Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:20 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 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

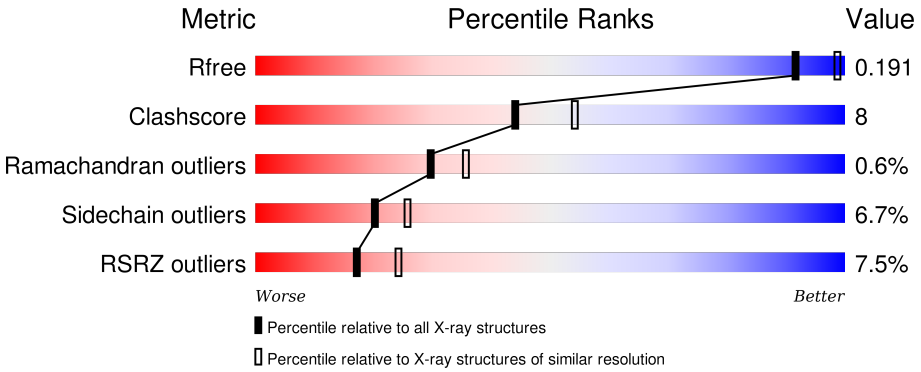
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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. 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 <=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	3% 83% 14%
1	B	729	12% 73% 21%

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
2	MG	A	1002	-	-	-	X
2	MG	B	1003	-	-	-	X
3	MLT	A	900	X	-	-	-
3	MLT	B	901	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 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			

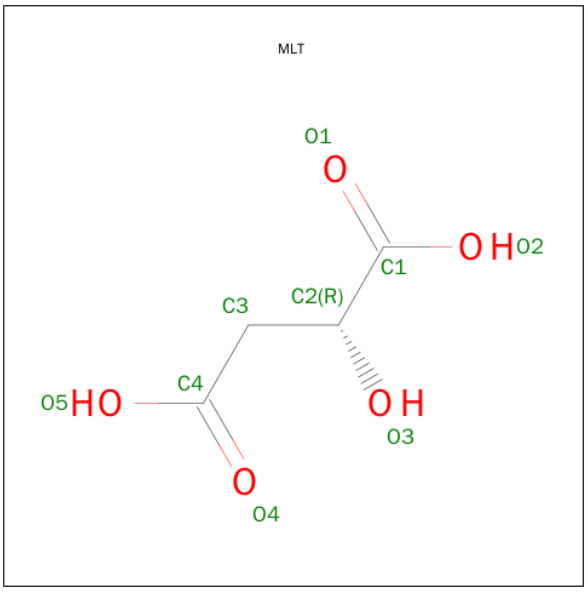
There are 4 discrepancies between the modelled and reference sequences:

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).

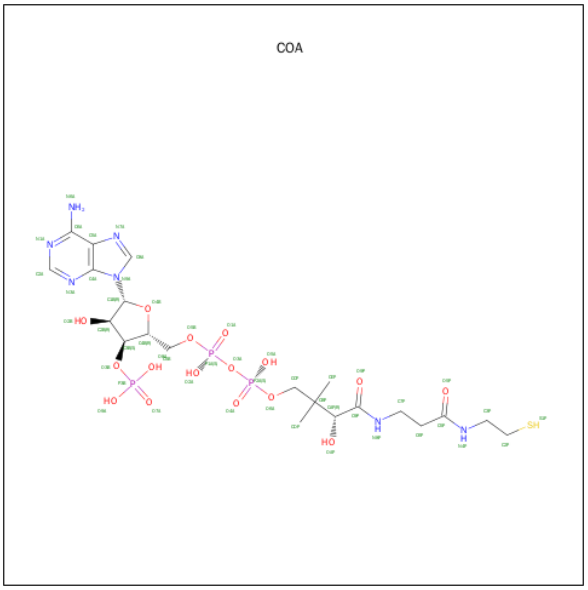
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is MALATE ION (three-letter code: MLT) (formula: $C_4H_6O_5$).



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

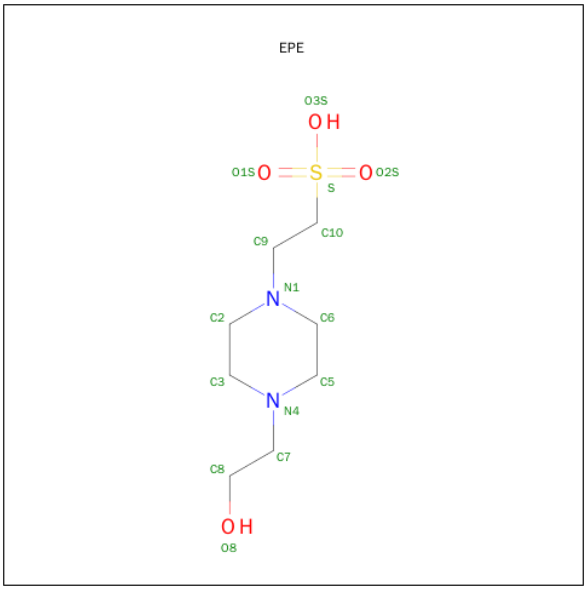
- Molecule 4 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID

(three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



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.

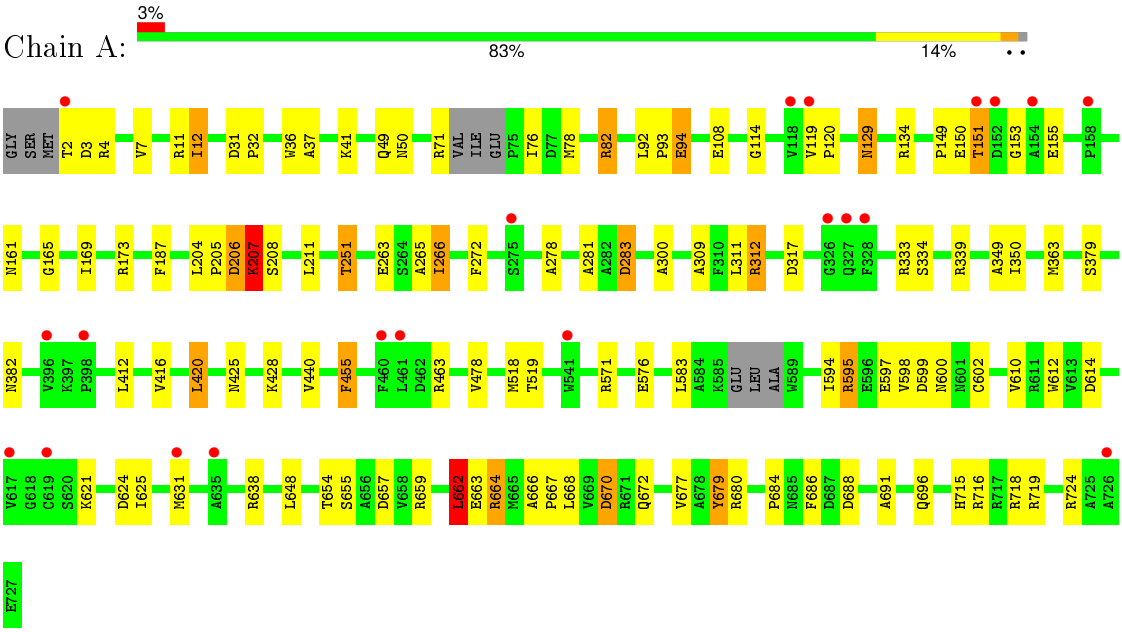
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	448	Total	O	0	0
			448	448		
6	B	169	Total	O	0	0
			169	169		

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 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.

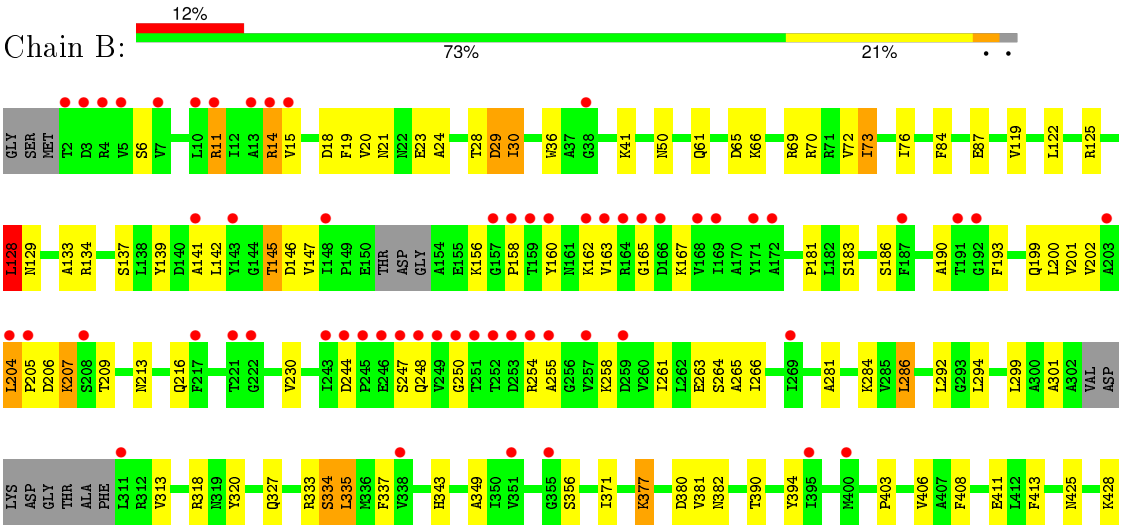
- Molecule 1: Malate synthase G

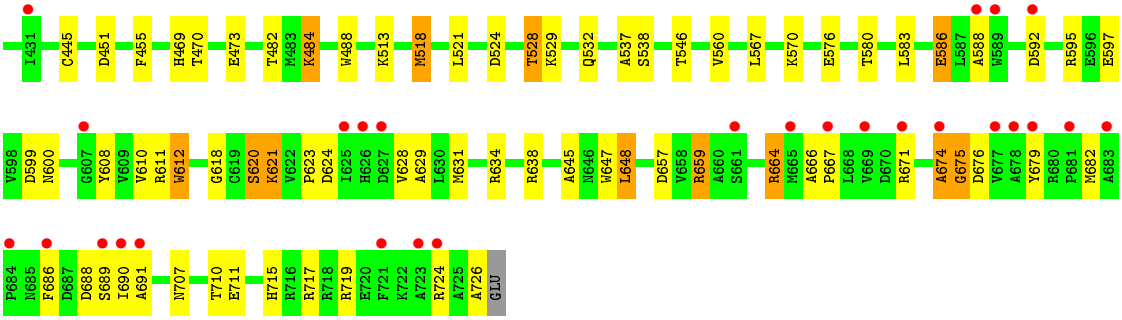
Chain A:



- Molecule 1: Malate synthase G

Chain B:




I431 C445 D451 F455 H469 T470 E473 T482 N483 K484 W488 K513 M518 L521 D524 T528 K529 Q532 A537 S538 T546 V560 L567 K570 E576 T580 L583 E586 L587 A588 W589 D592 R595 E596 E597
V598 D599 N600 G607 Y608 V609 V610 R611 W612 G618 C619 S620 K621 V622 P623 D624 I625 H626 D627 V628 A629 L630 M631 R634 R638 A645 N646 W647 L648 D657 V658 R659 A660 S661 R664 M665 A666 P667 L668 V669 D670 R671 A674 G675 D676 V677 A678 Y679 R680 P681 M682 A683
P684 N685 F686 D687 D688 S689 I690 A691 N707 T710 E711 H715 R716 R717 R718 R719 E720 F721 K722 A723 R724 A725 A726 GLU

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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)	0.30 , 44.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 78155 reflections	Xtriage
F_o,F_c correlation	0.95	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(^{o})	Ideal(^{o})
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 (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	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: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

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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: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

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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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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%)	56	68
1	B	708/729 (97%)	670 (95%)	31 (4%)	7 (1%)	19	21
All	All	1422/1458 (98%)	1371 (96%)	43 (3%)	8 (1%)	30	36

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%)	29	38
1	B	567/586 (97%)	521 (92%)	46 (8%)	15	18
All	All	1142/1172 (97%)	1066 (93%)	76 (7%)	20	26

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

There are no RNA molecules 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	-	14,15,15	0.95	1 (7%)	18,20,20	2.40	9 (50%)
4	COA	A	800	-	40,50,50	1.83	3 (7%)	50,75,75	2.72	17 (34%)
3	MLT	A	900	2	1,8,8	1.05	0	2,10,10	5.55	2 (100%)
5	EPE	B	6000	-	14,15,15	0.46	0	18,20,20	2.96	6 (33%)
3	MLT	B	901	2	1,8,8	0.93	0	2,10,10	4.44	2 (100%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	COA	C9P-N8P	2.01	1.37	1.33
5	A	5000	EPE	O1S-S	2.39	1.52	1.45
4	A	800	COA	C2A-N3A	3.03	1.37	1.32
4	A	800	COA	O9P-C9P	10.02	1.43	1.23

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	800	COA	N3A-C2A-N1A	-11.51	120.08	128.89
3	A	900	MLT	C3-C2-C1	-7.41	100.56	111.19
3	B	901	MLT	C3-C2-C1	-5.70	103.02	111.19
4	A	800	COA	C1B-N9A-C4A	-4.27	120.50	126.94
4	A	800	COA	C4A-C5A-N7A	-3.64	106.13	109.48
4	A	800	COA	C2B-C1B-N9A	-3.58	108.82	114.29
4	A	800	COA	O5P-C5P-C6P	-3.17	116.51	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	5000	EPE	O3S-S-O2S	-3.11	104.38	111.61
3	B	901	MLT	O3-C2-C1	-2.63	103.38	111.44
3	A	900	MLT	O3-C2-C1	-2.56	103.59	111.44
4	A	800	COA	CEP-CBP-CCP	-2.38	105.41	108.50
5	B	6000	EPE	C5-C6-N1	-2.37	106.39	110.63
4	A	800	COA	O3A-P2A-O6A	2.12	108.55	102.94
4	A	800	COA	CDP-CBP-CCP	2.15	111.29	108.50
4	A	800	COA	CAP-C9P-N8P	2.31	121.59	116.47
5	A	5000	EPE	C2-C3-N4	2.31	114.77	110.63
5	A	5000	EPE	C9-N1-C6	2.35	117.28	111.27
5	B	6000	EPE	C7-N4-C3	2.35	117.29	111.27
5	A	5000	EPE	C6-N1-C2	2.46	114.22	108.90
4	A	800	COA	C4B-O4B-C1B	2.47	112.43	109.72
4	A	800	COA	C7P-C6P-C5P	2.50	116.43	112.31
4	A	800	COA	C2A-N1A-C6A	2.50	123.23	118.77
5	A	5000	EPE	O2S-S-C10	2.75	109.25	106.91
4	A	800	COA	O6A-CCP-CBP	2.80	115.05	110.55
4	A	800	COA	C6P-C5P-N4P	2.86	121.43	116.46
5	A	5000	EPE	C7-N4-C5	3.23	119.56	111.27
5	B	6000	EPE	C6-N1-C2	3.24	115.91	108.90
5	B	6000	EPE	C7-N4-C5	3.30	119.72	111.27
5	A	5000	EPE	C9-N1-C2	3.38	119.92	111.27
5	B	6000	EPE	C5-N4-C3	3.57	116.62	108.90
4	A	800	COA	C6P-C7P-N8P	3.87	120.38	111.88
5	A	5000	EPE	C5-N4-C3	4.11	117.80	108.90
5	A	5000	EPE	C7-N4-C3	4.15	121.92	111.27
4	A	800	COA	OAP-CAP-C9P	5.22	122.35	110.38
4	A	800	COA	C7P-N8P-C9P	7.72	137.81	122.53
5	B	6000	EPE	O1S-S-C10	10.05	115.48	106.91

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

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, 95^{th} 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%)	0.26	21 (2%) 55 64	31, 38, 52, 75	1 (0%)
1	B	714/729 (97%)	0.64	86 (12%) 6 9	28, 39, 50, 64	0
All	All	1434/1458 (98%)	0.45	107 (7%) 17 24	28, 38, 50, 75	1 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	205	PRO	6.6
1	B	247	SER	5.2
1	B	204	LEU	5.0
1	B	251	THR	4.7
1	B	252	THR	4.5
1	B	245	PRO	4.5
1	B	588	ALA	4.3
1	B	674	ALA	4.3
1	B	679	TYR	4.1
1	B	248	GLN	4.1
1	B	38	GLY	4.0
1	B	160	TYR	4.0
1	B	678	ALA	4.0
1	B	665	MET	3.9
1	B	5	VAL	3.9
1	B	2	THR	3.8
1	B	255	ALA	3.8
1	B	11	ARG	3.7
1	B	169	ILE	3.7
1	B	158	PRO	3.6
1	B	203	ALA	3.6
1	B	187	PHE	3.6
1	B	243	ILE	3.6
1	A	327	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	157	GLY	3.5
1	B	677	VAL	3.5
1	B	191	THR	3.5
1	B	607	GLY	3.5
1	A	726	ALA	3.4
1	B	165	GLY	3.3
1	A	631	MET	3.3
1	B	166	ASP	3.3
1	B	684	PRO	3.2
1	B	143	TYR	3.2
1	B	168	VAL	3.2
1	B	250	GLY	3.1
1	B	15	VAL	3.1
1	B	3	ASP	3.1
1	A	2	THR	3.1
1	B	683	ALA	3.0
1	A	151	THR	3.0
1	B	395	ILE	3.0
1	B	253	ASP	3.0
1	B	222	GLY	2.9
1	B	269	ILE	2.9
1	B	4	ARG	2.9
1	A	152	ASP	2.9
1	A	158	PRO	2.8
1	B	257	VAL	2.8
1	B	162	LYS	2.8
1	A	154	ALA	2.8
1	B	259	ASP	2.8
1	B	686	PHE	2.8
1	B	163	VAL	2.8
1	B	148	ILE	2.8
1	B	217	PHE	2.8
1	B	208	SER	2.7
1	B	14	ARG	2.7
1	B	681	PRO	2.7
1	B	691	ALA	2.7
1	B	689	SER	2.7
1	B	249	VAL	2.7
1	A	326	GLY	2.6
1	B	244	ASP	2.6
1	B	592	ASP	2.6
1	B	246	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	328	PHE	2.5
1	B	669	VAL	2.5
1	B	254	ARG	2.5
1	B	355	GLY	2.5
1	B	667	PRO	2.5
1	B	671	ARG	2.5
1	B	171	TYR	2.4
1	A	619	CYS	2.4
1	B	724	ARG	2.4
1	A	460	PHE	2.4
1	B	141	ALA	2.4
1	B	192	GLY	2.4
1	B	627	ASP	2.4
1	B	431	ILE	2.3
1	A	635	ALA	2.3
1	A	275	SER	2.3
1	A	541	TRP	2.3
1	A	118	VAL	2.2
1	B	7	VAL	2.2
1	B	13	ALA	2.2
1	A	617	VAL	2.2
1	B	626	HIS	2.2
1	B	661	SER	2.2
1	B	221	THR	2.2
1	B	172	ALA	2.2
1	B	338	VAL	2.2
1	B	10	LEU	2.2
1	B	690	ILE	2.2
1	B	589	TRP	2.2
1	B	400	MET	2.1
1	A	396	VAL	2.1
1	A	461	LEU	2.1
1	B	311	LEU	2.1
1	B	164	ARG	2.1
1	A	398	PRO	2.1
1	B	351	VAL	2.1
1	B	159	THR	2.1
1	B	625	ILE	2.1
1	A	119	VAL	2.1
1	B	721	PHE	2.0
1	B	723	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^{th} 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(Å^2)	Q<0.9
2	MG	A	1002	1/1	0.94	0.24	6.24	40,40,40,40	0
2	MG	B	1003	1/1	0.93	0.29	4.32	76,76,76,76	0
5	EPE	B	6000	15/15	0.94	0.24	2.61	80,93,97,97	0
4	COA	A	800	48/48	0.90	0.20	-0.25	23,41,52,56	48
5	EPE	A	5000	15/15	0.93	0.13	-1.51	52,55,61,62	0
3	MLT	B	901	9/9	0.95	0.08	-2.09	29,37,49,53	0
2	MG	B	1001	1/1	0.97	0.04	-2.62	37,37,37,37	0
3	MLT	A	900	9/9	0.97	0.12	-5.41	19,23,43,49	0
2	MG	A	1000	1/1	0.98	0.08	-5.78	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.