



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 01:43 AM GMT

PDB ID : 2GQ3
Title : mycobacterium tuberculosis malate synthase in complex with magnesium, malate, and coenzyme A
Authors : Anstrom, D.M.; Remington, S.J.
Deposited on : 2006-04-19
Resolution : 2.30 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>

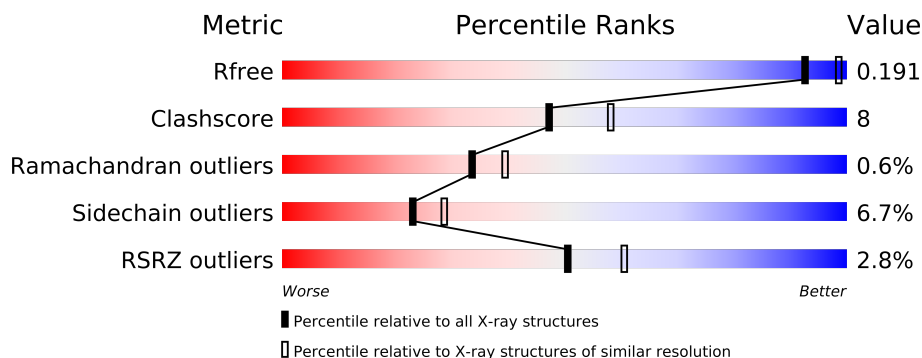
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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))
R_{free}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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 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	729	
1	B	729	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	COA	A	800	-	X
5	EPE	B	6000	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11633 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 Malate synthase G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	720	Total	C	N	O	S	0	0	0
			5487	3444	964	1057	22			
1	B	714	Total	C	N	O	S	0	0	0
			5429	3411	953	1043	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP P0A5J4
A	0	SER	-	CLONING ARTIFACT	UNP P0A5J4
B	-1	GLY	-	CLONING ARTIFACT	UNP P0A5J4
B	0	SER	-	CLONING ARTIFACT	UNP P0A5J4

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is MALATE ION (three-letter code: MLT) (formula: C₄H₆O₅).

Image for chem-comp MLT is not available.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	4	5		
3	B	1	Total	C	O	0	0
			9	4	5		

- Molecule 4 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).

Image for chem-comp COA is not available.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).

Image for chem-comp EPE is not available.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	448	Total	O	0	0
			448	448		
6	B	169	Total	O	0	0
			169	169		

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.38Å 120.38Å 238.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 2.30 49.08 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.09-2.30) 99.4 (49.08-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.178 , 0.244 0.181 , 0.191	Depositor DCC
R_{free} test set	7746 reflections (11.00%)	DCC
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 78155 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11633	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: COA, MG, EPE, MLT

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	1.17	8/5591 (0.1%)	1.07	18/7605 (0.2%)
1	B	0.98	8/5532 (0.1%)	0.96	12/7530 (0.2%)
All	All	1.08	16/11123 (0.1%)	1.02	30/15135 (0.2%)

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	2
1	B	0	4
All	All	0	6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	14	ARG	CZ-NH2	14.31	1.51	1.33
1	B	686	PHE	CG-CD1	6.75	1.48	1.38
1	B	14	ARG	NE-CZ	6.36	1.41	1.33
1	B	686	PHE	CE2-CZ	6.33	1.49	1.37
1	A	478	VAL	CB-CG1	6.24	1.66	1.52
1	B	686	PHE	CE1-CZ	6.22	1.49	1.37
1	A	37	ALA	CA-CB	6.22	1.65	1.52
1	B	726	ALA	C-O	5.91	1.34	1.23
1	A	94	GLU	CD-OE2	5.81	1.32	1.25
1	A	300	ALA	CA-CB	5.75	1.64	1.52
1	A	597	GLU	CB-CG	5.55	1.62	1.52
1	B	686	PHE	CG-CD2	5.45	1.47	1.38
1	A	679	TYR	CD1-CE1	5.41	1.47	1.39
1	A	94	GLU	CD-OE1	5.11	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	139	TYR	CD2-CE2	5.05	1.47	1.39
1	A	440	VAL	CB-CG1	5.03	1.63	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	638	ARG	NE-CZ-NH1	14.83	127.71	120.30
1	A	638	ARG	NE-CZ-NH2	-12.60	114.00	120.30
1	B	14	ARG	NE-CZ-NH1	-12.57	114.02	120.30
1	A	312	ARG	NE-CZ-NH2	-10.37	115.12	120.30
1	B	638	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	B	638	ARG	NE-CZ-NH2	-8.93	115.83	120.30
1	A	664	ARG	NE-CZ-NH1	-7.93	116.34	120.30
1	A	664	ARG	NE-CZ-NH2	7.84	124.22	120.30
1	A	638	ARG	CB-CG-CD	7.75	131.75	111.60
1	B	657	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	B	648	LEU	CA-CB-CG	7.20	131.85	115.30
1	A	4	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	B	335	LEU	CA-CB-CG	6.25	129.68	115.30
1	A	648	LEU	CA-CB-CG	6.20	129.56	115.30
1	B	717	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	614	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	670	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	283	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	595	ARG	NE-CZ-NH1	-5.87	117.37	120.30
1	A	518	MET	CG-SD-CE	-5.78	90.96	100.20
1	A	312	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	69	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	B	318	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	662	LEU	CA-CB-CG	5.56	128.09	115.30
1	B	128	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	716	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	B	688	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	A	463	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	A	82	ARG	CB-CA-C	-5.02	100.35	110.40
1	B	451	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	THR	Peptide

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Mol	Chain	Res	Type	Group
1	A	206	ASP	Peptide
1	B	183	SER	Peptide
1	B	586	GLU	Peptide
1	B	674	ALA	Peptide
1	B	675	GLY	Peptide

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	5487	0	5407	78	0
1	B	5429	0	5345	100	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	9	0	3	0	0
3	B	9	0	3	0	0
4	A	48	0	31	20	0
5	A	15	0	17	1	0
5	B	15	0	17	1	0
6	A	448	0	0	1	0
6	B	169	0	0	2	0
All	All	11633	0	10823	175	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 8.

All (175) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:206:ASP:HB2	1:A:207:LYS:HB2	1.33	1.11
1:B:11:ARG:HH21	1:B:11:ARG:HG2	1.13	1.06
1:A:631:MET:SD	4:A:800:COA:H62	2.04	0.97
1:B:204:LEU:HB3	1:B:205:PRO:HD2	1.55	0.88
1:A:206:ASP:HB2	1:A:207:LYS:CB	2.04	0.86
1:B:11:ARG:CG	1:B:11:ARG:HH21	1.89	0.86
1:A:153:GLY:HA2	1:A:155:GLU:OE1	1.76	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:11:ARG:HG2	1:B:11:ARG:NH2	1.90	0.84
1:B:145:THR:CG2	1:B:147:VAL:HG23	2.08	0.83
1:B:21:ASN:HD21	1:B:36:TRP:HE1	1.22	0.82
1:A:206:ASP:CB	1:A:207:LYS:HB2	2.09	0.82
1:B:518:MET:HG3	1:B:521:LEU:HD12	1.65	0.79
1:B:30:ILE:N	1:B:30:ILE:HD13	1.98	0.79
1:B:610:VAL:HA	1:B:691:ALA:HB1	1.65	0.78
1:B:134:ARG:O	1:B:263:GLU:HA	1.84	0.77
1:A:599:ASP:OD1	1:A:664:ARG:NH1	2.18	0.76
1:A:631:MET:CE	4:A:800:COA:C6P	2.63	0.76
1:B:145:THR:HG21	1:B:147:VAL:HG23	1.66	0.75
1:B:141:ALA:O	1:B:145:THR:HB	1.87	0.74
1:B:620:SER:OG	6:B:2179:HOH:O	2.07	0.73
1:A:631:MET:SD	4:A:800:COA:H21	2.30	0.72
1:A:631:MET:HG2	4:A:800:COA:S1P	2.30	0.71
1:A:631:MET:HE1	4:A:800:COA:H71	1.72	0.71
1:B:199:GLN:OE1	1:B:199:GLN:HA	1.90	0.70
1:B:621:LYS:HZ2	1:B:629:ALA:HB1	1.55	0.70
1:A:114:GLY:HA3	1:A:266:ILE:HD11	1.72	0.70
1:A:631:MET:CE	4:A:800:COA:H62	2.22	0.69
1:A:382:ASN:O	6:A:2801:HOH:O	2.09	0.69
1:B:30:ILE:H	1:B:30:ILE:HD13	1.58	0.69
1:B:524:ASP:O	1:B:528:THR:HG23	1.93	0.68
1:B:263:GLU:HG2	1:B:266:ILE:HD11	1.76	0.68
1:A:311:LEU:HB2	1:B:313:VAL:HG11	1.77	0.67
1:A:631:MET:SD	4:A:800:COA:C6P	2.82	0.66
1:B:621:LYS:NZ	1:B:629:ALA:HB1	2.10	0.66
1:A:668:LEU:O	1:A:672:GLN:HG3	1.95	0.66
1:A:12:ILE:HD12	1:A:36:TRP:CZ3	2.31	0.66
1:A:150:GLU:HG2	1:A:155:GLU:HA	1.77	0.65
1:A:129:ASN:HB3	4:A:800:COA:H2A	1.78	0.65
1:A:715:HIS:O	1:A:719:ARG:HG3	1.96	0.64
1:A:416:VAL:HG12	1:A:420:LEU:HD22	1.79	0.64
1:B:200:LEU:HD11	1:B:230:VAL:HG11	1.81	0.63
1:A:7:VAL:HG11	1:A:36:TRP:HB3	1.80	0.63
1:B:292:LEU:HA	1:B:371:ILE:HG23	1.81	0.63
1:B:292:LEU:HA	1:B:371:ILE:CG2	2.29	0.62
1:B:281:ALA:HB2	1:B:349:ALA:HA	1.81	0.62
1:B:145:THR:CG2	1:B:147:VAL:H	2.13	0.61
1:B:160:TYR:HE2	1:B:162:LYS:HG3	1.66	0.60
1:B:529:LYS:NZ	1:B:532:GLN:HE22	1.99	0.60
1:B:600:ASN:OD1	1:B:624:ASP:HB2	2.02	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:425:ASN:O	1:A:428:LYS:HE3	2.03	0.59
1:B:715:HIS:O	1:B:719:ARG:HG3	2.03	0.59
1:A:281:ALA:HB2	1:A:349:ALA:HA	1.85	0.59
1:B:204:LEU:HB3	1:B:205:PRO:CD	2.30	0.59
1:B:623:PRO:HA	1:B:628:VAL:O	2.03	0.59
1:B:294:LEU:HG	1:B:299:LEU:HD22	1.85	0.59
1:A:206:ASP:HB2	1:A:207:LYS:CG	2.33	0.58
1:B:599:ASP:OD1	1:B:664:ARG:NH1	2.37	0.58
1:B:425:ASN:O	1:B:428:LYS:NZ	2.29	0.57
1:A:108:GLU:CG	1:A:266:ILE:HG22	2.35	0.57
1:B:160:TYR:OH	1:B:165:GLY:HA3	2.04	0.57
1:B:265:ALA:O	1:B:334:SER:OG	2.23	0.57
1:A:631:MET:HE1	4:A:800:COA:C7P	2.35	0.57
1:A:631:MET:SD	4:A:800:COA:C2P	2.93	0.56
1:B:84:PHE:HA	1:B:87:GLU:HG2	1.88	0.56
1:A:631:MET:HE2	4:A:800:COA:C6P	2.34	0.56
1:B:206:ASP:CG	1:B:207:LYS:H	2.08	0.55
1:A:425:ASN:O	1:A:428:LYS:CE	2.54	0.55
1:B:244:ASP:O	1:B:250:GLY:HA3	2.07	0.55
1:B:19:PHE:O	1:B:23:GLU:HB2	2.05	0.55
1:A:631:MET:CG	4:A:800:COA:S1P	2.94	0.55
1:A:206:ASP:HB2	1:A:207:LYS:HG3	1.88	0.54
1:A:78:MET:HE2	1:A:576:GLU:HG3	1.89	0.54
1:B:244:ASP:O	1:B:247:SER:HB3	2.07	0.54
1:A:92:LEU:HB3	1:A:93:PRO:HD2	1.89	0.54
1:A:631:MET:CE	4:A:800:COA:C7P	2.86	0.53
1:A:312:ARG:NH2	4:A:800:COA:O7A	2.36	0.53
1:A:631:MET:HE2	4:A:800:COA:H61	1.90	0.52
1:A:519:THR:OG1	1:A:621:LYS:HD2	2.09	0.52
1:B:190:ALA:O	1:B:255:ALA:HB2	2.09	0.52
1:B:137:SER:HA	1:B:261:ILE:HD13	1.92	0.52
1:A:610:VAL:HA	1:A:691:ALA:HB1	1.92	0.51
1:B:28:THR:O	1:B:29:ASP:HB2	2.10	0.51
1:B:567:LEU:O	1:B:570:LYS:HB2	2.09	0.51
1:B:592:ASP:HA	1:B:595:ARG:HB3	1.91	0.51
1:B:676:ASP:O	1:B:679:TYR:N	2.42	0.51
1:B:213:ASN:HB3	1:B:216:GLN:HG3	1.92	0.51
1:A:631:MET:HE3	4:A:800:COA:H143	1.92	0.50
1:A:317:ASP:OD1	1:A:333:ARG:NH1	2.44	0.50
1:B:320:TYR:O	1:B:327:GLN:HA	2.11	0.50
1:A:149:PRO:HB2	1:A:151:THR:HB	1.94	0.49
1:A:663:GLU:HG2	1:A:686:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:114:GLY:CA	1:A:266:ILE:HD11	2.41	0.49
1:B:133:ALA:O	1:B:264:SER:HB2	2.12	0.49
1:A:309:ALA:O	1:B:313:VAL:HG22	2.13	0.49
1:A:631:MET:HG3	4:A:800:COA:H141	1.94	0.49
1:A:718:ARG:NH2	5:A:5000:EPE:H82	2.27	0.49
1:A:206:ASP:CA	1:A:207:LYS:HB2	2.43	0.48
1:B:128:LEU:HD12	1:B:301:ALA:HB3	1.95	0.48
1:B:411:GLU:OE1	1:B:411:GLU:HA	2.14	0.48
1:B:513:LYS:HG3	1:B:537:ALA:HB2	1.96	0.48
1:A:602:CYS:SG	1:A:662:LEU:HD13	2.54	0.48
5:B:6000:EPE:O8	5:B:6000:EPE:H52	2.13	0.48
1:B:529:LYS:HZ1	1:B:532:GLN:HE22	1.62	0.47
1:A:379:SER:OG	1:A:382:ASN:ND2	2.47	0.47
1:B:30:ILE:CD1	1:B:30:ILE:N	2.71	0.47
1:B:333:ARG:NH2	1:B:333:ARG:HB2	2.29	0.47
1:B:482:THR:HG22	1:B:482:THR:O	2.14	0.47
1:A:350:ILE:HD12	1:A:363:MET:SD	2.55	0.47
1:B:538:SER:HA	1:B:560:VAL:HG11	1.95	0.47
1:B:611:ARG:HE	1:B:620:SER:HB3	1.80	0.47
1:B:145:THR:HG22	1:B:147:VAL:H	1.79	0.46
1:B:61:GLN:OE1	1:B:470:THR:HA	2.15	0.46
1:A:311:LEU:HB2	1:B:313:VAL:CG1	2.44	0.46
1:B:145:THR:HG23	1:B:147:VAL:H	1.79	0.46
1:B:199:GLN:OE1	1:B:199:GLN:CA	2.63	0.46
1:B:206:ASP:CG	1:B:207:LYS:N	2.69	0.46
1:A:659:ARG:HD3	1:A:696:GLN:OE1	2.15	0.46
1:B:14:ARG:HG3	1:B:18:ASP:OD2	2.16	0.46
1:B:145:THR:HG23	1:B:146:ASP:N	2.31	0.46
1:A:119:VAL:CG2	1:A:120:PRO:HD2	2.46	0.45
1:A:631:MET:HE3	4:A:800:COA:CEP	2.47	0.45
1:B:666:ALA:N	1:B:667:PRO:HD2	2.32	0.45
1:B:244:ASP:CG	1:B:247:SER:HB2	2.36	0.45
1:A:455:PHE:CD1	1:A:455:PHE:C	2.90	0.45
1:A:680:ARG:O	1:A:680:ARG:HG3	2.17	0.45
1:B:200:LEU:HD23	1:B:201:VAL:N	2.32	0.44
1:A:204:LEU:HB3	1:A:205:PRO:HD2	1.99	0.44
1:A:666:ALA:HB3	1:A:667:PRO:HD3	1.99	0.44
1:A:165:GLY:O	1:A:169:ILE:HG13	2.17	0.44
1:B:682:MET:HG2	1:B:689:SER:OG	2.18	0.44
1:A:134:ARG:HD2	1:A:334:SER:HA	1.98	0.44
1:B:163:VAL:O	1:B:167:LYS:HG3	2.18	0.44
1:B:193:PHE:CE2	1:B:202:VAL:HG22	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:266:ILE:HG13	1:A:266:ILE:H	1.55	0.44
1:B:674:ALA:HA	1:B:675:GLY:HA2	1.67	0.44
1:B:403:PRO:HD2	6:B:2204:HOH:O	2.17	0.44
1:B:612:TRP:CD1	1:B:618:GLY:HA2	2.53	0.44
1:B:337:PHE:CD2	1:B:394:TYR:HB3	2.53	0.43
1:B:488:TRP:HB3	1:B:580:THR:O	2.19	0.43
1:A:594:ILE:O	1:A:598:VAL:HG23	2.18	0.43
1:A:134:ARG:O	1:A:263:GLU:HA	2.18	0.43
1:A:272:PHE:HB2	1:A:339:ARG:O	2.19	0.43
1:A:278:ALA:HA	1:A:283:ASP:HB3	2.00	0.43
1:B:469:HIS:CD2	1:B:707:ASN:HA	2.53	0.43
1:B:611:ARG:HH21	1:B:611:ARG:HG2	1.82	0.43
1:A:251:THR:HG21	1:B:158:PRO:HG2	2.00	0.42
1:B:122:LEU:HG	1:B:286:LEU:HD22	2.01	0.42
1:B:264:SER:O	1:B:266:ILE:HD12	2.18	0.42
1:A:631:MET:SD	4:A:800:COA:S1P	3.18	0.42
1:B:711:GLU:O	1:B:715:HIS:HB2	2.20	0.42
1:B:66:LYS:HE2	1:B:66:LYS:HB2	1.58	0.42
1:A:265:ALA:O	1:A:334:SER:HB2	2.19	0.42
1:A:129:ASN:HB3	4:A:800:COA:C2A	2.47	0.42
1:B:645:ALA:O	1:B:648:LEU:HB3	2.19	0.42
1:B:244:ASP:HB3	1:B:258:LYS:HB2	2.01	0.42
1:B:659:ARG:HA	1:B:659:ARG:HD2	1.78	0.42
1:A:670:ASP:OD1	1:A:679:TYR:OH	2.29	0.42
1:A:161:ASN:OD1	1:A:161:ASN:C	2.56	0.42
1:A:108:GLU:HG3	1:A:266:ILE:HG22	2.03	0.41
1:B:608:TYR:CZ	1:B:612:TRP:HD1	2.37	0.41
1:A:654:THR:O	1:A:657:ASP:HB2	2.20	0.41
1:B:21:ASN:HD22	1:B:21:ASN:N	2.17	0.41
1:B:20:VAL:HA	1:B:24:ALA:HB3	2.02	0.41
1:B:413:PHE:CD1	1:B:413:PHE:N	2.88	0.41
1:A:600:ASN:OD1	1:A:624:ASP:HB2	2.21	0.41
1:B:377:LYS:HG2	1:B:382:ASN:ND2	2.36	0.41
1:B:406:VAL:HG21	1:B:445:CYS:HB3	2.03	0.41
1:B:634:ARG:HG2	1:B:710:THR:OG1	2.20	0.40
1:A:412:LEU:O	1:A:416:VAL:HG23	2.22	0.40
1:B:484:LYS:HE3	1:B:484:LYS:HB3	1.74	0.40
1:B:65:ASP:HB3	1:B:473:GLU:HG3	2.03	0.40
1:A:31:ASP:HA	1:A:32:PRO:HD3	1.85	0.40
1:B:343:HIS:CE1	1:B:408:PHE:HD2	2.40	0.40
1:A:173:ARG:HD2	1:A:187:PHE:HB3	2.02	0.40
1:B:597:GLU:HG2	1:B:647:TRP:CH2	2.57	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	714/729 (98%)	701 (98%)	12 (2%)	1 (0%)	59	72
1	B	708/729 (97%)	670 (95%)	31 (4%)	7 (1%)	22	23
All	All	1422/1458 (98%)	1371 (96%)	43 (3%)	8 (1%)	33	39

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	LYS
1	B	586	GLU
1	B	588	ALA
1	B	207	LYS
1	B	29	ASP
1	B	15	VAL
1	B	204	LEU
1	B	73	ILE

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	575/586 (98%)	545 (95%)	30 (5%)	32	42
1	B	567/586 (97%)	521 (92%)	46 (8%)	17	20
All	All	1142/1172 (97%)	1066 (93%)	76 (7%)	23	29

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	11	ARG
1	A	12	ILE
1	A	41	LYS
1	A	49	GLN
1	A	50	ASN
1	A	71	ARG
1	A	76	ILE
1	A	82	ARG
1	A	94	GLU
1	A	129	ASN
1	A	151	THR
1	A	207	LYS
1	A	208	SER
1	A	211	LEU
1	A	251	THR
1	A	266	ILE
1	A	420	LEU
1	A	455	PHE
1	A	571	ARG
1	A	583	LEU
1	A	595	ARG
1	A	612	TRP
1	A	625	ILE
1	A	655	SER
1	A	662	LEU
1	A	677	VAL
1	A	684	PRO
1	A	688	ASP
1	A	724	ARG
1	B	6	SER
1	B	11	ARG
1	B	30	ILE
1	B	41	LYS
1	B	50	ASN
1	B	70	ARG
1	B	72	VAL
1	B	73	ILE
1	B	76	ILE
1	B	119	VAL
1	B	125	ARG
1	B	128	LEU
1	B	129	ASN

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Mol	Chain	Res	Type
1	B	142	LEU
1	B	145	THR
1	B	156	LYS
1	B	181	PRO
1	B	186	SER
1	B	209	THR
1	B	248	GLN
1	B	254	ARG
1	B	284	LYS
1	B	286	LEU
1	B	334	SER
1	B	335	LEU
1	B	356	SER
1	B	377	LYS
1	B	380	ASP
1	B	381	VAL
1	B	390	THR
1	B	455	PHE
1	B	484	LYS
1	B	518	MET
1	B	528	THR
1	B	546	THR
1	B	576	GLU
1	B	583	LEU
1	B	612	TRP
1	B	620	SER
1	B	621	LYS
1	B	631	MET
1	B	659	ARG
1	B	664	ARG
1	B	671	ARG
1	B	690	ILE
1	B	724	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	49	GLN
1	A	63	GLN
1	A	196	GLN
1	A	234	ASN

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Mol	Chain	Res	Type
1	A	340	ASN
1	A	382	ASN
1	B	21	ASN
1	B	340	ASN
1	B	382	ASN
1	B	495	HIS
1	B	532	GLN
1	B	672	GLN
1	B	673	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 ⓘ

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	EPE	A	5000	-	15,15,15	1.23	2 (13%)	20,20,20	2.22	9 (45%)
4	COA	A	800	-	50,50,50	1.68	3 (6%)	75,75,75	2.51	20 (26%)
3	MLT	A	900	2	8,8,8	1.23	1 (12%)	10,10,10	2.92	5 (50%)
5	EPE	B	6000	-	15,15,15	0.68	1 (6%)	20,20,20	2.91	9 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MLT	B	901	2	8,8,8	1.17	0	10,10,10	2.06	2 (20%)

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
5	EPE	A	5000	-	-	0/9/19/19	0/1/1/1
4	COA	A	800	-	-	1/48/64/64	0/1/3/3
3	MLT	A	900	2	1/1/3/3	0/8/8/8	0/0/0/0
5	EPE	B	6000	-	-	0/9/19/19	0/1/1/1
3	MLT	B	901	2	1/1/3/3	0/8/8/8	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	COA	O9P-C9P	9.91	1.43	1.23
5	A	5000	EPE	C10-S	3.33	1.82	1.77
4	A	800	COA	C2A-N3A	2.72	1.37	1.32
3	A	900	MLT	O2-C1	-2.26	1.22	1.30
5	A	5000	EPE	O1S-S	2.25	1.52	1.45
4	A	800	COA	P1A-O3A	2.08	1.63	1.59
5	B	6000	EPE	C10-S	2.07	1.80	1.77

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	COA	CBP-CAP-C9P	10.55	122.96	112.73
4	A	800	COA	N3A-C2A-N1A	-10.32	120.08	128.71
5	B	6000	EPE	O1S-S-C10	10.12	115.48	106.81
4	A	800	COA	C7P-N8P-C9P	7.42	137.81	122.57
3	A	900	MLT	C3-C2-C1	-7.03	100.56	109.88
3	B	901	MLT	C3-C2-C1	-5.17	103.02	109.88
4	A	800	COA	OAP-CAP-C9P	4.49	122.35	110.76
5	A	5000	EPE	C7-N4-C3	4.10	121.92	111.32
4	A	800	COA	C4A-C5A-N7A	-3.96	106.13	109.52
4	A	800	COA	C6P-C7P-N8P	3.95	120.38	111.87
5	B	6000	EPE	O3S-S-C10	-3.82	101.10	105.93
5	A	5000	EPE	C5-N4-C3	3.60	117.80	108.86
4	A	800	COA	C1B-N9A-C4A	-3.55	120.50	126.64
5	A	5000	EPE	O3S-S-O2S	-3.43	104.38	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	MLT	C2-C3-C4	3.36	119.86	112.16
5	A	5000	EPE	C9-N1-C2	3.33	119.92	111.32
5	B	6000	EPE	C7-N4-C5	3.25	119.72	111.32
5	A	5000	EPE	C7-N4-C5	3.19	119.56	111.32
5	B	6000	EPE	C5-N4-C3	3.12	116.62	108.86
3	B	901	MLT	O3-C2-C1	-2.98	103.38	110.44
4	A	800	COA	C8A-N9A-C1B	2.91	132.12	126.38
3	A	900	MLT	O3-C2-C1	-2.89	103.59	110.44
5	A	5000	EPE	O2S-S-C10	2.85	109.25	106.81
5	B	6000	EPE	C6-N1-C2	2.84	115.91	108.86
4	A	800	COA	O5P-C5P-C6P	-2.72	116.51	121.92
4	A	800	COA	C6P-C5P-N4P	2.71	121.43	116.50
4	A	800	COA	O6A-CCP-CBP	2.68	115.05	110.57
4	A	800	COA	C2A-N1A-C6A	2.47	123.23	118.77
4	A	800	COA	C4B-O4B-C1B	2.47	112.43	109.75
4	A	800	COA	C7P-C6P-C5P	2.45	116.43	112.25
4	A	800	COA	CDP-CBP-CAP	2.38	112.95	108.82
4	A	800	COA	CAP-C9P-N8P	2.34	121.59	116.57
4	A	800	COA	CEP-CBP-CCP	-2.32	105.41	108.76
5	B	6000	EPE	C7-N4-C3	2.31	117.29	111.32
5	A	5000	EPE	C9-N1-C6	2.31	117.28	111.32
5	A	5000	EPE	C6-N1-C2	2.16	114.22	108.86
5	B	6000	EPE	C5-C6-N1	-2.14	106.39	110.61
3	A	900	MLT	O2-C1-O1	-2.12	119.28	124.07
5	A	5000	EPE	C2-C3-N4	2.11	114.77	110.61
4	A	800	COA	O4B-C1B-N9A	2.08	110.37	108.44
5	B	6000	EPE	O2S-S-C10	2.06	108.58	106.81
4	A	800	COA	O8A-P3B-O3B	2.06	113.03	107.09
5	B	6000	EPE	O3S-S-O1S	-2.04	107.36	111.78
3	A	900	MLT	O3-C2-C3	2.04	114.86	109.86
4	A	800	COA	C5A-C6A-N6A	2.02	125.29	120.72

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	901	MLT	C2
3	A	900	MLT	C2

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	800	COA	CAP-C9P-N8P-C7P

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	720/729 (98%)	-0.28	1 (0%) 93 97	31, 38, 52, 75	1 (0%)
1	B	714/729 (97%)	0.17	39 (5%) 24 33	28, 39, 50, 64	0
All	All	1434/1458 (98%)	-0.06	40 (2%) 50 60	28, 38, 50, 75	1 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	245	PRO	4.4
1	B	160	TYR	4.4
1	B	158	PRO	4.3
1	B	205	PRO	4.1
1	B	588	ALA	3.9
1	B	678	ALA	3.9
1	B	247	SER	3.7
1	B	2	THR	3.6
1	B	204	LEU	3.5
1	B	679	TYR	3.4
1	B	251	THR	3.3
1	B	677	VAL	3.2
1	B	248	GLN	3.2
1	B	726	ALA	3.2
1	B	252	THR	3.2
1	B	166	ASP	3.1
1	B	11	ARG	3.0
1	B	607	GLY	3.0
1	B	169	ILE	3.0
1	B	157	GLY	2.8
1	B	203	ALA	2.8
1	B	187	PHE	2.7
1	B	674	ALA	2.7
1	B	141	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	159	THR	2.6
1	B	686	PHE	2.6
1	B	681	PRO	2.5
1	B	148	ILE	2.5
1	B	249	VAL	2.4
1	B	171	TYR	2.4
1	B	665	MET	2.4
1	B	259	ASP	2.3
1	B	168	VAL	2.3
1	B	627	ASP	2.3
1	B	683	ALA	2.2
1	B	671	ARG	2.1
1	B	202	VAL	2.1
1	A	353	THR	2.1
1	B	667	PRO	2.1
1	B	143	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

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
5	EPE	B	6000	15/15	0.18	2.40	80,93,97,97	0
4	COA	A	800	48/48	0.23	2.32	23,41,52,56	48
3	MLT	A	900	9/9	0.18	1.02	19,23,43,49	0
2	MG	B	1001	1/1	0.15	0.51	37,37,37,37	0
2	MG	A	1000	1/1	0.17	-0.24	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	A	1002	1/1	0.08	-0.29	40,40,40,40	0
3	MLT	B	901	9/9	0.12	-0.32	29,37,49,53	0
5	EPE	A	5000	15/15	0.12	-0.45	52,55,61,62	0
2	MG	B	1003	1/1	0.05	-2.69	76,76,76,76	0

6.5 Other polymers ⓘ

There are no such residues in this entry.