wwPDB X-ray Structure Validation Summary Report (i)

Jun 24, 2024 – 12:43 PM EDT

PDB ID	:	8STC
Title	:	S127A variant of LarB, a carboxylase/hydrolase involved in synthesis of the cofactor for lactate racemase, in complex with Zinc and soaked with bicarbonate.
Authors	:	Chatterjee, S.; Rankin, J.A.; Hu, J.; Hausinger, R.P.
Deposited on	:	2023-05-09
Resolution	:	2.80 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.

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 (1)) were used in the production of this report:

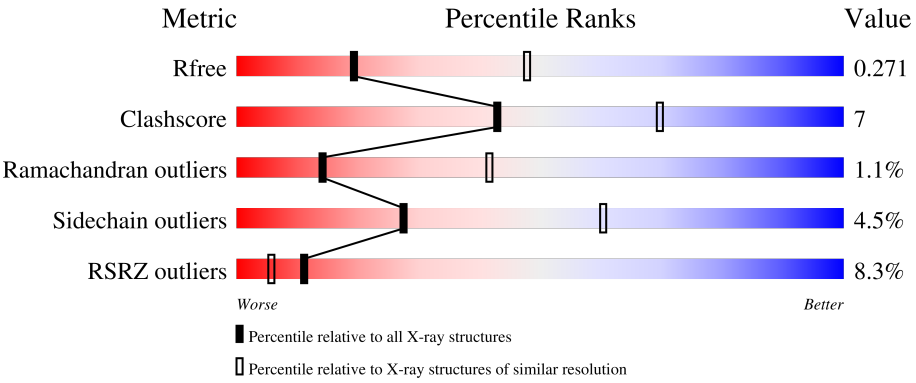
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	256	2% 63% 13% • 21%
1	B	256	2% 68% 10% • 21%
1	C	256	% 61% 16% • 21%
1	D	256	3% 69% 12% 19%
1	E	256	20% 69% 6% • 24%

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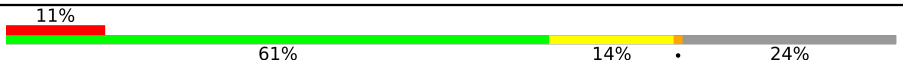
Mol	Chain	Length	Quality of chain
1	F	256	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8140 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 Pyridinium-3,5-biscarboxylic acid mononucleotide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	6	0
			1454	921	251	273	9			
1	B	203	Total	C	N	O	S	0	7	0
			1436	907	250	271	8			
1	C	201	Total	C	N	O	S	0	0	0
			1395	885	238	264	8			
1	D	207	Total	C	N	O	S	0	6	0
			1424	893	252	271	8			
1	E	195	Total	C	N	O	S	0	0	0
			1197	741	212	240	4			
1	F	195	Total	C	N	O	S	0	0	0
			1230	764	220	244	2			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	ALA	SER	engineered mutation	UNP F9UST0
A	247	ALA	-	expression tag	UNP F9UST0
A	248	SER	-	expression tag	UNP F9UST0
A	249	TRP	-	expression tag	UNP F9UST0
A	250	SER	-	expression tag	UNP F9UST0
A	251	HIS	-	expression tag	UNP F9UST0
A	252	PRO	-	expression tag	UNP F9UST0
A	253	GLN	-	expression tag	UNP F9UST0
A	254	PHE	-	expression tag	UNP F9UST0
A	255	GLU	-	expression tag	UNP F9UST0
A	256	LYS	-	expression tag	UNP F9UST0
B	127	ALA	SER	engineered mutation	UNP F9UST0
B	247	ALA	-	expression tag	UNP F9UST0
B	248	SER	-	expression tag	UNP F9UST0
B	249	TRP	-	expression tag	UNP F9UST0
B	250	SER	-	expression tag	UNP F9UST0
B	251	HIS	-	expression tag	UNP F9UST0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	252	PRO	-	expression tag	UNP F9UST0
B	253	GLN	-	expression tag	UNP F9UST0
B	254	PHE	-	expression tag	UNP F9UST0
B	255	GLU	-	expression tag	UNP F9UST0
B	256	LYS	-	expression tag	UNP F9UST0
C	127	ALA	SER	engineered mutation	UNP F9UST0
C	247	ALA	-	expression tag	UNP F9UST0
C	248	SER	-	expression tag	UNP F9UST0
C	249	TRP	-	expression tag	UNP F9UST0
C	250	SER	-	expression tag	UNP F9UST0
C	251	HIS	-	expression tag	UNP F9UST0
C	252	PRO	-	expression tag	UNP F9UST0
C	253	GLN	-	expression tag	UNP F9UST0
C	254	PHE	-	expression tag	UNP F9UST0
C	255	GLU	-	expression tag	UNP F9UST0
C	256	LYS	-	expression tag	UNP F9UST0
D	127	ALA	SER	engineered mutation	UNP F9UST0
D	247	ALA	-	expression tag	UNP F9UST0
D	248	SER	-	expression tag	UNP F9UST0
D	249	TRP	-	expression tag	UNP F9UST0
D	250	SER	-	expression tag	UNP F9UST0
D	251	HIS	-	expression tag	UNP F9UST0
D	252	PRO	-	expression tag	UNP F9UST0
D	253	GLN	-	expression tag	UNP F9UST0
D	254	PHE	-	expression tag	UNP F9UST0
D	255	GLU	-	expression tag	UNP F9UST0
D	256	LYS	-	expression tag	UNP F9UST0
E	127	ALA	SER	engineered mutation	UNP F9UST0
E	247	ALA	-	expression tag	UNP F9UST0
E	248	SER	-	expression tag	UNP F9UST0
E	249	TRP	-	expression tag	UNP F9UST0
E	250	SER	-	expression tag	UNP F9UST0
E	251	HIS	-	expression tag	UNP F9UST0
E	252	PRO	-	expression tag	UNP F9UST0
E	253	GLN	-	expression tag	UNP F9UST0
E	254	PHE	-	expression tag	UNP F9UST0
E	255	GLU	-	expression tag	UNP F9UST0
E	256	LYS	-	expression tag	UNP F9UST0
F	127	ALA	SER	engineered mutation	UNP F9UST0
F	247	ALA	-	expression tag	UNP F9UST0
F	248	SER	-	expression tag	UNP F9UST0
F	249	TRP	-	expression tag	UNP F9UST0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	250	SER	-	expression tag	UNP F9UST0
F	251	HIS	-	expression tag	UNP F9UST0
F	252	PRO	-	expression tag	UNP F9UST0
F	253	GLN	-	expression tag	UNP F9UST0
F	254	PHE	-	expression tag	UNP F9UST0
F	255	GLU	-	expression tag	UNP F9UST0
F	256	LYS	-	expression tag	UNP F9UST0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

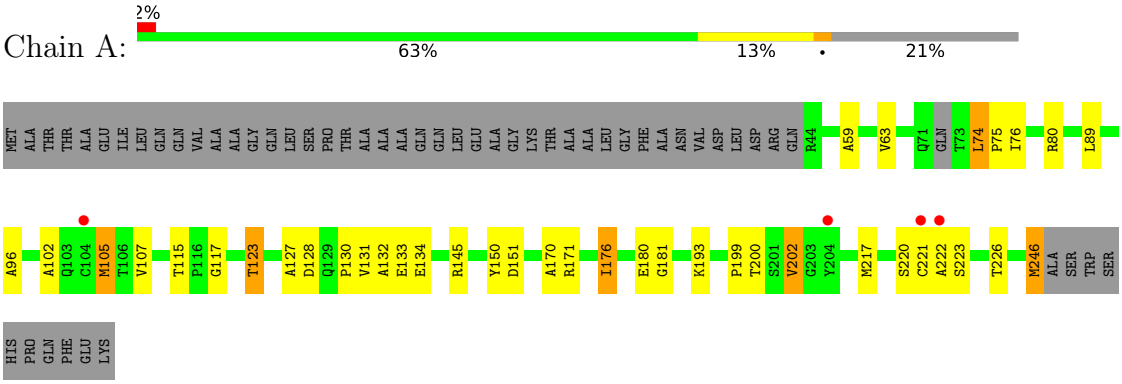
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

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.

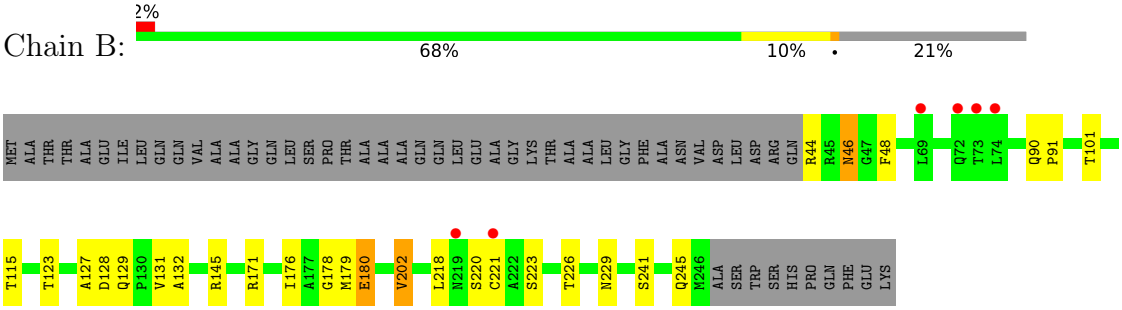
• Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase

Chain A:



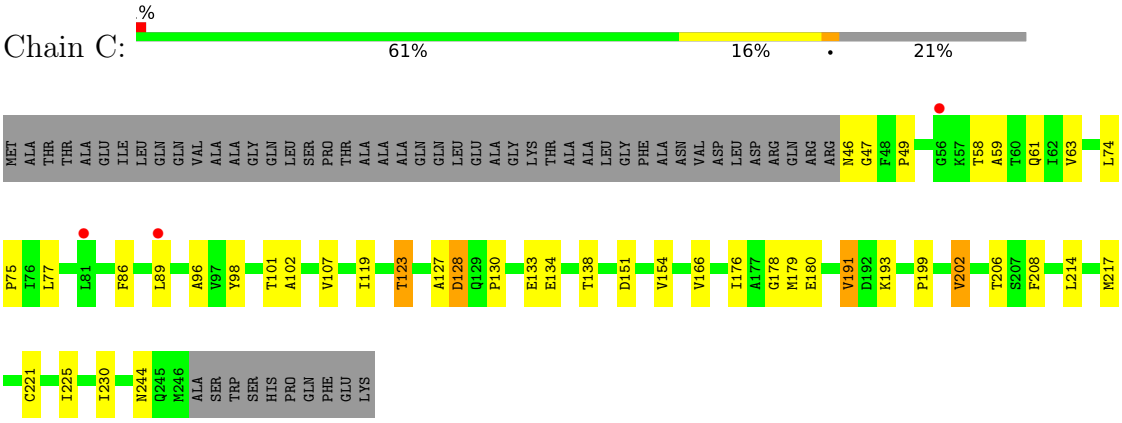
• Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase

Chain B:



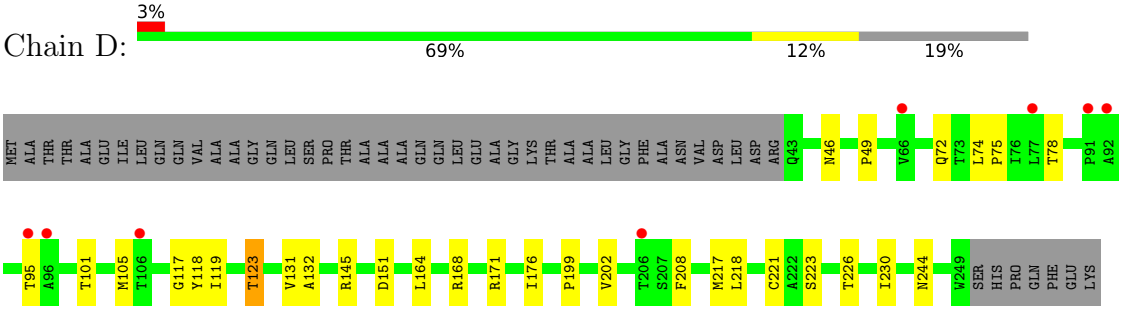
• Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase

Chain C:



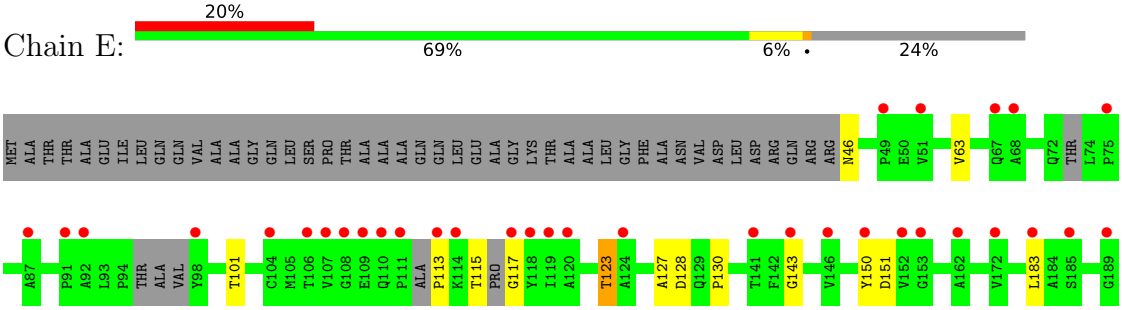
• Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase

Chain D:



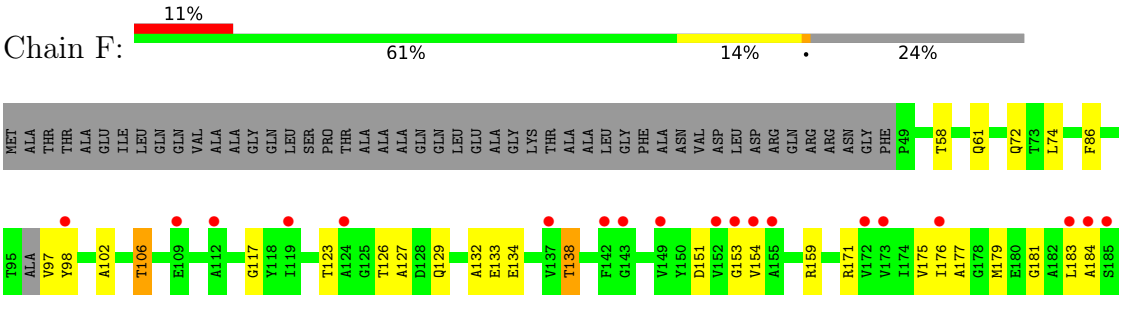
• Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase

Chain E:



• Molecule 1: Pyridinium-3,5-biscarboxylic acid mononucleotide synthase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	120.38Å 120.38Å 213.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.91 – 2.80 85.12 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.91-2.80) 99.6 (85.12-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.82Å)	Xtriage
Refinement program	PHENIX (1.19_4092: ???)	Depositor
R, R_{free}	0.237 , 0.273 0.236 , 0.271	Depositor DCC
R_{free} test set	2024 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	73.8	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 80.0	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	0.91	EDS
Total number of atoms	8140	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.50% 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: MG, ZN

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	0.30	0/1476	0.56	0/2018
1	B	0.31	0/1457	0.54	0/1998
1	C	0.30	0/1417	0.56	0/1941
1	D	0.28	0/1442	0.52	0/1977
1	E	0.30	0/1208	0.56	0/1662
1	F	0.26	0/1244	0.51	0/1715
All	All	0.29	0/8244	0.54	0/11311

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	1454	0	1442	25	0
1	B	1436	0	1404	14	0
1	C	1395	0	1389	25	0
1	D	1424	0	1340	15	0
1	E	1197	0	1013	11	0
1	F	1230	0	1084	26	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
All	All	8140	0	7672	108	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 7.

The worst 5 of 108 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:63:VAL:HG22	1:C:89:LEU:HD13	1.54	0.88
1:C:123:THR:HG22	1:C:151:ASP:H	1.53	0.74
1:C:127:ALA:HB1	1:C:202:VAL:HG21	1.70	0.72
1:E:127:ALA:O	1:E:130:PRO:HD2	1.91	0.70
1:C:77:LEU:HD21	1:C:138:THR:HG22	1.71	0.70

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	204/256 (80%)	183 (90%)	14 (7%)	7 (3%)	3 13
1	B	208/256 (81%)	188 (90%)	15 (7%)	5 (2%)	6 20
1	C	199/256 (78%)	186 (94%)	12 (6%)	1 (0%)	29 61
1	D	211/256 (82%)	194 (92%)	13 (6%)	4 (2%)	8 26
1	E	185/256 (72%)	172 (93%)	12 (6%)	1 (0%)	29 61
1	F	189/256 (74%)	176 (93%)	12 (6%)	1 (0%)	29 61
All	All	1196/1536 (78%)	1099 (92%)	78 (6%)	19 (2%)	14 31

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220[A]	SER
1	A	220[B]	SER
1	B	179	MET
1	A	128	ASP
1	B	221[A]	CYS

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	142/190 (75%)	136 (96%)	6 (4%)	30	63
1	B	136/190 (72%)	129 (95%)	7 (5%)	24	55
1	C	137/190 (72%)	131 (96%)	6 (4%)	28	61
1	D	126/190 (66%)	120 (95%)	6 (5%)	25	58
1	E	88/190 (46%)	83 (94%)	5 (6%)	20	50
1	F	96/190 (50%)	94 (98%)	2 (2%)	53	84
All	All	725/1140 (64%)	693 (96%)	32 (4%)	27	61

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	183	LEU
1	E	229	ASN
1	B	229	ASN
1	B	202	VAL
1	F	106	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	46	ASN
1	D	72	GLN

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Mol	Chain	Res	Type
1	D	244	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	202/256 (78%)	0.27	4 (1%)	65	56	36, 66, 137, 181	0
1	B	203/256 (79%)	0.29	6 (2%)	50	40	38, 65, 127, 214	0
1	C	201/256 (78%)	0.28	3 (1%)	73	68	37, 66, 138, 180	0
1	D	207/256 (80%)	0.34	8 (3%)	39	29	42, 81, 152, 205	0
1	E	195/256 (76%)	1.16	51 (26%)	0	0	123, 174, 225, 296	0
1	F	195/256 (76%)	0.79	28 (14%)	2	1	115, 163, 208, 273	0
All	All	1203/1536 (78%)	0.52	100 (8%)	11	6	36, 98, 194, 296	0

The worst 5 of 100 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	91	PRO	4.9
1	E	185	SER	4.9
1	E	143	GLY	4.7
1	E	221	CYS	4.7
1	E	193	LYS	4.6

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, 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
2	ZN	C	301	1/1	0.80	0.17	165,165,165,165	0
3	MG	D	301	1/1	0.84	0.27	88,88,88,88	0
3	MG	A	302	1/1	0.86	0.21	100,100,100,100	0
2	ZN	A	301	1/1	0.95	0.14	128,128,128,128	0

6.5 Other polymers

There are no such residues in this entry.