WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 19, 2020 – 04:50 am BST

PDB ID	:	4O7M
Title	:	Crystal structure of a trap periplasmic solute binding protein from shewanella loihica PV-4, target EFI-510273, with bound L-malate
Authors	:	Vetting, M.W.; Al Obaidi, N.F.; Morisco, L.L.; Wasserman, S.R.; Sojitra, S.; Stead, M.; Attonito, J.D.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hillerich, B.; Love, J.; Seidel, R.D.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on	:	2013-12-25
Resolution	:	1.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
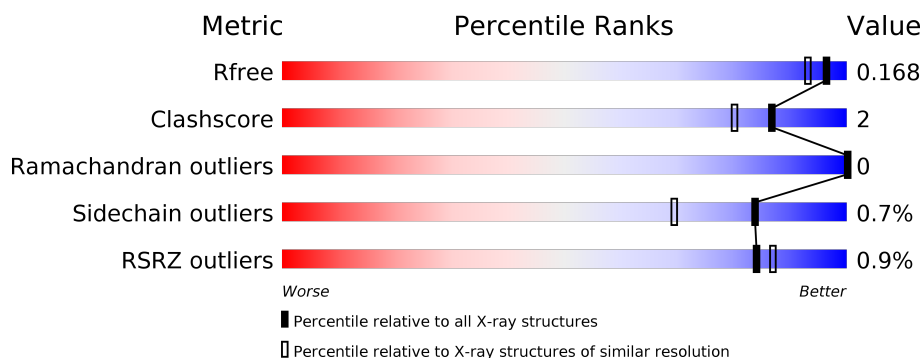with specific help available everywhere you see the (i) symbol.

---

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 1.50 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	Percentile Ranks	Value
Rfree		0.168
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		0.7%
RSRZ outliers		0.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 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	328	88% • 7%
1	B	328	89% • 7%
1	C	328	82% • 14%
1	D	328	88% • 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 21467 atoms, of which 9602 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 TRAP dicarboxylate transporter, DctP subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	304	Total 4866	C 1552	H 2434	N 412	O 461	Se 7	0	5	0
1	B	305	Total 4946	C 1573	H 2475	N 420	O 471	Se 7	0	14	0
1	C	283	Total 4533	C 1448	H 2266	N 384	O 428	Se 7	0	8	0
1	D	303	Total 4852	C 1548	H 2427	N 409	O 461	Se 7	0	10	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MSE	-	EXPRESSION TAG	UNP A3QCW5
A	10	HIS	-	EXPRESSION TAG	UNP A3QCW5
A	11	HIS	-	EXPRESSION TAG	UNP A3QCW5
A	12	HIS	-	EXPRESSION TAG	UNP A3QCW5
A	13	HIS	-	EXPRESSION TAG	UNP A3QCW5
A	14	HIS	-	EXPRESSION TAG	UNP A3QCW5
A	15	HIS	-	EXPRESSION TAG	UNP A3QCW5
A	16	SER	-	EXPRESSION TAG	UNP A3QCW5
A	17	SER	-	EXPRESSION TAG	UNP A3QCW5
A	18	GLY	-	EXPRESSION TAG	UNP A3QCW5
A	19	VAL	-	EXPRESSION TAG	UNP A3QCW5
A	20	ASP	-	EXPRESSION TAG	UNP A3QCW5
A	21	LEU	-	EXPRESSION TAG	UNP A3QCW5
A	22	GLY	-	EXPRESSION TAG	UNP A3QCW5
A	23	THR	-	EXPRESSION TAG	UNP A3QCW5
A	24	GLU	-	EXPRESSION TAG	UNP A3QCW5
A	25	ASN	-	EXPRESSION TAG	UNP A3QCW5
A	26	LEU	-	EXPRESSION TAG	UNP A3QCW5
A	27	TYR	-	EXPRESSION TAG	UNP A3QCW5
A	28	PHE	-	EXPRESSION TAG	UNP A3QCW5
A	29	GLN	-	EXPRESSION TAG	UNP A3QCW5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	SER	-	EXPRESSION TAG	UNP A3QCW5
A	31	MSE	-	EXPRESSION TAG	UNP A3QCW5
B	9	MSE	-	EXPRESSION TAG	UNP A3QCW5
B	10	HIS	-	EXPRESSION TAG	UNP A3QCW5
B	11	HIS	-	EXPRESSION TAG	UNP A3QCW5
B	12	HIS	-	EXPRESSION TAG	UNP A3QCW5
B	13	HIS	-	EXPRESSION TAG	UNP A3QCW5
B	14	HIS	-	EXPRESSION TAG	UNP A3QCW5
B	15	HIS	-	EXPRESSION TAG	UNP A3QCW5
B	16	SER	-	EXPRESSION TAG	UNP A3QCW5
B	17	SER	-	EXPRESSION TAG	UNP A3QCW5
B	18	GLY	-	EXPRESSION TAG	UNP A3QCW5
B	19	VAL	-	EXPRESSION TAG	UNP A3QCW5
B	20	ASP	-	EXPRESSION TAG	UNP A3QCW5
B	21	LEU	-	EXPRESSION TAG	UNP A3QCW5
B	22	GLY	-	EXPRESSION TAG	UNP A3QCW5
B	23	THR	-	EXPRESSION TAG	UNP A3QCW5
B	24	GLU	-	EXPRESSION TAG	UNP A3QCW5
B	25	ASN	-	EXPRESSION TAG	UNP A3QCW5
B	26	LEU	-	EXPRESSION TAG	UNP A3QCW5
B	27	TYR	-	EXPRESSION TAG	UNP A3QCW5
B	28	PHE	-	EXPRESSION TAG	UNP A3QCW5
B	29	GLN	-	EXPRESSION TAG	UNP A3QCW5
B	30	SER	-	EXPRESSION TAG	UNP A3QCW5
B	31	MSE	-	EXPRESSION TAG	UNP A3QCW5
C	9	MSE	-	EXPRESSION TAG	UNP A3QCW5
C	10	HIS	-	EXPRESSION TAG	UNP A3QCW5
C	11	HIS	-	EXPRESSION TAG	UNP A3QCW5
C	12	HIS	-	EXPRESSION TAG	UNP A3QCW5
C	13	HIS	-	EXPRESSION TAG	UNP A3QCW5
C	14	HIS	-	EXPRESSION TAG	UNP A3QCW5
C	15	HIS	-	EXPRESSION TAG	UNP A3QCW5
C	16	SER	-	EXPRESSION TAG	UNP A3QCW5
C	17	SER	-	EXPRESSION TAG	UNP A3QCW5
C	18	GLY	-	EXPRESSION TAG	UNP A3QCW5
C	19	VAL	-	EXPRESSION TAG	UNP A3QCW5
C	20	ASP	-	EXPRESSION TAG	UNP A3QCW5
C	21	LEU	-	EXPRESSION TAG	UNP A3QCW5
C	22	GLY	-	EXPRESSION TAG	UNP A3QCW5
C	23	THR	-	EXPRESSION TAG	UNP A3QCW5
C	24	GLU	-	EXPRESSION TAG	UNP A3QCW5
C	25	ASN	-	EXPRESSION TAG	UNP A3QCW5

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	26	LEU	-	EXPRESSION TAG	UNP A3QCW5
C	27	TYR	-	EXPRESSION TAG	UNP A3QCW5
C	28	PHE	-	EXPRESSION TAG	UNP A3QCW5
C	29	GLN	-	EXPRESSION TAG	UNP A3QCW5
C	30	SER	-	EXPRESSION TAG	UNP A3QCW5
C	31	MSE	-	EXPRESSION TAG	UNP A3QCW5
D	9	MSE	-	EXPRESSION TAG	UNP A3QCW5
D	10	HIS	-	EXPRESSION TAG	UNP A3QCW5
D	11	HIS	-	EXPRESSION TAG	UNP A3QCW5
D	12	HIS	-	EXPRESSION TAG	UNP A3QCW5
D	13	HIS	-	EXPRESSION TAG	UNP A3QCW5
D	14	HIS	-	EXPRESSION TAG	UNP A3QCW5
D	15	HIS	-	EXPRESSION TAG	UNP A3QCW5
D	16	SER	-	EXPRESSION TAG	UNP A3QCW5
D	17	SER	-	EXPRESSION TAG	UNP A3QCW5
D	18	GLY	-	EXPRESSION TAG	UNP A3QCW5
D	19	VAL	-	EXPRESSION TAG	UNP A3QCW5
D	20	ASP	-	EXPRESSION TAG	UNP A3QCW5
D	21	LEU	-	EXPRESSION TAG	UNP A3QCW5
D	22	GLY	-	EXPRESSION TAG	UNP A3QCW5
D	23	THR	-	EXPRESSION TAG	UNP A3QCW5
D	24	GLU	-	EXPRESSION TAG	UNP A3QCW5
D	25	ASN	-	EXPRESSION TAG	UNP A3QCW5
D	26	LEU	-	EXPRESSION TAG	UNP A3QCW5
D	27	TYR	-	EXPRESSION TAG	UNP A3QCW5
D	28	PHE	-	EXPRESSION TAG	UNP A3QCW5
D	29	GLN	-	EXPRESSION TAG	UNP A3QCW5
D	30	SER	-	EXPRESSION TAG	UNP A3QCW5
D	31	MSE	-	EXPRESSION TAG	UNP A3QCW5

- Molecule 2 is (2S)-2-hydroxybutanedioic acid (three-letter code: LMR) (formula: $C_4H_6O_5$).
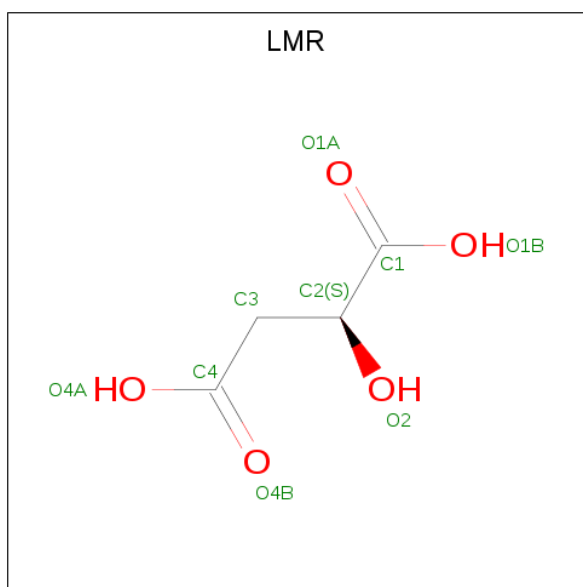
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 9	C 4	O 5	0	0
2	B	1	Total 9	C 4	O 5	0	0
2	C	1	Total 9	C 4	O 5	0	0
2	D	1	Total 9	C 4	O 5	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	554	Total O 554 554		0	0
4	B	582	Total O 582 582		0	0
4	C	557	Total O 557 557		0	0
4	D	536	Total O 536 536		0	0

3 Residue-property plots ⓘ

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.
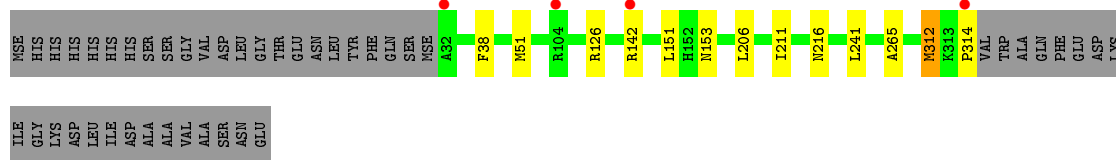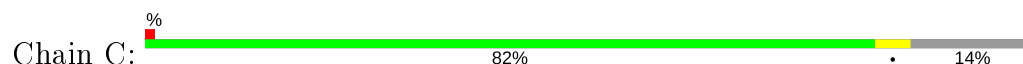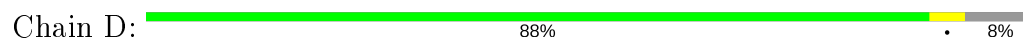
- Molecule 1: TRAP dicarboxylate transporter, DctP subunit

- Molecule 1: TRAP dicarboxylate transporter, DctP subunit
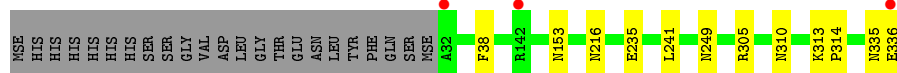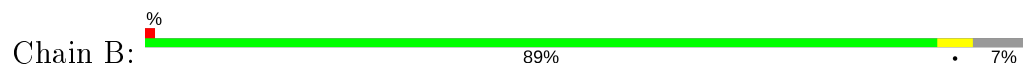
- Molecule 1: TRAP dicarboxylate transporter, DctP subunit

- Molecule 1: TRAP dicarboxylate transporter, DctP subunit

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.52Å 118.64Å 89.90Å 90.00° 93.18° 90.00°	Depositor
Resolution (Å)	22.60 – 1.50 22.60 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (22.60-1.50) 100.0 (22.60-1.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$<I/\sigma(I)>$ [1]	2.82 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.138 , 0.158 0.151 , 0.168	Depositor DCC
R_{free} test set	13518 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	9.7	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 55.6	EDS
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21467	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LMR, 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	0.48	1/2497 (0.0%)	0.61	0/3362
1	B	0.44	0/2558	0.59	0/3445
1	C	0.49	2/2339 (0.1%)	0.62	1/3150 (0.0%)
1	D	0.45	0/2513	0.59	1/3386 (0.0%)
All	All	0.46	3/9907 (0.0%)	0.60	2/13343 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	312	MSE	CG-SE	6.53	2.17	1.95
1	C	312	MSE	CG-SE	6.45	2.17	1.95
1	C	314	PRO	N-CD	5.11	1.55	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	312	MSE	CB-CA-C	6.93	124.25	110.40
1	D	312	MSE	CG-SE-CE	-6.60	84.39	98.90

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	2432	2434	2412	10	0
1	B	2471	2475	2425	10	0
1	C	2267	2266	2251	9	0
1	D	2425	2427	2379	11	0
2	A	9	0	4	0	0
2	B	9	0	4	0	0
2	C	9	0	4	0	0
2	D	9	0	4	0	0
3	B	5	0	0	0	0
4	A	554	0	0	3	1
4	B	582	0	0	7	1
4	C	557	0	0	2	0
4	D	536	0	0	6	2
All	All	11865	9602	9483	40	2

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.

The worst 5 of 40 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:312:MSE:SE	1:A:312:MSE:CG	2.17	1.43
1:C:312:MSE:SE	1:C:312:MSE:CG	2.17	1.42
1:D:312:MSE:SE	1:D:312:MSE:CE	2.17	1.41
1:A:76:GLN:NE2	4:A:847:HOH:O	2.04	0.90
1:B:305[B]:ARG:NH2	4:B:986:HOH:O	2.13	0.81

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:941:HOH:O	4:D:848:HOH:O[2_656]	2.16	0.04
4:A:904:HOH:O	4:D:1019:HOH:O[2_756]	2.17	0.03

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	307/328 (94%)	301 (98%)	6 (2%)	0	100	100
1	B	317/328 (97%)	314 (99%)	3 (1%)	0	100	100
1	C	289/328 (88%)	286 (99%)	3 (1%)	0	100	100
1	D	311/328 (95%)	308 (99%)	3 (1%)	0	100	100
All	All	1224/1312 (93%)	1209 (99%)	15 (1%)	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	266/274 (97%)	265 (100%)	1 (0%)	91	82
1	B	272/274 (99%)	270 (99%)	2 (1%)	84	69
1	C	251/274 (92%)	249 (99%)	2 (1%)	81	66
1	D	268/274 (98%)	266 (99%)	2 (1%)	84	69
All	All	1057/1096 (96%)	1050 (99%)	7 (1%)	84	69

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	142	ARG
1	D	216	ASN
1	C	216	ASN
1	B	38	PHE
1	D	38	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	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)

5 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	LMR	A	401	-	2,8,8	1.90	1 (50%)	3,10,10	0.71	0
2	LMR	D	401	-	2,8,8	1.75	1 (50%)	3,10,10	0.30	0
3	SO4	B	401	-	4,4,4	0.18	0	6,6,6	0.11	0
2	LMR	B	402	-	2,8,8	2.14	1 (50%)	3,10,10	0.79	0
2	LMR	C	401	-	2,8,8	1.80	1 (50%)	3,10,10	1.09	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
2	LMR	A	401	-	-	0/2/8/8	-
2	LMR	D	401	-	-	0/2/8/8	-
2	LMR	C	401	-	-	0/2/8/8	-
2	LMR	B	402	-	-	0/2/8/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	LMR	C3-C2	-2.66	1.49	1.53
2	B	402	LMR	C3-C2	-2.61	1.49	1.53
2	C	401	LMR	C3-C2	-2.40	1.50	1.53
2	D	401	LMR	C3-C2	-2.20	1.50	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	297/328 (90%)	-0.60	2 (0%)	87	90	4, 9, 21, 33	0
1	B	298/328 (90%)	-0.57	3 (1%)	82	85	4, 9, 20, 38	0
1	C	276/328 (84%)	-0.56	4 (1%)	75	79	4, 9, 21, 33	0
1	D	296/328 (90%)	-0.51	1 (0%)	94	95	5, 11, 23, 31	0
All	All	1167/1312 (88%)	-0.56	10 (0%)	84	87	4, 9, 21, 38	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	ALA	5.3
1	B	336	GLU	4.0
1	C	142	ARG	3.8
1	A	142	ARG	3.7
1	B	142	ARG	3.3

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. 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	B-factors(Å²)	Q<0.9
3	SO4	B	401	5/5	0.95	0.21	25,35,37,42	0
2	LMR	A	401	9/9	0.99	0.06	3,4,6,8	0
2	LMR	D	401	9/9	0.99	0.07	4,5,7,10	0
2	LMR	C	401	9/9	0.99	0.07	3,4,5,10	0
2	LMR	B	402	9/9	0.99	0.06	2,4,6,7	0

6.5 Other polymers (i)

There are no such residues in this entry.