



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 01:05 AM GMT

PDB ID : 1XR2
Title : Crystal Structure of oxidized T. maritima Cobalamin-IndependentMethionine
Synthase complexed with Methyltetrahydrofolate
Authors : Pejchal, R.; Ludwig, M.L.
Deposited on : 2004-10-13
Resolution : 2.35 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

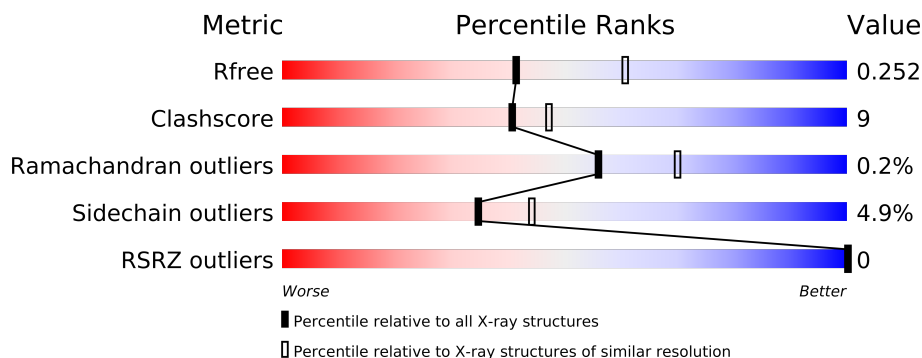
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.35 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}	66092	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	766	
1	B	766	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	C2F	A	1200	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11505 atoms, of which 0 are hydrogen and 0 are deuterium.

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--homocysteinemethyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	0	0	0
			5535	3597	903	1012	23			
1	B	728	Total	C	N	O	S	0	0	0
			5640	3660	919	1037	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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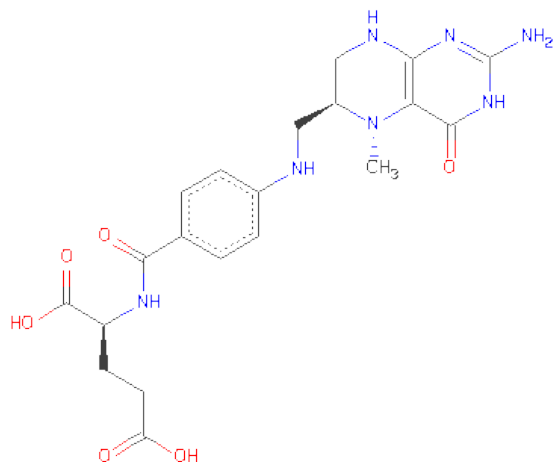
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	TYR	-	EXPRESSION TAG	UNP Q9X112
A	-6	PHE	-	EXPRESSION TAG	UNP Q9X112
A	-5	GLN	-	EXPRESSION TAG	UNP Q9X112
A	-4	GLY	-	EXPRESSION TAG	UNP Q9X112
A	-3	ILE	-	EXPRESSION TAG	UNP Q9X112
A	-2	ASP	-	EXPRESSION TAG	UNP Q9X112
A	-1	PRO	-	EXPRESSION TAG	UNP Q9X112
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	GLY	-	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).



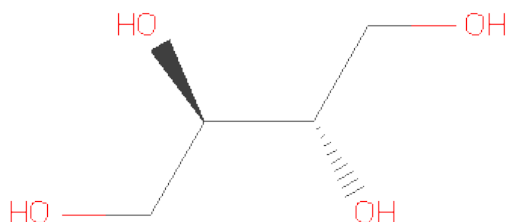
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 5-METHYL-5,6,7,8-TETRAHYDROFOLICACID (three-letter code: C2F) (formula: C₂₀H₂₅N₇O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	20	7	6		
3	B	1	Total	C	N	O	0	0
			33	20	7	6		

- Molecule 4 is MESO-ERYTHRITOL (three-letter code: MRY) (formula: C₄H₁₀O₄).



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

- Molecule 5 is water.

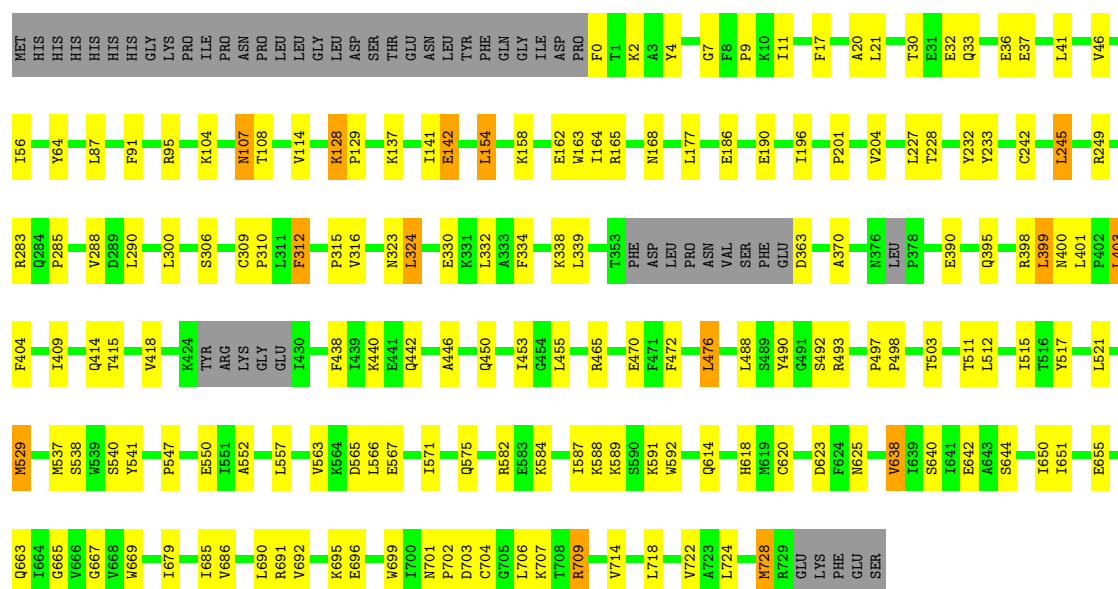
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	124	Total	O	0	0
			124	124		
5	B	114	Total	O	0	0
			114	114		

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.

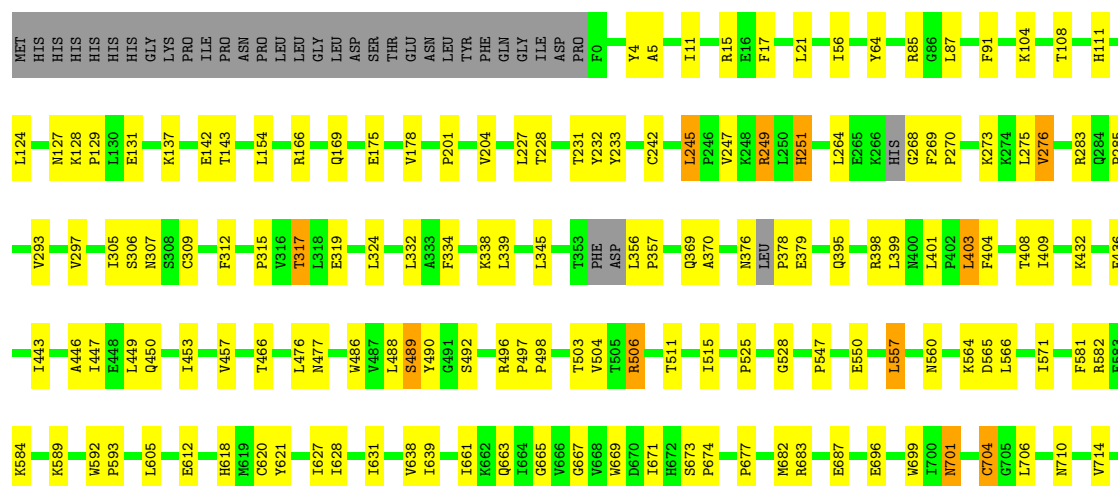
- Molecule 1: 5-methyltetrahydropteroyltriglutamate--homocysteinemethyltransferase

Chain A:



- Molecule 1: 5-methyltetrahydropteroyltriglutamate--homocysteinemethyltransferase

Chain B:



L718	R719	N720	A725	R729	E730	K731	PHE	GLU	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	164.06Å 159.01Å 64.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.35 19.95 – 2.07	Depositor EDS
% Data completeness (in resolution range)	97.5 (19.95-2.35) 95.9 (19.95-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.07Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.254 0.206 , 0.252	Depositor DCC
R_{free} test set	3465 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.0	EDS
Estimated twinning fraction	0.049 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 98786 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11505	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C2F, 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	0.36	0/5674	0.56	0/7722
1	B	0.36	0/5780	0.58	1/7869 (0.0%)
All	All	0.36	0/11454	0.57	1/15591 (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	B	528	GLY	N-CA-C	-6.03	98.03	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5535	0	5241	106	0
1	B	5640	0	5335	95	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	33	0	23	1	0
3	B	33	0	23	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	8	0	10	0	0
4	B	8	0	10	0	0
5	A	124	0	0	5	0
5	B	114	0	0	2	0
All	All	11505	0	10642	203	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (203) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:107:ASN:HD22	1:A:107:ASN:H	1.22	0.84
1:A:21:LEU:HD23	1:A:492:SER:HB3	1.61	0.82
1:B:403:LEU:O	1:B:729:ARG:HD3	1.83	0.78
1:B:557:LEU:HD23	1:B:605:LEU:HD21	1.69	0.75
1:A:114:VAL:HG11	1:A:158:LYS:HD2	1.69	0.74
1:A:37:GLU:O	1:A:41:LEU:HD13	1.90	0.72
1:B:449:LEU:O	1:B:453:ILE:HG12	1.91	0.71
1:A:201:PRO:O	1:A:204:VAL:HG22	1.89	0.71
1:A:283:ARG:HG3	1:A:309:CYS:SG	2.34	0.68
1:A:669:TRP:CH2	1:A:706:LEU:HD11	2.29	0.67
1:B:683:ARG:O	1:B:687:GLU:HG3	1.94	0.67
1:A:56:ILE:N	1:A:56:ILE:HD12	2.10	0.67
1:A:20:ALA:HB2	1:A:37:GLU:HG2	1.76	0.66
1:B:665:GLY:HA2	1:B:699:TRP:HB2	1.76	0.66
1:A:706:LEU:HD23	5:A:1011:HOH:O	1.96	0.65
1:A:679:ILE:HG23	1:A:724:LEU:HB2	1.79	0.64
1:A:512:LEU:HD11	1:A:565:ASP:HB3	1.78	0.64
1:B:638:VAL:HG22	1:B:663:GLN:HB2	1.80	0.64
1:A:186:GLU:O	1:A:190:GLU:HG3	1.97	0.64
1:B:4:TYR:HB2	1:B:306:SER:HB3	1.80	0.64
1:A:691:ARG:HG3	1:A:692:VAL:HG23	1.80	0.62
1:B:127:ASN:O	1:B:131:GLU:HG3	1.99	0.62
3:B:1201:C2F:O4	3:B:1201:C2F:H112	2.01	0.61
3:A:1200:C2F:H112	3:A:1200:C2F:O4	2.01	0.61
1:A:669:TRP:CE3	1:A:702:PRO:HB3	2.35	0.61
1:A:538:SER:HB3	1:A:584:LYS:HD2	1.83	0.61
1:A:644:SER:HA	1:A:685:ILE:HD13	1.83	0.61
1:B:232:TYR:O	1:B:233:TYR:HB2	2.01	0.60
1:A:618:HIS:CE1	1:A:704:CYS:SG	2.93	0.60
1:B:376:ASN:C	1:B:378:PRO:HD3	2.21	0.60
1:A:163:TRP:HB3	1:A:165:ARG:HG3	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:701:ASN:HB2	1:A:702:PRO:HD2	1.84	0.60
1:A:30:THR:HG23	1:A:33:GLN:OE1	2.01	0.59
1:A:667:GLY:HA2	1:A:701:ASN:O	2.02	0.59
1:B:432:LYS:O	1:B:436:GLU:HG3	2.02	0.59
1:B:581:PHE:HE2	1:B:631:ILE:HD12	1.66	0.59
1:B:571:ILE:HD12	1:B:571:ILE:N	2.19	0.58
1:A:232:TYR:O	1:A:233:TYR:HB2	2.04	0.58
1:A:107:ASN:ND2	1:A:587:ILE:HD11	2.19	0.58
1:B:283:ARG:HG2	1:B:309:CYS:SG	2.44	0.57
1:B:557:LEU:CD2	1:B:605:LEU:HD21	2.35	0.57
1:B:627:ILE:HD12	1:B:631:ILE:HD11	1.87	0.57
1:B:15:ARG:HG3	1:B:15:ARG:HH11	1.70	0.56
1:A:128:LYS:NZ	1:A:128:LYS:HB2	2.21	0.56
1:A:571:ILE:N	1:A:571:ILE:HD12	2.20	0.56
1:A:709:ARG:HA	1:A:709:ARG:NE	2.20	0.56
1:B:582:ARG:HB3	1:B:621:TYR:CZ	2.41	0.56
1:B:137:LYS:HD3	1:B:142:GLU:OE2	2.06	0.56
1:A:228:THR:HG23	1:A:249:ARG:HG3	1.87	0.55
1:A:665:GLY:HA2	1:A:699:TRP:HB2	1.87	0.55
1:B:270:PRO:HB2	1:B:273:LYS:HG2	1.89	0.53
1:A:409:ILE:HG22	1:A:575:GLN:OE1	2.09	0.53
1:A:404:PHE:CD2	1:A:728:MET:HB3	2.44	0.53
1:A:511:THR:O	1:A:515:ILE:HG12	2.07	0.53
1:A:32:GLU:O	1:A:36:GLU:HG3	2.09	0.53
1:A:686:VAL:O	1:A:690:LEU:HG	2.09	0.53
1:A:154:LEU:HD13	1:A:177:LEU:HD22	1.90	0.52
1:B:231:THR:H	1:B:251:HIS:HD2	1.57	0.52
1:B:395:GLN:O	1:B:399:LEU:HD23	2.09	0.52
1:B:571:ILE:HD12	1:B:571:ILE:H	1.74	0.52
1:B:443:ILE:O	1:B:447:ILE:HG12	2.10	0.52
1:A:4:TYR:HB2	1:A:306:SER:HB3	1.90	0.52
1:B:725:ALA:O	1:B:729:ARG:HG3	2.10	0.51
1:A:453:ILE:HG22	1:A:722:VAL:HG21	1.92	0.51
1:B:486:TRP:CE3	1:B:496:ARG:HG3	2.45	0.51
1:A:168:ASN:HB3	1:B:589:LYS:O	2.11	0.51
1:A:638:VAL:HB	1:A:663:GLN:HB2	1.91	0.51
1:A:547:PRO:HG2	1:A:550:GLU:HB2	1.93	0.51
1:B:315:PRO:HB2	1:B:334:PHE:CD2	2.46	0.50
1:B:166:ARG:HB2	1:B:169:GLN:OE1	2.11	0.50
1:A:288:VAL:O	1:A:290:LEU:HD22	2.12	0.50
1:A:644:SER:HA	1:A:685:ILE:CD1	2.42	0.50
1:A:104:LYS:HE3	1:A:108:THR:O	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:517:TYR:CE1	1:A:521:LEU:HD11	2.47	0.49
1:B:682:MET:HE1	1:B:720:ASN:HB3	1.95	0.49
1:A:0:PHE:HE1	1:A:2:LYS:HB2	1.77	0.49
1:A:228:THR:OG1	1:A:249:ARG:HD2	2.11	0.49
1:A:87:LEU:HD22	1:A:91:PHE:CE1	2.48	0.49
1:B:409:ILE:HD11	1:B:704:CYS:HA	1.95	0.49
1:B:201:PRO:O	1:B:204:VAL:HG22	2.12	0.49
1:A:414:GLN:NE2	1:A:707:LYS:HE2	2.28	0.49
1:B:403:LEU:HD23	1:B:404:PHE:H	1.78	0.49
1:B:566:LEU:O	1:B:571:ILE:HD13	2.13	0.49
1:B:251:HIS:HA	1:B:276:VAL:HG13	1.95	0.49
1:B:175:GLU:O	1:B:178:VAL:HG22	2.13	0.48
1:B:661:ILE:HG13	5:B:960:HOH:O	2.13	0.48
1:B:399:LEU:HB3	1:B:401:LEU:HG	1.95	0.48
1:A:158:LYS:HB2	1:A:162:GLU:O	2.14	0.48
1:A:618:HIS:NE2	1:A:704:CYS:SG	2.87	0.48
1:B:669:TRP:HZ3	1:B:718:LEU:HD13	1.78	0.48
1:B:242:CYS:O	1:B:245:LEU:HB2	2.14	0.48
1:A:91:PHE:O	1:A:95:ARG:HG2	2.12	0.48
1:A:588:LYS:HD2	1:A:591:LYS:NZ	2.29	0.48
1:A:128:LYS:HZ2	1:A:128:LYS:HB2	1.79	0.48
1:B:409:ILE:HD11	1:B:704:CYS:CA	2.44	0.48
1:A:330:GLU:H	1:A:330:GLU:CD	2.17	0.47
1:B:618:HIS:NE2	1:B:620:CYS:SG	2.87	0.47
1:B:511:THR:O	1:B:515:ILE:HG12	2.15	0.47
1:A:618:HIS:ND1	1:A:640:SER:OG	2.48	0.47
1:A:623:ASP:OD2	1:A:625:ASN:HB2	2.14	0.47
1:A:30:THR:OG1	1:A:33:GLN:HG3	2.13	0.47
1:B:488:LEU:C	1:B:488:LEU:HD13	2.35	0.47
1:A:415:THR:OG1	1:A:418:VAL:HG23	2.15	0.47
1:A:107:ASN:HD22	1:A:107:ASN:N	1.99	0.46
1:B:557:LEU:HD22	1:B:605:LEU:HD11	1.97	0.46
1:A:196:ILE:HB	1:A:227:LEU:HD23	1.97	0.46
1:A:584:LYS:HG2	1:A:584:LYS:O	2.15	0.46
1:B:584:LYS:O	1:B:584:LYS:HG3	2.16	0.46
1:B:228:THR:HG23	1:B:249:ARG:HB3	1.98	0.46
1:A:128:LYS:N	1:A:129:PRO:CD	2.79	0.46
1:B:696:GLU:H	1:B:696:GLU:CD	2.19	0.46
1:B:710:ASN:O	1:B:714:VAL:HG23	2.16	0.46
1:B:714:VAL:HG12	1:B:718:LEU:HD22	1.97	0.46
1:A:415:THR:HG23	5:A:1010:HOH:O	2.16	0.46
1:A:56:ILE:CD1	1:A:56:ILE:N	2.78	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:488:LEU:HD13	1:B:489:SER:N	2.31	0.46
1:B:560:ASN:OD1	1:B:564:LYS:HE2	2.16	0.45
1:B:334:PHE:O	1:B:338:LYS:HG2	2.17	0.45
1:B:399:LEU:HD22	1:B:399:LEU:N	2.31	0.45
1:A:242:CYS:O	1:A:245:LEU:HB2	2.15	0.45
1:A:465:ARG:HH22	1:A:529:MET:HB3	1.81	0.45
1:A:11:ILE:HA	1:A:17:PHE:HB3	1.98	0.45
1:A:650:ILE:HG12	1:A:650:ILE:O	2.17	0.45
1:B:293:VAL:O	1:B:297:VAL:HG23	2.17	0.45
1:A:696:GLU:H	1:A:696:GLU:CD	2.20	0.45
1:B:11:ILE:HA	1:B:17:PHE:HB3	1.99	0.45
1:B:497:PRO:HA	1:B:498:PRO:HD3	1.82	0.44
1:B:232:TYR:O	1:B:233:TYR:CB	2.65	0.44
1:B:15:ARG:NH1	1:B:15:ARG:HG3	2.30	0.44
1:B:87:LEU:HD22	1:B:91:PHE:CE1	2.52	0.44
1:B:506:ARG:HG3	1:B:506:ARG:O	2.18	0.44
1:A:537:MET:CE	1:A:552:ALA:HB2	2.47	0.44
1:A:107:ASN:ND2	1:A:107:ASN:H	2.01	0.44
1:A:324:LEU:HD13	5:A:812:HOH:O	2.17	0.44
1:B:403:LEU:HD22	1:B:404:PHE:CD2	2.52	0.44
1:B:581:PHE:CE2	1:B:631:ILE:HD12	2.49	0.44
1:A:370:ALA:HB3	1:A:503:THR:HG21	2.00	0.44
1:A:618:HIS:NE2	1:A:620:CYS:SG	2.91	0.44
1:A:334:PHE:O	1:A:338:LYS:HG2	2.18	0.44
1:A:395:GLN:OE1	1:A:614:GLN:HG3	2.18	0.43
1:A:709:ARG:HA	1:A:709:ARG:HE	1.83	0.43
1:B:718:LEU:HD12	1:B:718:LEU:HA	1.85	0.43
1:A:315:PRO:HB2	1:A:334:PHE:CD2	2.52	0.43
1:B:669:TRP:CZ3	1:B:718:LEU:HD13	2.52	0.43
1:B:5:ALA:HA	1:B:307:ASN:OD1	2.18	0.43
1:B:21:LEU:HD23	1:B:492:SER:HB3	1.99	0.43
1:B:408:THR:HB	5:B:955:HOH:O	2.18	0.43
1:B:669:TRP:CD1	1:B:677:PRO:HG2	2.54	0.43
1:B:639:ILE:O	1:B:639:ILE:HG23	2.18	0.43
1:B:547:PRO:HG2	1:B:550:GLU:HB2	2.00	0.43
1:B:477:ASN:O	1:B:504:VAL:HA	2.19	0.43
1:B:128:LYS:N	1:B:129:PRO:CD	2.81	0.43
1:B:269:PHE:CZ	1:B:275:LEU:HB2	2.54	0.43
1:A:232:TYR:O	1:A:233:TYR:CB	2.67	0.43
1:B:671:ILE:HG21	1:B:706:LEU:HD12	2.00	0.43
1:B:247:VAL:O	1:B:273:LYS:HE3	2.19	0.42
1:A:403:LEU:HD11	1:A:695:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:438:PHE:O	1:A:442:GLN:HG2	2.19	0.42
1:B:667:GLY:HA2	1:B:701:ASN:O	2.19	0.42
1:A:706:LEU:HD12	1:A:714:VAL:HG22	2.00	0.42
1:A:440:LYS:HD2	1:A:517:TYR:CD2	2.54	0.42
1:A:490:TYR:CZ	1:A:493:ARG:HG3	2.54	0.42
1:B:111:HIS:HB2	1:B:490:TYR:HB3	2.01	0.42
1:A:158:LYS:HD3	5:A:823:HOH:O	2.19	0.42
1:A:315:PRO:HD3	1:A:541:TYR:OH	2.19	0.42
1:A:589:LYS:HA	1:A:592:TRP:CD1	2.54	0.42
1:A:455:LEU:HD13	5:A:1013:HOH:O	2.18	0.42
1:A:446:ALA:O	1:A:450:GLN:HG3	2.20	0.42
1:A:158:LYS:HA	1:A:164:ILE:HG13	2.01	0.42
1:A:309:CYS:HB2	1:A:310:PRO:HD2	2.02	0.42
1:A:7:GLY:O	1:A:312:PHE:N	2.52	0.42
1:B:582:ARG:HD3	1:B:627:ILE:HG21	2.02	0.42
1:A:472:PHE:O	1:A:476:LEU:HD13	2.19	0.41
1:B:370:ALA:HB3	1:B:503:THR:HG21	2.02	0.41
1:B:264:LEU:HD23	1:B:264:LEU:C	2.40	0.41
1:A:0:PHE:CE1	1:A:2:LYS:HB2	2.54	0.41
1:A:114:VAL:HG11	1:A:158:LYS:CD	2.44	0.41
1:B:317:THR:HG22	1:B:319:GLU:H	1.85	0.41
1:B:264:LEU:O	1:B:268:GLY:HA2	2.19	0.41
3:B:1201:C2F:C11	3:B:1201:C2F:O4	2.68	0.41
1:B:476:LEU:HD23	1:B:506:ARG:HB3	2.03	0.41
1:B:592:TRP:N	1:B:593:PRO:CD	2.83	0.41
1:A:46:VAL:HG11	1:A:141:ILE:HD13	2.02	0.41
1:B:356:LEU:HA	1:B:357:PRO:HD3	1.93	0.41
1:B:506:ARG:NH1	1:B:565:ASP:OD2	2.49	0.41
1:A:563:VAL:O	1:A:567:GLU:HG3	2.21	0.41
1:A:399:LEU:HB3	1:A:401:LEU:HG	2.03	0.41
1:B:446:ALA:O	1:B:450:GLN:HG3	2.21	0.41
1:B:457:VAL:HG22	1:B:525:PRO:HG2	2.03	0.41
1:A:497:PRO:HA	1:A:498:PRO:HD3	1.97	0.41
1:B:56:ILE:O	1:B:143:THR:HA	2.21	0.41
1:A:651:ILE:O	1:A:655:GLU:HG3	2.20	0.41
1:A:620:CYS:HB3	1:A:642:GLU:OE2	2.21	0.40
1:B:251:HIS:CA	1:B:276:VAL:HG13	2.51	0.40
1:A:9:PRO:HB2	1:A:316:VAL:HG22	2.04	0.40
1:B:376:ASN:O	1:B:378:PRO:HD3	2.21	0.40
1:B:104:LYS:HD2	1:B:108:THR:O	2.21	0.40
1:B:305:ILE:HD12	1:B:345:LEU:HD23	2.03	0.40
1:B:673:SER:HA	1:B:674:PRO:HD3	1.82	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:137:LYS:HE3	1:A:142:GLU:OE1	2.21	0.40
1:A:41:LEU:N	1:A:41:LEU:CD1	2.84	0.40
1:A:703:ASP:O	1:A:704:CYS:SG	2.80	0.40
1:A:566:LEU:O	1:A:571:ILE:HD13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	707/766 (92%)	671 (95%)	35 (5%)	1 (0%)	59	75
1	B	720/766 (94%)	690 (96%)	28 (4%)	2 (0%)	50	62
All	All	1427/1532 (93%)	1361 (95%)	63 (4%)	3 (0%)	56	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	379	GLU
1	B	64	TYR
1	A	64	TYR

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	555/687 (81%)	526 (95%)	29 (5%)	32	40
1	B	568/687 (83%)	542 (95%)	26 (5%)	37	47
All	All	1123/1374 (82%)	1068 (95%)	55 (5%)	35	44

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	128	LYS
1	A	142	GLU
1	A	154	LEU
1	A	245	LEU
1	A	285	PRO
1	A	300	LEU
1	A	312	PHE
1	A	323	ASN
1	A	324	LEU
1	A	332	LEU
1	A	339	LEU
1	A	363	ASP
1	A	390	GLU
1	A	398	ARG
1	A	399	LEU
1	A	400	ASN
1	A	403	LEU
1	A	470	GLU
1	A	476	LEU
1	A	488	LEU
1	A	529	MET
1	A	540	SER
1	A	557	LEU
1	A	582	ARG
1	A	638	VAL
1	A	709	ARG
1	A	718	LEU
1	A	728	MET
1	B	85	ARG
1	B	124	LEU
1	B	154	LEU
1	B	227	LEU
1	B	245	LEU
1	B	249	ARG
1	B	251	HIS
1	B	276	VAL
1	B	285	PRO
1	B	312	PHE
1	B	317	THR
1	B	324	LEU
1	B	332	LEU

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Mol	Chain	Res	Type
1	B	339	LEU
1	B	369	GLN
1	B	398	ARG
1	B	403	LEU
1	B	466	THR
1	B	489	SER
1	B	506	ARG
1	B	557	LEU
1	B	612	GLU
1	B	628	ILE
1	B	701	ASN
1	B	704	CYS
1	B	718	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	323	ASN
1	A	720	ASN
1	B	251	HIS
1	B	263	ASN
1	B	369	GLN
1	B	376	ASN
1	B	400	ASN
1	B	601	ASN
1	B	608	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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$
3	C2F	A	1200	-	35,35,35	1.44	2 (5%)	47,49,49	1.24	6 (12%)
2	SO4	A	1202	-	4,4,4	0.27	0	6,6,6	0.08	0
4	MRY	A	1205	-	7,7,7	0.28	0	8,8,8	0.40	0
3	C2F	B	1201	-	35,35,35	1.45	2 (5%)	47,49,49	1.22	6 (12%)
2	SO4	B	1203	-	4,4,4	0.23	0	6,6,6	0.08	0
4	MRY	B	1204	-	7,7,7	0.28	0	8,8,8	0.38	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	C2F	A	1200	-	-	0/22/35/35	0/1/3/3
2	SO4	A	1202	-	-	0/0/0/0	0/0/0/0
4	MRY	A	1205	-	-	0/8/8/8	0/0/0/0
3	C2F	B	1201	-	-	0/22/35/35	0/1/3/3
2	SO4	B	1203	-	-	0/0/0/0	0/0/0/0
4	MRY	B	1204	-	-	0/8/8/8	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1200	C2F	O4-C4	6.26	1.36	1.24
3	B	1201	C2F	O4-C4	6.26	1.36	1.24
3	B	1201	C2F	C8A-N8	2.59	1.40	1.34
3	A	1200	C2F	C8A-N8	2.58	1.40	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1200	C2F	C9-C6-N5	-3.53	107.86	111.75
3	B	1201	C2F	C9-C6-N5	-3.26	108.17	111.75
3	B	1201	C2F	C4-C4A-C8A	2.97	116.89	114.43
3	A	1200	C2F	C4-C4A-C8A	2.95	116.87	114.43
3	A	1200	C2F	C7-C6-N5	2.50	110.98	108.42
3	B	1201	C2F	C2-N1-C8A	2.46	121.10	117.61
3	A	1200	C2F	C2-N1-C8A	2.39	121.00	117.61
3	B	1201	C2F	C7-C6-N5	2.36	110.84	108.42
3	B	1201	C2F	N8-C8A-N1	2.27	119.15	115.82
3	A	1200	C2F	N8-C8A-N1	2.19	119.03	115.82
3	B	1201	C2F	NA2-C2-N3	2.10	120.17	117.86
3	A	1200	C2F	NA2-C2-N3	2.09	120.16	117.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	715/766 (93%)	-0.44	0 100 100	14, 29, 48, 68	0
1	B	728/766 (95%)	-0.50	0 100 100	13, 27, 44, 60	0
All	All	1443/1532 (94%)	-0.47	0 100 100	13, 28, 47, 68	0

There are no RSRZ outliers to report.

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	C2F	A	1200	33/33	0.18	2.07	36,46,57,58	0
4	MRY	B	1204	8/8	0.15	1.39	42,48,49,50	0
3	C2F	B	1201	33/33	0.13	0.55	33,37,47,47	0
4	MRY	A	1205	8/8	0.11	-0.03	31,39,40,40	0
2	SO4	A	1202	5/5	0.11	-0.06	27,28,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	B	1203	5/5	0.09	-0.76	31,31,32,33	0

6.5 Other polymers ⓘ

There are no such residues in this entry.