Full wwPDB X-ray Structure Validation Report ⓘ

Jul 11, 2022 – 01:09 pm BST

PDB ID	:	7ZA4
Title	:	GSTF sh155 mutant
Authors	:	Papageorgiou, A.C.
Deposited on	:	2022-03-22
Resolution	:	2.05 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 ⓘ 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 ⓘ) were used in the production of this report:

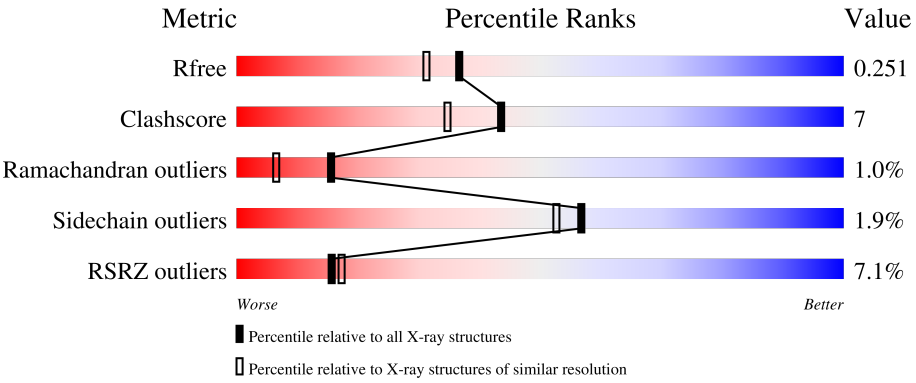
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	225	6% 80% 16%
1	B	225	5% 75% 14% 10%
1	C	225	9% 72% 16% 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5124 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 Glutathione transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1752	1137	289	316	10			
1	B	203	Total	C	N	O	S	0	0	0
			1621	1056	263	294	8			
1	C	200	Total	C	N	O	S	0	0	0
			1602	1042	260	291	9			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	ASP	ASN	variant	UNP Q9ZS17
A	37	LYS	ASN	variant	UNP Q9ZS17
A	38	ALA	THR	variant	UNP Q9ZS17
A	48	VAL	ALA	variant	UNP Q9ZS17
A	66	PHE	TRP	variant	UNP Q9ZS17
A	72	ALA	SER	variant	UNP Q9ZS17
A	90	GLY	SER	variant	UNP Q9ZS17
A	93	LYS	GLU	variant	UNP Q9ZS17
A	119	GLU	GLN	variant	UNP Q9ZS17
A	122	ILE	PHE	variant	UNP Q9ZS17
A	125	LEU	MET	variant	UNP Q9ZS17
A	132	ASN	ASP	variant	UNP Q9ZS17
A	133	GLN	GLU	variant	UNP Q9ZS17
A	134	THR	LYS	variant	UNP Q9ZS17
A	137	ASP	ALA	variant	UNP Q9ZS17
A	156	GLN	LYS	variant	UNP Q9ZS17
A	158	LYS	SER	variant	UNP Q9ZS17
A	220	HIS	-	expression tag	UNP Q9ZS17
A	221	HIS	-	expression tag	UNP Q9ZS17
A	222	HIS	-	expression tag	UNP Q9ZS17
A	223	HIS	-	expression tag	UNP Q9ZS17
A	224	HIS	-	expression tag	UNP Q9ZS17
A	225	HIS	-	expression tag	UNP Q9ZS17

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Chain	Residue	Modelled	Actual	Comment	Reference
B	33	ASP	ASN	variant	UNP Q9ZS17
B	37	LYS	ASN	variant	UNP Q9ZS17
B	38	ALA	THR	variant	UNP Q9ZS17
B	48	VAL	ALA	variant	UNP Q9ZS17
B	66	PHE	TRP	variant	UNP Q9ZS17
B	72	ALA	SER	variant	UNP Q9ZS17
B	90	GLY	SER	variant	UNP Q9ZS17
B	93	LYS	GLU	variant	UNP Q9ZS17
B	119	GLU	GLN	variant	UNP Q9ZS17
B	122	ILE	PHE	variant	UNP Q9ZS17
B	125	LEU	MET	variant	UNP Q9ZS17
B	132	ASN	ASP	variant	UNP Q9ZS17
B	133	GLN	GLU	variant	UNP Q9ZS17
B	134	THR	LYS	variant	UNP Q9ZS17
B	137	ASP	ALA	variant	UNP Q9ZS17
B	156	GLN	LYS	variant	UNP Q9ZS17
B	158	LYS	SER	variant	UNP Q9ZS17
B	220	HIS	-	expression tag	UNP Q9ZS17
B	221	HIS	-	expression tag	UNP Q9ZS17
B	222	HIS	-	expression tag	UNP Q9ZS17
B	223	HIS	-	expression tag	UNP Q9ZS17
B	224	HIS	-	expression tag	UNP Q9ZS17
B	225	HIS	-	expression tag	UNP Q9ZS17
C	33	ASP	ASN	variant	UNP Q9ZS17
C	37	LYS	ASN	variant	UNP Q9ZS17
C	38	ALA	THR	variant	UNP Q9ZS17
C	48	VAL	ALA	variant	UNP Q9ZS17
C	66	PHE	TRP	variant	UNP Q9ZS17
C	72	ALA	SER	variant	UNP Q9ZS17
C	90	GLY	SER	variant	UNP Q9ZS17
C	93	LYS	GLU	variant	UNP Q9ZS17
C	119	GLU	GLN	variant	UNP Q9ZS17
C	122	ILE	PHE	variant	UNP Q9ZS17
C	125	LEU	MET	variant	UNP Q9ZS17
C	132	ASN	ASP	variant	UNP Q9ZS17
C	133	GLN	GLU	variant	UNP Q9ZS17
C	134	THR	LYS	variant	UNP Q9ZS17
C	137	ASP	ALA	variant	UNP Q9ZS17
C	156	GLN	LYS	variant	UNP Q9ZS17
C	158	LYS	SER	variant	UNP Q9ZS17
C	220	HIS	-	expression tag	UNP Q9ZS17
C	221	HIS	-	expression tag	UNP Q9ZS17

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Chain	Residue	Modelled	Actual	Comment	Reference
C	222	HIS	-	expression tag	UNP Q9ZS17
C	223	HIS	-	expression tag	UNP Q9ZS17
C	224	HIS	-	expression tag	UNP Q9ZS17
C	225	HIS	-	expression tag	UNP Q9ZS17

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Na 2 2	0	0

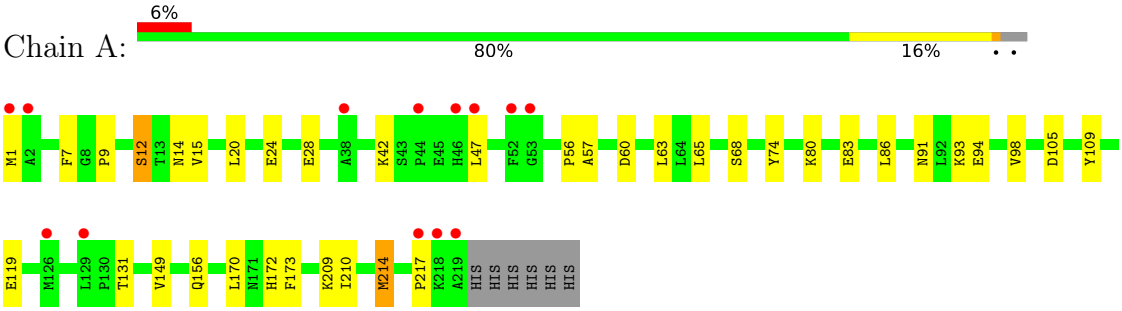
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	61	Total O 61 61	0	0
3	B	43	Total O 43 43	0	0
3	C	43	Total O 43 43	0	0

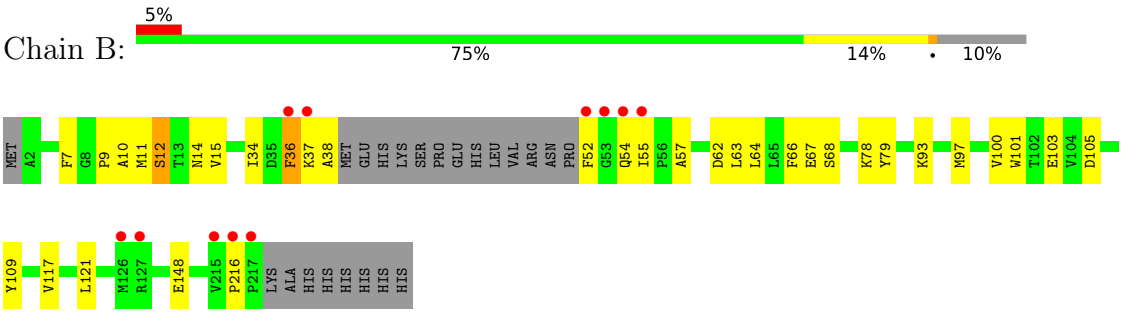
3 Residue-property plots (i)

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.

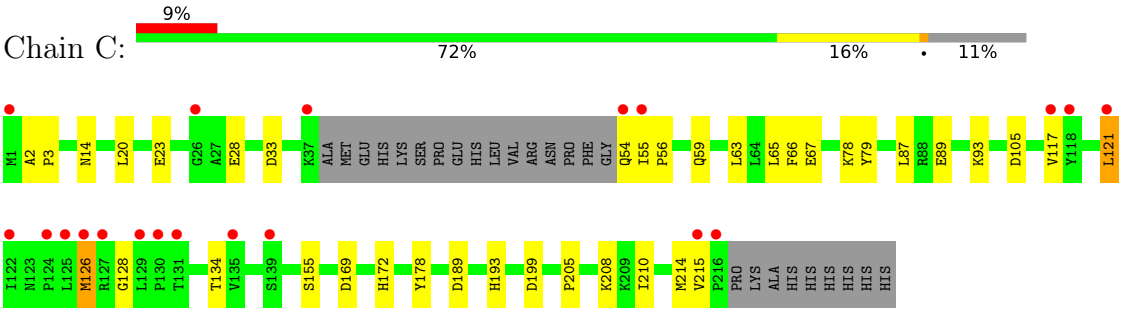
• Molecule 1: Glutathione transferase



• Molecule 1: Glutathione transferase



• Molecule 1: Glutathione transferase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	46.48Å 99.00Å 153.21Å 90.00° 93.73° 90.00°	Depositor
Resolution (Å)	45.31 – 2.05 45.31 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.31-2.05) 99.9 (45.31-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.216 , 0.252 0.215 , 0.251	Depositor DCC
R_{free} test set	2163 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5124	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 5.56% 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: NA

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	0.43	0/1800	0.60	1/2449 (0.0%)
1	B	0.41	0/1664	0.57	0/2265
1	C	0.39	0/1643	0.56	0/2235
All	All	0.41	0/5107	0.58	1/6949 (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	A	214	MET	CG-SD-CE	-5.24	91.81	100.20

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	1752	0	1748	28	0
1	B	1621	0	1611	23	0
1	C	1602	0	1599	20	0
2	B	2	0	0	0	0
3	A	61	0	0	2	1
3	B	43	0	0	4	0
3	C	43	0	0	5	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5124	0	4958	67	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 7.

All (67) 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:199:ASP:O	3:C:302:HOH:O	1.99	0.81
1:C:33:ASP:OD1	3:C:301:HOH:O	1.98	0.80
1:A:24:GLU:OE1	3:A:301:HOH:O	2.00	0.79
1:C:3:PRO:HB3	1:C:28:GLU:HG3	1.66	0.78
1:B:38:ALA:O	3:B:401:HOH:O	2.05	0.74
1:C:169:ASP:OD2	3:C:303:HOH:O	2.07	0.72
1:A:1:MET:HE2	1:A:28:GLU:HB2	1.76	0.68
1:B:37:LYS:O	1:B:37:LYS:HG3	1.92	0.68
1:C:117:VAL:HG23	1:C:121:LEU:HD13	1.75	0.67
1:C:59:GLN:OE1	3:C:304:HOH:O	2.12	0.67
1:B:148:GLU:OE2	3:B:403:HOH:O	2.15	0.64
1:B:54:GLN:NE2	3:B:402:HOH:O	2.12	0.64
1:A:93:LYS:HE2	1:B:63:LEU:HB2	1.82	0.60
1:C:54:GLN:HB2	1:C:66:PHE:HB3	1.81	0.60
1:A:7:PHE:HB2	1:A:57:ALA:HB3	1.85	0.58
1:C:155:SER:HB3	1:C:193:HIS:ND1	2.21	0.56
1:C:14:ASN:HB3	1:C:56:PRO:HD3	1.87	0.56
1:A:210:ILE:HG22	1:A:214:MET:CE	2.36	0.55
1:C:20:LEU:HA	1:C:210:ILE:HG13	1.87	0.55
1:A:9:PRO:O	1:A:12:SER:HB3	2.07	0.55
1:A:86:LEU:HD13	1:A:170:LEU:HD11	1.88	0.54
1:C:117:VAL:HG21	1:C:178:TYR:HB3	1.91	0.52
1:A:1:MET:HE1	1:A:28:GLU:H	1.75	0.52
1:B:100:VAL:HG13	1:B:101:TRP:CD1	2.44	0.52
1:A:105:ASP:HB2	1:A:172:HIS:CE1	2.44	0.52
1:B:14:ASN:HB3	1:B:68:SER:HB3	1.92	0.51
1:B:54:GLN:HB2	1:B:66:PHE:HB3	1.92	0.50
1:B:11:MET:SD	1:B:216:PRO:HG3	2.52	0.49
1:C:105:ASP:HB2	1:C:172:HIS:CE1	2.47	0.49
1:A:149:VAL:HG11	1:B:52:PHE:CE2	2.48	0.49
1:A:20:LEU:HA	1:A:210:ILE:HG13	1.95	0.48
1:A:173:PHE:CE2	1:A:214:MET:HE1	2.47	0.48
1:B:78:LYS:HD3	1:B:79:TYR:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LYS:HG2	1:B:63:LEU:HD13	1.94	0.48
1:A:156:GLN:HE21	1:A:156:GLN:HB3	1.49	0.47
1:A:1:MET:CE	1:A:28:GLU:H	2.27	0.47
1:A:119:GLU:O	1:A:131:THR:HG22	2.15	0.47
1:B:10:ALA:HA	1:B:15:VAL:HG11	1.97	0.46
1:A:15:VAL:HG22	1:A:56:PRO:HB3	1.98	0.46
1:B:97:MET:HA	1:B:100:VAL:HG12	1.98	0.46
1:C:210:ILE:HG22	1:C:214:MET:CE	2.45	0.45
1:B:54:GLN:OE1	1:B:67:GLU:HB2	2.17	0.45
1:A:91:ASN:HB3	1:A:94:GLU:HB2	1.99	0.45
1:C:14:ASN:ND2	1:C:55:ILE:HB	2.32	0.45
1:C:78:LYS:HD3	1:C:79:TYR:CE1	2.51	0.45
1:C:87:LEU:HB3	1:C:89:GLU:HG3	1.99	0.45
1:A:209:LYS:HD2	3:A:302:HOH:O	2.16	0.44
1:A:210:ILE:HG22	1:A:214:MET:HE2	1.99	0.44
1:B:117:VAL:O	1:B:121:LEU:HB2	2.18	0.44
1:A:60:ASP:OD2	1:A:74:TYR:OH	2.34	0.43
1:A:105:ASP:HA	1:A:109:TYR:HB3	2.01	0.43
1:B:7:PHE:HB2	1:B:57:ALA:HB3	2.00	0.43
1:A:14:ASN:HB3	1:A:68:SER:HB3	1.99	0.43
1:A:83:GLU:OE1	1:A:83:GLU:N	2.51	0.43
1:B:105:ASP:HA	1:B:109:TYR:HB3	2.00	0.42
1:C:63:LEU:HD11	1:C:65:LEU:HD21	2.00	0.42
1:A:63:LEU:HB2	1:B:93:LYS:HE2	2.02	0.42
1:B:9:PRO:O	1:B:12:SER:HB3	2.20	0.41
1:C:93:LYS:HG3	3:C:321:HOH:O	2.19	0.41
1:C:23:GLU:HG3	1:C:210:ILE:HD11	2.01	0.41
1:C:205:PRO:O	1:C:208:LYS:HG2	2.19	0.41
1:B:63:LEU:HG	1:B:64:LEU:N	2.36	0.41
1:A:65:LEU:HA	1:A:65:LEU:HD23	1.85	0.40
1:B:34:ILE:HD13	1:B:36:PHE:CE1	2.56	0.40
1:B:103:GLU:OE2	3:B:404:HOH:O	2.22	0.40
1:A:42:LYS:HG3	1:A:47:LEU:HD21	2.03	0.40
1:A:94:GLU:O	1:A:98:VAL:HG23	2.21	0.40

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)
3:C:336:HOH:O	3:C:336:HOH:O[2_456]	2.09	0.11
3:A:349:HOH:O	3:A:358:HOH:O[1_655]	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	217/225 (96%)	205 (94%)	11 (5%)	1 (0%)	29 18
1	B	199/225 (88%)	189 (95%)	10 (5%)	0	100 100
1	C	196/225 (87%)	179 (91%)	12 (6%)	5 (3%)	5 1
All	All	612/675 (91%)	573 (94%)	33 (5%)	6 (1%)	15 6

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	126	MET
1	C	2	ALA
1	C	128	GLY
1	C	215	VAL
1	A	217	PRO
1	C	67	GLU

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	188/194 (97%)	186 (99%)	2 (1%)	73 73
1	B	173/194 (89%)	169 (98%)	4 (2%)	50 44
1	C	172/194 (89%)	168 (98%)	4 (2%)	50 44
All	All	533/582 (92%)	523 (98%)	10 (2%)	57 53

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	80	LYS
1	B	12	SER
1	B	36	PHE
1	B	55	ILE
1	B	62	ASP
1	C	121	LEU
1	C	126	MET
1	C	134	THR
1	C	189	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	156	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 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 (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	219/225 (97%)	0.25	13 (5%) 22 24	29, 43, 77, 114	0
1	B	203/225 (90%)	0.19	11 (5%) 25 28	32, 47, 77, 131	0
1	C	200/225 (88%)	0.53	20 (10%) 7 7	35, 56, 116, 138	0
All	All	622/675 (92%)	0.32	44 (7%) 16 17	29, 49, 85, 138	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	PRO	11.3
1	A	1	MET	10.9
1	A	219	ALA	10.0
1	C	126	MET	7.6
1	C	215	VAL	5.3
1	B	53	GLY	4.8
1	C	216	PRO	4.6
1	C	121	LEU	4.6
1	C	1	MET	4.5
1	A	53	GLY	4.5
1	B	216	PRO	4.3
1	A	38	ALA	4.1
1	B	52	PHE	4.1
1	C	135	VAL	3.9
1	B	36	PHE	3.9
1	C	54	GLN	3.6
1	C	55	ILE	3.4
1	B	54	GLN	3.3
1	A	218	LYS	3.3
1	C	129	LEU	3.3
1	C	125	LEU	3.3
1	A	47	LEU	3.2
1	A	52	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	127	ARG	3.1
1	C	118	TYR	3.0
1	B	215	VAL	2.9
1	C	124	PRO	2.8
1	C	117	VAL	2.5
1	A	129	LEU	2.4
1	C	26	GLY	2.4
1	B	55	ILE	2.4
1	C	130	PRO	2.4
1	A	217	PRO	2.4
1	A	44	PRO	2.3
1	B	37	LYS	2.3
1	B	127	ARG	2.3
1	C	122	ILE	2.2
1	C	37	LYS	2.2
1	A	2	ALA	2.1
1	A	46	HIS	2.1
1	C	131	THR	2.1
1	A	126	MET	2.1
1	C	139	SER	2.0
1	B	126	MET	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
2	NA	B	302	1/1	0.90	0.10	55,55,55,55	0
2	NA	B	301	1/1	0.96	0.13	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.