



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:18 PM UTC

PDB ID : 2YXD / pdb_00002yxd
Title : Crystal Structure of Cobalamin biosynthesis precorrin 8W decarboxylase (cbiT)
Authors : Padmanabhan, B.; Bessho, Y.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-04-26
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

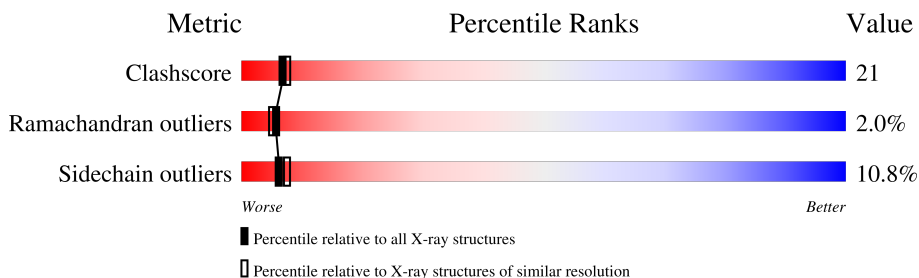
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	183	
1	B	183	

2 Entry composition [i](#)

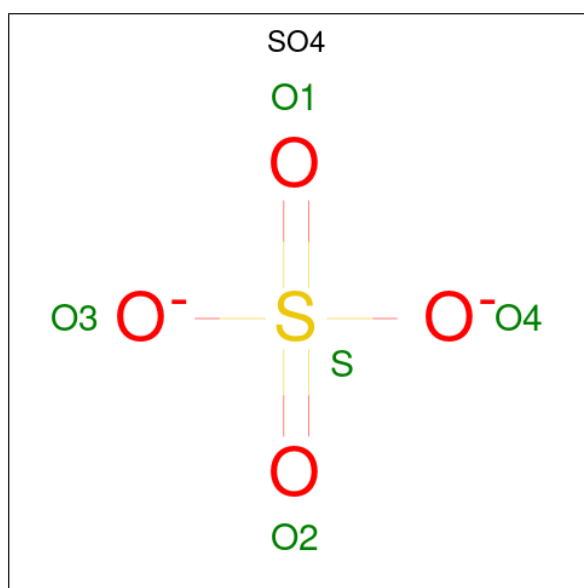
There are 4 unique types of molecules in this entry. The entry contains 2893 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Probable cobalt-precorrin-6Y C(15)-methyltransferase [decarboxylating].

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	Se	0	0	0
			1378	881	235	257	3	2			
1	B	180	Total	C	N	O	S	Se	0	0	0
			1385	886	235	259	3	2			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is water.

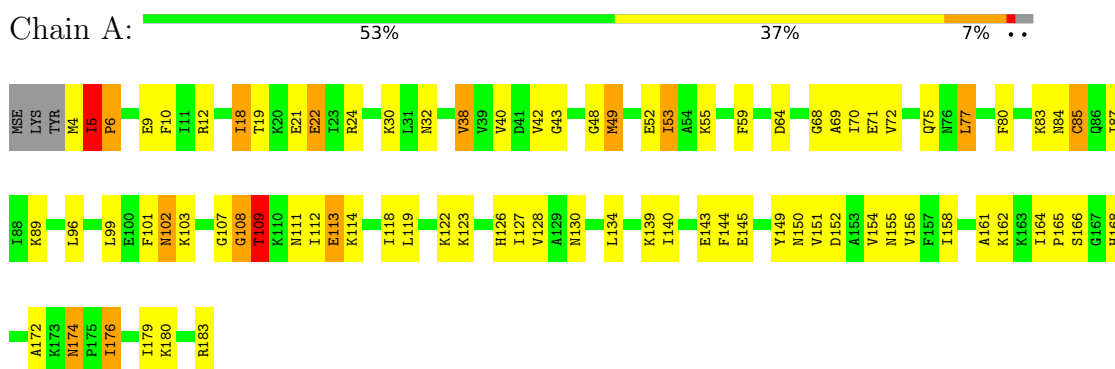
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total	O	0	0
			61	61		
4	B	47	Total	O	0	0
			47	47		

3 Residue-property plots

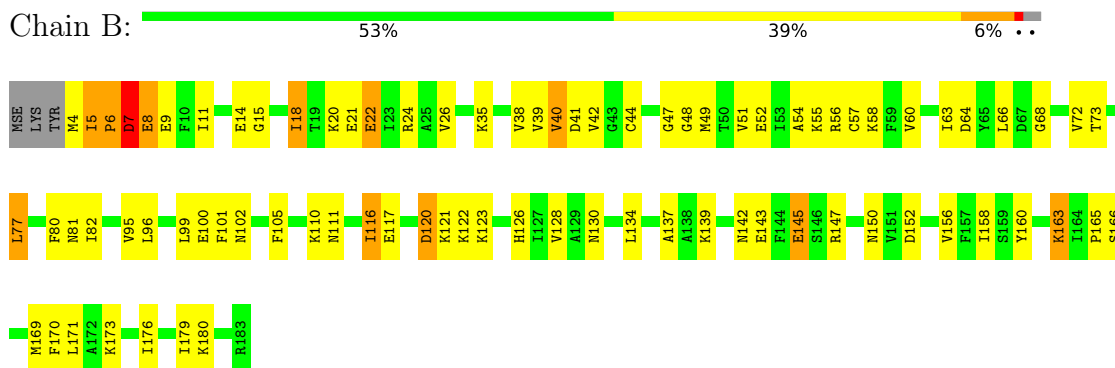
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

- Molecule 1: Probable cobalt-precorrin-6Y C(15)-methyltransferase [decarboxylating]



- Molecule 1: Probable cobalt-precorrin-6Y C(15)-methyltransferase [decarboxylating]



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	93.44Å 93.44Å 81.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	94.2 (20.00-2.30)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2893	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MES, SO4

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	1.66	11/1392 (0.8%)	1.47	12/1870 (0.6%)
1	B	1.72	13/1399 (0.9%)	1.50	14/1879 (0.7%)
All	All	1.69	24/2791 (0.9%)	1.49	26/3749 (0.7%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	ILE	CA-C	10.71	1.64	1.52
1	B	145	GLU	CB-CG	10.30	1.83	1.52
1	A	5	ILE	CA-CB	9.08	1.65	1.54
1	B	145	GLU	CD-OE2	8.98	1.42	1.25
1	B	150	ASN	N-CA	-6.97	1.37	1.46
1	B	5	ILE	CA-CB	6.96	1.63	1.54
1	B	145	GLU	CA-C	6.92	1.61	1.52
1	A	12	ARG	CA-CB	6.34	1.63	1.53
1	A	109	THR	CA-C	6.14	1.60	1.52
1	B	145	GLU	CA-CB	5.92	1.62	1.53
1	B	145	GLU	N-CA	5.83	1.53	1.46
1	A	156	VAL	CA-CB	5.74	1.61	1.54
1	B	142	ASN	C-O	-5.66	1.17	1.24
1	A	176	ILE	C-O	-5.57	1.18	1.24
1	A	69	ALA	C-O	5.35	1.30	1.24
1	A	38	VAL	CA-CB	5.35	1.60	1.54
1	B	156	VAL	CA-CB	5.33	1.60	1.54
1	B	18	ILE	CA-CB	5.29	1.61	1.54
1	B	170	PHE	C-O	-5.27	1.17	1.24
1	A	145	GLU	C-O	-5.22	1.18	1.24
1	B	24	ARG	C-O	5.13	1.30	1.24
1	A	172	ALA	CA-CB	-5.08	1.44	1.53
1	B	116	ILE	CA-CB	5.03	1.60	1.54
1	A	49	MSE	C-O	-5.01	1.18	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	GLU	CG-CD-OE1	-8.96	97.80	118.40
1	A	109	THR	N-CA-C	8.95	129.86	110.80
1	B	145	GLU	N-CA-C	-8.80	101.69	111.28
1	B	145	GLU	CG-CD-OE2	7.73	136.19	118.40
1	A	174	ASN	N-CA-C	7.64	126.69	109.81
1	B	110	LYS	N-CA-C	-6.62	101.62	110.55
1	A	149	TYR	CA-C-N	-6.45	113.59	122.30
1	A	149	TYR	C-N-CA	-6.45	113.59	122.30
1	A	151	VAL	N-CA-C	6.18	117.19	108.36
1	A	112	ILE	N-CA-C	-6.15	103.40	111.09
1	A	5	ILE	CA-C-N	6.04	127.39	119.84
1	A	5	ILE	C-N-CA	6.04	127.39	119.84
1	B	111	ASN	N-CA-C	5.97	119.47	111.24
1	B	39	VAL	N-CA-C	5.94	116.48	108.17
1	B	126	HIS	N-CA-C	5.75	117.50	107.49
1	B	145	GLU	CA-CB-CG	5.53	125.16	114.10
1	B	40	VAL	CB-CA-C	-5.44	103.76	111.21
1	B	137	ALA	N-CA-C	-5.43	105.36	111.28
1	B	6	PRO	N-CA-C	5.26	119.47	111.15
1	A	85	CYS	N-CA-C	5.19	117.87	108.69
1	B	120	ASP	CA-C-N	5.18	127.47	120.38
1	B	120	ASP	C-N-CA	5.18	127.47	120.38
1	A	53	ILE	N-CA-C	-5.14	105.39	111.00
1	A	155	ASN	N-CA-C	-5.12	100.90	109.24
1	B	42	VAL	CB-CA-C	-5.04	104.07	110.98
1	A	64	ASP	N-CA-C	-5.02	100.53	109.06

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	1378	0	1421	63	0
1	B	1385	0	1434	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	B	12	0	12	0	0
4	A	61	0	0	3	0
4	B	47	0	0	3	0
All	All	2893	0	2867	121	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 21.

All (121) 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:145:GLU:CB	1:B:145:GLU:CG	1.83	1.57
1:B:169:MSE:HE2	1:B:171:LEU:CD1	1.75	1.16
1:B:169:MSE:HE2	1:B:171:LEU:HD12	1.05	1.04
1:B:169:MSE:CE	1:B:171:LEU:HD12	1.96	0.91
1:A:38:VAL:H	1:A:102:ASN:HD21	1.14	0.87
1:B:6:PRO:HD2	1:B:52:GLU:OE2	1.77	0.84
1:A:154:VAL:HG12	1:B:160:TYR:CD1	2.16	0.80
1:A:38:VAL:H	1:A:102:ASN:ND2	1.82	0.78
1:B:160:TYR:HE2	1:B:173:LYS:HG3	1.50	0.76
1:B:20:LYS:HD2	1:B:160:TYR:OH	1.87	0.74
1:A:24:ARG:HB3	1:A:49:MSE:HE1	1.69	0.73
1:B:121:LYS:O	1:B:123:LYS:HD2	1.90	0.72
1:B:38:VAL:H	1:B:102:ASN:HD21	1.37	0.71
1:A:70:ILE:CD1	1:A:89:LYS:HG3	2.21	0.70
1:A:102:ASN:HD22	1:A:102:ASN:H	1.41	0.69
1:A:68:GLY:O	1:A:72:VAL:HG23	1.92	0.68
1:B:163:LYS:HG2	4:B:2008:HOH:O	1.93	0.67
1:A:4:MSE:O	1:A:5:ILE:CG1	2.41	0.67
1:A:4:MSE:O	1:A:5:ILE:CB	2.44	0.65
1:A:70:ILE:HD13	1:A:89:LYS:HG3	1.78	0.64
1:A:162:LYS:NZ	4:A:1058:HOH:O	2.31	0.64
1:A:24:ARG:HB3	1:A:49:MSE:CE	2.27	0.64
1:A:32:ASN:O	1:A:103:LYS:NZ	2.31	0.63
1:B:63:ILE:HD11	1:B:99:LEU:CD1	2.29	0.62
1:A:5:ILE:H	1:A:6:PRO:HD2	1.64	0.62
1:A:168:HIS:NE2	1:B:145:GLU:OE2	2.20	0.61
1:B:120:ASP:OD2	1:B:147:ARG:NH1	2.29	0.60
1:B:40:VAL:HG23	1:B:101:PHE:CG	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:CYS:SG	1:B:64:ASP:OD1	2.60	0.60
1:B:8:GLU:OE1	1:B:8:GLU:HA	1.94	0.60
1:B:160:TYR:HE2	1:B:173:LYS:CG	2.14	0.59
1:A:102:ASN:HD22	1:A:102:ASN:N	2.01	0.59
1:A:130:ASN:HB3	1:A:176:ILE:HD11	1.85	0.58
1:B:7:ASP:OD1	1:B:8:GLU:N	2.36	0.58
1:A:4:MSE:O	1:A:5:ILE:HG12	2.02	0.58
1:A:4:MSE:O	1:A:5:ILE:HB	2.04	0.58
1:B:38:VAL:H	1:B:102:ASN:ND2	2.02	0.58
1:B:121:LYS:O	1:B:123:LYS:CD	2.52	0.58
1:B:180:LYS:NZ	4:B:2012:HOH:O	2.33	0.58
1:A:42:VAL:HG12	1:A:43:GLY:N	2.17	0.57
1:B:163:LYS:CG	4:B:2008:HOH:O	2.49	0.57
1:B:14:GLU:CD	1:B:15:GLY:H	2.12	0.57
1:B:73:THR:HG22	1:B:77:LEU:HD22	1.86	0.57
1:A:5:ILE:N	1:A:6:PRO:HD2	2.20	0.56
1:B:48:GLY:O	1:B:52:GLU:HG2	2.06	0.56
1:A:154:VAL:HG12	1:B:160:TYR:HD1	1.68	0.56
1:B:35:LYS:O	1:B:58:LYS:HB2	2.06	0.56
1:B:57:CYS:SG	1:B:60:VAL:HG22	2.46	0.55
1:B:80:PHE:HB2	1:B:82:ILE:CD1	2.37	0.55
1:A:77:LEU:HD22	1:A:87:ILE:HD11	1.90	0.54
1:B:145:GLU:CB	1:B:145:GLU:OE1	2.55	0.54
1:B:6:PRO:HD2	1:B:52:GLU:CD	2.33	0.54
1:B:160:TYR:CE2	1:B:173:LYS:CG	2.92	0.53
1:A:22:GLU:H	1:A:22:GLU:CD	2.18	0.51
1:A:140:ILE:HG23	1:A:144:PHE:CE2	2.45	0.51
1:B:117:GLU:OE2	1:B:121:LYS:HE2	2.11	0.51
1:B:7:ASP:OD1	1:B:8:GLU:CB	2.59	0.51
1:B:80:PHE:O	1:B:82:ILE:HD12	2.11	0.51
1:B:63:ILE:HD11	1:B:99:LEU:HD12	1.92	0.51
1:B:123:LYS:HD2	1:B:123:LYS:N	2.26	0.51
1:A:19:THR:HG21	1:A:49:MSE:HE1	1.93	0.51
1:A:180:LYS:NZ	4:A:1044:HOH:O	2.26	0.50
1:A:40:VAL:HG11	1:A:96:LEU:HD21	1.93	0.50
1:B:22:GLU:HG3	1:B:158:ILE:HD13	1.94	0.50
1:A:6:PRO:HB2	1:A:9:GLU:HG2	1.94	0.50
1:A:161:ALA:O	1:A:162:LYS:HD2	2.12	0.49
1:A:113:GLU:H	1:A:113:GLU:CD	2.21	0.49
1:A:102:ASN:ND2	1:A:102:ASN:H	2.07	0.49
1:A:49:MSE:O	1:A:53:ILE:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:HD21	1:A:85:CYS:SG	2.53	0.48
1:A:18:ILE:HA	2:A:1001:SO4:O2	2.12	0.48
1:A:111:ASN:HB3	1:A:114:LYS:HD2	1.96	0.48
1:B:81:ASN:O	1:B:81:ASN:CG	2.51	0.48
1:B:99:LEU:O	1:B:122:LYS:NZ	2.42	0.47
1:A:71:GLU:HG3	1:A:75:GLN:HE21	1.78	0.47
1:A:38:VAL:N	1:A:102:ASN:HD21	1.96	0.46
1:A:139:LYS:O	1:A:143:GLU:HB2	2.15	0.46
1:A:59:PHE:HA	1:A:84:ASN:ND2	2.29	0.46
1:A:126:HIS:C	1:A:127:ILE:HG13	2.40	0.46
1:B:38:VAL:O	1:B:101:PHE:HB2	2.16	0.46
1:A:9:GLU:O	1:A:80:PHE:HZ	1.99	0.46
1:A:10:PHE:CE2	1:A:48:GLY:HA2	2.51	0.46
1:B:68:GLY:O	1:B:72:VAL:HG23	2.15	0.46
1:A:70:ILE:HD11	1:A:89:LYS:HG3	1.95	0.46
1:B:4:MSE:O	1:B:6:PRO:HD3	2.16	0.45
1:A:99:LEU:O	1:A:122:LYS:HE2	2.16	0.45
1:A:5:ILE:O	1:A:6:PRO:O	2.34	0.45
1:B:160:TYR:CE2	1:B:173:LYS:HG3	2.40	0.45
1:A:123:LYS:HE3	1:A:123:LYS:HB3	1.75	0.45
1:A:5:ILE:HA	1:A:52:GLU:OE2	2.18	0.44
1:A:102:ASN:ND2	1:A:102:ASN:N	2.64	0.44
1:A:71:GLU:O	1:A:75:GLN:HG3	2.17	0.44
1:B:139:LYS:O	1:B:143:GLU:HB2	2.18	0.44
1:A:118:ILE:O	1:A:119:LEU:C	2.59	0.44
1:A:128:VAL:HA	1:A:179:ILE:O	2.18	0.44
1:B:54:ALA:C	1:B:56:ARG:H	2.26	0.44
1:B:121:LYS:HD3	1:B:121:LYS:HA	1.58	0.44
1:A:84:ASN:HD22	1:A:84:ASN:HA	1.53	0.43
1:B:169:MSE:CE	1:B:171:LEU:CD1	2.68	0.43
1:B:6:PRO:HD3	1:B:55:LYS:NZ	2.32	0.43
1:A:42:VAL:CG1	1:A:43:GLY:N	2.82	0.43
1:B:44:CYS:HA	1:B:64:ASP:CG	2.44	0.42
1:B:47:GLY:O	1:B:51:VAL:HG23	2.18	0.42
1:A:154:VAL:CG1	1:B:160:TYR:CD1	2.96	0.42
1:B:128:VAL:HA	1:B:179:ILE:O	2.18	0.42
1:A:22:GLU:HB3	1:B:26:VAL:HG13	2.01	0.42
1:B:130:ASN:HB3	1:B:176:ILE:HD11	2.01	0.42
1:A:30:LYS:HE3	4:A:1005:HOH:O	2.19	0.41
1:A:164:ILE:O	1:A:165:PRO:C	2.63	0.41
1:B:49:MSE:HG2	1:B:105:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ILE:HG21	1:B:143:GLU:HG2	2.02	0.41
1:B:40:VAL:HG12	1:B:41:ASP:N	2.33	0.41
1:B:160:TYR:CE2	1:B:173:LYS:HG2	2.56	0.41
1:B:20:LYS:HD2	1:B:160:TYR:CZ	2.55	0.41
1:A:107:GLY:O	1:A:108:GLY:C	2.64	0.41
1:A:168:HIS:HE2	1:B:145:GLU:CD	2.25	0.41
1:B:51:VAL:HG13	1:B:82:ILE:HD11	2.04	0.40
1:A:55:LYS:HB3	1:A:55:LYS:HE2	1.91	0.40
1:A:38:VAL:HG12	1:A:101:PHE:CB	2.51	0.40
1:B:22:GLU:CG	1:B:158:ILE:HD13	2.52	0.40
1:A:111:ASN:CG	1:A:114:LYS:HD2	2.47	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	178/183 (97%)	171 (96%)	2 (1%)	5 (3%)	4	2
1	B	178/183 (97%)	166 (93%)	10 (6%)	2 (1%)	11	13
All	All	356/366 (97%)	337 (95%)	12 (3%)	7 (2%)	6	5

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	6	PRO
1	A	108	GLY
1	A	109	THR
1	A	174	ASN
1	B	7	ASP
1	B	21	GLU

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	147/153 (96%)	132 (90%)	15 (10%)	7	8
1	B	149/153 (97%)	132 (89%)	17 (11%)	5	6
All	All	296/306 (97%)	264 (89%)	32 (11%)	6	7

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	18	ILE
1	A	21	GLU
1	A	22	GLU
1	A	77	LEU
1	A	83	LYS
1	A	102	ASN
1	A	109	THR
1	A	113	GLU
1	A	134	LEU
1	A	150	ASN
1	A	152	ASP
1	A	158	ILE
1	A	166	SER
1	A	183	ARG
1	B	5	ILE
1	B	7	ASP
1	B	8	GLU
1	B	9	GLU
1	B	11	ILE
1	B	18	ILE
1	B	22	GLU
1	B	66	LEU
1	B	77	LEU
1	B	95	VAL
1	B	96	LEU
1	B	100	GLU

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Mol	Chain	Res	Type
1	B	134	LEU
1	B	152	ASP
1	B	163	LYS
1	B	165	PRO
1	B	166	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	75	GLN
1	A	84	ASN
1	A	86	GLN
1	A	102	ASN
1	A	136	ASN
1	A	155	ASN
1	A	174	ASN
1	B	32	ASN
1	B	102	ASN
1	B	130	ASN
1	B	136	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	SO4	A	1001	-	4,4,4	0.57	0	6,6,6	0.83	0
2	SO4	B	1002	-	4,4,4	0.43	0	6,6,6	1.18	0
3	MES	B	2001	-	12,12,12	1.54	3 (25%)	15,16,16	5.27	8 (53%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	B	2001	-	-	3/6/14/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	MES	O2S-S	2.39	1.51	1.45
3	B	2001	MES	C7-C8	2.15	1.58	1.52
3	B	2001	MES	O1S-S	2.02	1.50	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	MES	O3S-S-C8	-13.28	80.02	106.00
3	B	2001	MES	O2S-S-C8	-8.65	93.66	106.73
3	B	2001	MES	O3S-S-O2S	6.70	128.15	111.40
3	B	2001	MES	C5-N4-C3	6.65	123.17	108.84
3	B	2001	MES	O1S-S-C8	-5.64	98.21	106.73
3	B	2001	MES	C7-N4-C5	3.79	121.35	111.24
3	B	2001	MES	O3S-S-O1S	3.35	119.78	111.40
3	B	2001	MES	O1-C6-C5	3.01	118.26	111.77

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2001	MES	C8-C7-N4-C5
3	B	2001	MES	N4-C7-C8-S
3	B	2001	MES	C8-C7-N4-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	SO4	1	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.