Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2024 – 07:57 pm GMT

PDB ID	:	6SE8
Title	:	Cold-adapted beta-D-galactosidase from Arthrobacter sp. 32cB mutant E441Q
Authors	:	Rutkiewicz, M.; Bujacz, A.; Bujacz, G.
Deposited on	:	2019-07-29
Resolution	:	1.83 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

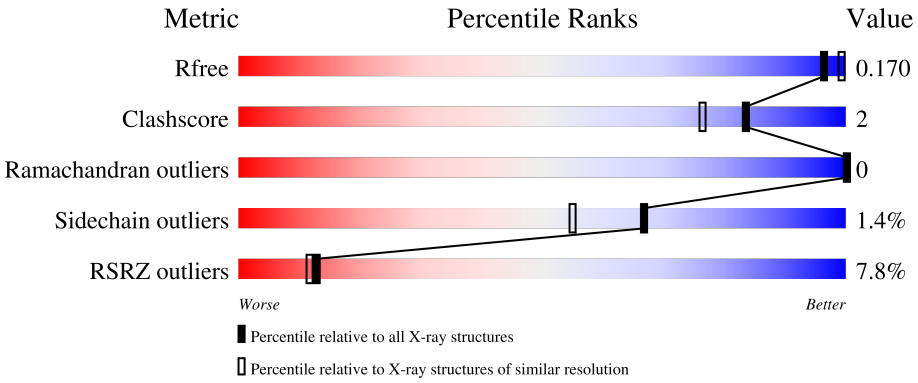
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.83 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}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	1010	8% 95%

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	ACT	A	1103	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	1104	-	-	X	-
2	ACT	A	1105	-	-	-	X
2	ACT	A	1106	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8760 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.

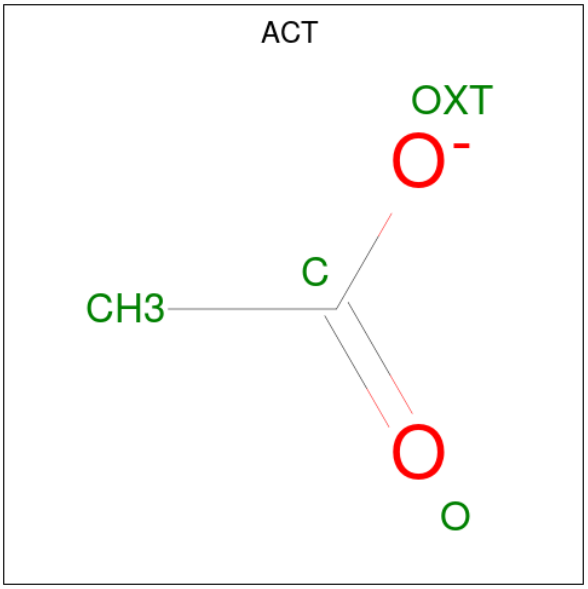
- Molecule 1 is a protein called Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1001	Total	C	N	O	S	0	18	0
			7794	4909	1393	1473	19			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	441	GLN	GLU	engineered mutation	UNP A0A023UGN9

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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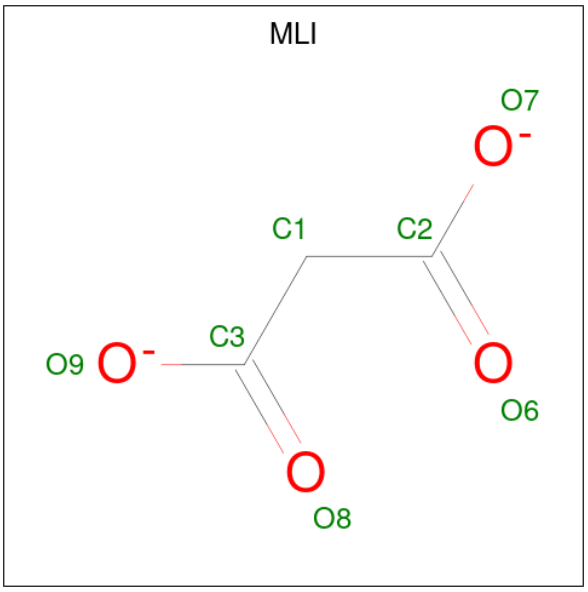
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

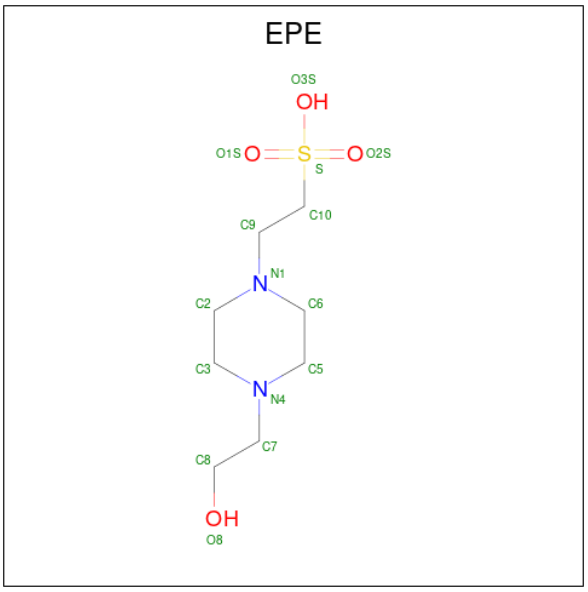
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total Na 6 6	0	0

- Molecule 4 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



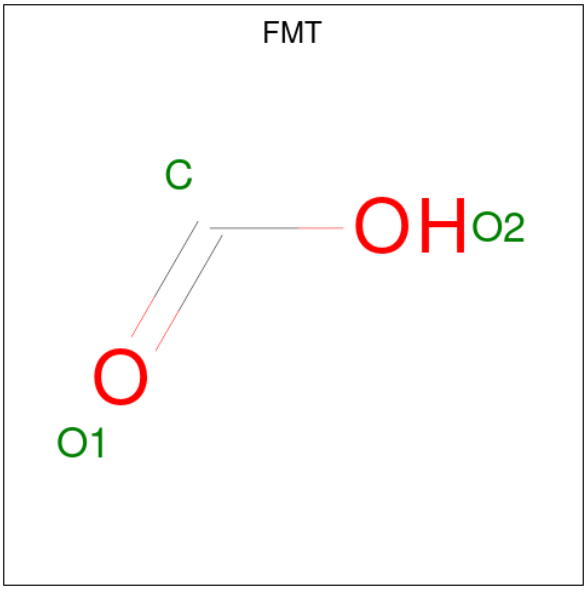
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 3 4	0	0
4	A	1	Total C O 7 3 4	0	0
4	A	1	Total C O 7 3 4	0	0
4	A	1	Total C O 7 3 4	0	0
4	A	1	Total C O 7 3 4	0	0
4	A	1	Total C O 7 3 4	0	0
4	A	1	Total C O 7 3 4	0	0

- 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		

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O		0	0
			3	1	2			
6	A	1	Total	C	O		0	0
			3	1	2			

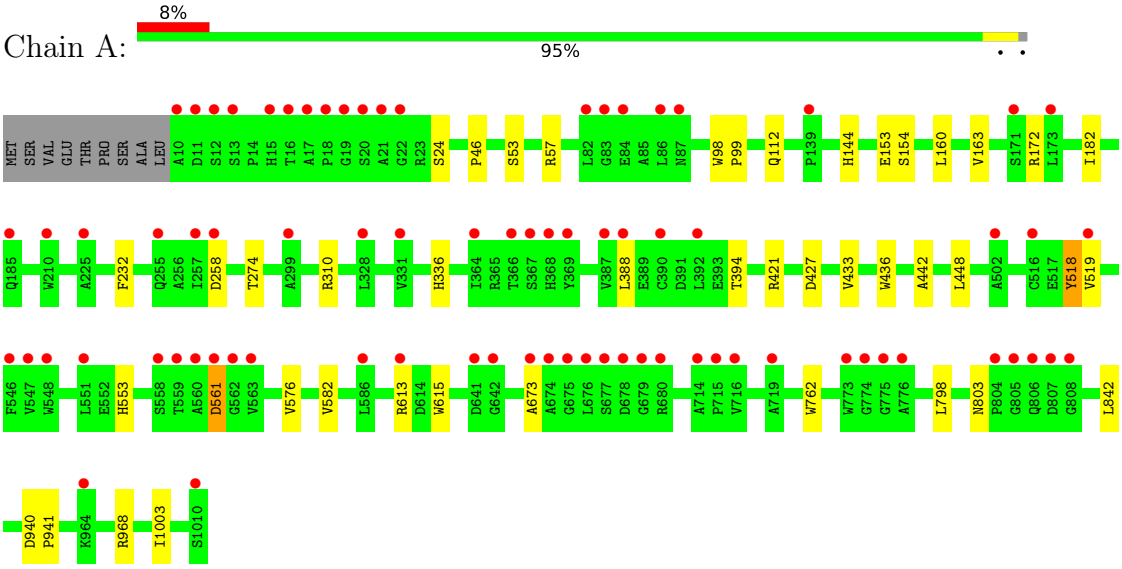
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	826	Total	O	0	4
			826	826		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Beta-galactosidase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	136.86Å 136.86Å 127.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.56 – 1.83 46.56 – 1.84	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.56-1.83) 98.8 (46.56-1.84)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 1.83Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.135 , 0.165 0.145 , 0.170	Depositor DCC
R_{free} test set	2101 reflections (1.77%)	wwPDB-VP
Wilson B-factor (Å^2)	30.3	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	8760	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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, 0.333 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: ACT, EPE, MLI, NA, FMT

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	0.44	0/8042	0.63	0/10957

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	7794	0	7527	28	0
2	A	64	0	48	12	0
3	A	6	0	0	0	0
4	A	49	0	14	1	0
5	A	15	0	17	4	0
6	A	6	0	2	0	0
7	A	826	0	0	9	0
All	All	8760	0	7608	37	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 2.

All (37) 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:561:ASP:N	1:A:561:ASP:OD1	2.07	0.86
2:A:1111:ACT:H2	7:A:1798:HOH:O	1.76	0.86
1:A:518:TYR:CD1	1:A:519:VAL:HG13	2.14	0.83
2:A:1104:ACT:C	5:A:1130:EPE:H52	2.19	0.72
1:A:46:PRO:HG2	2:A:1106:ACT:H2	1.77	0.67
1:A:421:ARG:HD2	2:A:1101:ACT:H2	1.81	0.61
1:A:519:VAL:O	1:A:519:VAL:HG23	2.01	0.59
2:A:1104:ACT:OXT	5:A:1130:EPE:H71	2.02	0.59
2:A:1104:ACT:OXT	5:A:1130:EPE:H52	2.01	0.59
2:A:1103:ACT:H1	7:A:1941:HOH:O	2.03	0.57
1:A:388[B]:LEU:HD21	1:A:427:ASP:OD2	2.05	0.57
2:A:1104:ACT:O	5:A:1130:EPE:H52	2.05	0.56
1:A:388[B]:LEU:HD23	1:A:436:TRP:HZ3	1.70	0.56
1:A:518:TYR:CE1	1:A:519:VAL:HG13	2.42	0.55
1:A:803:ASN:ND2	7:A:1215:HOH:O	2.36	0.53
1:A:553:HIS:HB2	1:A:582:VAL:HG22	1.90	0.53
1:A:388[B]:LEU:HD23	1:A:436:TRP:CZ3	2.44	0.52
1:A:274:THR:HG23	7:A:1510:HOH:O	2.10	0.52
1:A:613[A]:ARG:HG2	7:A:1808:HOH:O	2.11	0.51
1:A:160:LEU:O	1:A:163[A]:VAL:HG12	2.11	0.50
4:A:1128:MLI:O8	7:A:1201:HOH:O	2.20	0.49
1:A:394:THR:OG1	1:A:442:ALA:HA	2.12	0.49
1:A:144:HIS:H	2:A:1105:ACT:H2	1.78	0.48
2:A:1106:ACT:CH3	7:A:1935:HOH:O	2.62	0.47
1:A:448:LEU:HB3	2:A:1113:ACT:H3	1.99	0.45
1:A:112:GLN:CD	1:A:576[B]:VAL:CG1	2.86	0.44
1:A:388[B]:LEU:HD22	1:A:433:VAL:HG21	1.99	0.44
1:A:615:TRP:CE3	1:A:673:ALA:HB2	2.55	0.42
1:A:163[A]:VAL:CG1	1:A:182:ILE:HG21	2.49	0.42
1:A:388[B]:LEU:HD21	1:A:427:ASP:CB	2.49	0.42
1:A:940:ASP:O	1:A:941:PRO:C	2.58	0.42
1:A:153:GLU:HA	1:A:154:SER:HA	1.77	0.42
1:A:98:TRP:N	1:A:99:PRO:CD	2.83	0.41
1:A:258:ASP:HA	7:A:1587:HOH:O	2.19	0.41
1:A:336:HIS:CD2	1:A:553:HIS:HA	2.55	0.41
1:A:842:LEU:O	1:A:1003:ILE:HD12	2.21	0.40
2:A:1103:ACT:CH3	7:A:1474:HOH:O	2.70	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	1017/1010 (101%)	990 (97%)	27 (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	802/793 (101%)	790 (98%)	12 (2%)	65 52

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	SER
1	A	53	SER
1	A	57[A]	ARG
1	A	57[B]	ARG
1	A	172	ARG
1	A	232	PHE
1	A	310	ARG
1	A	518	TYR
1	A	561	ASP
1	A	762	TRP
1	A	798	LEU
1	A	968	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 6 are monoatomic - leaving 26 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	$\#\|Z\| > 2$
4	MLI	A	1126	-	6,6,6	1.33	0	7,7,7	1.22	0
2	ACT	A	1106	-	3,3,3	0.96	0	3,3,3	0.78	0
2	ACT	A	1114	-	3,3,3	0.96	0	3,3,3	0.76	0
2	ACT	A	1101	-	3,3,3	1.24	0	3,3,3	0.71	0
2	ACT	A	1103	-	3,3,3	1.01	0	3,3,3	0.94	0
2	ACT	A	1105	-	3,3,3	0.93	0	3,3,3	1.11	0
2	ACT	A	1108	-	3,3,3	0.93	0	3,3,3	0.96	0
4	MLI	A	1125	-	6,6,6	1.32	0	7,7,7	1.14	0
6	FMT	A	1131	-	2,2,2	0.59	0	1,1,1	0.40	0
2	ACT	A	1112	-	3,3,3	0.80	0	3,3,3	1.08	0
2	ACT	A	1104	-	3,3,3	1.00	0	3,3,3	0.87	0
5	EPE	A	1130	-	15,15,15	2.37	1 (6%)	18,20,20	1.93	3 (16%)
6	FMT	A	1132	-	2,2,2	0.66	0	1,1,1	0.43	0
4	MLI	A	1124	-	6,6,6	1.25	0	7,7,7	1.42	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MLI	A	1123	-	6,6,6	1.36	0	7,7,7	1.34	0
2	ACT	A	1102	-	3,3,3	1.11	0	3,3,3	0.64	0
4	MLI	A	1127	-	6,6,6	1.30	0	7,7,7	1.26	0
2	ACT	A	1109	-	3,3,3	1.05	0	3,3,3	0.65	0
4	MLI	A	1128	-	6,6,6	1.37	0	7,7,7	1.23	0
2	ACT	A	1113	-	3,3,3	1.14	0	3,3,3	0.64	0
2	ACT	A	1115	-	3,3,3	1.29	0	3,3,3	1.41	0
2	ACT	A	1107	-	3,3,3	1.31	0	3,3,3	0.64	0
2	ACT	A	1111	-	3,3,3	1.07	0	3,3,3	0.82	0
4	MLI	A	1129	-	6,6,6	1.30	0	7,7,7	1.24	0
2	ACT	A	1110	-	3,3,3	0.86	0	3,3,3	0.96	0
2	ACT	A	1116	-	3,3,3	0.90	0	3,3,3	0.99	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MLI	A	1128	-	-	2/4/4/4	-
4	MLI	A	1124	-	-	2/4/4/4	-
4	MLI	A	1126	-	-	2/4/4/4	-
4	MLI	A	1123	-	-	2/4/4/4	-
4	MLI	A	1125	-	-	0/4/4/4	-
4	MLI	A	1129	-	-	0/4/4/4	-
4	MLI	A	1127	-	-	1/4/4/4	-
5	EPE	A	1130	-	-	4/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1130	EPE	C10-S	-8.95	1.64	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1130	EPE	O2S-S-C10	4.65	112.51	106.92
5	A	1130	EPE	O1S-S-C10	4.51	112.34	106.92
5	A	1130	EPE	O3S-S-O1S	-2.72	104.64	111.27
4	A	1124	MLI	O9-C3-C1	2.01	120.95	114.54

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1130	EPE	N4-C7-C8-O8
5	A	1130	EPE	C9-C10-S-O2S
5	A	1130	EPE	C9-C10-S-O3S
4	A	1128	MLI	C3-C1-C2-O6
4	A	1128	MLI	C3-C1-C2-O7
4	A	1123	MLI	C3-C1-C2-O6
4	A	1126	MLI	C3-C1-C2-O6
4	A	1123	MLI	C3-C1-C2-O7
5	A	1130	EPE	C9-C10-S-O1S
4	A	1126	MLI	C3-C1-C2-O7
4	A	1124	MLI	C3-C1-C2-O6
4	A	1124	MLI	C3-C1-C2-O7
4	A	1127	MLI	C2-C1-C3-O8

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1106	ACT	2	0
2	A	1101	ACT	1	0
2	A	1103	ACT	2	0
2	A	1105	ACT	1	0
2	A	1104	ACT	4	0
5	A	1130	EPE	4	0
4	A	1128	MLI	1	0
2	A	1113	ACT	1	0
2	A	1111	ACT	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^{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	1001/1010 (99%)	0.13	78 (7%)	13	12	23, 34, 71, 145	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	PRO	12.4
1	A	17	ALA	11.1
1	A	560	ALA	10.9
1	A	563	VAL	9.2
1	A	20	SER	9.0
1	A	21	ALA	8.7
1	A	19	GLY	8.3
1	A	559	THR	8.2
1	A	561	ASP	7.6
1	A	562	GLY	6.7
1	A	87	ASN	6.0
1	A	775	GLY	5.9
1	A	15	HIS	5.3
1	A	678	ASP	5.2
1	A	22	GLY	4.9
1	A	11	ASP	4.6
1	A	83	GLY	4.4
1	A	776	ALA	4.4
1	A	716	VAL	4.4
1	A	16	THR	4.2
1	A	677	SER	4.1
1	A	676	LEU	4.0
1	A	388[A]	LEU	3.8
1	A	558	SER	3.8
1	A	1010	SER	3.8
1	A	804	PRO	3.7
1	A	674	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	86	LEU	3.6
1	A	673	ALA	3.5
1	A	806	GLN	3.4
1	A	719	ALA	3.4
1	A	10	ALA	3.2
1	A	84	GLU	3.1
1	A	12	SER	3.1
1	A	258	ASP	3.1
1	A	679	GLY	3.0
1	A	366	THR	3.0
1	A	364	ILE	2.9
1	A	369	TYR	2.9
1	A	675	GLY	2.9
1	A	392	LEU	2.8
1	A	13	SER	2.8
1	A	715	PRO	2.8
1	A	331	VAL	2.8
1	A	808	GLY	2.7
1	A	774	GLY	2.7
1	A	367	SER	2.6
1	A	387	VAL	2.6
1	A	299	ALA	2.6
1	A	613[A]	ARG	2.6
1	A	547	VAL	2.5
1	A	642	GLY	2.5
1	A	641	ASP	2.5
1	A	502	ALA	2.5
1	A	773	TRP	2.5
1	A	551	LEU	2.5
1	A	225	ALA	2.4
1	A	390	CYS	2.4
1	A	807	ASP	2.3
1	A	546	PHE	2.3
1	A	82	LEU	2.3
1	A	185	GLN	2.2
1	A	368	HIS	2.2
1	A	173	LEU	2.2
1	A	516	CYS	2.2
1	A	714	ALA	2.2
1	A	519	VAL	2.2
1	A	586	LEU	2.2
1	A	139	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	257	ILE	2.1
1	A	548	TRP	2.1
1	A	255	GLN	2.1
1	A	210	TRP	2.1
1	A	680	ARG	2.1
1	A	328	LEU	2.1
1	A	805	GLY	2.1
1	A	171	SER	2.1
1	A	964	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
4	MLI	A	1123	7/7	0.63	0.33	76,101,105,113	0
2	ACT	A	1110	4/4	0.65	0.20	55,78,79,87	0
2	ACT	A	1105	4/4	0.72	0.47	52,63,65,74	0
2	ACT	A	1109	4/4	0.72	0.23	51,56,64,65	0
2	ACT	A	1114	4/4	0.73	0.34	71,93,97,110	0
2	ACT	A	1108	4/4	0.79	0.26	45,59,70,83	0
2	ACT	A	1116	4/4	0.81	0.31	62,67,74,76	0
3	NA	A	1120	1/1	0.82	0.29	78,78,78,78	0
2	ACT	A	1115	4/4	0.85	0.20	64,74,75,94	0
2	ACT	A	1112	4/4	0.85	0.30	53,54,68,73	0
4	MLI	A	1126	7/7	0.85	0.50	69,88,113,117	0
2	ACT	A	1102	4/4	0.86	0.15	64,70,72,74	0
3	NA	A	1122	1/1	0.86	0.11	60,60,60,60	0
4	MLI	A	1127	7/7	0.86	0.14	47,82,92,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACT	A	1106	4/4	0.87	0.15	53,67,69,71	0
4	MLI	A	1128	7/7	0.87	0.12	43,58,68,72	0
5	EPE	A	1130	15/15	0.87	0.21	45,81,112,112	0
4	MLI	A	1129	7/7	0.88	0.17	73,89,106,110	0
2	ACT	A	1103	4/4	0.88	0.12	29,39,49,59	0
4	MLI	A	1124	7/7	0.90	0.12	63,70,120,124	0
2	ACT	A	1111	4/4	0.91	0.18	63,65,69,83	0
2	ACT	A	1113	4/4	0.92	0.12	34,39,54,64	0
6	FMT	A	1131	3/3	0.93	0.14	46,46,52,55	0
6	FMT	A	1132	3/3	0.93	0.17	42,42,59,61	0
4	MLI	A	1125	7/7	0.95	0.16	38,46,62,64	0
2	ACT	A	1104	4/4	0.96	0.18	31,33,34,37	0
2	ACT	A	1101	4/4	0.96	0.09	28,35,40,58	0
2	ACT	A	1107	4/4	0.97	0.12	29,29,39,43	0
3	NA	A	1119	1/1	0.97	0.23	39,39,39,39	0
3	NA	A	1118	1/1	0.98	0.05	29,29,29,29	0
3	NA	A	1121	1/1	0.99	0.08	29,29,29,29	0
3	NA	A	1117	1/1	0.99	0.10	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.