Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:26 AM GMT

PDB ID : 3IGJ

Title : Crystal Structure of Maltose O-acetyltransferase Complexed with Acetyl Coenzyme A from Bacillus anthracis

Authors : Maltseva, N.; Kim, Y.; Papazisi, L.; Anderson, W.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)

Deposited on : 2009-07-27

Resolution : 2.60 Å(reported)

The following versions of software and data (see references (i)) 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 2.60 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.
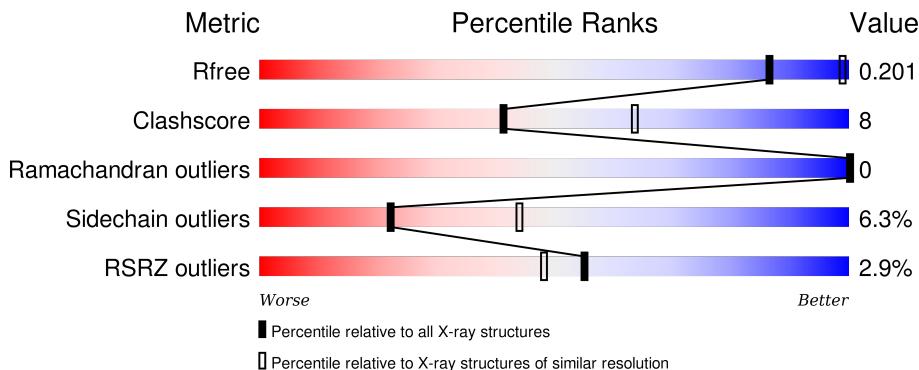
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	190	
1	B	190	
1	C	190	
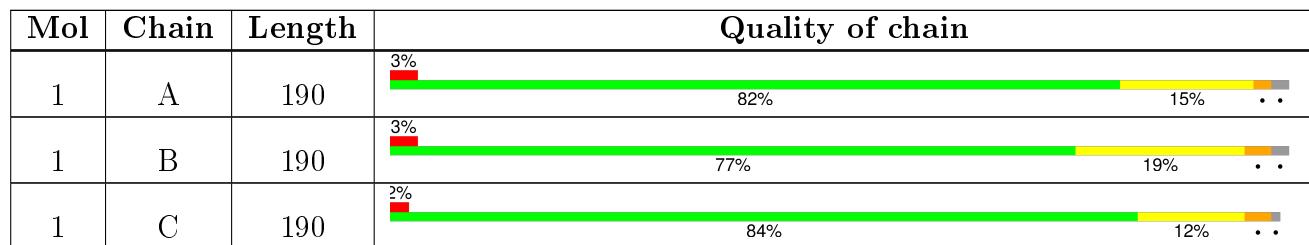
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACO	A	188	X	-	-	-
2	ACO	A	189	X	-	-	-
2	ACO	B	188	X	-	-	-
3	SO4	B	191	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4731 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 Maltose O-acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	Se	0	1	0
			1428	896	250	275	4	3			
1	B	187	Total	C	N	O	S	Se	0	3	0
			1453	910	253	282	4	4			
1	C	188	Total	C	N	O	S	Se	0	2	0
			1452	910	256	278	4	4			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q81N16
A	-1	ASN	-	EXPRESSION TAG	UNP Q81N16
A	0	ALA	-	EXPRESSION TAG	UNP Q81N16
B	-2	SER	-	EXPRESSION TAG	UNP Q81N16
B	-1	ASN	-	EXPRESSION TAG	UNP Q81N16
B	0	ALA	-	EXPRESSION TAG	UNP Q81N16
C	-2	SER	-	EXPRESSION TAG	UNP Q81N16
C	-1	ASN	-	EXPRESSION TAG	UNP Q81N16
C	0	ALA	-	EXPRESSION TAG	UNP Q81N16

- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).
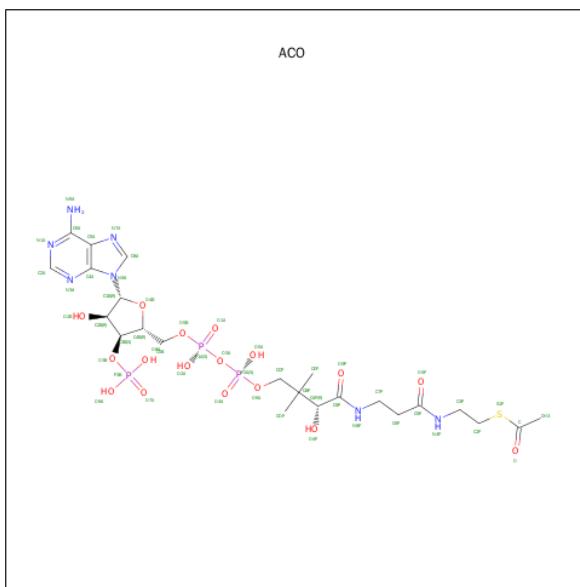
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
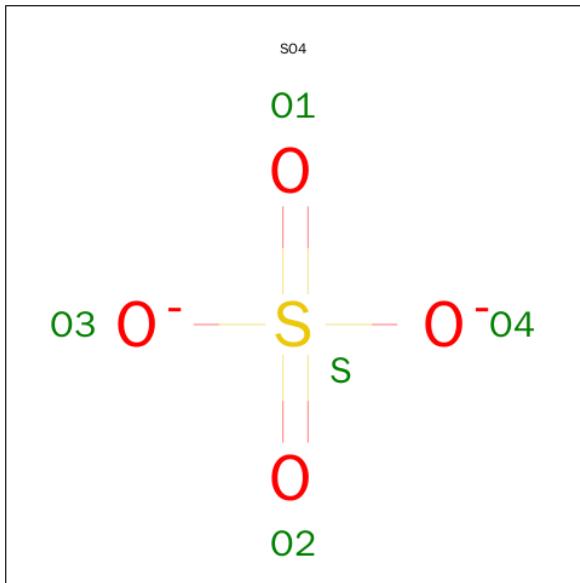
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
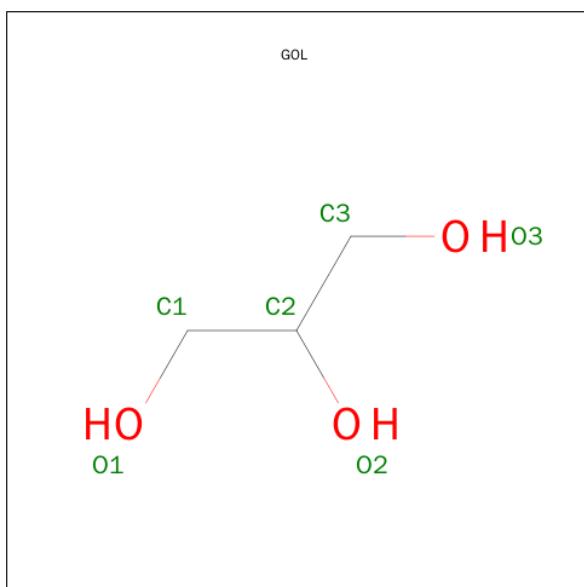
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).
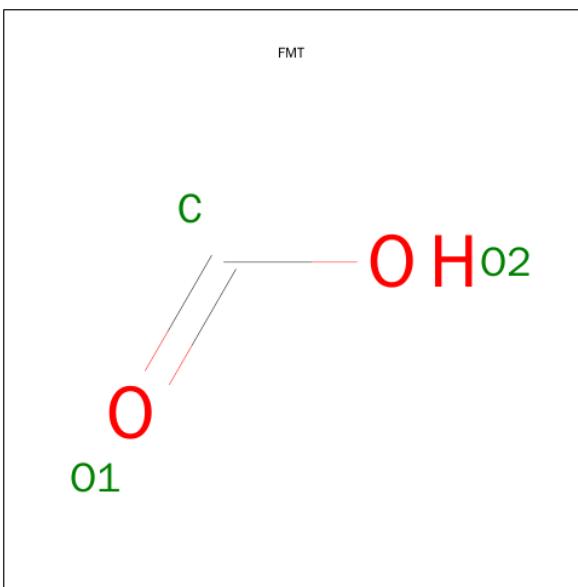
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 3	C 1	O 2	0	0
5	A	1	Total 3	C 1	O 2	0	0
5	B	1	Total 3	C 1	O 2	0	0
5	B	1	Total 3	C 1	O 2	0	0
5	B	1	Total 3	C 1	O 2	0	0
5	B	1	Total 3	C 1	O 2	0	0
5	C	1	Total 3	C 1	O 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	54	Total 54	O 54	0	0
6	B	51	Total 51	O 51	0	0
6	C	71	Total 71	O 71	0	0

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: Maltose O-acetyltransferase
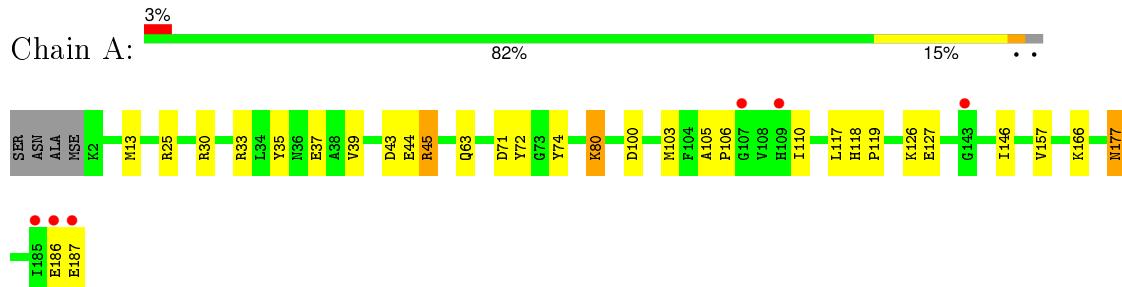
Chain A:

- Molecule 1: Maltose O-acetyltransferase

Chain B:

- Molecule 1: Maltose O-acetyltransferase

Chain C:
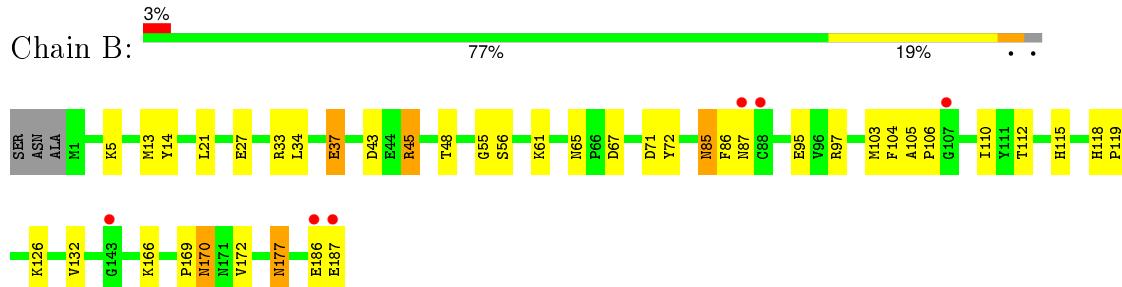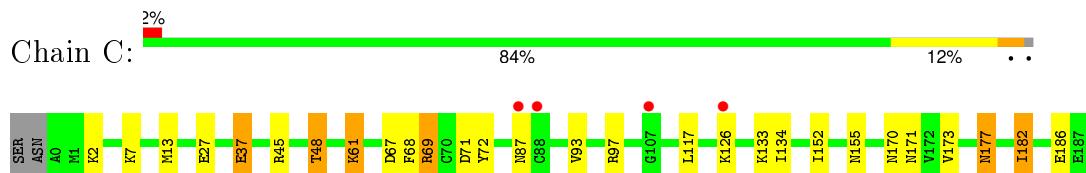
4 Data and refinement statistics (i)

| Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	121.97Å 121.97Å 142.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.59 – 2.60 41.59 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (41.59-2.60) 98.3 (41.59-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.26 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.173 , 0.213 0.171 , 0.201	Depositor DCC
R_{free} test set	1679 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	51.5	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 47.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 33137 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4731	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FMT, ACO, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.57	0/1451	0.67	0/1961
1	B	0.52	0/1476	0.64	0/1994
1	C	0.55	0/1474	0.72	1/1989 (0.1%)
All	All	0.55	0/4401	0.68	1/5944 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	69	ARG	NE-CZ-NH1	-5.77	117.42	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1428	0	1406	24	0
1	B	1453	0	1426	39	0
1	C	1452	0	1435	21	0
2	A	102	0	62	0	0
2	B	51	0	30	3	0
3	A	5	0	0	0	0
3	B	20	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	5	0	0	0	0
4	A	12	0	16	1	0
4	C	6	0	8	1	0
5	A	6	0	2	1	0
5	B	12	0	4	0	0
5	C	3	0	1	0	0
6	A	54	0	0	1	0
6	B	51	0	0	2	0
6	C	71	0	0	3	0
All	All	4731	0	4390	76	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 (76) 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:C:13:MSE:HE3	1:C:126:LYS:HB3	1.49	0.93
1:B:170:ASN:H	1:B:170:ASN:HD22	1.16	0.91
1:C:170:ASN:HB3	1:C:171:ASN:HD22	1.54	0.73
1:B:170:ASN:ND2	1:B:170:ASN:H	1.86	0.71
1:A:103:MSE:HE1	1:B:115:HIS:CE1	2.27	0.69
1:B:85:ASN:HD22	1:B:86:PHE:H	1.41	0.68
1:A:103:MSE:HE1	1:B:115:HIS:CG	2.30	0.67
1:C:67:ASP:H	1:C:87:ASN:HD22	1.43	0.66
1:A:25:ARG:HE	4:A:191:GOL:H2	1.61	0.65
1:C:117:LEU:H	4:C:189:GOL:H2	1.61	0.64
1:A:103:MSE:HE1	1:B:115:HIS:CD2	2.36	0.60
1:C:67:ASP:H	1:C:87:ASN:ND2	2.00	0.60
1:B:177:ASN:C	1:B:177:ASN:HD22	2.05	0.60
1:A:43:ASP:OD2	1:A:45:ARG:HB2	2.04	0.58
1:B:85:ASN:HD22	1:B:86:PHE:N	2.02	0.58
1:B:105:ALA:HB1	2:B:188:ACO:H31	1.86	0.57
1:A:13:MSE:HE3	1:A:126:LYS:HB3	1.86	0.57
1:C:173:VAL:HG12	1:C:182:ILE:HD11	1.87	0.57
1:B:13:MSE:HE3	1:B:126:LYS:HB2	1.87	0.56
1:A:33:ARG:NH1	1:C:37:GLU:HG2	2.21	0.56
1:B:104:PHE:CE2	1:B:110:ILE:HD11	2.40	0.56
1:B:170:ASN:N	1:B:170:ASN:ND2	2.50	0.55
1:A:71:ASP:HB3	1:A:72:TYR:CD1	2.41	0.55
1:B:85:ASN:ND2	1:B:86:PHE:H	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:THR:HG22	1:B:132:VAL:HG23	1.90	0.53
1:A:13:MSE:HE3	1:A:126:LYS:CB	2.38	0.53
1:B:43:ASP:OD2	1:B:45:ARG:HB2	2.08	0.53
1:A:103:MSE:HE1	1:B:115:HIS:ND1	2.23	0.53
1:A:63:GLN:NE2	3:B:190:SO4:O1	2.41	0.53
1:C:97[A]:ARG:HD3	6:C:231:HOH:O	2.08	0.52
1:B:65:ASN:HD22	1:B:85:ASN:ND2	2.07	0.52
1:C:177:ASN:HD22	1:C:177:ASN:C	2.13	0.52
1:B:13:MSE:HE3	1:B:126:LYS:CB	2.40	0.51
1:B:170:ASN:N	1:B:170:ASN:HD22	1.94	0.51
1:C:97[B]:ARG:NH2	1:C:133:LYS:HZ2	2.08	0.51
1:C:155:ASN:HD22	1:C:171:ASN:HD21	1.59	0.50
1:B:33:ARG:O	1:B:37[B]:GLU:HG3	2.11	0.50
1:C:71:ASP:HB3	1:C:72:TYR:CD1	2.47	0.50
1:B:71:ASP:HB3	1:B:72:TYR:CD1	2.47	0.50
1:A:37:GLU:HG3	6:A:239:HOH:O	2.13	0.49
1:A:105:ALA:HB1	1:A:106:PRO:CD	2.42	0.49
1:B:48:THR:HG23	3:B:192:SO4:O4	2.13	0.48
1:C:68:PHE:O	1:C:69:ARG:HG2	2.14	0.48
1:A:177:ASN:HD22	1:A:177:ASN:C	2.16	0.47
1:A:103:MSE:CE	1:B:115:HIS:CE1	2.96	0.47
1:C:2:LYS:HE3	1:C:7:LYS:HG2	1.97	0.47
1:B:177:ASN:C	1:B:177:ASN:ND2	2.69	0.47
1:B:104:PHE:CZ	1:B:110:ILE:HD11	2.51	0.46
1:B:14:TYR:O	1:B:126:LYS:HA	2.16	0.46
1:C:48:THR:CG2	6:C:258:HOH:O	2.63	0.45
1:C:155:ASN:HD22	1:C:171:ASN:ND2	2.14	0.45
1:A:33:ARG:NH1	1:C:37:GLU:CG	2.79	0.45
1:A:110:ILE:HD13	1:A:146:ILE:HB	1.99	0.45
1:A:187:GLU:OE1	1:B:119:PRO:HD2	2.18	0.43
1:B:105:ALA:CB	2:B:188:ACO:H31	2.49	0.43
1:B:61:LYS:HE2	6:B:218:HOH:O	2.17	0.43
1:A:35:TYR:CZ	1:A:39:VAL:CG2	3.03	0.42
2:B:188:ACO:N7A	2:B:188:ACO:OAP	2.46	0.42
1:C:61:LYS:HA	1:C:61:LYS:HD2	1.76	0.42
1:C:182:ILE:HD13	1:C:182:ILE:HG23	1.85	0.42
1:A:80:LYS:HG2	1:A:100:ASP:OD1	2.19	0.42
1:A:103:MSE:HE1	1:B:115:HIS:NE2	2.34	0.42
1:B:67:ASP:H	1:B:87:ASN:HD22	1.68	0.42
1:A:118:HIS:HA	1:A:119:PRO:HD3	1.90	0.42
1:B:169:PRO:HD2	1:B:172:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ILE:HG12	1:C:152:ILE:HG13	2.01	0.41
1:A:110:ILE:CD1	1:A:146:ILE:HD12	2.50	0.41
1:A:30:ARG:HH12	5:A:193:FMT:C	2.33	0.41
1:B:5:LYS:NZ	6:B:246:HOH:O	2.53	0.41
1:B:118:HIS:HA	1:B:119:PRO:HD3	1.75	0.41
1:B:105:ALA:HB1	1:B:106:PRO:CD	2.51	0.41
1:C:48:THR:HG22	6:C:258:HOH:O	2.21	0.41
1:B:95:GLU:OE2	1:B:97:ARG:HD2	2.22	0.40
1:B:55:GLY:O	1:B:56:SER:HB3	2.20	0.40
1:B:21:LEU:HA	1:B:21:LEU:HD23	1.75	0.40
1:B:166:LYS:HB2	1:B:166:LYS:HE2	1.79	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	185/190 (97%)	177 (96%)	8 (4%)	0	100	100
1	B	188/190 (99%)	182 (97%)	6 (3%)	0	100	100
1	C	188/190 (99%)	183 (97%)	5 (3%)	0	100	100
All	All	561/570 (98%)	542 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	153/151 (101%)	142 (93%)	11 (7%)	18	35
1	B	156/151 (103%)	145 (93%)	11 (7%)	18	36
1	C	155/151 (103%)	146 (94%)	9 (6%)	25	49
All	All	464/453 (102%)	433 (93%)	31 (7%)	22	40

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44[A]	GLU
1	A	44[B]	GLU
1	A	45	ARG
1	A	74	TYR
1	A	80	LYS
1	A	117	LEU
1	A	127	GLU
1	A	157	VAL
1	A	166	LYS
1	A	177	ASN
1	A	186	GLU
1	B	27	GLU
1	B	34	LEU
1	B	37[A]	GLU
1	B	37[B]	GLU
1	B	45	ARG
1	B	85	ASN
1	B	103	MSE
1	B	170	ASN
1	B	177	ASN
1	B	186	GLU
1	B	187	GLU
1	C	27	GLU
1	C	37	GLU
1	C	45	ARG
1	C	48	THR
1	C	61	LYS
1	C	93	VAL
1	C	177	ASN
1	C	182	ILE
1	C	186	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	177	ASN
1	B	63	GLN
1	B	85	ASN
1	B	87	ASN
1	B	147	ASN
1	B	170	ASN
1	B	177	ASN
1	C	87	ASN
1	C	171	ASN
1	C	177	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 ⓘ

19 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	ACO	A	188	-	43,53,53	4.53	22 (51%)	55,79,79	2.50	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z|$ > 2	Counts	RMSZ	#$|Z|$ > 2
2	ACO	A	189	-	43,53,53	4.62	21 (48%)	55,79,79	2.31	14 (25%)
3	SO4	A	190	-	4,4,4	0.20	0	6,6,6	0.72	0
4	GOL	A	191	-	5,5,5	0.47	0	5,5,5	0.82	0
4	GOL	A	192	-	5,5,5	0.36	0	5,5,5	0.79	0
5	FMT	A	193	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	194	-	0,2,2	0.00	-	0,1,1	0.00	-
2	ACO	B	188	-	43,53,53	4.70	21 (48%)	55,79,79	2.20	12 (21%)
3	SO4	B	189	-	4,4,4	0.27	0	6,6,6	0.59	0
3	SO4	B	190	-	4,4,4	0.21	0	6,6,6	0.43	0
3	SO4	B	191	-	4,4,4	0.06	0	6,6,6	2.15	2 (33%)
3	SO4	B	192	-	4,4,4	0.25	0	6,6,6	0.29	0
5	FMT	B	193	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	194	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	195	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	196	-	0,2,2	0.00	-	0,1,1	0.00	-
3	SO4	C	188	-	4,4,4	0.24	0	6,6,6	0.68	0
4	GOL	C	189	-	5,5,5	0.25	0	5,5,5	1.10	1 (20%)
5	FMT	C	190	-	0,2,2	0.00	-	0,1,1	0.00	-

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
2	ACO	A	188	-	1/1/12/14	1/47/67/67	0/3/3/3
2	ACO	A	189	-	1/1/12/14	1/47/67/67	0/3/3/3
3	SO4	A	190	-	-	0/0/0/0	0/0/0/0
4	GOL	A	191	-	-	0/4/4/4	0/0/0/0
4	GOL	A	192	-	-	0/4/4/4	0/0/0/0
5	FMT	A	193	-	-	0/0/0/0	0/0/0/0
5	FMT	A	194	-	-	0/0/0/0	0/0/0/0
2	ACO	B	188	-	1/1/12/14	2/47/67/67	0/3/3/3
3	SO4	B	189	-	-	0/0/0/0	0/0/0/0
3	SO4	B	190	-	-	0/0/0/0	0/0/0/0
3	SO4	B	191	-	-	0/0/0/0	0/0/0/0
3	SO4	B	192	-	-	0/0/0/0	0/0/0/0
5	FMT	B	193	-	-	0/0/0/0	0/0/0/0
5	FMT	B	194	-	-	0/0/0/0	0/0/0/0
5	FMT	B	195	-	-	0/0/0/0	0/0/0/0
5	FMT	B	196	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	C	188	-	-	0/0/0/0	0/0/0/0
4	GOL	C	189	-	-	0/4/4/4	0/0/0/0
5	FMT	C	190	-	-	0/0/0/0	0/0/0/0

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	188	ACO	O4B-C1B	-20.78	1.14	1.41
2	A	189	ACO	O4B-C1B	-20.52	1.15	1.41
2	A	188	ACO	O4B-C1B	-19.72	1.16	1.41
2	A	188	ACO	C3B-C4B	-10.49	1.22	1.52
2	A	189	ACO	C3B-C4B	-10.46	1.22	1.52
2	B	188	ACO	C3B-C4B	-10.19	1.23	1.52
2	A	189	ACO	O4B-C4B	-5.47	1.32	1.45
2	B	188	ACO	O4B-C4B	-5.31	1.32	1.45
2	A	188	ACO	O4B-C4B	-5.25	1.32	1.45
2	A	189	ACO	C5B-C4B	-4.99	1.35	1.51
2	B	188	ACO	C5B-C4B	-4.97	1.35	1.51
2	A	188	ACO	C5B-C4B	-4.95	1.35	1.51
2	A	189	ACO	C5A-C4A	-4.82	1.29	1.40
2	A	188	ACO	C5A-C4A	-4.61	1.30	1.40
2	B	188	ACO	C5A-C4A	-4.33	1.30	1.40
2	A	189	ACO	C2B-C3B	-3.69	1.44	1.53
2	A	188	ACO	C2B-C3B	-3.59	1.44	1.53
2	B	188	ACO	C8A-N7A	-3.59	1.27	1.34
2	A	189	ACO	C8A-N7A	-3.58	1.27	1.34
2	A	188	ACO	C8A-N7A	-3.46	1.28	1.34
2	B	188	ACO	C2B-C3B	-3.43	1.45	1.53
2	A	188	ACO	C6A-N1A	-2.49	1.25	1.37
2	A	189	ACO	C6A-N1A	-2.48	1.25	1.37
2	A	189	ACO	O9P-C9P	-2.30	1.18	1.23
2	A	188	ACO	O9P-C9P	-2.29	1.18	1.23
2	B	188	ACO	C6A-N1A	-2.21	1.26	1.37
2	A	188	ACO	P2A-O5A	2.03	1.63	1.54
2	A	188	ACO	P1A-O5B	2.08	1.68	1.59
2	B	188	ACO	P1A-O5B	2.23	1.69	1.59
2	A	189	ACO	P1A-O5B	2.25	1.69	1.59
2	A	188	ACO	O2B-C2B	2.30	1.48	1.43
2	A	189	ACO	P2A-O5A	2.38	1.65	1.54
2	B	188	ACO	P3B-O3B	2.43	1.67	1.60
2	B	188	ACO	O2B-C2B	2.44	1.48	1.43
2	A	188	ACO	P3B-O3B	2.49	1.67	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	189	ACO	P3B-O3B	2.60	1.67	1.60
2	B	188	ACO	P2A-O5A	2.60	1.66	1.54
2	B	188	ACO	P1A-O2A	2.74	1.66	1.54
2	A	188	ACO	P1A-O2A	2.76	1.66	1.54
2	A	189	ACO	P1A-O2A	2.79	1.66	1.54
2	A	189	ACO	P3B-O9A	3.05	1.65	1.54
2	A	188	ACO	P3B-O8A	3.10	1.65	1.54
2	B	188	ACO	P3B-O8A	3.10	1.65	1.54
2	A	188	ACO	C5A-N7A	3.15	1.50	1.39
2	B	188	ACO	P3B-O9A	3.17	1.66	1.54
2	A	189	ACO	P3B-O8A	3.20	1.66	1.54
2	A	188	ACO	P3B-O9A	3.21	1.66	1.54
2	A	189	ACO	C5A-N7A	3.27	1.50	1.39
2	A	188	ACO	C6A-N6A	3.33	1.45	1.34
2	A	189	ACO	C6A-N6A	3.44	1.45	1.34
2	B	188	ACO	C5A-N7A	3.49	1.51	1.39
2	B	188	ACO	C6A-N6A	4.04	1.47	1.34
2	A	188	ACO	C5P-N4P	5.69	1.47	1.33
2	A	189	ACO	C5P-N4P	5.83	1.47	1.33
2	B	188	ACO	C5P-N4P	5.97	1.47	1.33
2	A	188	ACO	C9P-N8P	6.44	1.47	1.33
2	A	189	ACO	C9P-N8P	6.54	1.47	1.33
2	B	188	ACO	C9P-N8P	6.85	1.48	1.33
2	A	189	ACO	C4A-N3A	7.16	1.46	1.35
2	A	189	ACO	C2A-N1A	7.21	1.47	1.33
2	A	188	ACO	C4A-N3A	7.27	1.46	1.35
2	A	188	ACO	C2A-N1A	7.67	1.48	1.33
2	B	188	ACO	C2A-N1A	7.92	1.49	1.33
2	B	188	ACO	C4A-N3A	8.05	1.47	1.35

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	188	ACO	N3A-C2A-N1A	-11.12	120.38	128.89
2	A	189	ACO	N3A-C2A-N1A	-10.01	121.23	128.89
2	B	188	ACO	N3A-C2A-N1A	-8.76	122.19	128.89
2	A	188	ACO	P2A-O3A-P1A	-5.31	117.81	132.73
2	A	189	ACO	P2A-O3A-P1A	-4.81	119.22	132.73
2	B	188	ACO	P2A-O3A-P1A	-4.58	119.86	132.73
3	B	191	SO4	O4-S-O1	-3.82	74.65	110.19
2	B	188	ACO	C3P-C2P-S1P	-3.59	101.74	111.36
2	A	188	ACO	CEP-CBP-CCP	-3.59	103.85	108.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	188	ACO	C2P-C3P-N4P	-3.07	106.22	112.36
2	A	189	ACO	C3P-C2P-S1P	-2.98	103.39	111.36
2	B	188	ACO	CEP-CBP-CCP	-2.91	104.73	108.50
2	A	188	ACO	O5P-C5P-C6P	-2.83	117.10	121.98
2	A	188	ACO	O6A-CCP-CBP	-2.65	106.28	110.55
4	C	189	GOL	O1-C1-C2	-2.15	99.76	110.18
2	A	189	ACO	CEP-CBP-CCP	-2.07	105.82	108.50
2	A	189	ACO	O9P-C9P-N8P	-2.03	119.01	123.08
2	B	188	ACO	P3B-O3B-C3B	2.01	126.39	121.56
2	B	188	ACO	C2P-S1P-C	2.01	114.30	101.83
2	A	189	ACO	O5B-C5B-C4B	2.04	116.63	109.12
2	A	189	ACO	C1B-N9A-C4A	2.05	130.04	126.94
2	B	188	ACO	CDP-CBP-CCP	2.09	111.21	108.50
2	A	189	ACO	CAP-C9P-N8P	2.13	121.19	116.47
3	B	191	SO4	O2-S-O1	2.22	116.53	109.50
2	B	188	ACO	O3A-P2A-O6A	2.34	109.15	102.94
2	A	188	ACO	C2P-S1P-C	2.34	116.34	101.83
2	A	189	ACO	CEP-CBP-CAP	2.39	113.71	109.34
2	B	188	ACO	C1B-N9A-C4A	2.46	130.65	126.94
2	A	189	ACO	O3A-P2A-O6A	2.48	109.51	102.94
2	A	188	ACO	O5B-C5B-C4B	2.49	118.29	109.12
2	A	189	ACO	O4B-C4B-C5B	2.56	118.47	109.32
2	A	189	ACO	O3A-P1A-O5B	3.07	111.08	102.94
2	A	188	ACO	O4B-C4B-C5B	3.23	120.87	109.32
2	A	188	ACO	O3A-P1A-O5B	4.01	113.56	102.94
2	B	188	ACO	C2B-C1B-N9A	4.03	120.45	114.29
2	B	188	ACO	O3A-P1A-O5B	4.15	113.95	102.94
2	A	189	ACO	C2B-C1B-N9A	4.70	121.47	114.29
2	A	188	ACO	C2B-C1B-N9A	4.76	121.57	114.29
2	A	188	ACO	O4B-C1B-N9A	7.17	123.11	108.10
2	B	188	ACO	O4B-C1B-N9A	7.20	123.16	108.10
2	A	189	ACO	O4B-C1B-N9A	7.59	123.99	108.10

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	188	ACO	C1B
2	A	189	ACO	C1B
2	A	188	ACO	C1B

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	189	ACO	O-C-S1P-C2P
2	A	188	ACO	O-C-S1P-C2P
2	B	188	ACO	CH3-C-S1P-C2P
2	B	188	ACO	O-C-S1P-C2P

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	191	GOL	1	0
5	A	193	FMT	1	0
2	B	188	ACO	3	0
3	B	190	SO4	1	0
3	B	192	SO4	1	0
4	C	189	GOL	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	183/190 (96%)	-0.04	6 (3%)	50	43	36, 50, 66, 98	0
1	B	183/190 (96%)	-0.08	6 (3%)	50	43	38, 51, 69, 112	0
1	C	184/190 (96%)	-0.25	4 (2%)	65	59	34, 45, 61, 73	0
All	All	550/570 (96%)	-0.12	16 (2%)	55	48	34, 48, 67, 112	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	187	GLU	5.2
1	A	187	GLU	4.7
1	A	186	GLU	2.6
1	A	107	GLY	2.5
1	B	107	GLY	2.5
1	A	185	ILE	2.5
1	B	88	CYS	2.5
1	C	107	GLY	2.4
1	A	143	GLY	2.4
1	A	109	HIS	2.3
1	B	87	ASN	2.2
1	B	186	GLU	2.1
1	C	88	CYS	2.1
1	C	87	ASN	2.1
1	B	143	GLY	2.1
1	C	126	LYS	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	B	191	5/5	0.88	0.51	18.79	87,87,90,96	5
3	SO4	B	190	5/5	0.89	0.19	1.73	65,82,99,114	0
4	GOL	A	191	6/6	0.96	0.21	1.72	44,58,62,72	0
2	ACO	A	189	51/51	0.85	0.19	0.87	43,82,114,129	0
2	ACO	B	188	51/51	0.81	0.21	0.73	46,94,131,153	0
4	GOL	C	189	6/6	0.88	0.20	0.35	67,79,85,86	0
3	SO4	B	189	5/5	0.91	0.18	0.14	63,81,106,116	0
3	SO4	C	188	5/5	0.95	0.12	0.02	67,69,77,102	0
2	ACO	A	188	51/51	0.89	0.16	-0.08	40,65,94,116	0
3	SO4	A	190	5/5	0.95	0.13	-0.23	51,65,91,95	0
5	FMT	B	193	3/3	0.74	0.19	-	75,75,81,83	0
5	FMT	B	196	3/3	0.66	0.26	-	85,85,88,91	0
5	FMT	A	194	3/3	0.84	0.17	-	72,72,75,79	0
3	SO4	B	192	5/5	0.91	0.40	-	77,86,119,123	0
5	FMT	B	194	3/3	0.60	0.23	-	94,94,95,96	0
5	FMT	A	193	3/3	0.77	0.25	-	79,79,79,79	3
5	FMT	B	195	3/3	0.61	0.27	-	75,75,82,86	0
4	GOL	A	192	6/6	0.72	0.22	-	80,85,91,93	0
5	FMT	C	190	3/3	0.91	0.20	-	63,63,70,73	0

6.5 Other polymers (i)

There are no such residues in this entry.