



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:56 pm BST

PDB ID : 1T7L
Title : Crystal Structure of Cobalamin-Independent Methionine Synthase from *T. maritima*
Authors : Pejchal, R.; Ludwig, M.L.
Deposited on : 2004-05-10
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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

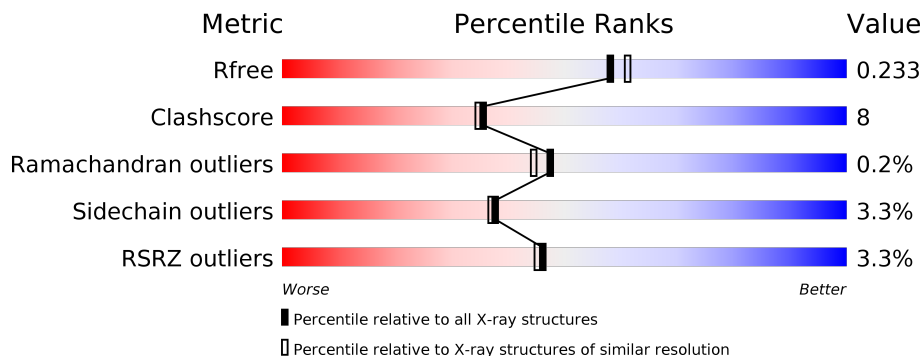
1 Overall quality at a glance

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 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 $\leq 5\%$. 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	766	 3% 78% 15% • •
1	B	766	 3% 77% 17% • 5%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 12255 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 5-methyltetrahydropteroyltriglutamate--homocysteine methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	734	Total	C	N	O	S	0	0	0
			5831	3780	950	1077	24			
1	B	731	Total	C	N	O	S	0	0	0
			5780	3743	950	1063	24			

There are 66 discrepancies between the modelled and reference sequences:

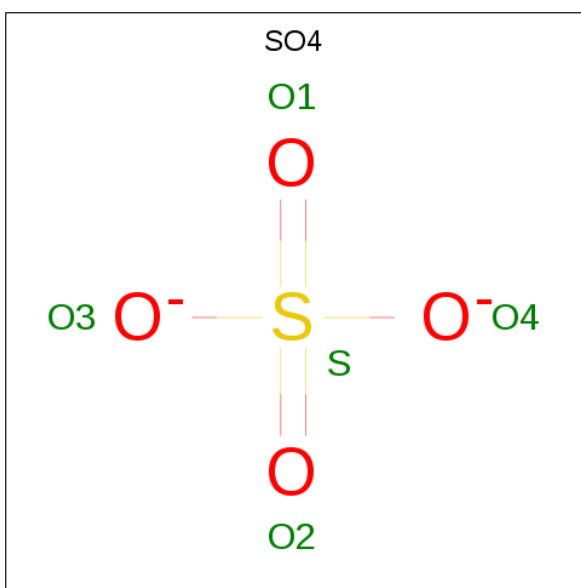
Chain	Residue	Modelled	Actual	Comment	Reference
A	-31	MET	-	EXPRESSION TAG	UNP Q9X112
A	-30	HIS	-	EXPRESSION TAG	UNP Q9X112
A	-29	HIS	-	EXPRESSION TAG	UNP Q9X112
A	-28	HIS	-	EXPRESSION TAG	UNP Q9X112
A	-27	HIS	-	EXPRESSION TAG	UNP Q9X112
A	-26	HIS	-	EXPRESSION TAG	UNP Q9X112
A	-25	HIS	-	EXPRESSION TAG	UNP Q9X112
A	-24	GLY	-	EXPRESSION TAG	UNP Q9X112
A	-23	LYS	-	EXPRESSION TAG	UNP Q9X112
A	-22	PRO	-	EXPRESSION TAG	UNP Q9X112
A	-21	ILE	-	EXPRESSION TAG	UNP Q9X112
A	-20	PRO	-	EXPRESSION TAG	UNP Q9X112
A	-19	ASN	-	EXPRESSION TAG	UNP Q9X112
A	-18	PRO	-	EXPRESSION TAG	UNP Q9X112
A	-17	LEU	-	EXPRESSION TAG	UNP Q9X112
A	-16	LEU	-	EXPRESSION TAG	UNP Q9X112
A	-15	GLY	-	EXPRESSION TAG	UNP Q9X112
A	-14	LEU	-	EXPRESSION TAG	UNP Q9X112
A	-13	ASP	-	EXPRESSION TAG	UNP Q9X112
A	-12	SER	-	EXPRESSION TAG	UNP Q9X112
A	-11	THR	-	EXPRESSION TAG	UNP Q9X112
A	-10	GLU	-	EXPRESSION TAG	UNP Q9X112
A	-9	ASN	-	EXPRESSION TAG	UNP Q9X112
A	-8	LEU	-	EXPRESSION TAG	UNP Q9X112

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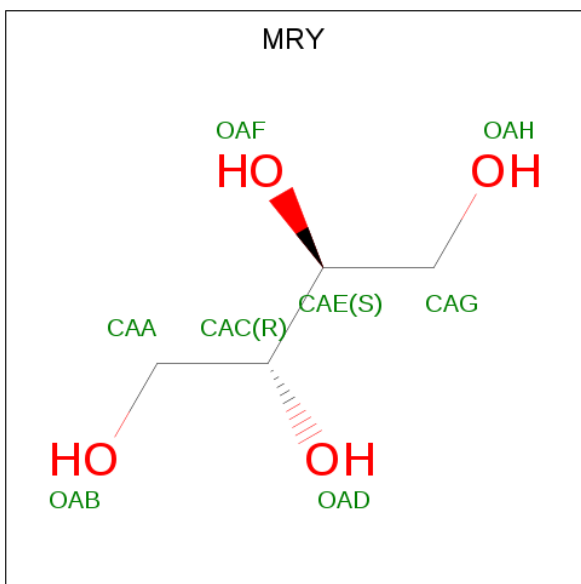
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	TYR	-	EXPRESSION TAG	UNP Q9X112
A	-6	PHE	-	EXPRESSION TAG	UNP Q9X112
A	-5	GLN	-	EXPRESSION TAG	UNP Q9X112
A	-4	GLN	-	EXPRESSION TAG	UNP Q9X112
A	-3	ILE	-	EXPRESSION TAG	UNP Q9X112
A	-2	ASP	-	EXPRESSION TAG	UNP Q9X112
A	-1	PRO	-	EXPRESSION TAG	UNP Q9X112
A	0	PHE	-	EXPRESSION TAG	UNP Q9X112
A	1	THR	-	EXPRESSION TAG	UNP Q9X112
B	-31	MET	-	EXPRESSION TAG	UNP Q9X112
B	-30	HIS	-	EXPRESSION TAG	UNP Q9X112
B	-29	HIS	-	EXPRESSION TAG	UNP Q9X112
B	-28	HIS	-	EXPRESSION TAG	UNP Q9X112
B	-27	HIS	-	EXPRESSION TAG	UNP Q9X112
B	-26	HIS	-	EXPRESSION TAG	UNP Q9X112
B	-25	HIS	-	EXPRESSION TAG	UNP Q9X112
B	-24	GLY	-	EXPRESSION TAG	UNP Q9X112
B	-23	LYS	-	EXPRESSION TAG	UNP Q9X112
B	-22	PRO	-	EXPRESSION TAG	UNP Q9X112
B	-21	ILE	-	EXPRESSION TAG	UNP Q9X112
B	-20	PRO	-	EXPRESSION TAG	UNP Q9X112
B	-19	ASN	-	EXPRESSION TAG	UNP Q9X112
B	-18	PRO	-	EXPRESSION TAG	UNP Q9X112
B	-17	LEU	-	EXPRESSION TAG	UNP Q9X112
B	-16	LEU	-	EXPRESSION TAG	UNP Q9X112
B	-15	GLY	-	EXPRESSION TAG	UNP Q9X112
B	-14	LEU	-	EXPRESSION TAG	UNP Q9X112
B	-13	ASP	-	EXPRESSION TAG	UNP Q9X112
B	-12	SER	-	EXPRESSION TAG	UNP Q9X112
B	-11	THR	-	EXPRESSION TAG	UNP Q9X112
B	-10	GLU	-	EXPRESSION TAG	UNP Q9X112
B	-9	ASN	-	EXPRESSION TAG	UNP Q9X112
B	-8	LEU	-	EXPRESSION TAG	UNP Q9X112
B	-7	TYR	-	EXPRESSION TAG	UNP Q9X112
B	-6	PHE	-	EXPRESSION TAG	UNP Q9X112
B	-5	GLN	-	EXPRESSION TAG	UNP Q9X112
B	-4	GLN	-	EXPRESSION TAG	UNP Q9X112
B	-3	ILE	-	EXPRESSION TAG	UNP Q9X112
B	-2	ASP	-	EXPRESSION TAG	UNP Q9X112
B	-1	PRO	-	EXPRESSION TAG	UNP Q9X112
B	0	PHE	-	EXPRESSION TAG	UNP Q9X112
B	1	THR	-	EXPRESSION TAG	UNP Q9X112

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is MESO-ERYTHRITOL (three-letter code: MRY) (formula: C₄H₁₀O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 4 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			8	4	4		

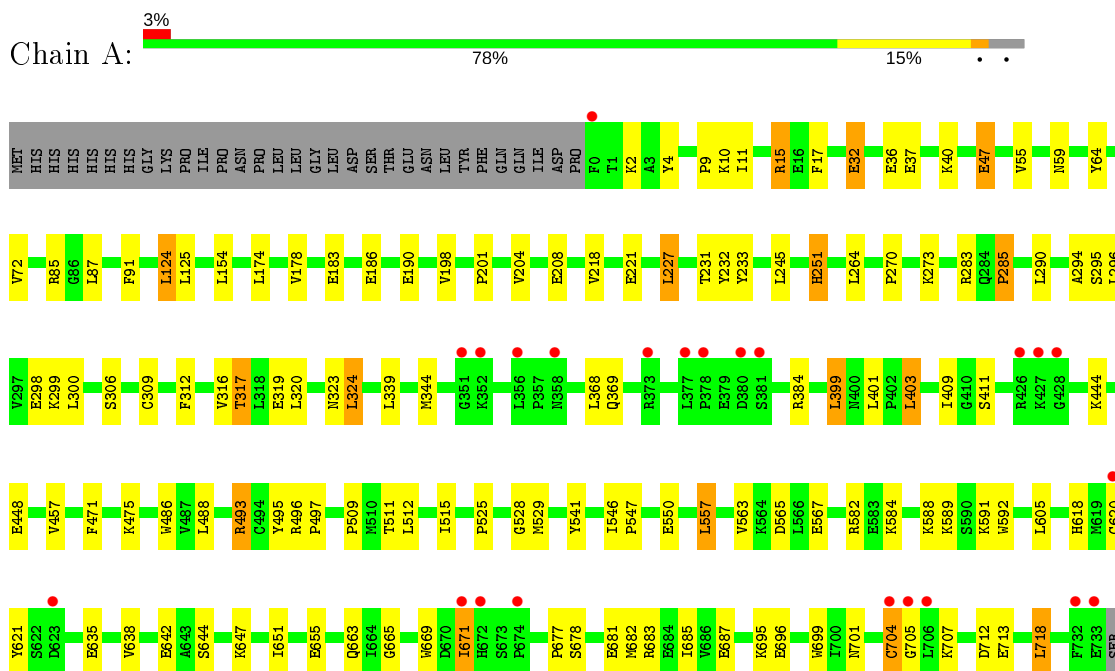
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	331	Total	O	0	0
			331	331		
4	B	287	Total	O	0	0
			287	287		

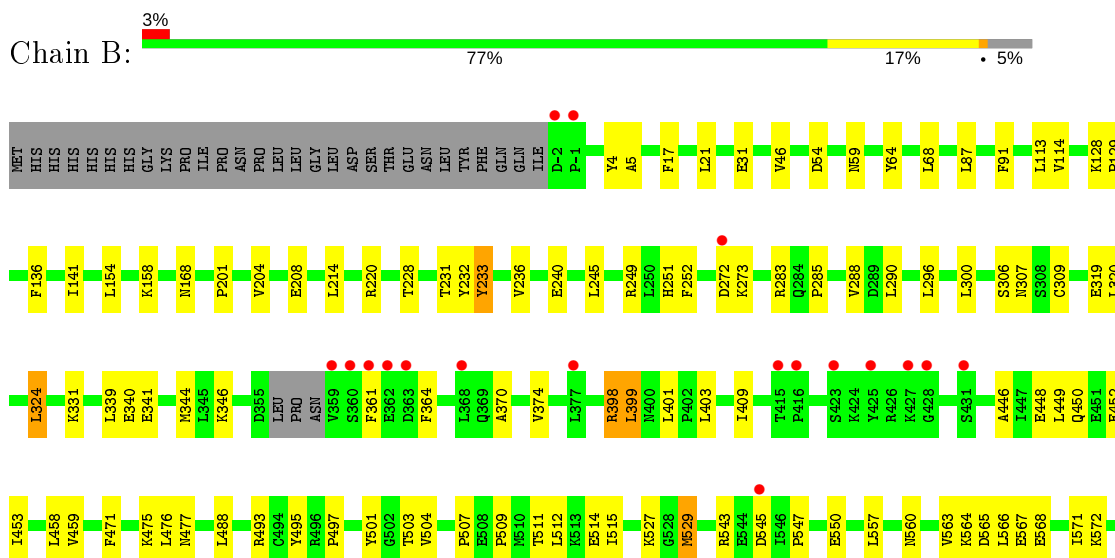
3 Residue-property plots

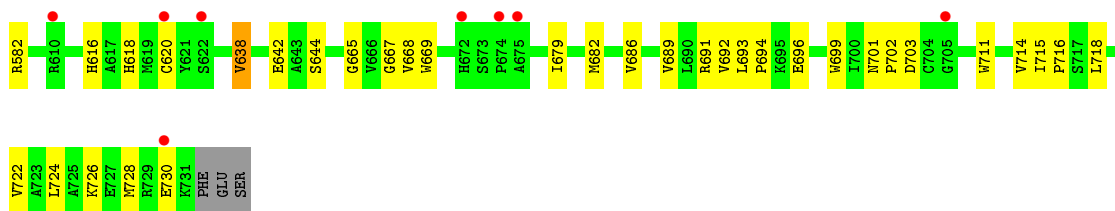
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 5-methyltetrahydropteroyltriglutamate--homocysteine methyltransferase



- Molecule 1: 5-methyltetrahydropteroyltriglutamate--homocysteine methyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	163.56Å 158.76Å 64.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.00 19.91 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.91-2.00) 99.3 (19.91-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 2.01Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.240 0.200 , 0.233	Depositor DCC
R_{free} test set	11263 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtrriage
Anisotropy	0.202	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.023 for k,h,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12255	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MRY, 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	0.33	0/5977	0.57	1/8117 (0.0%)
1	B	0.34	0/5924	0.56	0/8046
All	All	0.33	0/11901	0.57	1/16163 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	528	GLY	N-CA-C	-5.84	98.50	113.10

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	5831	0	5632	91	0
1	B	5780	0	5551	97	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	8	0	10	0	0
3	B	8	0	10	0	0
4	A	331	0	0	7	0
4	B	287	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12255	0	11203	185	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 8.

All (185) 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:557:LEU:HD22	1:A:605:LEU:HD21	1.44	0.97
1:B:331:LYS:HE3	1:B:361:PHE:HB3	1.65	0.79
1:B:283:ARG:HG3	1:B:309:CYS:SG	2.24	0.78
1:B:319:GLU:HG3	1:B:320:LEU:HD13	1.69	0.73
1:B:296:LEU:O	1:B:300:LEU:HD13	1.88	0.73
1:B:495:TYR:CE2	1:B:497:PRO:HG3	2.24	0.72
1:A:294:ALA:O	1:A:298:GLU:HG3	1.90	0.72
1:A:444:LYS:O	1:A:448:GLU:HG3	1.89	0.71
1:A:317:THR:HG21	4:A:1251:HOH:O	1.91	0.70
1:B:228:THR:OG1	1:B:249:ARG:HD2	1.92	0.69
1:B:409:ILE:HD12	1:B:618:HIS:CE1	2.28	0.68
1:B:114:VAL:HG11	1:B:158:LYS:HD2	1.76	0.67
1:A:4:TYR:HB2	1:A:306:SER:HB3	1.75	0.67
1:B:4:TYR:HB2	1:B:306:SER:HB3	1.76	0.66
1:B:448:GLU:O	1:B:452:GLU:HG3	1.95	0.66
1:B:511:THR:O	1:B:515:ILE:HG12	1.96	0.65
1:B:618:HIS:CE1	1:B:620:CYS:SG	2.90	0.65
1:B:501:TYR:O	1:B:543:ARG:HD2	1.96	0.65
1:B:711:TRP:O	1:B:715:ILE:HG12	1.97	0.64
1:A:409:ILE:HD11	1:A:704:CYS:HA	1.80	0.64
1:A:495:TYR:CE1	1:A:497:PRO:HG3	2.32	0.64
1:B:529:MET:HG3	4:B:1622:HOH:O	1.96	0.63
1:A:283:ARG:HG2	1:A:309:CYS:SG	2.39	0.63
1:B:679:ILE:HG23	1:B:724:LEU:HB2	1.81	0.62
1:A:665:GLY:HA2	1:A:699:TRP:HB2	1.82	0.61
1:B:228:THR:HG23	1:B:249:ARG:HG3	1.82	0.61
1:B:54:ASP:OD2	1:B:346:LYS:HE2	2.01	0.61
1:A:409:ILE:HD11	1:A:704:CYS:CA	2.31	0.60
1:B:665:GLY:HA2	1:B:699:TRP:HB2	1.83	0.60
1:B:543:ARG:HB3	1:B:545:ASP:OD1	2.02	0.60
1:B:331:LYS:HE2	1:B:364:PHE:CD2	2.37	0.60
1:B:691:ARG:HG3	1:B:692:VAL:HG23	1.84	0.60
1:A:557:LEU:CD2	1:A:605:LEU:HD21	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:ARG:NH1	1:B:572:LYS:HG2	2.17	0.59
1:A:678:SER:OG	1:A:681:GLU:HG3	2.02	0.59
1:A:201:PRO:O	1:A:204:VAL:HG22	2.03	0.59
1:A:47:GLU:HG3	4:A:853:HOH:O	2.02	0.58
1:A:32:GLU:O	1:A:36:GLU:HG3	2.04	0.58
1:B:509:PRO:HB3	1:B:512:LEU:HD12	1.86	0.58
1:B:560:ASN:OD1	1:B:564:LYS:HE2	2.04	0.57
1:A:563:VAL:O	1:A:567:GLU:HG3	2.04	0.57
1:A:232:TYR:O	1:A:233:TYR:HB2	2.05	0.57
1:A:15:ARG:HH21	1:A:15:ARG:HB2	1.69	0.56
1:A:512:LEU:HD11	1:A:565:ASP:HB3	1.86	0.56
1:B:232:TYR:O	1:B:233:TYR:HB2	2.06	0.56
1:A:696:GLU:H	1:A:696:GLU:CD	2.09	0.56
1:B:616:HIS:CE1	1:B:638:VAL:HG21	2.42	0.56
1:A:557:LEU:HD22	1:A:605:LEU:CD2	2.27	0.55
1:A:671:ILE:HD12	1:A:704:CYS:H	1.71	0.55
1:A:620:CYS:HB3	1:A:642:GLU:CD	2.27	0.55
1:B:512:LEU:HD11	1:B:565:ASP:HB3	1.87	0.55
1:B:714:VAL:O	1:B:718:LEU:HD13	2.07	0.55
1:B:87:LEU:HD22	1:B:91:PHE:CE1	2.42	0.54
1:A:509:PRO:HB3	1:A:512:LEU:HD12	1.90	0.54
1:B:571:ILE:HD12	1:B:571:ILE:N	2.22	0.54
1:A:671:ILE:HD13	4:A:1122:HOH:O	2.08	0.53
1:A:124:LEU:HD12	1:A:183:GLU:HG2	1.91	0.53
1:B:31:GLU:OE2	1:B:87:LEU:HB2	2.08	0.53
1:B:493:ARG:HD2	4:B:1477:HOH:O	2.08	0.53
1:A:493:ARG:HH11	1:A:493:ARG:HG2	1.74	0.52
1:B:509:PRO:CB	1:B:512:LEU:HD12	2.39	0.52
1:A:584:LYS:HG3	1:A:584:LYS:O	2.10	0.52
1:A:186:GLU:O	1:A:190:GLU:HG3	2.09	0.52
1:A:324:LEU:HD13	4:A:790:HOH:O	2.09	0.52
1:A:638:VAL:HG22	1:A:663:GLN:HB2	1.91	0.52
1:A:409:ILE:HD11	1:A:704:CYS:C	2.30	0.52
1:A:618:HIS:CE1	1:A:620:CYS:SG	3.03	0.52
1:A:683:ARG:O	1:A:687:GLU:HG3	2.10	0.52
1:B:240:GLU:HG3	4:B:1535:HOH:O	2.09	0.52
1:A:677:PRO:HB2	1:A:682:MET:CE	2.40	0.52
1:A:231:THR:H	1:A:251:HIS:HD2	1.57	0.51
1:A:317:THR:HG22	1:A:319:GLU:H	1.75	0.51
1:A:588:LYS:HD2	1:A:591:LYS:HE3	1.93	0.51
1:A:399:LEU:HB3	1:A:401:LEU:HG	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:PRO:HG2	1:A:550:GLU:HB2	1.92	0.51
1:A:471:PHE:CZ	1:A:475:LYS:HE3	2.46	0.51
1:B:59:ASN:HB2	4:B:1486:HOH:O	2.09	0.51
1:A:270:PRO:HB2	1:A:273:LYS:HG2	1.94	0.50
1:B:701:ASN:HB2	1:B:702:PRO:HD2	1.92	0.50
1:B:288:VAL:O	1:B:290:LEU:HD22	2.11	0.50
1:A:368:LEU:C	1:A:368:LEU:HD13	2.32	0.50
1:A:671:ILE:HG13	1:A:705:GLY:O	2.12	0.50
1:B:399:LEU:HB3	1:B:401:LEU:HG	1.92	0.50
1:A:9:PRO:HB2	1:A:316:VAL:HG22	1.94	0.49
1:A:296:LEU:O	1:A:300:LEU:HD13	2.13	0.49
1:A:290:LEU:HD11	1:A:344:MET:HE3	1.95	0.49
1:B:715:ILE:HB	1:B:716:PRO:CD	2.43	0.49
1:B:686:VAL:O	1:B:689:VAL:HG22	2.13	0.49
1:B:214:LEU:HD13	4:B:1526:HOH:O	2.13	0.49
1:B:696:GLU:H	1:B:696:GLU:CD	2.14	0.49
1:A:2:LYS:HE2	1:A:55:VAL:CG2	2.44	0.48
1:B:272:ASP:OD1	1:B:273:LYS:HG3	2.12	0.48
1:B:477:ASN:HD21	1:B:507:PRO:HB3	1.78	0.48
1:A:409:ILE:C	1:A:409:ILE:HD12	2.34	0.47
1:A:707:LYS:HE2	4:A:1181:HOH:O	2.14	0.47
1:B:667:GLY:HA2	1:B:701:ASN:O	2.14	0.47
1:B:563:VAL:O	1:B:567:GLU:HG3	2.15	0.47
1:B:724:LEU:O	1:B:728:MET:HG2	2.13	0.47
1:B:201:PRO:O	1:B:204:VAL:HG22	2.14	0.47
1:A:582:ARG:HB3	1:A:621:TYR:CZ	2.50	0.47
1:A:546:ILE:HG13	1:A:547:PRO:HD2	1.97	0.47
1:B:620:CYS:HB3	1:B:642:GLU:CD	2.34	0.47
1:B:114:VAL:HG11	1:B:158:LYS:CD	2.45	0.46
1:A:589:LYS:O	1:B:168:ASN:HB3	2.15	0.46
1:A:486:TRP:CE3	1:A:496:ARG:HG3	2.51	0.46
1:A:671:ILE:HD12	1:A:704:CYS:N	2.31	0.46
1:A:677:PRO:HB2	1:A:682:MET:HE2	1.96	0.46
1:A:174:LEU:O	1:A:178:VAL:HG22	2.15	0.46
1:B:370:ALA:O	1:B:374:VAL:HG23	2.16	0.46
1:B:453:ILE:HG22	1:B:722:VAL:HG21	1.97	0.46
1:A:178:VAL:HG21	1:A:221:GLU:OE2	2.15	0.46
1:A:707:LYS:HG2	1:A:707:LYS:O	2.16	0.46
1:A:712:ASP:OD1	1:A:713:GLU:HG3	2.15	0.46
1:B:319:GLU:HG3	1:B:320:LEU:CD1	2.43	0.46
1:B:331:LYS:HE3	1:B:361:PHE:CB	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:VAL:HG21	1:A:227:LEU:HG	1.97	0.45
1:A:618:HIS:NE2	1:A:620:CYS:SG	2.89	0.45
1:B:46:VAL:HG11	1:B:141:ILE:HD13	1.97	0.45
1:B:471:PHE:CZ	1:B:475:LYS:HE3	2.51	0.45
1:B:564:LYS:O	1:B:568:GLU:HG3	2.16	0.45
1:A:589:LYS:HA	1:A:592:TRP:CD1	2.51	0.45
1:A:671:ILE:HD13	1:A:671:ILE:H	1.81	0.45
1:B:514:GLU:HG3	4:B:1554:HOH:O	2.17	0.45
1:A:647:LYS:HD2	1:B:691:ARG:CZ	2.47	0.45
1:A:320:LEU:HD12	1:A:320:LEU:N	2.32	0.45
1:B:370:ALA:HB3	1:B:503:THR:HG21	1.99	0.45
1:A:264:LEU:C	1:A:264:LEU:HD23	2.37	0.45
1:B:449:LEU:HD11	1:B:715:ILE:HD12	1.98	0.45
1:B:547:PRO:HG2	1:B:550:GLU:HB2	1.98	0.45
1:B:31:GLU:OE2	1:B:87:LEU:HD12	2.18	0.44
1:A:11:ILE:HA	1:A:17:PHE:HB3	1.99	0.44
1:B:495:TYR:O	1:B:497:PRO:HD3	2.18	0.44
1:B:669:TRP:CE3	1:B:702:PRO:HB3	2.52	0.44
1:B:324:LEU:HD13	4:B:1463:HOH:O	2.18	0.44
1:A:669:TRP:HZ3	1:A:718:LEU:HD13	1.82	0.44
1:B:616:HIS:ND1	1:B:638:VAL:HG21	2.32	0.44
1:A:285:PRO:HD3	1:A:541:TYR:CD1	2.53	0.43
1:B:158:LYS:HD3	4:B:1404:HOH:O	2.17	0.43
1:A:295:SER:O	1:A:299:LYS:HG3	2.18	0.43
1:B:644:SER:HB3	1:B:703:ASP:OD1	2.18	0.43
1:B:68:LEU:HD22	1:B:113:LEU:CD1	2.48	0.43
1:B:341:GLU:HA	1:B:344:MET:CE	2.48	0.43
1:B:331:LYS:HE2	1:B:364:PHE:CG	2.54	0.43
1:A:457:VAL:HG22	1:A:525:PRO:HG2	2.00	0.43
1:A:589:LYS:HG2	1:A:592:TRP:CZ2	2.53	0.43
1:A:208:GLU:HA	1:B:208:GLU:HA	2.00	0.43
1:B:616:HIS:CG	1:B:638:VAL:HG22	2.53	0.43
1:A:178:VAL:HG11	1:A:218:VAL:HG13	2.00	0.43
1:A:72:VAL:O	1:A:125:LEU:HB3	2.18	0.43
1:B:128:LYS:N	1:B:129:PRO:CD	2.82	0.43
1:B:340:GLU:O	1:B:344:MET:HG3	2.18	0.43
1:A:511:THR:O	1:A:515:ILE:HG12	2.19	0.43
1:A:87:LEU:HD22	1:A:91:PHE:CE1	2.54	0.43
1:B:477:ASN:O	1:B:504:VAL:HA	2.19	0.43
1:A:232:TYR:O	1:A:233:TYR:CB	2.67	0.42
1:B:231:THR:H	1:B:251:HIS:HD2	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:LEU:HD23	4:A:1115:HOH:O	2.18	0.42
1:A:409:ILE:CD1	1:A:704:CYS:HA	2.49	0.42
1:B:341:GLU:HA	1:B:344:MET:HE2	2.01	0.42
1:B:566:LEU:O	1:B:571:ILE:HD13	2.19	0.42
1:B:5:ALA:HA	1:B:307:ASN:OD1	2.19	0.42
1:B:693:LEU:HA	1:B:694:PRO:HD3	1.93	0.42
1:B:477:ASN:ND2	1:B:507:PRO:HD3	2.34	0.41
1:B:236:VAL:HG21	1:B:252:PHE:HE2	1.85	0.41
1:B:446:ALA:O	1:B:450:GLN:HG3	2.21	0.41
1:A:10:LYS:HE2	1:A:488:LEU:HD22	2.02	0.41
1:A:644:SER:HA	1:A:685:ILE:HD13	2.01	0.41
1:B:220:ARG:HG2	1:B:220:ARG:HH21	1.86	0.41
1:A:37:GLU:HA	1:A:40:LYS:HD3	2.03	0.41
1:B:232:TYR:O	1:B:233:TYR:CB	2.69	0.41
1:B:668:VAL:HG23	1:B:682:MET:CE	2.50	0.41
1:A:651:ILE:O	1:A:655:GLU:HG2	2.20	0.41
1:B:409:ILE:HD12	1:B:618:HIS:HE1	1.82	0.41
1:B:724:LEU:HD13	1:B:724:LEU:C	2.41	0.41
1:A:384:ARG:HG3	1:A:635:GLU:OE1	2.20	0.41
1:B:459:VAL:HG12	1:B:527:LYS:HD3	2.01	0.41
1:A:403:LEU:HD11	1:A:695:LYS:HD2	2.03	0.40
1:B:17:PHE:O	1:B:21:LEU:HD13	2.21	0.40
1:B:726:LYS:O	1:B:730:GLU:HG3	2.20	0.40
1:B:46:VAL:HG21	1:B:136:PHE:CE2	2.57	0.40
1:A:411:SER:HB2	1:A:707:LYS:HB2	2.04	0.40
1:A:59:ASN:HB2	4:A:820:HOH:O	2.20	0.40
1:A:669:TRP:CD1	1:A:677:PRO:HG2	2.56	0.40
1:A:178:VAL:CG1	1:A:218:VAL:HG13	2.52	0.40
1:B:228:THR:OG1	1:B:249:ARG:CD	2.66	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	732/766 (96%)	703 (96%)	28 (4%)	1 (0%)	51	49
1	B	727/766 (95%)	696 (96%)	29 (4%)	2 (0%)	41	37
All	All	1459/1532 (95%)	1399 (96%)	57 (4%)	3 (0%)	47	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	TYR
1	B	233	TYR
1	B	64	TYR

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	608/688 (88%)	583 (96%)	25 (4%)	30	28
1	B	595/688 (86%)	580 (98%)	15 (2%)	47	49
All	All	1203/1376 (87%)	1163 (97%)	40 (3%)	38	37

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	32	GLU
1	A	47	GLU
1	A	85	ARG
1	A	124	LEU
1	A	154	LEU
1	A	227	LEU
1	A	245	LEU
1	A	251	HIS
1	A	285	PRO
1	A	312	PHE
1	A	317	THR
1	A	323	ASN

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Mol	Chain	Res	Type
1	A	324	LEU
1	A	339	LEU
1	A	369	GLN
1	A	399	LEU
1	A	403	LEU
1	A	493	ARG
1	A	529	MET
1	A	557	LEU
1	A	671	ILE
1	A	701	ASN
1	A	704	CYS
1	A	718	LEU
1	B	154	LEU
1	B	245	LEU
1	B	285	PRO
1	B	324	LEU
1	B	339	LEU
1	B	398	ARG
1	B	399	LEU
1	B	403	LEU
1	B	458	LEU
1	B	476	LEU
1	B	488	LEU
1	B	529	MET
1	B	557	LEU
1	B	582	ARG
1	B	638	VAL

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

Mol	Chain	Res	Type
1	A	251	HIS
1	A	323	ASN
1	A	369	GLN
1	A	400	ASN
1	A	710	ASN
1	B	251	HIS
1	B	267	HIS
1	B	323	ASN
1	B	477	ASN
1	B	601	ASN
1	B	625	ASN

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Mol	Chain	Res	Type
1	B	710	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	1351	-	4,4,4	0.21	0	6,6,6	0.08	0
3	MRY	B	1352	-	7,7,7	0.30	0	8,8,8	0.47	0
3	MRY	A	1353	-	7,7,7	0.31	0	8,8,8	0.45	0
2	SO4	A	1350	-	4,4,4	0.23	0	6,6,6	0.06	0

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	MRY	B	1352	-	-	0/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MRY	A	1353	-	-	0/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	734/766 (95%)	0.06	23 (3%) 49 48	12, 25, 43, 58	0
1	B	731/766 (95%)	0.16	26 (3%) 42 42	13, 26, 46, 68	0
All	All	1465/1532 (95%)	0.11	49 (3%) 46 45	12, 25, 45, 68	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	361	PHE	7.8
1	B	428	GLY	6.0
1	B	377	LEU	4.9
1	B	674	PRO	4.6
1	B	359	VAL	4.4
1	B	362	GLU	4.2
1	B	425	TYR	3.9
1	A	704	CYS	3.8
1	A	672	HIS	3.8
1	B	431	SER	3.8
1	A	377	LEU	3.6
1	A	380	ASP	3.6
1	A	732	PHE	3.5
1	A	427	LYS	3.4
1	B	620	CYS	3.3
1	B	-1	PRO	3.3
1	A	381	SER	3.2
1	B	368	LEU	3.1
1	A	428	GLY	3.0
1	A	351	GLY	3.0
1	B	705	GLY	3.0
1	B	363	ASP	2.9
1	A	358	ASN	2.9
1	B	672	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	426	ARG	2.7
1	B	423	SER	2.7
1	B	360	SER	2.7
1	A	373	ARG	2.7
1	B	427	LYS	2.6
1	A	0	PHE	2.6
1	B	416	PRO	2.6
1	B	415	THR	2.6
1	B	730	GLU	2.5
1	B	675	ALA	2.4
1	B	272	ASP	2.4
1	A	620	CYS	2.4
1	B	622	SER	2.3
1	A	352	LYS	2.3
1	A	356	LEU	2.3
1	A	705	GLY	2.2
1	A	733	GLU	2.2
1	A	706	LEU	2.1
1	A	378	PRO	2.1
1	A	671	ILE	2.1
1	A	623	ASP	2.1
1	B	-2	ASP	2.1
1	B	545	ASP	2.0
1	B	610	ARG	2.0
1	A	674	PRO	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. 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	B-factors(\AA^2)	Q<0.9
3	MRY	A	1353	8/8	0.89	0.19	24,37,39,42	0
3	MRY	B	1352	8/8	0.93	0.15	23,34,36,39	0
2	SO4	B	1351	5/5	0.99	0.10	24,25,27,29	0
2	SO4	A	1350	5/5	0.99	0.09	26,27,27,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.