



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:34 PM GMT

PDB ID : 4COO
Title : Crystal structure of human cystathionine beta-synthase (delta516-525) at 2.0 angstrom resolution
Authors : McCorvie, T.J.; Kopec, J.; Vollamar, M.; Strain-Damerell, C.; Bushell, S.; Bradley, A.; Tallant, C.; Kiyani, W.; Froese, D.S.; Carpenter, E.S.; Burgess-Brown, N.; von Delft, F.; Arrowsmith, C.; Edwards, A.; Bountra, C.; Yue, W.W.
Deposited on : 2014-01-29
Resolution : 2.00 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

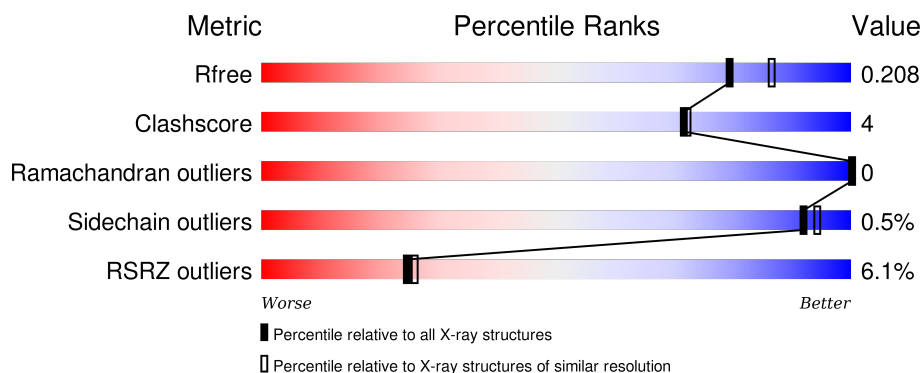
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


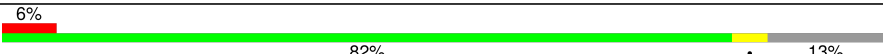
The reported resolution of this entry is 2.00 Å.

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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	563	
1	B	563	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	A	1550	-	-	X	X
3	ACT	B	1540	-	-	X	-
3	ACT	B	1541	-	-	-	X
3	ACT	B	1542	-	-	X	X
3	ACT	B	1546	-	-	X	X
5	EDO	A	1552	-	-	-	X
5	EDO	A	1553	-	-	-	X
5	EDO	A	1554	-	-	X	X
5	EDO	A	1559	-	-	-	X
5	EDO	B	1544	-	-	-	X
6	PE4	A	1557	-	-	-	X
7	NA	A	1558	-	-	-	X
7	NA	B	1545	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8055 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	5	0
			3822	2424	668	708	22			
1	B	487	Total	C	N	O	S	0	5	0
			3766	2392	657	695	22			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	EXPRESSION TAG	UNP P35520
A	-20	HIS	-	EXPRESSION TAG	UNP P35520
A	-19	HIS	-	EXPRESSION TAG	UNP P35520
A	-18	HIS	-	EXPRESSION TAG	UNP P35520
A	-17	HIS	-	EXPRESSION TAG	UNP P35520
A	-16	HIS	-	EXPRESSION TAG	UNP P35520
A	-15	HIS	-	EXPRESSION TAG	UNP P35520
A	-14	SER	-	EXPRESSION TAG	UNP P35520
A	-13	SER	-	EXPRESSION TAG	UNP P35520
A	-12	GLY	-	EXPRESSION TAG	UNP P35520
A	-11	VAL	-	EXPRESSION TAG	UNP P35520
A	-10	ASP	-	EXPRESSION TAG	UNP P35520
A	-9	LEU	-	EXPRESSION TAG	UNP P35520
A	-8	GLY	-	EXPRESSION TAG	UNP P35520
A	-7	THR	-	EXPRESSION TAG	UNP P35520
A	-6	GLU	-	EXPRESSION TAG	UNP P35520
A	-5	ASN	-	EXPRESSION TAG	UNP P35520
A	-4	LEU	-	EXPRESSION TAG	UNP P35520
A	-3	TYR	-	EXPRESSION TAG	UNP P35520
A	-2	PHE	-	EXPRESSION TAG	UNP P35520
A	-1	GLN	-	EXPRESSION TAG	UNP P35520
A	0	SER	-	EXPRESSION TAG	UNP P35520
A	.	-	ILE	DELETION	UNP P35520
A	.	-	GLN	DELETION	UNP P35520
A	.	-	TYR	DELETION	UNP P35520

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Chain	Residue	Modelled	Actual	Comment	Reference
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
B	-21	MET	-	EXPRESSION TAG	UNP P35520
B	-20	HIS	-	EXPRESSION TAG	UNP P35520
B	-19	HIS	-	EXPRESSION TAG	UNP P35520
B	-18	HIS	-	EXPRESSION TAG	UNP P35520
B	-17	HIS	-	EXPRESSION TAG	UNP P35520
B	-16	HIS	-	EXPRESSION TAG	UNP P35520
B	-15	HIS	-	EXPRESSION TAG	UNP P35520
B	-14	SER	-	EXPRESSION TAG	UNP P35520
B	-13	SER	-	EXPRESSION TAG	UNP P35520
B	-12	GLY	-	EXPRESSION TAG	UNP P35520
B	-11	VAL	-	EXPRESSION TAG	UNP P35520
B	-10	ASP	-	EXPRESSION TAG	UNP P35520
B	-9	LEU	-	EXPRESSION TAG	UNP P35520
B	-8	GLY	-	EXPRESSION TAG	UNP P35520
B	-7	THR	-	EXPRESSION TAG	UNP P35520
B	-6	GLU	-	EXPRESSION TAG	UNP P35520
B	-5	ASN	-	EXPRESSION TAG	UNP P35520
B	-4	LEU	-	EXPRESSION TAG	UNP P35520
B	-3	TYR	-	EXPRESSION TAG	UNP P35520
B	-2	PHE	-	EXPRESSION TAG	UNP P35520
B	-1	GLN	-	EXPRESSION TAG	UNP P35520
B	0	SER	-	EXPRESSION TAG	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

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0

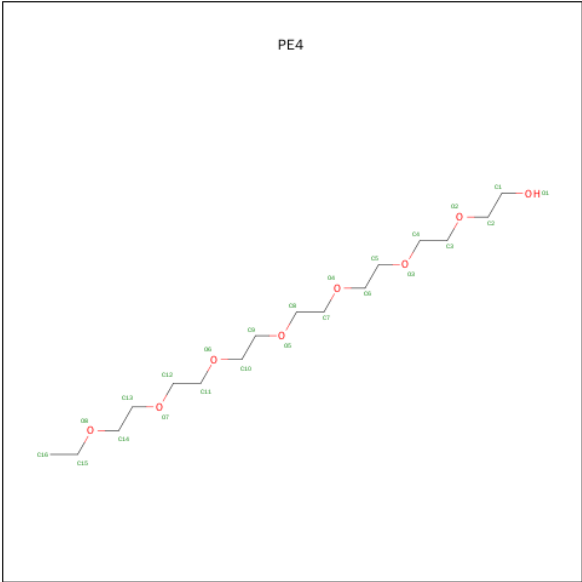
- PLP
-
- The chemical structure of PLP (Pyridoxal phosphate) is shown. It consists of a pyridine ring substituted with a hydroxyl group at C3, a hydroxymethyl group at C5, and an aldehyde group at C4. The aldehyde group is linked to a phosphate group. The atoms are labeled as follows: N1 (Nitrogen), C2, C3, C4, C5, C6 (Ring carbons); C2A (Hydroxymethyl carbon), C3A (Hydroxyl oxygen), C4A (Aldehyde carbon), C5A (Hydroxymethyl carbon), C6A (Hydroxyl oxygen); O1P, O2P, O3P, O4P (Phosphate oxygens); and P (Phosphorus).

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C₁₆H₃₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	5	2		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Na	0	0
			1	1		
7	A	1	Total	Na	0	0
			1	1		

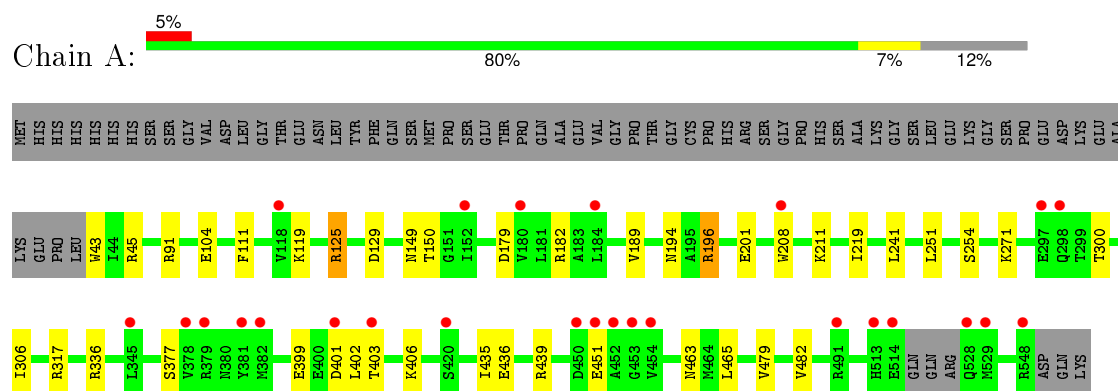
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	191	Total	O	0	0
			191	191		
8	B	103	Total	O	0	0
			103	103		

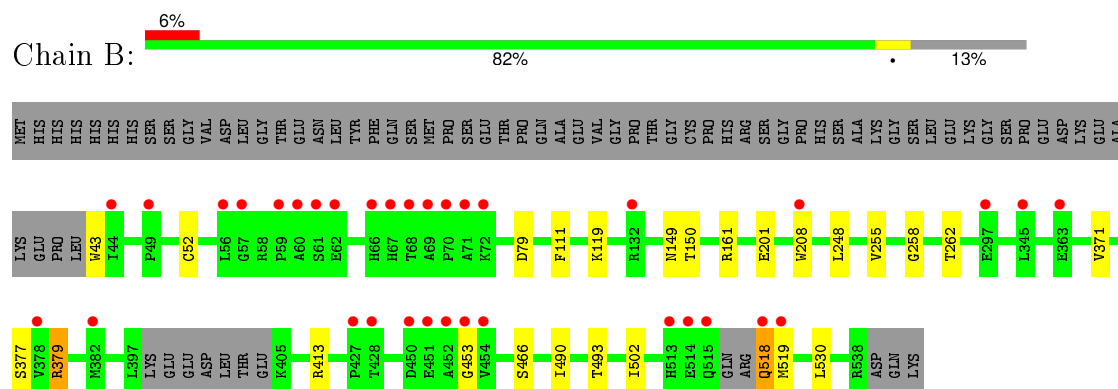
3 Residue-property plots

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	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.26Å 116.19Å 167.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.56 – 2.00 48.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (95.56-2.00) 99.7 (48.89-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.174 , 0.201 0.184 , 0.208	Depositor DCC
R_{free} test set	4662 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 93225 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8055	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PLP, PE4, NA, EDO, ACT, HEM

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	0.53	0/3905	0.76	6/5295 (0.1%)
1	B	0.46	0/3846	0.66	1/5216 (0.0%)
All	All	0.50	0/7751	0.71	7/10511 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	A	125	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	A	336	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	A	196	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	A	317	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	A	196	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	B	379	ARG	NE-CZ-NH1	5.09	122.85	120.30

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	3822	0	3856	32	0
1	B	3766	0	3778	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	43	0	30	3	0
2	B	43	0	30	4	0
3	A	4	0	3	4	0
3	B	16	0	12	13	0
4	A	15	0	6	1	0
4	B	15	0	6	3	0
5	A	24	0	36	5	0
5	B	4	0	6	1	0
6	A	7	0	6	2	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	191	0	0	8	0
8	B	103	0	0	4	0
All	All	8055	0	7769	66	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 4.

All (66) 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:379:ARG:NH2	8:B:2011:HOH:O	1.81	1.09
1:B:119:LYS:HZ3	4:B:1543:PLP:C4A	1.81	0.90
1:B:150:THR:H	3:B:1540:ACT:H1	1.40	0.87
1:A:150:THR:H	3:A:1550:ACT:H1	1.41	0.85
5:A:1554:EDO:O2	3:B:1542:ACT:H2	1.83	0.79
8:A:2190:HOH:O	3:B:1542:ACT:H1	1.83	0.77
1:B:530:LEU:HA	3:B:1542:ACT:H3	1.66	0.74
1:A:194[B]:ASN:ND2	8:A:2082:HOH:O	2.19	0.74
1:B:201:GLU:OE1	8:B:2041:HOH:O	2.06	0.72
1:A:201:GLU:OE1	8:A:2086:HOH:O	2.07	0.72
2:A:1549:HEM:HMC2	2:A:1549:HEM:HBC2	1.74	0.69
1:A:91:ARG:NH1	1:A:104:GLU:OE2	2.26	0.69
1:A:194[B]:ASN:CG	8:A:2082:HOH:O	2.32	0.67
2:B:1539:HEM:HMC2	2:B:1539:HEM:HBC2	1.75	0.67
5:A:1554:EDO:H11	3:B:1546:ACT:CH3	2.28	0.64
1:A:208[A]:TRP:CZ3	1:A:211:LYS:HE2	2.33	0.63
3:A:1550:ACT:H3	8:A:2047:HOH:O	2.00	0.60
1:A:43:TRP:CZ3	1:A:45[A]:ARG:HG2	2.38	0.59
1:B:530:LEU:CA	3:B:1542:ACT:H3	2.32	0.58
1:A:211:LYS:HD3	1:A:219:ILE:HG13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194[A]:ASN:OD1	1:A:300:THR:CG2	2.52	0.57
1:B:119:LYS:NZ	3:B:1540:ACT:H2	2.21	0.56
1:A:403:THR:HA	1:A:406:LYS:HG2	1.88	0.56
1:A:125:ARG:HD2	1:A:129:ASP:OD2	2.07	0.55
1:A:150:THR:H	3:A:1550:ACT:CH3	2.15	0.55
3:B:1540:ACT:H3	8:B:2019:HOH:O	2.07	0.55
1:B:111:PHE:HB2	1:B:377:SER:HB3	1.89	0.54
1:A:196:ARG:HD3	1:B:466:SER:OG	2.08	0.53
1:A:196:ARG:NH2	8:A:2084:HOH:O	2.29	0.53
1:A:439:ARG:HH21	6:A:1557:PE4:C6	2.22	0.53
2:B:1539:HEM:HMB1	2:B:1539:HEM:HBB2	1.89	0.52
1:A:111:PHE:HB2	1:A:377:SER:HB3	1.92	0.51
1:B:119:LYS:CE	4:B:1543:PLP:C4A	2.81	0.51
2:A:1549:HEM:HBC2	2:A:1549:HEM:CMC	2.40	0.51
1:A:479:VAL:HG22	8:A:2162:HOH:O	2.12	0.49
1:A:119:LYS:HG3	3:A:1550:ACT:H2	1.94	0.49
1:B:453:GLY:HA3	1:B:518:GLN:OE1	2.13	0.48
1:B:262:THR:HG21	5:B:1544:EDO:H22	1.95	0.48
5:A:1554:EDO:C1	3:B:1546:ACT:CH3	2.91	0.48
1:A:194[A]:ASN:OD1	1:A:300:THR:HG22	2.12	0.48
1:A:403:THR:HA	1:A:406:LYS:CG	2.43	0.48
1:A:189:VAL:HG22	3:B:1546:ACT:H2	1.95	0.47
1:B:255:VAL:HG13	1:B:258:GLY:HA2	1.98	0.46
2:A:1549:HEM:HBB2	2:A:1549:HEM:HHC	1.97	0.46
1:A:435:ILE:HD12	1:A:465:LEU:HG	1.97	0.45
1:A:179:ASP:OD2	8:A:2074:HOH:O	2.21	0.45
1:B:79:ASP:OD2	1:B:161[B]:ARG:NH1	2.43	0.44
1:A:463:ASN:HB2	1:B:201:GLU:OE2	2.17	0.43
1:B:52:CYS:HA	2:B:1539:HEM:C1A	2.53	0.43
1:B:413:ARG:HD2	1:B:493:THR:O	2.19	0.43
1:A:399:GLU:HA	1:A:402:LEU:HB3	2.01	0.43
1:B:490:ILE:HD12	1:B:502:ILE:HD12	2.00	0.43
1:A:182:ARG:HD3	8:B:2096:HOH:O	2.19	0.42
1:A:451:GLU:H	1:A:451:GLU:CD	2.22	0.42
5:A:1554:EDO:O2	3:B:1542:ACT:CH3	2.59	0.42
1:B:150:THR:H	3:B:1540:ACT:CH3	2.22	0.42
1:A:436:GLU:HG2	6:A:1557:PE4:H31	2.00	0.42
1:B:43:TRP:N	1:B:208[B]:TRP:CZ2	2.88	0.42
1:A:482:VAL:O	1:A:482:VAL:HG12	2.20	0.42
1:A:241:LEU:HD13	1:A:271:LYS:HE3	2.02	0.42
2:B:1539:HEM:CMC	2:B:1539:HEM:HBC2	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:SER:HB2	1:A:306:ILE:HG21	2.02	0.41
1:B:248:LEU:HD13	1:B:371:VAL:HG23	2.01	0.41
1:A:149:ASN:ND2	4:A:1551:PLP:H2A1	2.36	0.41
1:B:149:ASN:ND2	4:B:1543:PLP:H2A1	2.37	0.40
5:A:1554:EDO:H11	3:B:1546:ACT:H1	2.01	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	494/563 (88%)	484 (98%)	10 (2%)	0	100	100
1	B	486/563 (86%)	475 (98%)	11 (2%)	0	100	100
All	All	980/1126 (87%)	959 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	412/476 (87%)	410 (100%)	2 (0%)	92	94
1	B	402/476 (84%)	400 (100%)	2 (0%)	92	94
All	All	814/952 (86%)	810 (100%)	4 (0%)	92	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	LEU
1	A	401	ASP
1	B	518	GLN
1	B	519	MET

Some 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	B	222	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 for Mogul analysis.

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	HEM	A	1549	1	30,50,50	2.12	7 (23%)	24,82,82	2.44	9 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	A	1550	-	1,3,3	4.17	1 (100%)	0,3,3	0.00	-
4	PLP	A	1551	1	15,15,16	2.51	4 (26%)	21,22,23	2.32	9 (42%)
5	EDO	A	1552	-	3,3,3	0.52	0	2,2,2	0.33	0
5	EDO	A	1553	-	3,3,3	0.38	0	2,2,2	0.23	0
5	EDO	A	1554	-	3,3,3	0.37	0	2,2,2	0.44	0
5	EDO	A	1555	-	3,3,3	0.37	0	2,2,2	0.48	0
5	EDO	A	1556	-	3,3,3	0.44	0	2,2,2	0.27	0
6	PE4	A	1557	-	6,6,23	0.79	0	5,5,22	0.61	0
5	EDO	A	1559	-	3,3,3	0.47	0	2,2,2	0.43	0
2	HEM	B	1539	1	30,50,50	2.18	7 (23%)	24,82,82	2.43	10 (41%)
3	ACT	B	1540	-	1,3,3	2.42	1 (100%)	0,3,3	0.00	-
3	ACT	B	1541	-	1,3,3	0.40	0	0,3,3	0.00	-
3	ACT	B	1542	-	1,3,3	0.68	0	0,3,3	0.00	-
4	PLP	B	1543	1	15,15,16	2.57	4 (26%)	21,22,23	2.44	10 (47%)
5	EDO	B	1544	-	3,3,3	0.48	0	2,2,2	0.26	0
3	ACT	B	1546	-	1,3,3	0.41	0	0,3,3	0.00	-

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	HEM	A	1549	1	-	0/10/54/54	0/0/8/8
3	ACT	A	1550	-	-	0/0/0/0	0/0/0/0
4	PLP	A	1551	1	-	0/6/6/8	0/1/1/1
5	EDO	A	1552	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1553	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1554	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1555	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1556	-	-	0/1/1/1	0/0/0/0
6	PE4	A	1557	-	-	0/4/4/21	0/0/0/0
5	EDO	A	1559	-	-	0/1/1/1	0/0/0/0
2	HEM	B	1539	1	-	0/10/54/54	0/0/8/8
3	ACT	B	1540	-	-	0/0/0/0	0/0/0/0
3	ACT	B	1541	-	-	0/0/0/0	0/0/0/0
3	ACT	B	1542	-	-	0/0/0/0	0/0/0/0
4	PLP	B	1543	1	-	0/6/6/8	0/1/1/1
5	EDO	B	1544	-	-	0/1/1/1	0/0/0/0
3	ACT	B	1546	-	-	0/0/0/0	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1539	HEM	C2D-C3D	-6.55	1.34	1.54
2	A	1549	HEM	C2D-C3D	-6.52	1.34	1.54
2	A	1549	HEM	C2C-C1C	-6.35	1.40	1.52
2	B	1539	HEM	C2C-C1C	-6.21	1.40	1.52
3	A	1550	ACT	CH3-C	-4.17	1.43	1.48
4	A	1551	PLP	C4A-C4	-4.09	1.43	1.51
4	B	1543	PLP	C4A-C4	-3.98	1.43	1.51
2	B	1539	HEM	C3D-C4D	-3.83	1.46	1.51
2	A	1549	HEM	C2B-C1B	-3.04	1.41	1.51
2	A	1549	HEM	C3D-C4D	-3.02	1.47	1.51
2	B	1539	HEM	C2B-C1B	-2.48	1.43	1.51
3	B	1540	ACT	CH3-C	-2.42	1.45	1.48
2	B	1539	HEM	C3B-C4B	-2.14	1.50	1.51
2	A	1549	HEM	C3B-CAB	-2.14	1.47	1.51
2	A	1549	HEM	FE-NB	2.22	2.09	1.97
2	A	1549	HEM	FE-NC	2.52	2.05	1.95
4	B	1543	PLP	C3-C4	2.72	1.46	1.40
2	B	1539	HEM	FE-NB	2.74	2.12	1.97
4	A	1551	PLP	C3-C4	3.13	1.47	1.40
4	A	1551	PLP	C5-C4	3.46	1.44	1.40
2	B	1539	HEM	FE-NC	3.49	2.09	1.95
4	B	1543	PLP	C5-C4	5.39	1.46	1.40
4	B	1543	PLP	C3-C2	6.14	1.45	1.40
4	A	1551	PLP	C3-C2	7.01	1.45	1.40

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1551	PLP	C4A-C4-C5	-4.50	116.19	120.88
4	B	1543	PLP	C6-C5-C4	-3.84	114.89	118.15
4	A	1551	PLP	C6-C5-C4	-3.65	115.06	118.15
2	B	1539	HEM	CAA-CBA-CGA	-3.59	106.17	112.75
2	B	1539	HEM	CBD-CAD-C3D	-3.26	104.07	113.55
2	A	1549	HEM	CBD-CAD-C3D	-3.22	104.18	113.55
2	A	1549	HEM	C3B-C4B-NB	-3.14	105.63	111.63
2	A	1549	HEM	C4B-CHC-C1C	-3.03	120.75	125.82
4	B	1543	PLP	C4-C3-C2	-2.94	115.04	120.05
4	B	1543	PLP	C4A-C4-C5	-2.81	117.95	120.88
4	A	1551	PLP	C3-C2-N1	-2.60	117.03	120.61
2	B	1539	HEM	C3B-C4B-NB	-2.22	107.39	111.63
4	A	1551	PLP	C4-C3-C2	-2.20	116.31	120.05
4	B	1543	PLP	O2P-P-O4P	-2.14	100.40	106.56
2	B	1539	HEM	CBA-CAA-C2A	2.13	116.36	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1543	PLP	O3P-P-O2P	2.33	116.26	107.38
2	B	1539	HEM	CMD-C2D-C3D	2.50	125.42	114.35
2	A	1549	HEM	C3B-C4B-CHC	2.66	126.90	123.16
4	B	1543	PLP	O2P-P-O1P	2.73	119.38	110.58
2	B	1539	HEM	C2D-C3D-C4D	2.74	106.14	101.50
4	A	1551	PLP	C5A-C5-C6	2.80	124.57	119.28
2	A	1549	HEM	CMB-C2B-C3B	2.80	123.53	116.53
2	A	1549	HEM	CMD-C2D-C3D	2.88	127.07	114.35
4	B	1543	PLP	C6-N1-C2	3.14	125.69	119.28
4	A	1551	PLP	C3-C4-C5	3.23	122.31	118.78
4	B	1543	PLP	O3-C3-C2	3.29	123.39	117.66
4	A	1551	PLP	O4P-C5A-C5	3.31	114.46	108.99
4	A	1551	PLP	O3-C3-C2	3.36	123.50	117.66
4	A	1551	PLP	C6-N1-C2	3.59	126.61	119.28
2	A	1549	HEM	CAD-C3D-C4D	3.68	125.44	112.47
2	B	1539	HEM	CAD-C3D-C4D	3.79	125.84	112.47
4	B	1543	PLP	C3-C4-C5	3.94	123.08	118.78
2	B	1539	HEM	CMB-C2B-C3B	4.31	127.30	116.53
2	B	1539	HEM	CMC-C2C-C3C	4.85	128.64	116.53
4	B	1543	PLP	O4P-C5A-C5	4.95	117.17	108.99
2	B	1539	HEM	CAD-C3D-C2D	5.13	127.96	113.22
2	A	1549	HEM	CMC-C2C-C3C	5.20	129.52	116.53
2	A	1549	HEM	CAD-C3D-C2D	5.84	130.02	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1549	HEM	3	0
3	A	1550	ACT	4	0
4	A	1551	PLP	1	0
5	A	1554	EDO	5	0
6	A	1557	PE4	2	0
2	B	1539	HEM	4	0
3	B	1540	ACT	4	0
3	B	1542	ACT	5	0
4	B	1543	PLP	3	0
5	B	1544	EDO	1	0
3	B	1546	ACT	4	0

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	493/563 (87%)	0.21	26 (5%)	30 32	24, 36, 64, 107	0
1	B	487/563 (86%)	0.30	34 (6%)	19 21	26, 45, 76, 126	0
All	All	980/1126 (87%)	0.26	60 (6%)	25 26	24, 40, 74, 126	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	ALA	8.4
1	B	70	PRO	8.2
1	B	60	ALA	5.9
1	B	69	ALA	5.8
1	B	61	SER	5.0
1	B	68	THR	4.3
1	A	548	ARG	4.1
1	B	515	GLN	4.1
1	B	297	GLU	3.9
1	B	72	LYS	3.9
1	A	403	THR	3.9
1	B	518	GLN	3.9
1	B	66	HIS	3.7
1	A	513	HIS	3.7
1	B	513	HIS	3.6
1	A	452	ALA	3.5
1	B	59	PRO	3.5
1	B	452	ALA	3.5
1	B	451	GLU	3.4
1	A	451	GLU	3.3
1	A	454	VAL	3.3
1	B	57	GLY	3.3
1	A	528	GLN	3.2
1	B	56	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	519	MET	3.1
1	A	297	GLU	3.1
1	A	514	GLU	3.0
1	A	529	MET	3.0
1	A	152	ILE	3.0
1	A	378	VAL	2.9
1	B	62	GLU	2.9
1	B	428	THR	2.9
1	B	514	GLU	2.8
1	A	453	GLY	2.8
1	B	453	GLY	2.7
1	B	363	GLU	2.7
1	B	44	ILE	2.7
1	B	450	ASP	2.6
1	A	381	TYR	2.6
1	A	401	ASP	2.6
1	A	379	ARG	2.5
1	A	208[A]	TRP	2.5
1	B	454	VAL	2.4
1	B	49	PRO	2.4
1	A	118	VAL	2.4
1	B	427	PRO	2.4
1	B	345	LEU	2.4
1	A	420	SER	2.4
1	B	67	HIS	2.3
1	B	382	MET	2.3
1	A	345	LEU	2.3
1	B	378	VAL	2.3
1	A	180	VAL	2.2
1	A	382	MET	2.1
1	B	208[A]	TRP	2.1
1	A	298	GLN	2.1
1	A	184	LEU	2.1
1	A	450	ASP	2.1
1	A	491	ARG	2.0
1	B	132	ARG	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 [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(\AA^2)	Q<0.9
5	EDO	A	1559	4/4	0.78	0.37	11.03	20,20,20,20	0
3	ACT	B	1546	4/4	0.86	0.37	10.12	42,64,65,67	0
3	ACT	B	1542	4/4	0.94	0.18	7.81	57,62,62,64	0
5	EDO	B	1544	4/4	0.93	0.19	5.79	51,53,53,57	0
7	NA	A	1558	1/1	0.99	0.33	5.74	28,28,28,28	0
7	NA	B	1545	1/1	0.99	0.27	5.27	34,34,34,34	0
6	PE4	A	1557	7/24	0.67	0.24	5.08	50,56,63,66	0
3	ACT	A	1550	4/4	0.91	0.27	4.46	24,28,29,42	0
5	EDO	A	1553	4/4	0.88	0.19	3.35	34,46,47,49	0
3	ACT	B	1541	4/4	0.90	0.16	3.14	52,53,55,56	0
5	EDO	A	1552	4/4	0.94	0.15	3.08	43,43,45,45	0
5	EDO	A	1554	4/4	0.94	0.15	2.69	44,45,47,47	0
3	ACT	B	1540	4/4	0.90	0.19	1.81	29,34,39,47	0
2	HEM	A	1549	43/43	0.96	0.13	0.90	26,33,46,60	0
2	HEM	B	1539	43/43	0.92	0.23	0.68	48,60,71,74	0
4	PLP	A	1551	15/16	0.99	0.17	-0.24	23,26,28,31	0
4	PLP	B	1543	15/16	0.98	0.13	-0.31	29,32,34,35	0
5	EDO	A	1556	4/4	0.93	0.17	-	41,45,47,47	0
5	EDO	A	1555	4/4	0.91	0.28	-	54,54,55,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.