



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2017 – 01:48 PM EDT

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 : unknown  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

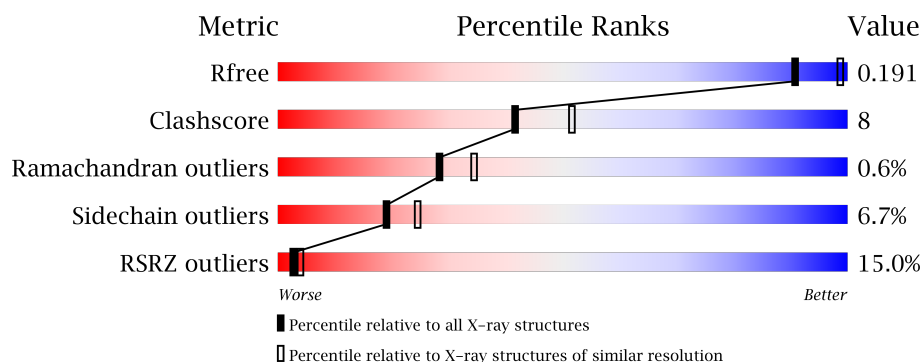
# 1 Overall quality at a glance

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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	729	<div> <div>11%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	B	729	<div> <div>19%</div> <div>73%</div> <div>21%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MLT	A	900	X	-	-	-
3	MLT	B	901	X	-	-	-

## 2 Entry composition

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

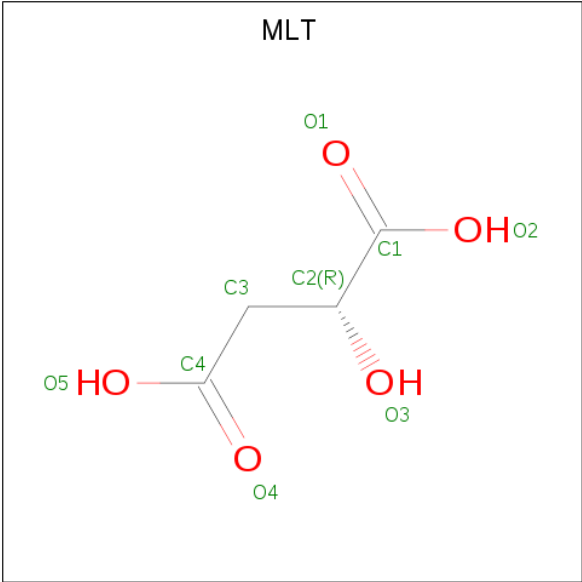
There are 4 discrepancies between the modelled and reference sequences:

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).

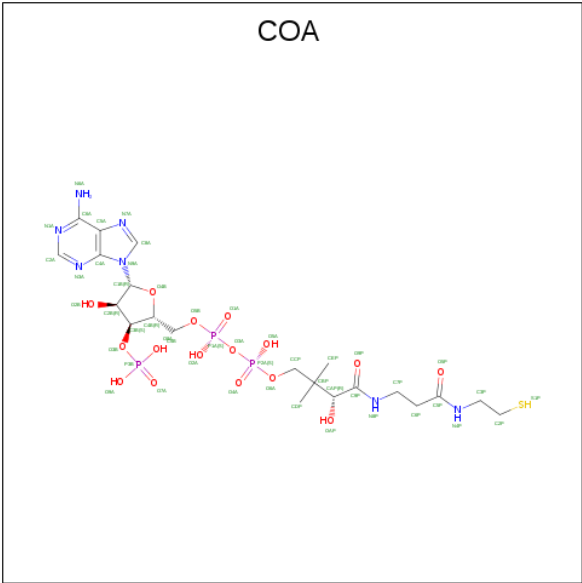
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is D-MALATE (three-letter code: MLT) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>5</sub>).



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		

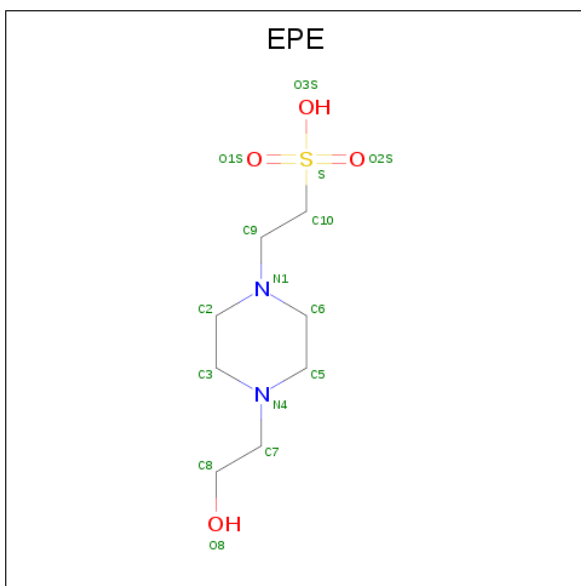
- Molecule 4 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).



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-PIPERAZINE ETHANESULFONIC ACID

(three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



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		

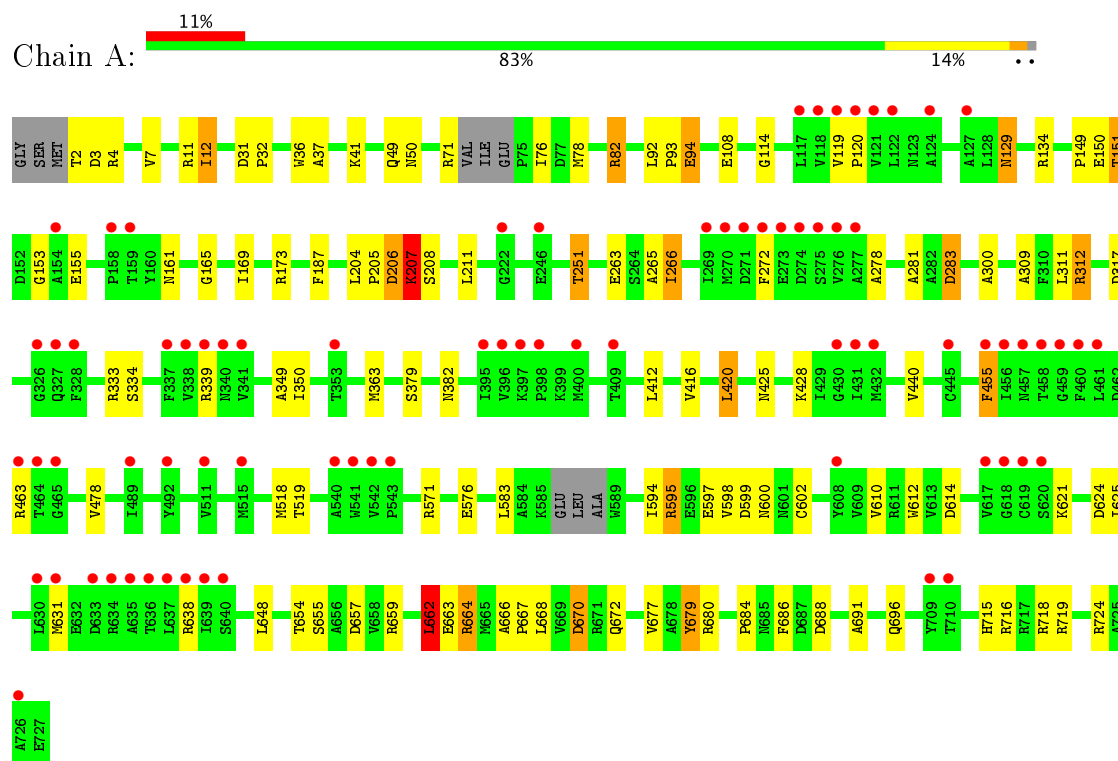
- Molecule 6 is water.

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

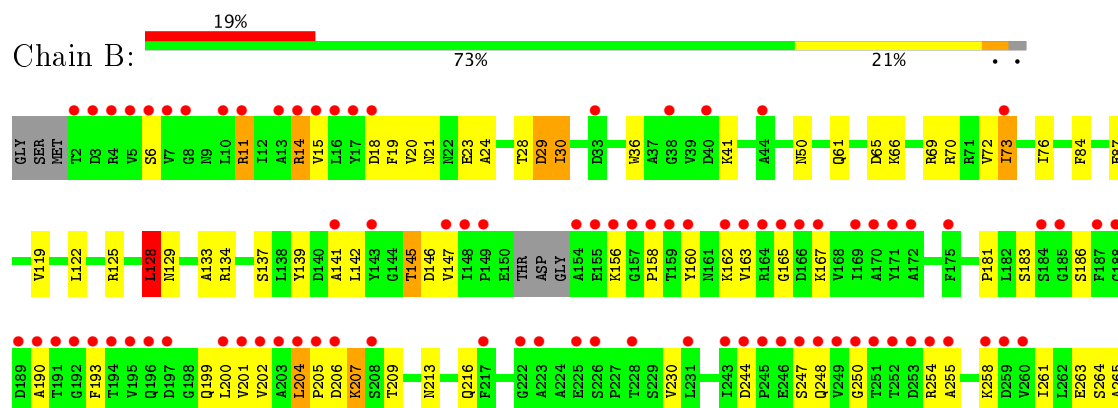
### 3 Residue-property plots [i](#)

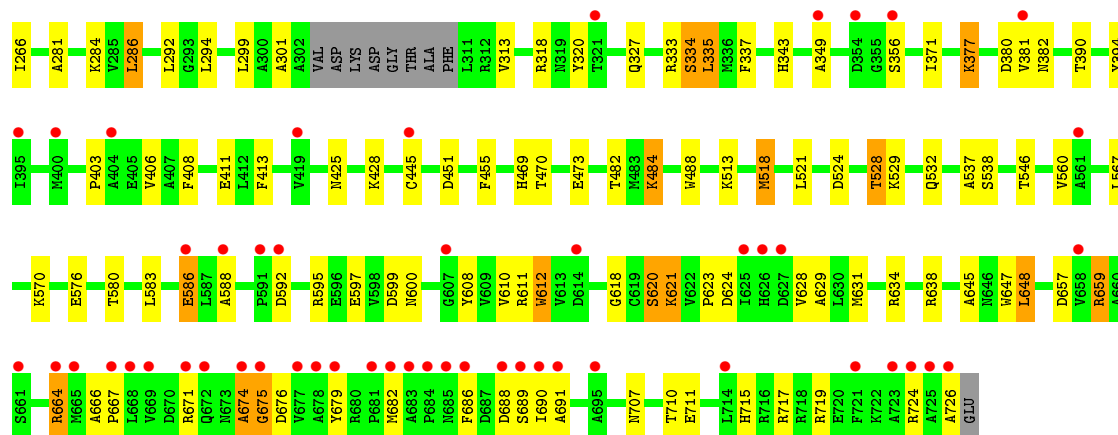
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



#### • Molecule 1: Malate synthase G







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.38 Å   120.38 Å   238.89 Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.97 (at 2.29 Å)	Xtriage
Refinement program	REFMAC	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 <sup>2</sup> )	36.4	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11633	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 ⓘ

### 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 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	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

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 (175) 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: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	Interatomic distance (Å)	Clash overlap (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:A:668:LEU:O	1:A:672:GLN:HG3	1.95	0.66
1:B:621:LYS:NZ	1:B:629:ALA:HB1	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:ASN:OD1	1:B:624:ASP:HB2	2.02	0.59
1:A:425:ASN:O	1:A:428:LYS:HE3	2.03	0.59
1:A:281:ALA:HB2	1:A:349:ALA:HA	1.85	0.59
1:B:715:HIS:O	1:B:719:ARG:HG3	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:718:ARG:NH2	5:A:5000:EPE:H82	2.27	0.49
1:A:631:MET:HG3	4:A:800:COA:H141	1.94	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:A:602:CYS:SG	1:A:662:LEU:HD13	2.54	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
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:A:659:ARG:HD3	1:A:696:GLN:OE1	2.15	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: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:A:204:LEU:HB3	1:A:205:PRO:HD2	1.99	0.44
1:B:200:LEU:HD23	1:B:201:VAL:N	2.32	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:A:134:ARG:HD2	1:A:334:SER:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:682:MET:HG2	1:B:689:SER:OG	2.18	0.44
1:A:266:ILE:H	1:A:266:ILE:HG13	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:66:LYS:HE2	1:B:66:LYS:HB2	1.58	0.42
1:B:711:GLU:O	1:B:715:HIS:HB2	2.20	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:A:670:ASP:OD1	1:A:679:TYR:OH	2.29	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: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:N	1:B:21:ASN:HD22	2.17	0.41
1:B:20:VAL:HA	1:B:24:ALA:HB3	2.02	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:413:PHE:CD1	1:B:413:PHE:N	2.88	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:A:31:ASP:HA	1:A:32:PRO:HD3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ASP:HB3	1:B:473:GLU:HG3	2.03	0.40
1:A:173:ARG:HD2	1:A:187:PHE:HB3	2.02	0.40
1:B:343:HIS:CE1	1:B:408:PHE:HD2	2.40	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 [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	714/729 (98%)	701 (98%)	12 (2%)	1 (0%)	55	67
1	B	708/729 (97%)	670 (95%)	31 (4%)	7 (1%)	18	20
All	All	1422/1458 (98%)	1371 (96%)	43 (3%)	8 (1%)	28	34

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 [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	575/586 (98%)	545 (95%)	30 (5%)	27	36
1	B	567/586 (97%)	521 (92%)	46 (8%)	14	17
All	All	1142/1172 (97%)	1066 (93%)	76 (7%)	19	24

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 [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](#)

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	1.31	2 (13%)	18,20,20	2.35	9 (50%)
4	COA	A	800	-	43,50,50	1.79	3 (6%)	48,75,75	2.51	15 (31%)
3	MLT	A	900	2	2,8,8	0.95	0	4,10,10	4.99	4 (100%)
5	EPE	B	6000	-	15,15,15	0.73	1 (6%)	18,20,20	3.09	8 (44%)
3	MLT	B	901	2	2,8,8	0.68	0	4,10,10	3.51	2 (50%)

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	-	-	1/44/64/64	0/3/3/3
3	MLT	A	900	2	1/1/3/3	0/2/8/8	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	0/2/8/8	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	COA	C9P-N8P	2.05	1.37	1.33
5	B	6000	EPE	C10-S	2.12	1.80	1.77
5	A	5000	EPE	O1S-S	2.61	1.52	1.45
4	A	800	COA	C2A-N3A	3.22	1.37	1.32
5	A	5000	EPE	C10-S	3.41	1.82	1.77
4	A	800	COA	O9P-C9P	10.03	1.43	1.23

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	COA	N3A-C2A-N1A	-10.08	120.08	128.86
3	A	900	MLT	C3-C2-C1	-7.98	100.56	111.11
3	B	901	MLT	C3-C2-C1	-6.12	103.02	111.11
5	B	6000	EPE	O3S-S-C10	-4.03	101.10	106.06
4	A	800	COA	C1B-N9A-C4A	-3.55	120.50	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	COA	C4A-C5A-N7A	-3.40	106.13	109.41
5	A	5000	EPE	O3S-S-O2S	-3.05	104.38	111.37
4	A	800	COA	O5P-C5P-C6P	-2.93	116.51	122.01
3	B	901	MLT	O3-C2-C1	-2.69	103.38	111.46
3	A	900	MLT	O3-C2-C1	-2.62	103.59	111.46
5	B	6000	EPE	C5-C6-N1	-2.10	106.39	110.63
4	A	800	COA	CEP-CBP-CCP	-2.01	105.41	108.37
5	A	5000	EPE	C2-C3-N4	2.04	114.77	110.63
5	B	6000	EPE	O2S-S-C10	2.08	108.58	106.79
5	A	5000	EPE	C9-N1-C6	2.35	117.28	111.26
5	B	6000	EPE	C7-N4-C3	2.36	117.29	111.26
5	A	5000	EPE	C6-N1-C2	2.36	114.22	108.87
4	A	800	COA	C5A-C6A-N6A	2.36	125.29	120.47
4	A	800	COA	CDP-CBP-CAP	2.38	112.95	108.82
4	A	800	COA	CAP-C9P-N8P	2.41	121.59	116.58
4	A	800	COA	C4B-O4B-C1B	2.50	112.43	109.77
4	A	800	COA	C2A-N1A-C6A	2.55	123.23	118.77
4	A	800	COA	C7P-C6P-C5P	2.62	116.43	112.22
4	A	800	COA	O6A-CCP-CBP	2.80	115.05	110.55
3	A	900	MLT	O3-C2-C3	2.82	114.86	108.65
4	A	800	COA	C6P-C5P-N4P	2.86	121.43	116.49
5	A	5000	EPE	O2S-S-C10	2.87	109.25	106.79
5	B	6000	EPE	C6-N1-C2	3.11	115.91	108.87
5	A	5000	EPE	C7-N4-C5	3.24	119.56	111.26
5	B	6000	EPE	C7-N4-C5	3.30	119.72	111.26
5	A	5000	EPE	C9-N1-C2	3.38	119.92	111.26
5	B	6000	EPE	C5-N4-C3	3.42	116.62	108.87
5	A	5000	EPE	C5-N4-C3	3.94	117.80	108.87
4	A	800	COA	C6P-C7P-N8P	4.11	120.38	111.87
5	A	5000	EPE	C7-N4-C3	4.16	121.92	111.26
3	A	900	MLT	C4-C3-C2	4.61	119.86	113.96
4	A	800	COA	C7P-N8P-C9P	8.16	137.81	122.59
5	B	6000	EPE	O1S-S-C10	10.11	115.48	106.79

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.

3 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	5000	EPE	1	0
4	A	800	COA	20	0
5	B	6000	EPE	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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	720/729 (98%)	0.67	77 (10%) 7 9	31, 38, 52, 75	1 (0%)
1	B	714/729 (97%)	1.03	138 (19%) 1 2	28, 39, 50, 64	0
All	All	1434/1458 (98%)	0.85	215 (14%) 3 4	28, 38, 50, 75	1 (0%)

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	245	PRO	7.0
1	B	205	PRO	6.3
1	B	160	TYR	6.0
1	B	678	ALA	5.8
1	B	588	ALA	5.7
1	B	171	TYR	5.3
1	B	2	THR	5.3
1	B	251	THR	5.3
1	B	187	PHE	5.3
1	B	157	GLY	5.2
1	B	683	ALA	5.0
1	B	158	PRO	5.0
1	B	159	THR	5.0
1	B	247	SER	4.9
1	B	204	LEU	4.9
1	B	665	MET	4.7
1	B	255	ALA	4.7
1	B	252	THR	4.7
1	B	677	VAL	4.6
1	B	163	VAL	4.6
1	B	681	PRO	4.6
1	B	726	ALA	4.5
1	B	248	GLN	4.5
1	B	208	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	141	ALA	4.2
1	B	674	ALA	4.2
1	B	143	TYR	4.1
1	B	690	ILE	4.1
1	A	118	VAL	4.0
1	A	396	VAL	4.0
1	B	249	VAL	3.9
1	B	679	TYR	3.9
1	B	684	PRO	3.9
1	B	148	ILE	3.9
1	A	631	MET	3.8
1	B	203	ALA	3.8
1	B	667	PRO	3.7
1	B	3	ASP	3.7
1	B	194	THR	3.7
1	B	191	THR	3.6
1	B	169	ILE	3.6
1	A	636	THR	3.6
1	B	166	ASP	3.6
1	A	460	PHE	3.6
1	B	671	ARG	3.6
1	B	11	ARG	3.6
1	A	619	CYS	3.5
1	B	73	ILE	3.5
1	B	193	PHE	3.5
1	B	222	GLY	3.5
1	B	202	VAL	3.4
1	A	461	LEU	3.4
1	B	661	SER	3.4
1	A	275	SER	3.4
1	B	7	VAL	3.3
1	A	158	PRO	3.3
1	A	269	ILE	3.3
1	B	196	GLN	3.3
1	A	635	ALA	3.3
1	A	400	MET	3.3
1	A	398	PRO	3.3
1	B	243	ILE	3.3
1	B	259	ASP	3.2
1	B	627	ASP	3.2
1	B	10	LEU	3.2
1	A	327	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	669	VAL	3.2
1	B	688	ASP	3.2
1	B	5	VAL	3.2
1	A	120	PRO	3.2
1	B	381	VAL	3.1
1	B	607	GLY	3.1
1	A	119	VAL	3.1
1	B	149	PRO	3.1
1	B	724	ARG	3.1
1	B	206	ASP	3.1
1	B	6	SER	3.1
1	A	540	ALA	3.1
1	B	419	VAL	3.1
1	B	38	GLY	3.1
1	A	541	TRP	3.1
1	A	465	GLY	3.1
1	B	723	ALA	3.1
1	A	637	LEU	3.0
1	B	165	GLY	3.0
1	B	689	SER	3.0
1	B	184	SER	3.0
1	B	217	PHE	3.0
1	B	254	ARG	3.0
1	B	672	GLN	3.0
1	A	274	ASP	3.0
1	B	253	ASP	2.9
1	A	341	VAL	2.9
1	B	195	VAL	2.9
1	B	192	GLY	2.9
1	B	658	VAL	2.9
1	A	459	GLY	2.9
1	B	225	GLU	2.9
1	B	4	ARG	2.9
1	B	686	PHE	2.9
1	B	197	ASP	2.8
1	B	188	GLY	2.8
1	A	272	PHE	2.8
1	B	691	ALA	2.8
1	A	710	THR	2.8
1	A	276	VAL	2.8
1	A	338	VAL	2.8
1	B	15	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	13	ALA	2.7
1	B	685	ASN	2.7
1	A	456	ILE	2.7
1	B	17	TYR	2.7
1	B	725	ALA	2.7
1	A	639	ILE	2.7
1	B	154	ALA	2.7
1	A	432	MET	2.7
1	B	250	GLY	2.7
1	B	721	PHE	2.7
1	B	591	PRO	2.7
1	A	608	TYR	2.7
1	A	515	MET	2.7
1	A	339	ARG	2.6
1	B	614	ASP	2.6
1	B	223	ALA	2.6
1	B	695	ALA	2.6
1	A	431	ILE	2.6
1	A	159	THR	2.6
1	B	354	ASP	2.6
1	A	121	VAL	2.6
1	A	542	VAL	2.6
1	B	682	MET	2.6
1	A	633	ASP	2.6
1	A	455	PHE	2.5
1	B	147	VAL	2.5
1	B	190	ALA	2.5
1	B	200	LEU	2.5
1	B	231	LEU	2.5
1	B	586	GLU	2.5
1	B	14	ARG	2.5
1	B	162	LYS	2.5
1	B	164	ARG	2.5
1	A	638	ARG	2.5
1	A	617	VAL	2.5
1	A	445	CYS	2.4
1	B	201	VAL	2.4
1	A	458	THR	2.4
1	B	625	ILE	2.4
1	A	270	MET	2.4
1	A	337	PHE	2.4
1	A	543	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	630	LEU	2.4
1	A	277	ALA	2.4
1	B	675	GLY	2.4
1	A	511	VAL	2.4
1	A	430	GLY	2.4
1	A	271	ASP	2.3
1	B	8	GLY	2.3
1	A	273	GLU	2.3
1	B	349	ALA	2.3
1	A	464	THR	2.3
1	B	258	LYS	2.3
1	A	154	ALA	2.3
1	B	260	VAL	2.3
1	A	222	GLY	2.3
1	B	172	ALA	2.3
1	A	117	LEU	2.3
1	B	244	ASP	2.3
1	B	561	ALA	2.3
1	A	122	LEU	2.3
1	B	226	SER	2.3
1	A	353	THR	2.2
1	A	634	ARG	2.2
1	B	170	ALA	2.2
1	B	228	THR	2.2
1	B	668	LEU	2.2
1	A	492	TYR	2.2
1	A	709	TYR	2.2
1	B	18	ASP	2.2
1	A	640	SER	2.2
1	B	356	SER	2.2
1	A	340	ASN	2.2
1	B	714	LEU	2.2
1	B	185	GLY	2.2
1	B	33	ASP	2.2
1	B	155	GLU	2.2
1	B	44	ALA	2.2
1	B	40	ASP	2.2
1	A	397	LYS	2.1
1	A	328	PHE	2.1
1	B	592	ASP	2.1
1	B	626	HIS	2.1
1	A	326	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	618	GLY	2.1
1	A	124	ALA	2.1
1	B	175	PHE	2.1
1	A	463	ARG	2.1
1	A	489	ILE	2.1
1	B	395	ILE	2.1
1	A	726	ALA	2.1
1	A	620	SER	2.1
1	B	156	LYS	2.1
1	B	246	GLU	2.1
1	A	409	THR	2.1
1	B	189	ASP	2.1
1	B	664	ARG	2.1
1	A	457	ASN	2.1
1	A	395	ILE	2.0
1	A	127	ALA	2.0
1	B	16	LEU	2.0
1	B	400	MET	2.0
1	B	321	THR	2.0
1	B	167	LYS	2.0
1	B	445	CYS	2.0
1	A	246	GLU	2.0
1	B	404	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EPE	B	6000	15/15	0.90	0.21	0.33	80,93,97,97	0
2	MG	B	1001	1/1	0.93	0.17	0.16	37,37,37,37	0
3	MLT	B	901	9/9	0.94	0.17	0.13	29,37,49,53	0
4	COA	A	800	48/48	0.89	0.26	-0.08	23,41,52,56	48
2	MG	A	1002	1/1	0.93	0.12	-0.65	40,40,40,40	0
2	MG	B	1003	1/1	0.80	0.12	-1.28	76,76,76,76	0
5	EPE	A	5000	15/15	0.91	0.17	-1.33	52,55,61,62	0
3	MLT	A	900	9/9	0.97	0.23	-2.83	19,23,43,49	0
2	MG	A	1000	1/1	0.98	0.17	-4.80	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.