WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 29, 2023 – 03:28 AM EDT

PDB ID	:	3N6H
Title	:	Crystal structure of Mandelate racemase/muconate lactonizing protein from Actinobacillus succinogenes 130Z complexed with magnesium/sulfate
Authors	:	Malashkevich, V.N.; Patskovsky, Y.; Toro, R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYS-GXRC)
Deposited on	:	2010-05-25
Resolution	:	2.30 Å(reported)

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

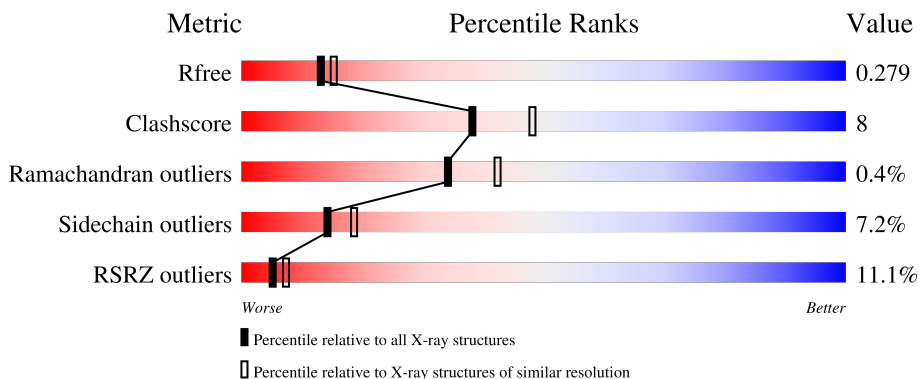|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.279
Clashscore		8
Ramachandran outliers		0.4%
Sidechain outliers		7.2%
RSRZ outliers		11.1%

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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 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	455	3% / 72% 19% • 6%
1	B	455	.% / 77% 16% • 5%
1	C	455	12% / 73% 19% • 6%
1	D	455	24% / 74% 18% • 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13719 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 Mandelate racemase/muconate lactonizing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	Se	0	1	0
			3356	2136	581	619	6	14			
1	B	432	Total	C	N	O	S	Se	0	2	0
			3386	2155	587	624	6	14			
1	C	426	Total	C	N	O	S	Se	0	1	0
			3328	2117	577	614	6	14			
1	D	424	Total	C	N	O	S	Se	0	2	0
			3316	2108	574	614	6	14			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP A6VQF6
A	2	SER	-	expression tag	UNP A6VQF6
A	3	LEU	-	expression tag	UNP A6VQF6
A	448	GLU	-	expression tag	UNP A6VQF6
A	449	GLY	-	expression tag	UNP A6VQF6
A	450	HIS	-	expression tag	UNP A6VQF6
A	451	HIS	-	expression tag	UNP A6VQF6
A	452	HIS	-	expression tag	UNP A6VQF6
A	453	HIS	-	expression tag	UNP A6VQF6
A	454	HIS	-	expression tag	UNP A6VQF6
A	455	HIS	-	expression tag	UNP A6VQF6
B	1	MSE	-	expression tag	UNP A6VQF6
B	2	SER	-	expression tag	UNP A6VQF6
B	3	LEU	-	expression tag	UNP A6VQF6
B	448	GLU	-	expression tag	UNP A6VQF6
B	449	GLY	-	expression tag	UNP A6VQF6
B	450	HIS	-	expression tag	UNP A6VQF6
B	451	HIS	-	expression tag	UNP A6VQF6
B	452	HIS	-	expression tag	UNP A6VQF6
B	453	HIS	-	expression tag	UNP A6VQF6
B	454	HIS	-	expression tag	UNP A6VQF6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	455	HIS	-	expression tag	UNP A6VQF6
C	1	MSE	-	expression tag	UNP A6VQF6
C	2	SER	-	expression tag	UNP A6VQF6
C	3	LEU	-	expression tag	UNP A6VQF6
C	448	GLU	-	expression tag	UNP A6VQF6
C	449	GLY	-	expression tag	UNP A6VQF6
C	450	HIS	-	expression tag	UNP A6VQF6
C	451	HIS	-	expression tag	UNP A6VQF6
C	452	HIS	-	expression tag	UNP A6VQF6
C	453	HIS	-	expression tag	UNP A6VQF6
C	454	HIS	-	expression tag	UNP A6VQF6
C	455	HIS	-	expression tag	UNP A6VQF6
D	1	MSE	-	expression tag	UNP A6VQF6
D	2	SER	-	expression tag	UNP A6VQF6
D	3	LEU	-	expression tag	UNP A6VQF6
D	448	GLU	-	expression tag	UNP A6VQF6
D	449	GLY	-	expression tag	UNP A6VQF6
D	450	HIS	-	expression tag	UNP A6VQF6
D	451	HIS	-	expression tag	UNP A6VQF6
D	452	HIS	-	expression tag	UNP A6VQF6
D	453	HIS	-	expression tag	UNP A6VQF6
D	454	HIS	-	expression tag	UNP A6VQF6
D	455	HIS	-	expression tag	UNP A6VQF6

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2
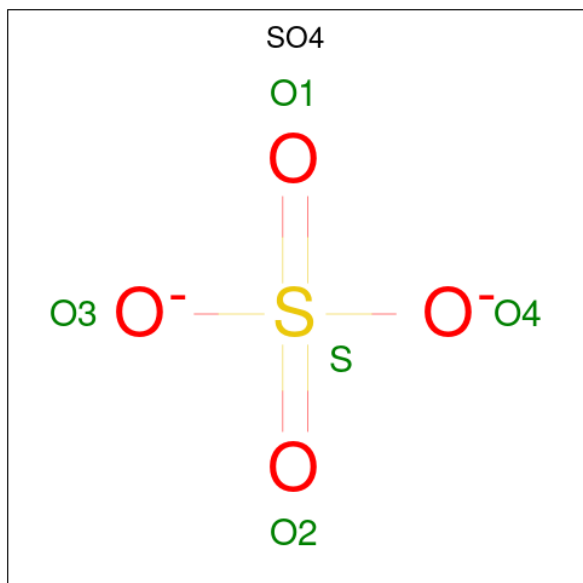
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0
3	B	1	Total 1	Mg 1	0	0
3	C	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	150	Total 150	O 150	0	0
5	B	105	Total 105	O 105	0	0
5	C	41	Total 41	O 41	0	0
5	D	12	Total 12	O 12	0	0

3 Residue-property plots ⓘ

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.
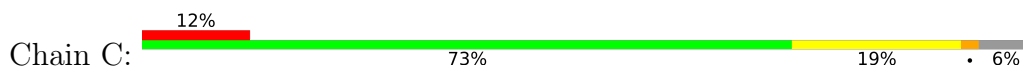
• Molecule 1: Mandelate racemase/muconate lactonizing protein
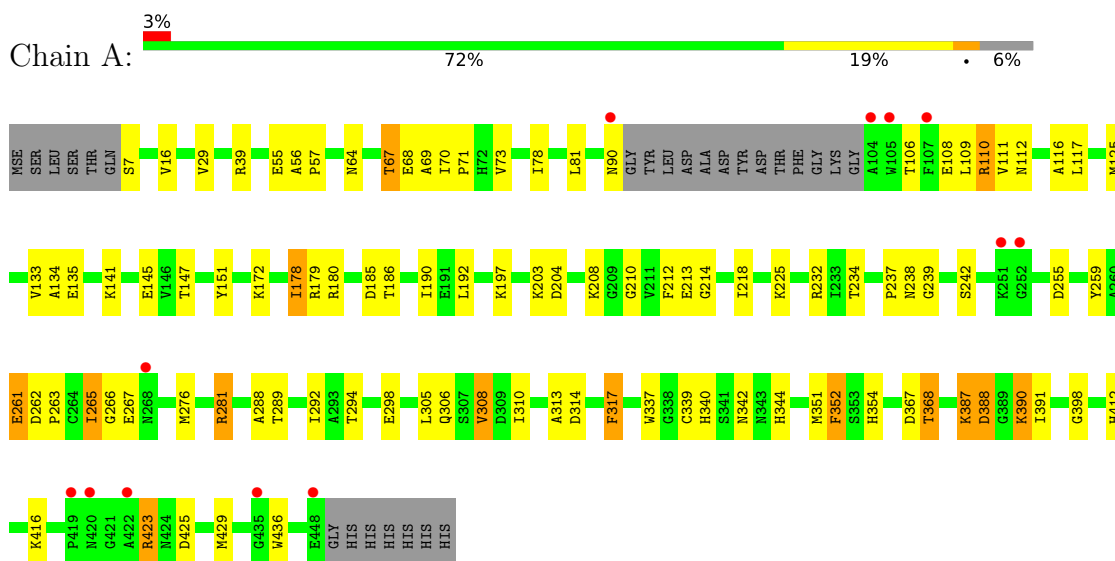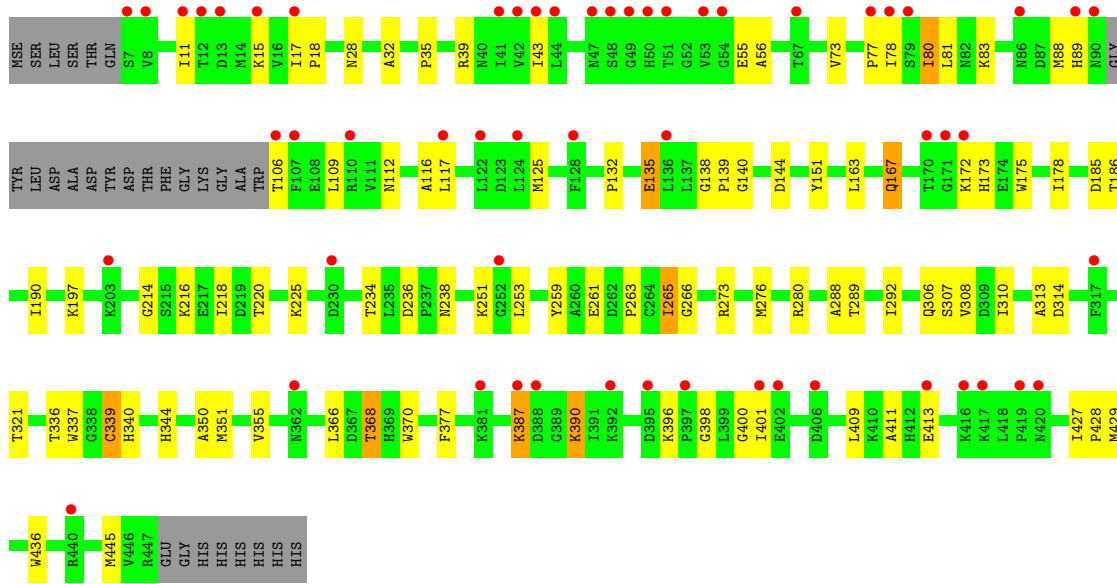
Chain A:

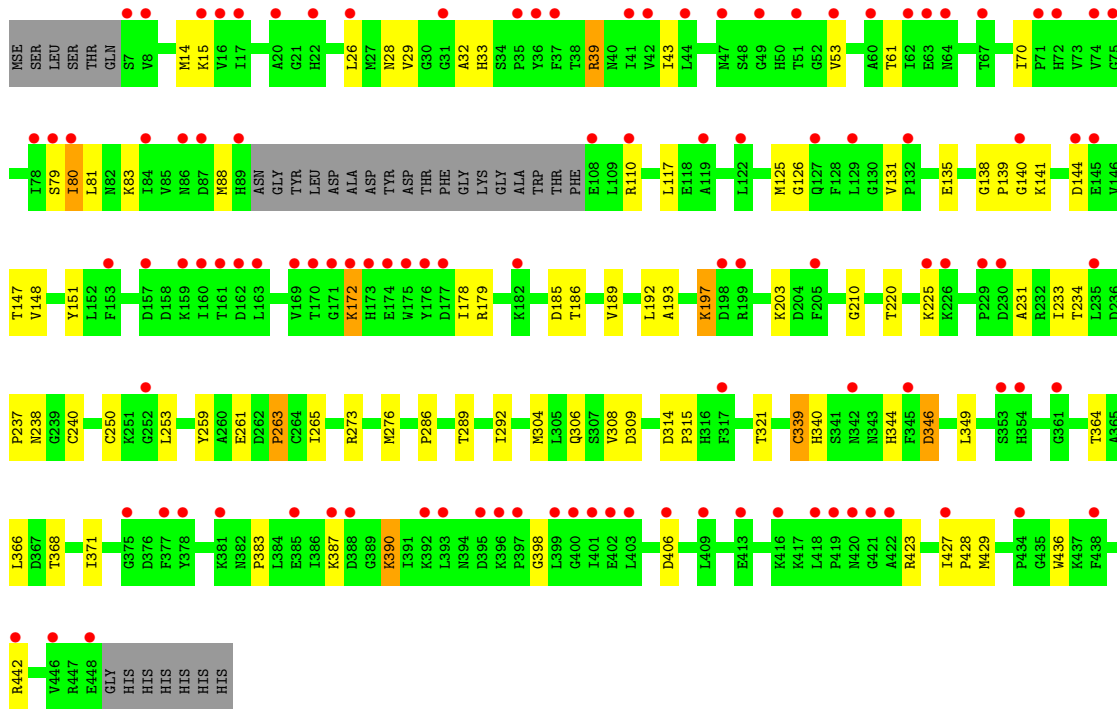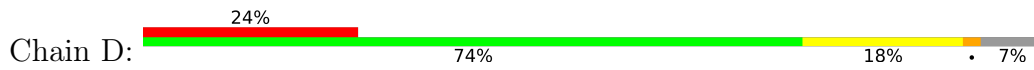• Molecule 1: Mandelate racemase/muconate lactonizing protein

Chain B:

• Molecule 1: Mandelate racemase/muconate lactonizing protein

Chain C:

• Molecule 1: Mandelate racemase/muconate lactonizing protein

Chain D:
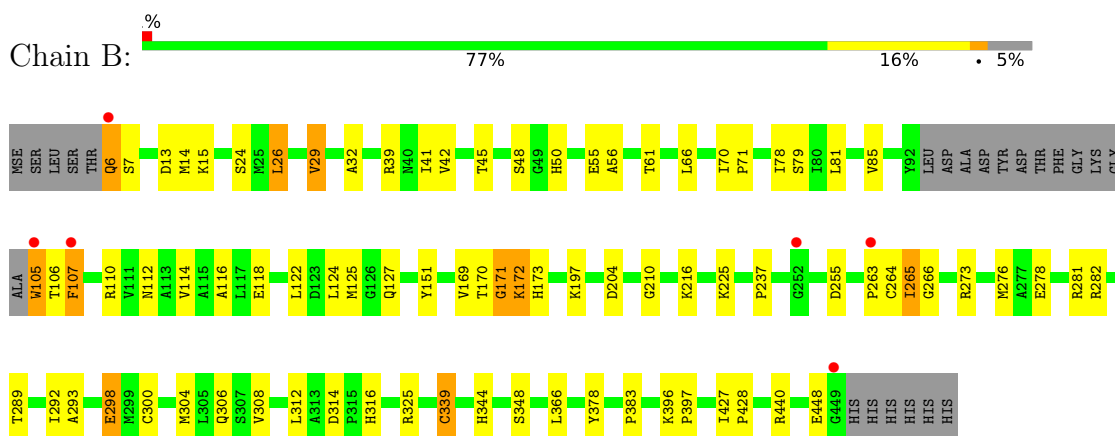
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	97.40Å 85.88Å 112.42Å 90.00° 96.03° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	77.9 (20.00-2.30) 77.9 (20.00-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.30Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.219 , 0.278 0.220 , 0.279	Depositor DCC
R_{free} test set	1907 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.7	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13719	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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, 0.333 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: SO4, CL, MG

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	0.49	0/3428	0.61	0/4632
1	B	0.44	0/3463	0.58	0/4679
1	C	0.38	0/3398	0.52	0/4590
1	D	0.37	0/3388	0.50	0/4576
All	All	0.43	0/13677	0.56	0/18477

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	3356	0	3307	65	0
1	B	3386	0	3330	46	0
1	C	3328	0	3286	47	0
1	D	3316	0	3274	46	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	1	0	0	0	0
5	A	150	0	0	3	0
5	B	105	0	0	3	0
5	C	41	0	0	1	0
5	D	12	0	0	1	0
All	All	13719	0	13197	201	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.

The worst 5 of 201 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:D:26:LEU:HB2	1:D:33:HIS:CD2	1.96	1.00
1:D:79:SER:HA	1:D:125:MSE:HE1	1.45	0.98
1:A:306:GLN:HG3	1:C:306:GLN:HG3	1.55	0.88
1:D:26:LEU:HB2	1:D:33:HIS:HD2	1.36	0.87
1:B:298:GLU:HG2	5:B:536:HOH:O	1.78	0.82

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	426/455 (94%)	401 (94%)	24 (6%)	1 (0%)	47	58
1	B	430/455 (94%)	413 (96%)	15 (4%)	2 (0%)	29	35
1	C	423/455 (93%)	407 (96%)	15 (4%)	1 (0%)	47	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	422/455 (93%)	399 (94%)	20 (5%)	3 (1%)	22	26
All	All	1701/1820 (94%)	1620 (95%)	74 (4%)	7 (0%)	34	42

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	448	GLU
1	D	172	LYS
1	A	425	ASP
1	C	81	LEU
1	B	171	GLY

5.3.2 Protein sidechains ⓘ

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	356/361 (99%)	330 (93%)	26 (7%)	14	18
1	B	359/361 (99%)	333 (93%)	26 (7%)	14	18
1	C	354/361 (98%)	329 (93%)	25 (7%)	14	19
1	D	353/361 (98%)	328 (93%)	25 (7%)	14	19
All	All	1422/1444 (98%)	1320 (93%)	102 (7%)	14	18

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	135	GLU
1	C	307	SER
1	D	390	LYS
1	C	151	TYR
1	C	216	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	173	HIS
1	C	238	ASN
1	D	328	GLN
1	D	33	HIS
1	D	89	HIS

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 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 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	$\#|Z| > 2$
2	SO4	D	500	-	4,4,4	0.17	0	6,6,6	0.06	0
2	SO4	B	500	-	4,4,4	0.13	0	6,6,6	0.27	0
2	SO4	C	500	-	4,4,4	0.14	0	6,6,6	0.30	0
2	SO4	A	500	-	4,4,4	0.21	0	6,6,6	0.20	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	SO4	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, 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	415/455 (91%)	-0.14	12 (2%)	51	58	13, 28, 48, 80	0
1	B	418/455 (91%)	-0.11	6 (1%)	75	80	15, 30, 47, 72	0
1	C	412/455 (90%)	0.65	56 (13%)	3	4	20, 51, 102, 122	0
1	D	410/455 (90%)	1.32	109 (26%)	0	0	25, 79, 109, 124	0
All	All	1655/1820 (90%)	0.43	183 (11%)	5	7	13, 39, 100, 124	0

The worst 5 of 183 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	TRP	9.7
1	D	419	PRO	7.1
1	D	170	THR	6.9
1	B	105	TRP	5.9
1	C	7	SER	5.6

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å^2)	Q<0.9
3	MG	C	501	1/1	0.92	0.10	40,40,40,40	0
4	CL	B	503	1/1	0.94	0.05	56,56,56,56	0
2	SO4	D	500	5/5	0.96	0.11	75,76,78,82	0
3	MG	D	501	1/1	0.96	0.10	49,49,49,49	0
3	MG	B	501	1/1	0.96	0.21	45,45,45,45	0
2	SO4	A	500	5/5	0.97	0.10	40,41,41,48	0
2	SO4	C	500	5/5	0.98	0.08	42,48,49,50	0
2	SO4	B	500	5/5	0.98	0.10	38,38,38,40	0
3	MG	A	501	1/1	0.99	0.04	28,28,28,28	0

6.5 Other polymers ⓘ

There are no such residues in this entry.