HG11	1:A:479:VAL:HG13	1.78	0.64
1:C:263:GLY:HA2	3:C:602:HEM:HBC1	1.79	0.64
1:C:81:LEU:HD21	1:C:157:ALA:HA	1.80	0.64
1:A:480:GLY:CA	1:A:483:ILE:CD1	2.62	0.64
1:A:191:THR:HG21	1:A:203:HIS:HA	1.80	0.64
1:A:180:VAL:HG21	1:A:379:ARG:NH1	2.13	0.63
1:D:58:ARG:NE	1:D:62:GLU:OE1	2.31	0.63
1:A:363:GLU:CG	1:A:364:LEU:N	2.62	0.63
1:C:397:LEU:HD13	1:C:398:LYS:C	2.19	0.63
1:D:232:HIS:CD2	1:D:260:THR:HA	2.33	0.63
3:C:602:HEM:HHA	3:C:602:HEM:HBD2	1.80	0.63
1:D:465:LEU:O	1:D:469:LEU:HD13	1.98	0.63
1:C:392:LEU:CD2	1:C:397:LEU:HD12	2.29	0.63
1:A:254:SER:HB3	1:A:306:ILE:HG21	1.81	0.62
1:A:429:ILE:CD1	1:A:434:THR:HG23	2.28	0.62
1:D:397:LEU:HD13	1:D:398:LYS:O	1.98	0.62
1:A:430:THR:HG1	1:A:476:SER:C	2.03	0.62
1:C:350:ALA:HB1	1:C:374:LEU:HD22	1.80	0.62
1:A:149:ASN:HD22	2:A:601:PLP:H2A1	1.65	0.62
1:B:94:LYS:NZ	1:D:159:ALA:O	2.33	0.62
1:D:264:ILE:O	1:D:268:LEU:CD1	2.43	0.62
1:A:338:LEU:HD12	1:A:344:LEU:HD12	1.82	0.62
1:B:350:ALA:HB1	1:B:374:LEU:HD22	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:LYS:HE3	1:C:410:TRP:CE2	2.35	0.61
1:A:467:SER:HB3	1:A:473:VAL:HG12	1.82	0.61
1:B:254:SER:HA	1:B:280:VAL:HB	1.82	0.61
1:B:458:MET:HE1	1:B:510:LEU:HD21	1.80	0.61
1:C:126:MET:HE2	1:C:220:LEU:HB3	1.82	0.61
1:D:415:GLN:HB3	1:D:492:LEU:HB3	1.82	0.61
1:A:363:GLU:HG3	1:A:364:LEU:N	2.16	0.60
1:A:512:VAL:HG12	1:A:513:HIS:H	1.66	0.60
1:C:226:ALA:HA	3:C:602:HEM:HMD2	1.83	0.60
1:C:64:PRO:HG3	3:C:602:HEM:HMA1	1.83	0.60
1:A:140:ASP:OD2	1:A:218:HIS:NE2	2.29	0.60
3:A:602:HEM:HBA2	3:A:602:HEM:HBD2	1.83	0.60
1:C:412:LEU:HD22	1:C:416:GLU:OE1	2.01	0.60
1:D:149:ASN:ND2	2:D:601:PLP:H2A1	2.16	0.60
1:A:122:ILE:HG21	1:A:228:ASN:OD1	2.02	0.60
1:B:543:VAL:O	1:B:547:GLU:HG2	2.02	0.60
1:C:226:ALA:HA	3:C:602:HEM:CMD	2.31	0.60
1:D:254:SER:HA	1:D:280:VAL:HB	1.84	0.60
1:A:479:VAL:C	1:A:483:ILE:HG13	2.22	0.59
1:C:264:ILE:O	1:C:268:LEU:CD1	2.44	0.59
1:A:543:VAL:O	1:A:547:GLU:HG2	2.03	0.59
1:A:363:GLU:CG	1:A:364:LEU:HD12	2.32	0.59
1:A:480:GLY:HA2	1:A:483:ILE:CG1	2.30	0.59
1:A:51:ARG:C	1:A:52:CYS:CA	2.71	0.59
1:C:122:ILE:O	1:C:126:MET:HG3	2.02	0.59
1:C:229:PRO:HB2	3:C:602:HEM:HAC	1.85	0.59
1:B:63:SER:CB	3:B:602:HEM:HAB	2.33	0.59
1:D:510:LEU:HD22	1:D:533:VAL:HG12	1.85	0.59
1:A:467:SER:CB	1:A:473:VAL:CG1	2.81	0.58
1:B:490:ILE:HG22	1:B:491:ARG:O	2.03	0.58
1:B:226:ALA:HA	3:B:602:HEM:HMD2	1.84	0.58
1:C:464:MET:O	1:C:468:LEU:CD1	2.50	0.58
1:C:397:LEU:CD1	1:C:397:LEU:C	2.72	0.58
1:C:191:THR:HG21	1:C:203:HIS:HA	1.85	0.58
1:B:510:LEU:HD22	1:B:533:VAL:HG22	1.85	0.58
1:B:431:CYS:O	1:B:434:THR:OG1	2.17	0.58
3:D:602:HEM:HBD2	3:D:602:HEM:HHA	1.86	0.58
1:A:338:LEU:HD21	1:A:354:VAL:HG21	1.84	0.57
1:A:435:ILE:HG13	1:A:464:MET:HE2	1.85	0.57
1:B:122:ILE:O	1:B:126:MET:HG3	2.04	0.57
1:C:490:ILE:HD12	1:C:502:ILE:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:THR:O	1:A:194:ASN:ND2	2.36	0.57
1:B:119:LYS:HB3	1:B:150:THR:HA	1.86	0.57
1:C:122:ILE:HG21	1:C:228:ASN:OD1	2.04	0.57
1:A:431:CYS:SG	1:A:464:MET:HE3	2.38	0.57
1:B:434:THR:HG21	1:B:479:VAL:HG21	1.87	0.57
1:D:451:GLU:C	1:D:453:GLY:H	2.08	0.57
1:B:430:THR:OG1	1:B:475:PRO:O	2.18	0.57
1:D:54:TRP:HD1	3:D:602:HEM:HAB	1.69	0.57
1:B:196:ARG:O	1:B:199:SER:OG	2.23	0.56
1:C:431:CYS:SG	1:C:435:ILE:CD1	2.89	0.56
1:C:119:LYS:HB3	1:C:150:THR:HA	1.87	0.56
1:C:254:SER:HA	1:C:280:VAL:HB	1.87	0.56
1:D:451:GLU:C	1:D:453:GLY:N	2.54	0.56
1:A:512:VAL:CG1	1:A:513:HIS:H	2.18	0.56
1:D:256:GLY:HA3	2:D:601:PLP:H5A1	1.88	0.56
1:D:193:THR:O	1:D:194:ASN:ND2	2.39	0.56
1:A:449:VAL:HG22	1:A:455:ILE:CG1	2.34	0.56
1:A:512:VAL:CG1	1:A:513:HIS:N	2.68	0.56
1:C:429:ILE:HG23	1:C:434:THR:OG1	2.06	0.56
1:C:419:LEU:HD21	1:C:534:VAL:HG22	1.88	0.56
1:D:403:THR:HA	1:D:406:LYS:HD2	1.88	0.56
1:A:200:PRO:HB2	1:A:209:ARG:NH1	2.21	0.55
1:A:430:THR:OG1	1:A:476:SER:C	2.45	0.55
1:C:334:PHE:O	1:C:338:LEU:HD22	2.06	0.55
1:D:423:LEU:HD22	1:D:441:LYS:HD2	1.87	0.55
1:C:54:TRP:HD1	3:C:602:HEM:CAB	2.20	0.55
1:D:338:LEU:HD21	1:D:354:VAL:HG21	1.87	0.55
1:B:431:CYS:HB3	1:B:464:MET:SD	2.46	0.55
1:A:504:GLU:OE1	1:C:182:ARG:NH1	2.40	0.55
1:B:102:LYS:HB2	1:B:365:GLN:HA	1.88	0.55
1:D:397:LEU:CD1	1:D:397:LEU:C	2.75	0.55
1:C:52:CYS:HA	3:C:602:HEM:C1A	2.42	0.55
1:A:467:SER:O	1:A:473:VAL:HG12	2.06	0.54
1:A:422:PRO:HA	1:A:443:PHE:CE2	2.42	0.54
1:B:264:ILE:O	1:B:268:LEU:CD1	2.52	0.54
1:B:264:ILE:CG2	1:B:268:LEU:HD13	2.37	0.54
1:B:149:ASN:HD22	2:B:601:PLP:H2A1	1.71	0.54
1:A:467:SER:CB	1:A:473:VAL:HG12	2.38	0.54
1:A:492:LEU:CD2	1:A:511:VAL:CG2	2.74	0.54
1:A:54:TRP:HD1	3:A:602:HEM:CBB	2.20	0.54
1:C:459:VAL:HG12	1:C:483:ILE:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:THR:HG21	1:B:203:HIS:HA	1.89	0.54
1:C:78:PRO:HG2	1:C:82:LYS:HD3	1.90	0.54
1:A:278:ILE:HD12	1:A:360:ALA:HB1	1.88	0.53
1:D:122:ILE:HG21	1:D:228:ASN:OD1	2.08	0.53
1:D:406:LYS:HD3	1:D:410:TRP:CE2	2.43	0.53
1:B:128:GLU:O	1:B:132:ARG:HG3	2.08	0.53
1:B:439:ARG:HH22	1:B:465:LEU:HD21	1.65	0.53
1:B:490:ILE:HG22	1:B:491:ARG:N	2.23	0.53
1:B:264:ILE:HG22	1:B:268:LEU:HD13	1.89	0.53
1:D:397:LEU:HD13	1:D:398:LYS:C	2.29	0.53
1:B:429:ILE:HD11	1:B:433:HIS:ND1	2.24	0.53
1:A:510:LEU:HD22	1:A:533:VAL:HG22	1.91	0.53
3:A:602:HEM:HBA2	3:A:602:HEM:HHA	1.91	0.53
1:B:119:LYS:HD2	1:B:150:THR:OG1	2.08	0.53
1:D:419:LEU:CD1	1:D:511:VAL:CG1	2.84	0.52
1:A:196:ARG:O	1:A:202:SER:HB3	2.09	0.52
1:A:436:GLU:O	1:A:440:GLU:HB2	2.10	0.52
1:D:111:PHE:HB2	1:D:377:SER:HB3	1.90	0.52
3:A:602:HEM:CHA	3:A:602:HEM:HBD1	2.19	0.52
1:A:527:ARG:HG3	1:A:528:GLN:H	1.73	0.52
1:B:433:HIS:O	1:B:437:ILE:HG12	2.10	0.52
1:D:119:LYS:HB3	1:D:150:THR:HA	1.90	0.52
1:D:353:THR:HG22	1:D:372:VAL:HG13	1.92	0.51
1:D:543:VAL:O	1:D:547:GLU:HG3	2.10	0.51
1:B:490:ILE:CG2	1:B:491:ARG:N	2.72	0.51
1:B:256:GLY:HA3	2:B:601:PLP:H5A1	1.91	0.51
1:B:284:GLY:HA2	1:B:296:THR:HG21	1.93	0.51
1:A:465:LEU:O	1:A:469:LEU:CD1	2.51	0.51
1:C:193:THR:HG22	1:C:194:ASN:N	2.25	0.51
1:A:449:VAL:HG22	1:A:455:ILE:HA	1.92	0.51
1:A:226:ALA:HA	3:A:602:HEM:HMD2	1.93	0.51
1:B:182:ARG:NH1	1:D:504:GLU:OE1	2.43	0.51
1:A:119:LYS:HG3	1:A:149:ASN:CB	2.41	0.51
1:B:226:ALA:HA	3:B:602:HEM:CMD	2.41	0.51
1:A:119:LYS:HB3	1:A:150:THR:HA	1.91	0.51
1:B:414:VAL:HG23	1:B:417:LEU:HD12	1.92	0.51
1:C:132:ARG:HG2	1:C:132:ARG:HH11	1.75	0.51
1:A:490:ILE:O	1:A:511:VAL:HA	2.11	0.51
1:A:122:ILE:O	1:A:126:MET:HG3	2.10	0.51
1:C:193:THR:O	1:C:194:ASN:ND2	2.43	0.51
1:A:126:MET:HG2	1:A:227:SER:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:602:HEM:HBC2	3:C:602:HEM:HMC2	1.93	0.50
1:B:411:HIS:O	1:B:412:LEU:HG	2.11	0.50
1:C:397:LEU:CD1	1:C:398:LYS:O	2.59	0.50
1:D:338:LEU:HD12	1:D:344:LEU:HD12	1.92	0.50
1:A:58:ARG:CZ	1:A:62:GLU:OE2	2.56	0.50
1:B:459:VAL:HG11	1:B:479:VAL:HG13	1.93	0.50
1:D:131:GLU:OE2	1:D:161:ARG:NH1	2.44	0.50
1:D:264:ILE:HG23	1:D:268:LEU:CD1	2.41	0.50
1:C:338:LEU:HD11	1:C:354:VAL:HG21	1.93	0.50
1:B:236:THR:HB	1:B:264:ILE:HD11	1.93	0.50
1:B:180:VAL:HG21	1:B:379:ARG:NH1	2.26	0.50
1:B:115:GLY:N	1:B:120:ASP:OD2	2.44	0.50
1:C:214:ILE:HG22	1:C:217:SER:HB3	1.94	0.50
1:A:419:LEU:HD13	1:A:511:VAL:HG11	1.93	0.50
1:B:126:MET:HG2	1:B:227:SER:HB2	1.94	0.49
1:C:102:LYS:HB2	1:C:365:GLN:HA	1.93	0.49
1:A:119:LYS:CG	1:A:149:ASN:HB3	2.42	0.49
1:A:426:LEU:CD1	1:A:426:LEU:C	2.80	0.49
1:D:223:TYR:O	1:D:314:VAL:HG13	2.13	0.49
1:B:425:VAL:HG13	1:B:448:VAL:HG22	1.95	0.49
1:D:115:GLY:O	1:D:379:ARG:NH2	2.45	0.49
1:A:467:SER:CB	1:A:473:VAL:HG11	2.43	0.49
1:A:455:ILE:HD11	1:A:530:VAL:CG2	2.43	0.49
1:B:52:CYS:HA	3:B:602:HEM:C1A	2.48	0.49
1:C:115:GLY:O	1:C:379:ARG:NH2	2.46	0.49
1:A:527:ARG:HG3	1:A:528:GLN:N	2.28	0.49
1:C:427:PRO:HG3	1:C:456:LEU:HD12	1.95	0.49
1:D:322:LYS:NZ	1:C:66:HIS:HB2	2.26	0.49
1:B:414:VAL:CG2	1:B:417:LEU:HD12	2.43	0.48
1:C:353:THR:HG22	1:C:372:VAL:HG13	1.95	0.48
1:D:461:LEU:O	1:D:465:LEU:HG	2.13	0.48
1:D:513:HIS:HB2	1:D:531:PHE:HE2	1.78	0.48
1:D:287:LEU:HD23	1:D:311:ILE:HD13	1.94	0.48
1:A:438:LEU:HD22	1:A:461:LEU:HD13	1.94	0.48
1:A:45:ARG:NH2	1:A:47:ASP:OD2	2.47	0.48
1:C:459:VAL:HG11	1:C:479:VAL:CG1	2.43	0.48
1:A:479:VAL:HG12	1:A:483:ILE:HD11	1.96	0.48
1:B:412:LEU:HD13	1:B:416:GLU:OE1	2.14	0.48
1:A:121:ARG:NH1	1:A:235:THR:OG1	2.47	0.47
1:A:200:PRO:HB2	1:A:209:ARG:HH11	1.79	0.47
1:B:54:TRP:HB2	3:B:602:HEM:C4B	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:LEU:HD12	1:C:293:LEU:N	2.28	0.47
1:D:122:ILE:O	1:D:126:MET:CG	2.62	0.47
1:B:81:LEU:HD21	1:B:157:ALA:HA	1.96	0.47
1:D:410:TRP:CE2	1:D:497:GLY:HA3	2.50	0.47
1:B:193:THR:HG22	1:B:194:ASN:N	2.29	0.47
1:C:87:THR:HB	1:C:109:CYS:O	2.14	0.47
1:D:448:VAL:CG2	1:D:459:VAL:HG13	2.45	0.47
1:A:544:ALA:HA	1:A:547:GLU:HG3	1.96	0.47
1:D:459:VAL:HG11	1:D:479:VAL:HG13	1.97	0.47
1:D:54:TRP:HB2	3:D:602:HEM:C4B	2.50	0.47
1:B:419:LEU:HD21	1:B:534:VAL:HG22	1.96	0.47
1:A:119:LYS:HG3	1:A:149:ASN:HB3	1.97	0.47
1:B:314:VAL:HG12	3:B:602:HEM:CMD	2.45	0.47
1:C:406:LYS:HE3	1:C:410:TRP:CD1	2.49	0.47
1:C:406:LYS:HE3	1:C:410:TRP:CD2	2.49	0.47
1:A:514:GLU:C	1:A:527:ARG:HH21	2.18	0.47
1:A:266:ARG:HD2	3:A:602:HEM:HBC2	1.97	0.46
1:C:419:LEU:HD11	1:C:511:VAL:HG21	1.96	0.46
1:C:149:ASN:HD22	2:C:601:PLP:H2A1	1.81	0.46
1:C:510:LEU:HD22	1:C:533:VAL:HG12	1.97	0.46
1:D:449:VAL:HA	1:D:455:ILE:HA	1.97	0.46
1:A:119:LYS:HD2	1:A:150:THR:OG1	2.16	0.46
1:A:386:LEU:HD23	1:C:179:ASP:HB3	1.98	0.46
1:C:432:GLY:O	1:C:436:GLU:HG2	2.16	0.46
1:D:103:CYS:HB2	1:D:368:GLN:O	2.14	0.46
1:A:197:PHE:CE2	1:A:310:PHE:HB3	2.51	0.46
1:C:314:VAL:HG12	3:C:602:HEM:CMD	2.45	0.46
1:A:287:LEU:HD23	1:A:311:ILE:HD13	1.97	0.46
1:A:537:ILE:HD12	1:C:209:ARG:CZ	2.46	0.46
1:D:226:ALA:HA	3:D:602:HEM:HMD2	1.97	0.46
1:D:264:ILE:CG2	1:D:268:LEU:HD13	2.46	0.46
1:A:353:THR:HG22	1:A:372:VAL:HG13	1.98	0.46
1:A:90:VAL:HG21	1:C:80:ILE:HD13	1.98	0.46
1:B:126:MET:HE2	1:B:220:LEU:HB3	1.98	0.46
1:A:434:THR:O	1:A:438:LEU:HB3	2.16	0.46
1:B:280:VAL:HG13	1:B:356:VAL:HG21	1.97	0.45
1:B:499:LEU:HD23	1:B:539:LEU:HD22	1.98	0.45
1:A:125:ARG:NE	1:A:129:ASP:OD1	2.50	0.45
1:A:495:THR:HG23	1:A:498:ARG:H	1.81	0.45
1:C:281:ASP:OD2	1:C:282:PRO:HD2	2.16	0.45
1:C:392:LEU:HD21	1:C:397:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:LEU:HD13	1:C:532:GLY:HA3	1.97	0.45
1:D:286:ILE:HD11	1:D:310:PHE:HA	1.98	0.45
1:A:95:ILE:HD12	1:A:338:LEU:HD13	1.98	0.45
1:A:384:LYS:O	1:A:390:TRP:HB3	2.17	0.45
1:B:166:ILE:HG12	1:B:187:GLU:HB2	1.97	0.45
1:A:449:VAL:HG11	1:A:528:GLN:HG3	1.98	0.45
1:C:106:LEU:HB2	1:C:371:VAL:HG22	1.98	0.45
1:C:178:VAL:HG13	1:C:188:ILE:HD13	1.99	0.45
1:A:455:ILE:O	1:A:455:ILE:HG22	2.15	0.45
1:B:544:ALA:HA	1:B:547:GLU:HG3	1.98	0.45
1:B:490:ILE:HG23	1:B:494:ASP:HB2	1.97	0.45
1:D:192:PRO:HG2	1:D:195:ALA:HB2	1.99	0.45
1:D:264:ILE:HG23	1:D:268:LEU:HD13	1.99	0.45
1:C:431:CYS:HG	1:C:435:ILE:HD11	1.76	0.45
1:D:451:GLU:O	1:D:452:ALA:C	2.53	0.45
1:A:434:THR:CG2	1:A:479:VAL:HG21	2.46	0.44
1:C:290:PRO:HD2	1:C:293:LEU:CD1	2.47	0.44
1:B:46:PRO:HB2	1:B:310:PHE:CE1	2.52	0.44
1:C:491:ARG:HB2	1:C:494:ASP:CG	2.37	0.44
1:B:504:GLU:OE1	1:D:182:ARG:NH1	2.51	0.44
1:D:64:PRO:HG3	3:D:602:HEM:CHB	2.48	0.44
1:B:406:LYS:HD3	1:B:410:TRP:CE2	2.53	0.44
1:A:198:ASP:HB2	1:C:466:SER:OG	2.17	0.44
1:D:226:ALA:HA	3:D:602:HEM:CMD	2.47	0.44
1:C:92:ILE:HD11	1:C:107:ALA:HB2	2.00	0.44
1:C:52:CYS:HA	3:C:602:HEM:NA	2.33	0.44
1:B:223:TYR:CE1	1:B:257:THR:HG22	2.52	0.44
1:D:542:PHE:O	1:D:546:GLN:HG2	2.18	0.44
1:A:131:GLU:HG3	1:A:136:LEU:HD23	2.00	0.44
1:A:363:GLU:HG3	1:A:364:LEU:HD12	2.00	0.44
1:B:468:LEU:HD23	1:B:473:VAL:O	2.18	0.44
1:A:461:LEU:O	1:A:464:MET:HB2	2.17	0.44
1:C:392:LEU:HD23	1:C:397:LEU:HD12	2.00	0.44
1:C:432:GLY:HA2	1:C:435:ILE:HD12	2.00	0.44
1:D:95:ILE:HD12	1:D:338:LEU:HD13	1.99	0.44
1:B:190:ARG:HG3	1:D:505:MET:C	2.38	0.44
1:D:54:TRP:HD1	3:D:602:HEM:CAB	2.29	0.43
1:B:413:ARG:HD2	1:B:493:THR:HA	1.99	0.43
1:C:285:SER:HG	1:C:308:TYR:H	1.63	0.43
1:D:111:PHE:HB3	1:D:376:ASP:C	2.38	0.43
1:A:63:SER:HB3	3:A:602:HEM:CAB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ILE:HD12	1:B:264:ILE:HD12	1.99	0.43
1:C:140:ASP:OD2	1:C:218:HIS:CE1	2.71	0.43
1:D:503:LEU:HD13	1:D:536:ALA:HA	2.00	0.43
1:A:146:THR:HG21	1:A:151:GLY:HA3	2.00	0.43
1:A:503:LEU:HA	1:A:506:ASP:O	2.19	0.43
1:C:423:LEU:HD12	1:C:424:THR:N	2.30	0.43
1:C:286:ILE:HD11	1:C:310:PHE:HA	2.00	0.43
1:D:220:LEU:HA	1:D:220:LEU:HD23	1.84	0.43
1:C:110:GLU:OE2	1:C:121:ARG:NH2	2.50	0.43
1:C:145:PRO:HB2	1:C:203:HIS:CD2	2.53	0.43
1:D:169:MET:O	1:D:190:ARG:HA	2.18	0.43
1:A:337:MET:HG2	1:A:341:GLN:HG3	2.01	0.43
1:C:248:LEU:HG	1:C:275:CYS:SG	2.58	0.43
1:B:119:LYS:HG3	1:B:149:ASN:CB	2.49	0.43
1:D:254:SER:HB2	1:D:306:ILE:HG21	2.01	0.43
1:A:54:TRP:CD1	3:A:602:HEM:CBB	3.02	0.43
1:B:102:LYS:HD2	1:B:365:GLN:HA	2.01	0.43
1:C:293:LEU:H	1:C:293:LEU:CD1	2.32	0.43
1:C:489:GLN:NE2	1:C:528:GLN:OE1	2.50	0.43
1:D:392:LEU:HD23	1:D:397:LEU:HD12	1.94	0.43
1:D:512:VAL:HG12	1:D:530:VAL:HG22	2.00	0.43
1:A:479:VAL:HG12	1:A:483:ILE:CG1	2.49	0.42
1:A:503:LEU:HD13	1:A:536:ALA:HA	2.01	0.42
1:B:397:LEU:HA	1:B:397:LEU:HD23	1.92	0.42
1:B:429:ILE:HG13	1:B:430:THR:N	2.33	0.42
1:C:111:PHE:HB2	1:C:377:SER:HB3	2.01	0.42
1:D:448:VAL:HG21	1:D:459:VAL:HG13	2.01	0.42
1:B:529:MET:HG2	1:B:531:PHE:CE1	2.54	0.42
1:C:445:GLN:HB3	1:C:460:THR:HG22	2.01	0.42
1:A:280:VAL:HG13	1:A:356:VAL:HG21	2.01	0.42
1:D:52:CYS:HA	3:D:602:HEM:C1A	2.54	0.42
1:A:467:SER:HB2	1:A:473:VAL:HG11	2.01	0.42
1:B:281:ASP:OD2	1:B:287:LEU:HD12	2.19	0.42
1:C:54:TRP:HB2	3:C:602:HEM:C4B	2.55	0.42
1:A:419:LEU:HD12	1:A:511:VAL:HG11	1.99	0.42
1:B:469:LEU:O	1:B:469:LEU:HD23	2.19	0.42
1:D:264:ILE:C	1:D:268:LEU:HD13	2.35	0.42
1:A:108:LYS:HB3	1:A:373:ILE:HD13	2.00	0.42
1:A:51:ARG:HB3	3:A:602:HEM:O1A	2.19	0.42
1:C:406:LYS:HE3	1:C:410:TRP:NE1	2.35	0.42
1:D:110:GLU:HG2	1:D:118:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:ARG:O	1:C:202:SER:HB3	2.20	0.42
1:C:293:LEU:CD1	1:C:293:LEU:N	2.82	0.42
1:C:397:LEU:CD1	1:C:397:LEU:O	2.68	0.42
1:C:499:LEU:HD21	1:C:534:VAL:HG11	2.02	0.42
1:B:264:ILE:HG23	1:B:268:LEU:CD1	2.49	0.42
1:D:446:ALA:O	1:D:459:VAL:HG22	2.20	0.42
1:C:412:LEU:O	1:C:495:THR:HA	2.20	0.42
1:D:281:ASP:OD1	1:D:285:SER:HB3	2.20	0.42
1:A:221:ASP:OD1	1:A:224:ARG:NH1	2.52	0.41
1:A:426:LEU:HB3	1:A:429:ILE:HG23	2.01	0.41
1:A:448:VAL:O	1:A:456:LEU:N	2.52	0.41
1:B:338:LEU:HD12	1:B:344:LEU:HD12	2.02	0.41
1:D:353:THR:CG2	1:D:372:VAL:HG13	2.50	0.41
1:B:301:TYR:CD2	1:B:301:TYR:N	2.88	0.41
3:C:602:HEM:HBC2	3:C:602:HEM:CMC	2.50	0.41
1:D:432:GLY:HA2	1:D:435:ILE:HD12	2.01	0.41
1:B:122:ILE:HG21	1:B:228:ASN:OD1	2.19	0.41
1:C:327:ASN:OD1	1:C:330:GLU:HB2	2.20	0.41
1:C:426:LEU:O	1:C:429:ILE:HG22	2.20	0.41
1:D:190:ARG:HD2	1:D:190:ARG:HA	1.89	0.41
1:C:190:ARG:HA	1:C:190:ARG:HD2	1.83	0.41
1:C:229:PRO:HB2	3:C:602:HEM:CAC	2.48	0.41
1:A:136:LEU:HG	1:A:163:TYR:HE2	1.85	0.41
1:D:233:TYR:O	1:D:267:LYS:HD2	2.20	0.41
1:D:180:VAL:HG21	1:D:379:ARG:NH1	2.36	0.41
1:D:406:LYS:HD3	1:D:410:TRP:NE1	2.35	0.41
1:A:435:ILE:HD11	1:A:464:MET:HB3	2.02	0.41
1:B:83:LYS:HD2	1:B:83:LYS:HA	1.82	0.41
1:C:110:GLU:OE2	1:C:121:ARG:NE	2.49	0.41
1:A:51:ARG:CB	3:A:602:HEM:O1A	2.68	0.41
1:D:214:ILE:HA	1:D:215:PRO:HD3	1.91	0.41
1:A:226:ALA:HA	3:A:602:HEM:CMD	2.51	0.41
1:A:263:GLY:HA2	3:A:602:HEM:HBC1	2.03	0.41
1:A:422:PRO:HA	1:A:443:PHE:HE2	1.86	0.41
1:B:264:ILE:CG2	1:B:268:LEU:CD1	2.99	0.41
1:C:302:GLU:OE2	1:C:394:LYS:NZ	2.42	0.41
1:D:180:VAL:HG21	1:D:379:ARG:HH11	1.86	0.41
1:A:180:VAL:HG21	1:A:379:ARG:HH11	1.83	0.40
1:B:338:LEU:HD21	1:B:354:VAL:HG21	2.03	0.40
1:C:103:CYS:HB2	1:C:368:GLN:O	2.21	0.40
1:A:190:ARG:NH1	1:C:504:GLU:O	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:PRO:HB2	1:D:203:HIS:CD2	2.56	0.40
1:A:260:THR:CB	2:A:601:PLP:O1P	2.69	0.40
1:B:82:LYS:N	1:B:82:LYS:HD2	2.36	0.40
1:D:322:LYS:NZ	1:C:132:ARG:HH12	2.19	0.40
1:C:255:VAL:HG13	1:C:258:GLY:HA2	2.04	0.40
1:A:64:PRO:HG3	3:A:602:HEM:CMA	2.51	0.40
1:C:180:VAL:HG21	1:C:379:ARG:NH1	2.37	0.40
1:A:191:THR:HB	1:A:201:GLU:O	2.21	0.40
1:B:258:GLY:HA3	1:B:315:LEU:HD13	2.03	0.40
1:B:337:MET:HG2	1:B:341:GLN:HG3	2.02	0.40
1:C:82:LYS:HD2	1:C:82:LYS:N	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LEU:CD2	1:C:421:ALA:CB[5_455]	2.13	0.07

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	467/548 (85%)	455 (97%)	12 (3%)	0	100	100
1	B	482/548 (88%)	475 (98%)	7 (2%)	0	100	100
1	C	485/548 (88%)	478 (99%)	7 (1%)	0	100	100
1	D	483/548 (88%)	475 (98%)	7 (1%)	1 (0%)	51	84
All	All	1917/2192 (88%)	1883 (98%)	33 (2%)	1 (0%)	55	87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	452	ALA

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	408/463 (88%)	404 (99%)	4 (1%)	80	91
1	B	413/463 (89%)	407 (98%)	6 (2%)	70	87
1	C	411/463 (89%)	409 (100%)	2 (0%)	91	96
1	D	411/463 (89%)	407 (99%)	4 (1%)	80	91
All	All	1643/1852 (89%)	1627 (99%)	16 (1%)	80	91

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

Mol	Chain	Res	Type
1	B	220	LEU
1	B	301	TYR
1	B	338	LEU
1	B	377	SER
1	B	479	VAL
1	B	493	THR
1	D	217	SER
1	D	338	LEU
1	D	414	VAL
1	D	451	GLU
1	A	127	ILE
1	A	338	LEU
1	A	386	LEU
1	A	455	ILE
1	C	414	VAL
1	C	464	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	194	ASN
1	A	194	ASN
1	A	232	HIS
1	C	194	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	PLP	A	601	1	15,15,16	1.34	1 (6%)	20,22,23	1.14	1 (5%)
3	HEM	A	602	1	28,50,50	2.16	6 (21%)	17,82,82	3.14	9 (52%)
2	PLP	B	601	1	15,15,16	1.22	1 (6%)	20,22,23	1.09	1 (5%)
3	HEM	B	602	1	28,50,50	2.22	7 (25%)	17,82,82	1.33	1 (5%)
2	PLP	C	601	1	15,15,16	1.24	1 (6%)	20,22,23	1.08	2 (10%)
3	HEM	C	602	1	28,50,50	2.25	10 (35%)	17,82,82	2.68	5 (29%)
2	PLP	D	601	1	15,15,16	1.32	1 (6%)	20,22,23	1.08	1 (5%)
3	HEM	D	602	1	28,50,50	2.22	8 (28%)	17,82,82	1.35	3 (17%)

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

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	HEM	C3C-C2C	-5.02	1.33	1.40
3	B	602	HEM	C3B-C2B	-5.02	1.33	1.40
3	C	602	HEM	C3C-C2C	-4.91	1.33	1.40
3	A	602	HEM	C3C-C2C	-4.82	1.34	1.40
3	D	602	HEM	C3C-C2C	-4.55	1.34	1.40
3	D	602	HEM	C3B-C2B	-4.26	1.34	1.40
3	A	602	HEM	C3B-C2B	-4.16	1.34	1.40
3	C	602	HEM	C3B-C2B	-4.13	1.34	1.40
2	A	601	PLP	C3-C2	-3.04	1.38	1.40
2	D	601	PLP	C3-C2	-3.01	1.38	1.40
2	C	601	PLP	C3-C2	-2.47	1.39	1.40
2	B	601	PLP	P-O3P	-2.06	1.46	1.54
3	D	602	HEM	CAD-C3D	2.00	1.56	1.52
3	C	602	HEM	CMB-C2B	2.03	1.55	1.51
3	D	602	HEM	C4D-ND	2.07	1.39	1.36
3	C	602	HEM	CMA-C3A	2.09	1.55	1.51
3	D	602	HEM	CAA-C2A	2.09	1.55	1.52
3	C	602	HEM	C1B-NB	2.12	1.39	1.36
3	B	602	HEM	CAD-C3D	2.15	1.56	1.52
3	A	602	HEM	C1B-NB	2.23	1.39	1.36
3	C	602	HEM	C4D-ND	2.40	1.39	1.36
3	B	602	HEM	C1B-NB	2.50	1.39	1.36
3	B	602	HEM	C3B-CAB	2.79	1.53	1.47
3	C	602	HEM	CAA-C2A	2.93	1.57	1.52
3	B	602	HEM	C3C-CAC	3.20	1.54	1.47
3	C	602	HEM	C3C-CAC	3.28	1.54	1.47
3	A	602	HEM	C3B-CAB	3.55	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	HEM	C3C-CAC	3.60	1.54	1.47
3	A	602	HEM	C3C-CAC	3.70	1.55	1.47
3	D	602	HEM	C3B-CAB	3.89	1.55	1.47
3	C	602	HEM	C3B-CAB	4.09	1.56	1.47
3	C	602	HEM	C3D-C2D	5.08	1.52	1.37
3	B	602	HEM	C3D-C2D	5.32	1.53	1.37
3	D	602	HEM	C3D-C2D	5.52	1.54	1.37
3	A	602	HEM	C3D-C2D	5.54	1.54	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	HEM	CAA-CBA-CGA	-9.97	95.62	112.66
3	C	602	HEM	CMA-C3A-C4A	-6.03	119.19	128.46
3	A	602	HEM	CAA-C2A-C3A	-2.84	120.91	129.00
3	A	602	HEM	C1D-C2D-C3D	-2.49	105.27	107.00
3	A	602	HEM	CMA-C3A-C4A	-2.05	125.31	128.46
3	A	602	HEM	C3B-C4B-NB	-2.03	106.59	109.21
2	C	601	PLP	O4P-C5A-C5	2.00	113.34	109.32
3	D	602	HEM	CMB-C2B-C3B	2.28	129.12	124.89
3	C	602	HEM	C4C-C3C-C2C	2.29	108.50	106.90
3	B	602	HEM	C4C-C3C-C2C	2.33	108.53	106.90
3	D	602	HEM	C4A-C3A-C2A	2.45	108.70	107.00
3	D	602	HEM	CMC-C2C-C3C	2.46	129.46	124.89
2	D	601	PLP	O3P-P-O1P	2.55	120.47	110.50
2	A	601	PLP	O3P-P-O1P	2.58	120.58	110.50
2	C	601	PLP	O3P-P-O1P	2.58	120.61	110.50
3	A	602	HEM	CMC-C2C-C3C	2.60	129.72	124.89
3	A	602	HEM	C4A-C3A-C2A	2.62	108.82	107.00
2	B	601	PLP	O3P-P-O1P	2.68	120.97	110.50
3	A	602	HEM	CAD-CBD-CGD	3.00	117.79	112.66
3	C	602	HEM	CMC-C2C-C3C	3.70	131.75	124.89
3	A	602	HEM	CBA-CAA-C2A	3.78	119.71	112.48
3	C	602	HEM	CMA-C3A-C2A	4.19	132.84	124.94
3	C	602	HEM	CAA-CBA-CGA	5.25	121.64	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	PLP	4	0
3	A	602	HEM	15	0
2	B	601	PLP	3	0
3	B	602	HEM	12	0
2	C	601	PLP	2	0
3	C	602	HEM	14	0
2	D	601	PLP	3	0
3	D	602	HEM	9	0

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	485/548 (88%)	0.72	72 (14%) 3 3	43, 83, 160, 205	0
1	B	490/548 (89%)	0.20	23 (4%) 32 30	40, 84, 141, 214	0
1	C	491/548 (89%)	0.23	15 (3%) 49 46	39, 78, 137, 185	0
1	D	491/548 (89%)	0.36	38 (7%) 14 14	34, 75, 159, 207	0
All	All	1957/2192 (89%)	0.38	148 (7%) 15 15	34, 80, 154, 214	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	57	GLY	12.0
1	A	443	PHE	6.9
1	B	427	PRO	6.5
1	A	41	PRO	6.2
1	A	417	LEU	6.1
1	A	446	ALA	5.6
1	A	456	LEU	5.5
1	C	427	PRO	5.4
1	A	512	VAL	5.4
1	A	56	LEU	5.2
1	A	298	GLN	5.1
1	A	409	TRP	5.1
1	A	496	LEU	5.1
1	A	414	VAL	4.9
1	A	532	GLY	4.9
1	D	532	GLY	4.8
1	A	545	ALA	4.8
1	A	548	ARG	4.7
1	D	452	ALA	4.6
1	D	533	VAL	4.6
1	A	448	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	531	PHE	4.5
1	D	417	LEU	4.5
1	A	109	CYS	4.4
1	A	450	ASP	4.4
1	D	456	LEU	4.4
1	A	278	ILE	4.3
1	A	370	CYS	4.3
1	D	427	PRO	4.3
1	D	457	GLY	4.2
1	D	539	LEU	4.0
1	A	529	MET	4.0
1	B	456	LEU	4.0
1	B	450	ASP	4.0
1	A	481	LYS	3.9
1	A	510	LEU	3.8
1	D	445	GLN	3.8
1	A	252	VAL	3.8
1	D	434	THR	3.8
1	A	415	GLN	3.8
1	A	477	ASP	3.7
1	B	531	PHE	3.7
1	A	533	VAL	3.7
1	A	546	GLN	3.7
1	A	459	VAL	3.7
1	B	423	LEU	3.7
1	C	298	GLN	3.6
1	A	514	GLU	3.6
1	D	455	ILE	3.6
1	A	70	PRO	3.5
1	D	458	MET	3.5
1	B	455	ILE	3.5
1	A	398	LYS	3.5
1	B	532	GLY	3.4
1	A	542	PHE	3.4
1	D	449	VAL	3.4
1	A	397	LEU	3.4
1	A	299	THR	3.3
1	A	549	ASP	3.3
1	B	399	GLU	3.2
1	B	481	LYS	3.2
1	C	399	GLU	3.2
1	D	479	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	499	LEU	3.2
1	C	398	LYS	3.1
1	A	492	LEU	3.1
1	A	104	GLU	3.1
1	A	451	GLU	3.1
1	C	299	THR	3.1
1	D	397	LEU	3.0
1	A	530	VAL	3.0
1	B	489	GLN	3.0
1	B	448	VAL	3.0
1	A	372	VAL	2.9
1	D	419	LEU	2.9
1	A	268	LEU	2.9
1	D	508	PHE	2.8
1	C	428	THR	2.8
1	A	430	THR	2.8
1	A	535	THR	2.8
1	D	534	VAL	2.8
1	A	508	PHE	2.8
1	B	425	VAL	2.7
1	A	264	ILE	2.7
1	C	443	PHE	2.6
1	D	482	VAL	2.6
1	A	534	VAL	2.6
1	A	106	LEU	2.6
1	A	253	ALA	2.6
1	A	358	VAL	2.6
1	B	446	ALA	2.6
1	A	324	PHE	2.6
1	A	449	VAL	2.6
1	D	411	HIS	2.6
1	A	408	TRP	2.6
1	B	482	VAL	2.6
1	D	428	THR	2.5
1	A	366	GLU	2.5
1	A	513	HIS	2.5
1	D	147	SER	2.5
1	A	63	SER	2.5
1	D	443	PHE	2.5
1	D	483	ILE	2.5
1	B	449	VAL	2.4
1	A	365	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	457	GLY	2.4
1	B	424	THR	2.4
1	A	476	SER	2.4
1	A	105	LEU	2.4
1	A	541	ASN	2.3
1	D	429	ILE	2.3
1	A	511	VAL	2.3
1	A	455	ILE	2.3
1	A	371	VAL	2.3
1	A	445	GLN	2.3
1	B	458	MET	2.2
1	D	416	GLU	2.2
1	D	478	GLN	2.2
1	A	361	ALA	2.2
1	D	438	LEU	2.2
1	C	456	LEU	2.2
1	B	533	VAL	2.2
1	D	441	LYS	2.2
1	A	279	GLY	2.2
1	B	492	LEU	2.2
1	D	512	VAL	2.2
1	D	403	THR	2.2
1	B	530	VAL	2.1
1	C	441	LYS	2.1
1	D	425	VAL	2.1
1	C	527	ARG	2.1
1	C	166	ILE	2.1
1	B	548	ARG	2.1
1	D	422	PRO	2.1
1	B	508	PHE	2.1
1	D	485	LYS	2.1
1	D	447	PRO	2.1
1	D	509	ALA	2.1
1	A	464	MET	2.1
1	B	490	ILE	2.1
1	C	528	GLN	2.1
1	A	280	VAL	2.1
1	C	72	LYS	2.1
1	C	434	THR	2.1
1	D	530	VAL	2.0
1	A	88	PRO	2.0
1	D	446	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	491	ARG	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	HEM	C	602	43/43	0.94	0.33	2.52	79,79,80,80	0
3	HEM	B	602	43/43	0.94	0.29	1.46	112,112,113,113	0
3	HEM	A	602	43/43	0.91	0.34	0.84	106,106,107,107	0
3	HEM	D	602	43/43	0.95	0.28	0.50	79,79,80,80	0
2	PLP	C	601	15/16	0.94	0.28	0.35	45,56,60,63	0
2	PLP	D	601	15/16	0.96	0.24	0.11	49,56,65,66	0
2	PLP	A	601	15/16	0.91	0.25	-0.03	50,67,77,77	0
2	PLP	B	601	15/16	0.94	0.23	-0.33	57,70,80,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.