WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:35 PM GMT

PDB ID : 4PCU

Title : Crystal structure of delta516-525 E201S human cystathionine beta-synthase with AdoMet

Authors : Ereno-Orbea, J.; Majtan, T.; Oyenarte, I.; Kraus, J.P.; Martinez-Cruz, L.A.

Deposited on : 2014-04-16
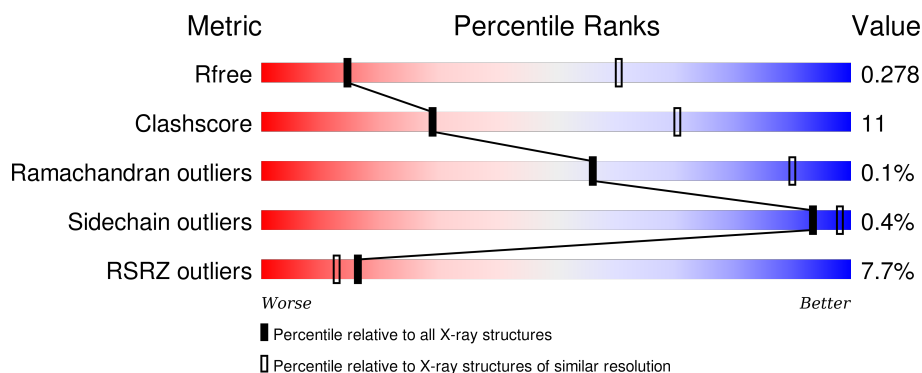
Resolution : 3.58 Å(reported)

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 3.58 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	Percentile Ranks	Value
Rfree		0.278
Clashscore		11
Ramachandran outliers		0.1%
Sidechain outliers		0.4%
RSRZ outliers		7.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1261 (3.76-3.40)
Clashscore	102246	1026 (3.72-3.44)
Ramachandran outliers	100387	1028 (3.74-3.42)
Sidechain outliers	100360	1028 (3.74-3.42)
RSRZ outliers	91569	1268 (3.76-3.40)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	549	4% — 71% — 17% — 11%
1	B	549	10% — 74% — 15% • 11%

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:

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SAM	A	603	-	-	-	X
4	SAM	B	603	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7565 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	486	Total 3681	C 2335	N 638	O 687	S 21	0	0	0
1	B	489	Total 3714	C 2352	N 644	O 697	S 21	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	PRO	conflict	UNP P35520
A	201	SER	GLU	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	conflict	UNP P35520
B	201	SER	GLU	engineered mutation	UNP P35520
B	?	-	ILE	deletion	UNP P35520
B	?	-	GLN	deletion	UNP P35520
B	?	-	TYR	deletion	UNP P35520

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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 PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
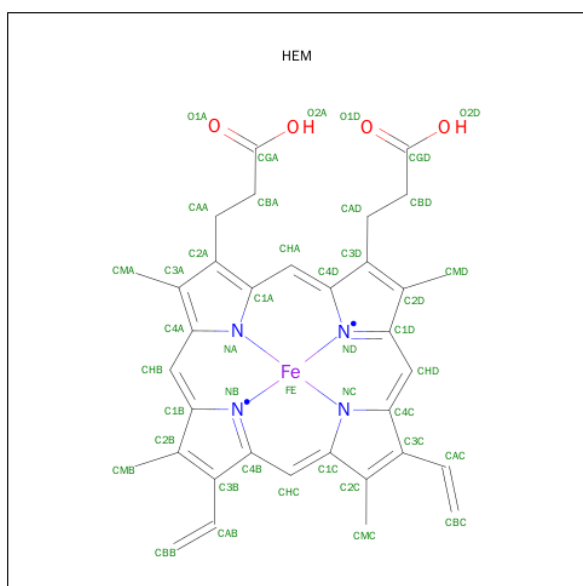
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).
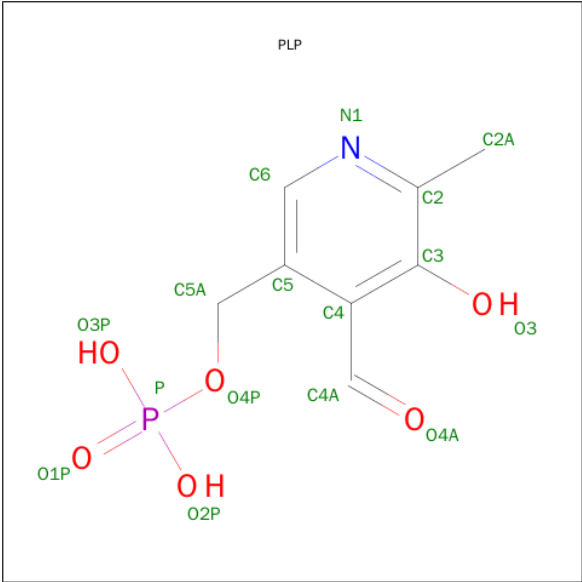
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).
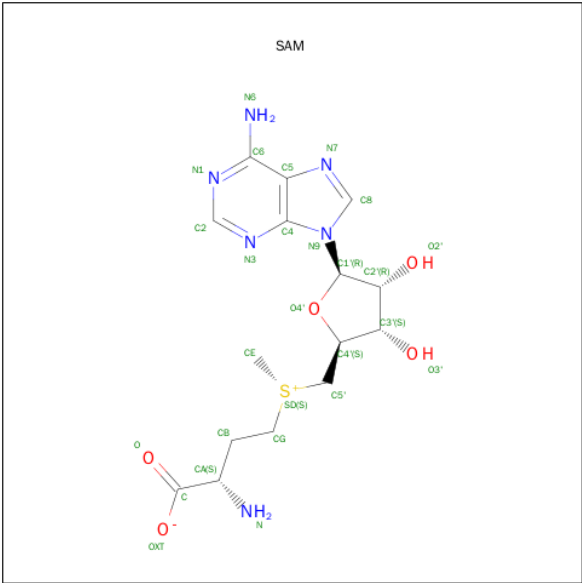
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

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 (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	141.35Å 141.35Å 108.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.80 – 3.58	Depositor
	46.27 – 3.58	EDS
% Data completeness	98.2 (40.80-3.58)	Depositor
(in resolution range)	98.5 (46.27-3.58)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.257 , 0.277	Depositor
	0.258 , 0.278	DCC
R_{free} test set	754 reflections (5.08%)	DCC
Wilson B-factor (Å²)	105.5	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.31 , 72.6	EDS
Estimated twinning fraction	0.057 for -h,-k,l	Xtriage
L-test for twinning [2]	$< |L| > = 0.44, < L^2 > = 0.27$	Xtriage
Outliers	0 of 14903 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	7565	wwPDB-VP
Average B, all atoms (Å²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: HEM, SAM, 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	0.35	1/3751 (0.0%)	0.58	5/5091 (0.1%)
1	B	0.32	0/3784	0.63	6/5135 (0.1%)
All	All	0.33	1/7535 (0.0%)	0.60	11/10226 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	408	TRP	C-N	11.12	1.59	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	428	THR	O-C-N	-19.05	92.21	122.70
1	B	428	THR	CA-C-N	14.19	148.41	117.20
1	A	399	GLU	N-CA-C	9.98	137.95	111.00
1	B	428	THR	C-N-CA	7.49	140.42	121.70
1	A	492	LEU	CA-CB-CG	7.38	132.28	115.30
1	A	510	LEU	CA-CB-CG	7.20	131.85	115.30
1	B	445	GLN	N-CA-C	6.74	129.19	111.00
1	B	307	GLY	N-CA-C	5.79	127.58	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	546	GLN	O-C-N	-5.40	114.06	122.70
1	A	456	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	490	ILE	C-N-CA	5.07	134.38	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	408	TRP	Mainchain
1	B	446	ALA	Peptide
1	B	546	GLN	Mainchain

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	3681	0	3659	100	1
1	B	3714	0	3700	82	3
2	A	43	0	30	4	0
2	B	43	0	30	4	0
3	A	15	0	7	1	0
3	B	15	0	6	0	0
4	A	27	0	22	4	0
4	B	27	0	22	5	0
All	All	7565	0	7476	172	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (172) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ILE:O	1:A:439:ARG:HG3	1.22	1.32
1:A:425:VAL:HG22	1:A:447:PRO:O	1.34	1.25
1:B:513:HIS:HD2	1:B:529:MET:HB3	1.06	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:GLN:HB3	1:A:492:LEU:CD1	1.80	1.09
1:A:414:VAL:HG13	1:A:417:LEU:HD12	1.20	1.08
1:B:513:HIS:CD2	1:B:529:MET:HB3	1.94	1.02
1:A:415:GLN:HB3	1:A:492:LEU:HD12	1.40	1.01
1:B:513:HIS:HD2	1:B:529:MET:CB	1.76	0.97
1:B:445:GLN:NE2	4:B:603:SAM:N7	2.21	0.88
1:B:427:PRO:CD	1:B:428:THR:H	1.87	0.87
1:A:504:GLU:OE2	1:B:469:LEU:HD12	1.75	0.85
1:A:540:LEU:HB3	1:B:435:ILE:HD13	1.60	0.83
1:B:427:PRO:HD2	1:B:428:THR:H	1.42	0.82
1:A:537:ILE:CD1	1:B:435:ILE:HG23	2.10	0.82
1:A:426:LEU:O	1:A:429:ILE:HG12	1.80	0.82
1:A:435:ILE:O	1:A:439:ARG:CG	2.19	0.81
1:A:504:GLU:OE2	1:B:469:LEU:CD1	2.29	0.81
1:A:146:THR:HG21	1:A:150:THR:HB	1.62	0.79
1:A:425:VAL:CG2	1:A:447:PRO:O	2.27	0.78
1:A:406:LYS:CB	1:A:407:PRO:HD2	2.15	0.77
1:A:415:GLN:HB3	1:A:492:LEU:HD11	1.63	0.76
1:A:491:ARG:NH1	1:A:493:THR:OG1	2.20	0.74
1:A:414:VAL:HG13	1:A:417:LEU:CD1	2.10	0.73
1:A:415:GLN:CB	1:A:492:LEU:CD1	2.64	0.72
1:B:425:VAL:HG13	1:B:446:ALA:HB2	1.72	0.72
1:A:436:GLU:HA	1:A:439:ARG:HD3	1.72	0.71
1:A:434:THR:HG22	1:A:438:LEU:HD12	1.71	0.71
1:A:537:ILE:HD11	1:B:435:ILE:HG23	1.74	0.70
1:A:406:LYS:CB	1:A:407:PRO:CD	2.70	0.70
1:A:415:GLN:CB	1:A:492:LEU:HD12	2.19	0.69
1:A:393:GLN:OE1	1:A:501:HIS:O	2.10	0.69
1:B:427:PRO:CD	1:B:428:THR:N	2.57	0.66
1:B:491:ARG:HA	1:B:511:VAL:HA	1.77	0.66
1:B:513:HIS:O	1:B:526:GLN:N	2.29	0.66
1:B:410:TRP:HD1	1:B:411:HIS:HD2	1.43	0.66
1:B:490:ILE:HB	1:B:494:ASP:OD2	1.96	0.66
1:A:425:VAL:HG23	1:A:448:VAL:HA	1.79	0.64
1:A:393:GLN:NE2	1:A:504:GLU:OE1	2.22	0.64
2:B:601:HEM:HBB2	2:B:601:HEM:HMB1	1.80	0.63
1:A:502:ILE:HG21	1:A:509:ALA:HB2	1.80	0.62
1:B:145:PRO:HB3	1:B:204:VAL:HA	1.82	0.62
1:A:431:CYS:HB3	1:A:464:MET:HE1	1.83	0.61
1:A:537:ILE:HD12	1:B:435:ILE:HG23	1.79	0.61
1:B:447:PRO:HA	1:B:458:MET:HG2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:ARG:O	1:A:393:GLN:HG2	2.01	0.60
1:A:415:GLN:CB	1:A:492:LEU:HD11	2.27	0.59
1:B:427:PRO:CG	1:B:428:THR:N	2.66	0.59
1:B:426:LEU:HB3	1:B:427:PRO:HD2	1.84	0.59
1:A:474:GLN:N	1:A:477:ASP:OD2	2.36	0.58
1:A:512:VAL:HG12	1:A:530:VAL:HA	1.84	0.58
1:B:450:ASP:HB3	1:B:456:LEU:HD21	1.85	0.58
1:B:513:HIS:CD2	1:B:529:MET:CB	2.69	0.57
1:A:436:GLU:HA	1:A:439:ARG:CD	2.34	0.57
1:A:436:GLU:O	1:A:439:ARG:HB2	2.04	0.57
1:B:490:ILE:HG12	1:B:509:ALA:HB1	1.85	0.57
2:A:601:HEM:HMB1	2:A:601:HEM:HBB2	1.87	0.57
1:A:254:SER:HA	1:A:280:VAL:HB	1.86	0.57
1:B:427:PRO:CG	1:B:428:THR:H	2.18	0.57
1:A:408:TRP:CZ3	1:A:409:TRP:HB3	2.39	0.56
1:B:148:GLY:HA3	1:B:177:LYS:HD3	1.86	0.56
1:B:254:SER:HA	1:B:280:VAL:HB	1.87	0.56
1:B:490:ILE:HD13	1:B:502:ILE:HD12	1.88	0.56
2:B:601:HEM:HBC2	2:B:601:HEM:HMC1	1.88	0.55
1:A:445:GLN:NE2	4:A:603:SAM:O	2.31	0.55
4:A:603:SAM:H5'2	4:A:603:SAM:OXT	2.07	0.55
1:A:540:LEU:HD13	1:B:435:ILE:HD13	1.89	0.55
1:A:474:GLN:HG3	1:A:477:ASP:OD2	2.07	0.54
1:A:429:ILE:CG1	1:A:479:VAL:HG11	2.37	0.54
1:B:435:ILE:HD11	1:B:464:MET:HG2	1.91	0.53
1:A:438:LEU:HD21	1:A:446:ALA:HB2	1.90	0.53
1:A:540:LEU:CB	1:B:435:ILE:HD13	2.37	0.52
1:B:507:HIS:HB2	1:B:508:PHE:HD2	1.74	0.52
1:A:74:PRO:HG2	1:A:77:LEU:HD23	1.90	0.52
1:A:52:CYS:HA	2:A:601:HEM:C1A	2.45	0.52
1:A:413:ARG:HD3	1:A:493:THR:O	2.10	0.52
1:B:267:LYS:HD2	1:B:271:LYS:HE2	1.92	0.52
1:B:427:PRO:HG2	1:B:428:THR:HG23	1.91	0.52
1:A:393:GLN:OE1	1:A:504:GLU:HB2	2.11	0.51
1:B:285:SER:OG	1:B:307:GLY:O	2.16	0.51
1:A:350:ALA:HB1	1:A:374:LEU:HD22	1.93	0.51
1:B:125:ARG:HG3	1:B:227:SER:HB3	1.92	0.50
1:B:74:PRO:HG2	1:B:77:LEU:HD23	1.92	0.50
1:B:410:TRP:CD1	1:B:411:HIS:HD2	2.25	0.50
1:A:287:LEU:HD12	1:A:307:GLY:HA2	1.92	0.50
1:B:448:VAL:O	1:B:456:LEU:N	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:GLU:O	1:B:440:GLU:HG3	2.12	0.50
1:A:414:VAL:HG12	1:A:414:VAL:O	2.11	0.50
2:A:601:HEM:HMC1	2:A:601:HEM:HBC2	1.91	0.50
1:A:267:LYS:HD2	1:A:271:LYS:HE2	1.93	0.50
1:B:435:ILE:O	1:B:435:ILE:HG22	2.12	0.50
1:B:510:LEU:HD11	1:B:530:VAL:HG12	1.93	0.50
1:B:350:ALA:HB1	1:B:374:LEU:HD22	1.93	0.49
1:B:502:ILE:O	1:B:506:ASP:N	2.33	0.49
1:B:410:TRP:CE2	1:B:497:GLY:HA3	2.47	0.49
1:A:475:PRO:HG2	1:B:547:GLU:HB2	1.95	0.49
1:A:414:VAL:HG22	1:A:499:LEU:HD22	1.94	0.49
1:B:489:GLN:HG3	1:B:489:GLN:O	2.13	0.49
1:A:394:LYS:HB3	1:A:396:PHE:CE2	2.48	0.49
4:B:603:SAM:H8	4:B:603:SAM:O	2.13	0.48
1:A:427:PRO:HD3	1:A:449:VAL:O	2.14	0.48
1:A:394:LYS:CB	1:A:396:PHE:CE2	2.97	0.48
1:B:46:PRO:HG3	1:B:197:PHE:HZ	1.77	0.48
1:A:490:ILE:HD13	1:A:499:LEU:HB2	1.94	0.48
1:A:530:VAL:HG12	1:A:531:PHE:N	2.29	0.48
1:A:490:ILE:HG21	1:A:499:LEU:HD13	1.96	0.47
1:B:413:ARG:HB2	1:B:415:GLN:HG2	1.95	0.47
1:B:535:THR:HG21	4:B:603:SAM:O	2.15	0.47
1:A:511:VAL:O	1:A:531:PHE:N	2.46	0.47
1:A:443:PHE:HD1	4:A:603:SAM:SD	2.38	0.46
1:A:463:ASN:HD22	1:A:484:TYR:HB2	1.79	0.46
1:A:540:LEU:HD13	1:B:435:ILE:CD1	2.45	0.46
4:B:603:SAM:H5'2	4:B:603:SAM:O	2.16	0.46
1:A:537:ILE:HD12	1:B:435:ILE:CG2	2.46	0.46
1:B:479:VAL:O	1:B:482:VAL:HG22	2.16	0.46
1:B:52:CYS:HA	2:B:601:HEM:C1A	2.51	0.46
1:A:448:VAL:HG11	1:A:483:ILE:HG12	1.98	0.45
1:A:378:VAL:HG21	1:A:386:LEU:HD13	1.99	0.45
1:B:446:ALA:HB3	1:B:459:VAL:HG12	1.98	0.45
1:B:450:ASP:OD2	1:B:454:VAL:HB	2.17	0.45
1:A:503:LEU:HD13	1:A:536:ALA:HA	1.99	0.45
1:A:425:VAL:CG2	1:A:448:VAL:HA	2.44	0.45
1:A:504:GLU:OE2	1:B:469:LEU:HD13	2.14	0.45
1:A:537:ILE:CD1	1:B:435:ILE:CG2	2.90	0.45
1:A:125:ARG:HG3	1:A:227:SER:HB3	1.98	0.45
1:B:111:PHE:HB2	1:B:377:SER:HB3	1.99	0.45
1:A:469:LEU:HD12	1:B:504:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ILE:HG22	1:A:509:ALA:CB	2.47	0.45
1:A:427:PRO:HD3	1:A:450:ASP:HA	1.99	0.44
1:A:196:ARG:HB3	1:A:199:SER:HB2	1.97	0.44
1:A:426:LEU:HB2	1:A:429:ILE:HG23	1.99	0.44
1:B:425:VAL:CG1	1:B:446:ALA:HB2	2.45	0.44
1:A:255:VAL:HG21	1:A:323:TRP:CZ3	2.53	0.44
4:A:603:SAM:H8	4:A:603:SAM:OXT	2.16	0.44
1:B:427:PRO:HG2	1:B:428:THR:N	2.32	0.44
1:B:310:PHE:O	1:B:312:PRO:HD3	2.18	0.44
1:B:378:VAL:HG21	1:B:386:LEU:HD13	1.99	0.44
1:A:434:THR:HG22	1:A:438:LEU:CD1	2.43	0.43
1:A:540:LEU:HB3	1:B:435:ILE:HG21	1.99	0.43
1:A:111:PHE:HB2	1:A:377:SER:HB3	2.00	0.43
1:A:126:MET:HG2	1:A:227:SER:HB2	2.00	0.43
1:B:445:GLN:HG2	4:B:603:SAM:HN61	1.84	0.43
1:B:168:VAL:HG11	1:B:206:VAL:HG13	2.00	0.43
1:B:374:LEU:HA	1:B:375:PRO:HD3	1.88	0.43
1:A:256:GLY:HA3	3:A:602:PLP:H5A1	2.01	0.43
1:A:419:LEU:HD12	1:A:511:VAL:HG21	2.00	0.42
1:B:287:LEU:HD12	1:B:307:GLY:HA2	2.01	0.42
1:A:425:VAL:HB	1:A:429:ILE:CD1	2.49	0.42
1:A:491:ARG:HG2	1:A:491:ARG:HH11	1.84	0.42
1:B:492:LEU:N	1:B:511:VAL:HG13	2.33	0.42
1:B:422:PRO:HD3	1:B:532:GLY:HA2	2.01	0.42
1:A:309:ASP:OD1	1:A:309:ASP:N	2.52	0.42
1:B:464:MET:HE1	1:B:479:VAL:HG23	2.00	0.42
1:B:229:PRO:HB2	2:B:601:HEM:HBC1	2.02	0.42
1:A:48:ALA:HB3	1:A:224:ARG:NH1	2.35	0.42
1:A:464:MET:HB3	1:A:464:MET:HE2	1.91	0.41
1:A:90:VAL:HG22	1:B:77:LEU:HD12	2.01	0.41
1:B:168:VAL:HG11	1:B:206:VAL:CG1	2.50	0.41
1:A:441:LYS:HB3	1:A:441:LYS:HE3	1.86	0.41
1:B:423:LEU:C	1:B:423:LEU:HD23	2.40	0.41
1:A:425:VAL:HB	1:A:429:ILE:HD11	2.01	0.41
1:A:414:VAL:HA	1:A:417:LEU:HG	2.03	0.41
1:A:159:ALA:HB1	1:B:340:ALA:O	2.20	0.41
1:A:429:ILE:HG12	1:A:479:VAL:HG11	2.03	0.41
1:A:463:ASN:ND2	1:A:484:TYR:HB2	2.36	0.41
1:A:252:VAL:HG22	1:A:278:ILE:HB	2.03	0.41
1:A:414:VAL:CG1	1:A:414:VAL:O	2.70	0.40
1:B:426:LEU:HB3	1:B:427:PRO:CD	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:GLU:HA	1:B:145:PRO:HD3	1.80	0.40
1:B:46:PRO:HG3	1:B:197:PHE:CZ	2.56	0.40
1:A:54:TRP:HB2	2:A:601:HEM:C4B	2.55	0.40
1:A:540:LEU:HD22	1:B:435:ILE:CD1	2.51	0.40
1:A:199:SER:HB3	1:A:202:SER:HB3	2.03	0.40

All (3) 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:B:416:GLU:OE1	1:B:416:GLU:OE1[6_555]	1.60	0.60
1:A:416:GLU:OE2	1:B:209:ARG:NE[5_554]	1.93	0.27
1:B:416:GLU:CD	1:B:416:GLU:OE1[6_555]	2.18	0.02

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	478/549 (87%)	460 (96%)	18 (4%)	0	100	100
1	B	483/549 (88%)	467 (97%)	15 (3%)	1 (0%)	52	87
All	All	961/1098 (88%)	927 (96%)	33 (3%)	1 (0%)	56	90

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	309	ASP

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	389/463 (84%)	388 (100%)	1 (0%)	94	99
1	B	396/463 (86%)	394 (100%)	2 (0%)	92	97
All	All	785/926 (85%)	782 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	397	LEU
1	B	248	LEU
1	B	477	ASP

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

Mol	Chain	Res	Type
1	B	411	HIS
1	B	445	GLN
1	B	474	GLN
1	B	513	HIS

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)

6 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	HEM	A	601	1	30,50,50	2.19	5 (16%)	24,82,82	2.39	7 (29%)
3	PLP	A	602	1	15,15,16	0.90	0	21,22,23	1.39	3 (14%)
4	SAM	A	603	-	21,29,29	1.38	4 (19%)	17,42,42	2.81	6 (35%)
2	HEM	B	601	1	30,50,50	2.20	7 (23%)	24,82,82	2.36	9 (37%)
3	PLP	B	602	-	15,15,16	0.98	1 (6%)	21,22,23	1.42	2 (9%)
4	SAM	B	603	-	21,29,29	1.67	4 (19%)	17,42,42	2.88	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	HEM	A	601	1	-	0/10/54/54	0/0/8/8
3	PLP	A	602	1	-	0/6/6/8	0/1/1/1
4	SAM	A	603	-	-	0/8/33/33	0/3/3/3
2	HEM	B	601	1	-	0/10/54/54	0/0/8/8
3	PLP	B	602	-	-	0/6/6/8	0/1/1/1
4	SAM	B	603	-	-	0/8/33/33	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEM	C3B-C4B	-7.22	1.45	1.51
2	A	601	HEM	C3B-C4B	-6.74	1.45	1.51
2	A	601	HEM	C3D-C4D	-6.18	1.43	1.51
2	B	601	HEM	C3D-C4D	-6.15	1.43	1.51
4	B	603	SAM	CG-SD	-5.77	1.68	1.80
2	A	601	HEM	C2C-C1C	-3.96	1.45	1.52
2	B	601	HEM	C2C-C1C	-3.87	1.45	1.52
4	A	603	SAM	CG-SD	-2.91	1.74	1.80
2	A	601	HEM	C2D-C1D	-2.35	1.44	1.51
2	B	601	HEM	C2D-C1D	-2.17	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	PLP	C3-C2	-2.13	1.39	1.40
4	A	603	SAM	C2'-C3'	-2.12	1.47	1.53
2	B	601	HEM	C2B-C1B	-2.12	1.44	1.51
2	B	601	HEM	C3B-CAB	2.04	1.55	1.51
2	B	601	HEM	C3C-CAC	2.07	1.55	1.51
4	A	603	SAM	C4-N3	2.11	1.38	1.35
4	B	603	SAM	CG-CB	2.18	1.55	1.52
4	B	603	SAM	C5-C4	2.19	1.45	1.40
2	A	601	HEM	C3B-CAB	2.38	1.55	1.51
4	B	603	SAM	O4'-C1'	2.82	1.44	1.41
4	A	603	SAM	C2-N3	3.14	1.37	1.32

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	603	SAM	N3-C2-N1	-10.37	120.95	128.89
4	A	603	SAM	N3-C2-N1	-9.36	121.72	128.89
4	B	603	SAM	C1'-N9-C4	-3.39	121.83	126.94
2	A	601	HEM	CAA-CBA-CGA	-3.14	107.00	112.75
4	A	603	SAM	C1'-N9-C4	-3.07	122.31	126.94
4	B	603	SAM	C4-C5-N7	-2.78	106.92	109.48
2	B	601	HEM	CAA-CBA-CGA	-2.73	107.75	112.75
2	B	601	HEM	CMA-C3A-C4A	-2.05	124.98	128.36
3	A	602	PLP	C4A-C4-C3	-2.02	116.70	120.36
2	B	601	HEM	C3B-C4B-CHC	2.05	126.05	123.16
2	A	601	HEM	C2D-C3D-C4D	2.21	105.24	101.50
2	B	601	HEM	C2D-C3D-C4D	2.25	105.31	101.50
4	A	603	SAM	N6-C6-N1	2.28	124.10	119.20
3	A	602	PLP	C6-C5-C4	2.37	120.15	118.15
4	A	603	SAM	C2-N1-C6	2.39	123.04	118.77
3	B	602	PLP	C6-C5-C4	2.64	120.38	118.15
2	B	601	HEM	CMD-C2D-C3D	2.70	126.27	114.35
4	A	603	SAM	O4'-C1'-N9	2.78	113.91	108.10
2	A	601	HEM	CMD-C2D-C3D	2.83	126.89	114.35
4	A	603	SAM	C4'-O4'-C1'	3.44	113.50	109.72
3	A	602	PLP	C4A-C4-C5	3.98	125.03	120.88
3	B	602	PLP	C4A-C4-C5	4.18	125.24	120.88
2	B	601	HEM	CAD-C3D-C4D	4.31	127.67	112.47
2	A	601	HEM	CAD-C3D-C4D	4.48	128.26	112.47
2	A	601	HEM	CAD-C3D-C2D	4.62	126.49	113.22
2	B	601	HEM	CAD-C3D-C2D	4.80	127.02	113.22
2	A	601	HEM	CMB-C2B-C3B	5.02	129.06	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	HEM	CMB-C2B-C3B	5.06	129.15	116.53
2	B	601	HEM	CMC-C2C-C3C	5.17	129.45	116.53
2	A	601	HEM	CMC-C2C-C3C	5.37	129.93	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	4	0
3	A	602	PLP	1	0
4	A	603	SAM	4	0
2	B	601	HEM	4	0
4	B	603	SAM	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	515:GLN	C	526:GLN	N	2.96

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	486/549 (88%)	0.33	22 (4%)	37	29	74, 95, 187, 212	0
1	B	489/549 (89%)	0.55	53 (10%)	8	7	74, 94, 222, 247	0
All	All	975/1098 (88%)	0.44	75 (7%)	16	13	74, 95, 211, 247	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	532	GLY	7.7
1	B	401	ASP	7.6
1	B	511	VAL	7.5
1	B	455	ILE	6.9
1	B	299	THR	5.8
1	B	528	GLN	5.8
1	B	416	GLU	5.6
1	B	546	GLN	5.4
1	A	475	PRO	4.9
1	B	530	VAL	4.4
1	B	547	GLU	4.3
1	B	480	GLY	4.3
1	B	482	VAL	4.2
1	A	426	LEU	4.0
1	B	421	ALA	4.0
1	A	442	GLY	3.8
1	A	422	PRO	3.8
1	B	423	LEU	3.7
1	B	531	PHE	3.7
1	B	422	PRO	3.7
1	B	447	PRO	3.6
1	A	528	GLN	3.3
1	B	411	HIS	3.3
1	B	512	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	477	ASP	3.1
1	B	419	LEU	3.1
1	B	438	LEU	3.0
1	A	474	GLN	3.0
1	B	425	VAL	3.0
1	B	435	ILE	3.0
1	B	527	ARG	3.0
1	B	491	ARG	3.0
1	B	539	LEU	3.0
1	A	203	HIS	2.9
1	B	439	ARG	2.9
1	B	424	THR	2.9
1	B	448	VAL	2.9
1	B	454	VAL	2.9
1	B	515	GLN	2.9
1	B	542	PHE	2.8
1	A	366	GLU	2.8
1	B	479	VAL	2.8
1	B	417	LEU	2.8
1	B	481	LYS	2.7
1	B	513	HIS	2.7
1	B	529	MET	2.7
1	B	457	GLY	2.7
1	B	453	GLY	2.7
1	B	540	LEU	2.6
1	A	438	LEU	2.6
1	B	477	ASP	2.6
1	A	513	HIS	2.6
1	B	420	SER	2.5
1	B	445	GLN	2.5
1	A	418	GLY	2.5
1	A	443	PHE	2.5
1	A	427	PRO	2.4
1	B	478	GLN	2.4
1	B	456	LEU	2.4
1	B	298	GLN	2.4
1	B	476	SER	2.3
1	B	461	LEU	2.3
1	A	478	GLN	2.3
1	A	470	ALA	2.3
1	B	449	VAL	2.3
1	B	428	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	425	VAL	2.2
1	A	451	GLU	2.2
1	B	475	PRO	2.2
1	A	531	PHE	2.1
1	A	73	SER	2.1
1	A	479	VAL	2.1
1	B	427	PRO	2.1
1	B	526	GLN	2.1
1	A	85	GLY	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
4	SAM	A	603	27/27	0.79	0.84	2.27	170,175,180,184	0
2	HEM	A	601	43/43	0.95	0.40	1.79	81,90,97,99	0
2	HEM	B	601	43/43	0.96	0.37	1.52	80,88,95,98	0
3	PLP	A	602	15/16	0.92	0.29	-0.21	82,83,84,84	0
4	SAM	B	603	27/27	0.68	0.43	-0.73	184,200,210,218	0
3	PLP	B	602	15/16	0.92	0.25	-0.74	87,88,90,91	0

6.5 Other polymers (i)

There are no such residues in this entry.