Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2022 – 01:07 am BST

PDB ID	:	5EFY
Title	:	Apo-form of SCO3201
Authors	:	Waack, P.; Hinrichs, W.
Deposited on	:	2015-10-26
Resolution	:	2.70 Å(reported)

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

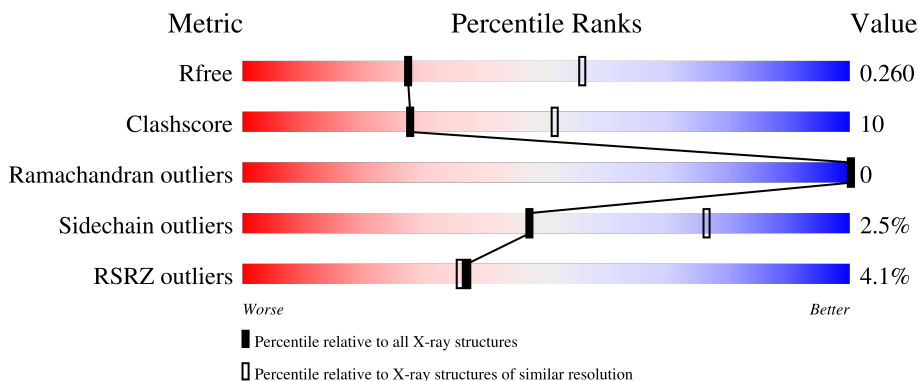|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.30
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 2.70 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		0.260
Clashscore		10
Ramachandran outliers		0
Sidechain outliers		2.5%
RSRZ outliers		4.1%

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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	216	3% / 72% 14% · 12%
1	B	216	% / 72% 17% 11%
1	C	216	4% / 74% 17% · 9%
1	D	216	6% / 69% 13% 18%

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 5332 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 Putative tetR-family transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	0	0
			1343	856	238	246	3			
1	B	193	Total	C	N	O	S	0	0	0
			1392	883	253	253	3			
1	C	197	Total	C	N	O	S	0	0	0
			1392	873	260	256	3			
1	D	178	Total	C	N	O	S	0	0	0
			1182	757	208	214	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	HIS	-	cloning artifact	UNP Q9KYU4
A	22	MET	-	cloning artifact	UNP Q9KYU4
B	21	HIS	-	cloning artifact	UNP Q9KYU4
B	22	MET	-	cloning artifact	UNP Q9KYU4
C	21	HIS	-	cloning artifact	UNP Q9KYU4
C	22	MET	-	cloning artifact	UNP Q9KYU4
D	21	HIS	-	cloning artifact	UNP Q9KYU4
D	22	MET	-	cloning artifact	UNP Q9KYU4

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	O	0	0
			7	7		
2	B	5	Total	O	0	0
			5	5		
2	C	5	Total	O	0	0
			5	5		
2	D	6	Total	O	0	0
			6	6		

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.
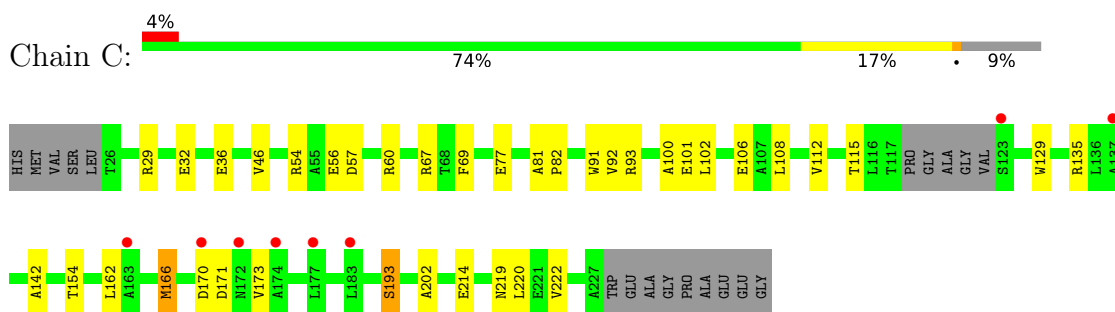
• Molecule 1: Putative tetR-family transcriptional regulator
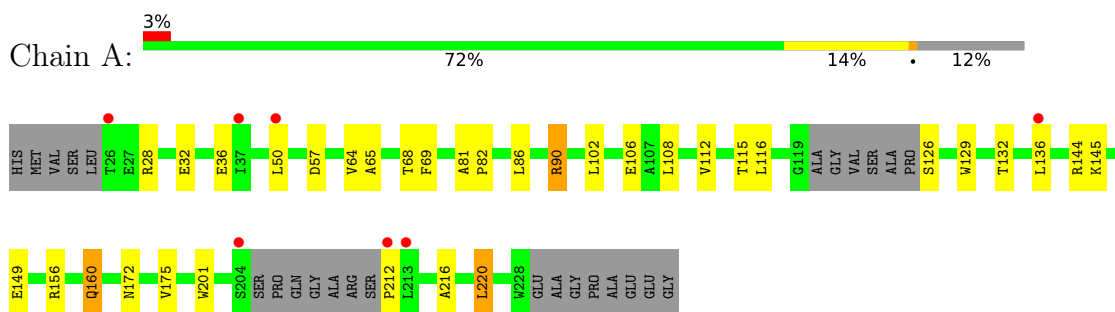
Chain A:

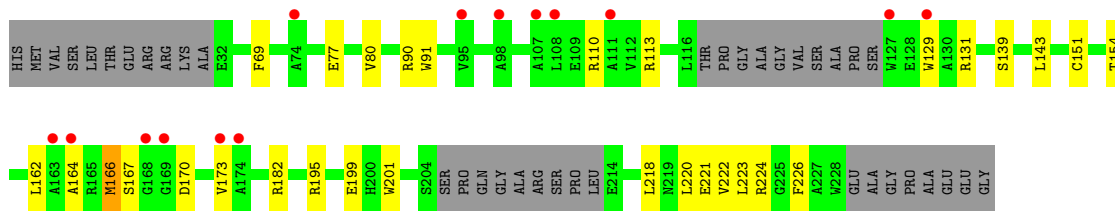• Molecule 1: Putative tetR-family transcriptional regulator

Chain B:

• Molecule 1: Putative tetR-family transcriptional regulator

Chain C:

• Molecule 1: Putative tetR-family transcriptional regulator

Chain D:
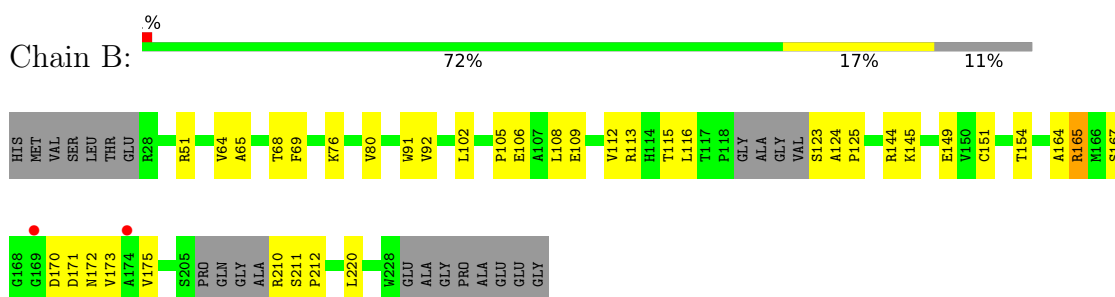
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.79Å 98.43Å 89.61Å 90.00° 100.78° 90.00°	Depositor
Resolution (Å)	88.03 – 2.70 48.12 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.7 (88.03-2.70) 97.0 (48.12-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.94 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.258 , 0.297 0.260 , 0.260	Depositor DCC
R_{free} test set	1155 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	71.0	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning [2]	$< \lvert L \rvert > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5332	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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)

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	0.61	0/1371	0.72	2/1876 (0.1%)
1	B	0.66	0/1419	0.81	3/1936 (0.2%)
1	C	0.62	0/1417	0.79	1/1938 (0.1%)
1	D	0.58	0/1203	0.72	0/1651
All	All	0.62	0/5410	0.76	6/7401 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	144	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	B	220	LEU	CA-CB-CG	5.63	128.26	115.30
1	B	165	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	144	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	220	LEU	CA-CB-CG	5.17	127.18	115.30
1	C	93	ARG	NE-CZ-NH2	5.05	122.82	120.30

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	1343	0	1259	26	0
1	B	1392	0	1346	31	0
1	C	1392	0	1323	26	0

Continued on next page...

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1182	0	1059	28	0
2	A	7	0	0	0	0
2	B	5	0	0	2	0
2	C	5	0	0	0	0
2	D	6	0	0	0	0
All	All	5332	0	4987	103	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 10.

All (103) 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:216:ALA:O	1:A:220:LEU:HD23	1.59	1.01
1:C:101:GLU:OE2	1:C:101:GLU:N	2.06	0.88
1:D:131:ARG:CG	1:D:201:TRP:CZ2	2.60	0.83
1:B:64:VAL:HB	1:B:68:THR:HG21	1.61	0.82
1:D:131:ARG:HG2	1:D:201:TRP:CH2	2.15	0.82
1:A:149:GLU:HG3	1:B:145:LYS:HD3	1.65	0.79
1:C:54:ARG:NH1	1:C:56:GLU:HB2	2.01	0.75
1:A:216:ALA:O	1:A:220:LEU:CD2	2.35	0.75
1:B:65:ALA:O	1:B:68:THR:HG22	1.86	0.75
1:D:195:ARG:O	1:D:199:GLU:HG3	1.86	0.74
1:D:131:ARG:HG2	1:D:201:TRP:CZ2	2.21	0.74
1:B:64:VAL:HB	1:B:68:THR:CG2	2.16	0.74
1:B:167:SER:O	1:B:173:VAL:HG11	1.92	0.70
1:D:167:SER:O	1:D:173:VAL:HG11	1.93	0.69
1:D:131:ARG:CG	1:D:201:TRP:CH2	2.76	0.68
1:C:222:VAL:O	1:D:222:VAL:HG13	1.96	0.67
1:B:76:LYS:HE2	2:B:303:HOH:O	1.93	0.66
1:C:92:VAL:CG2	1:C:154:THR:HG23	2.25	0.66
1:B:124:ALA:N	1:B:125:PRO:HD2	2.11	0.66
1:D:164:ALA:O	1:D:167:SER:HB3	1.96	0.65
1:C:135:ARG:NH2	1:C:202:ALA:O	2.30	0.65
1:D:221:GLU:O	1:D:224:ARG:HG2	1.96	0.65
1:D:131:ARG:HG3	1:D:201:TRP:CZ2	2.31	0.65
1:B:105:PRO:O	1:B:109:GLU:HG3	1.97	0.64
1:C:77:GLU:HG3	1:C:142:ALA:HB1	1.78	0.64
1:B:164:ALA:O	1:B:167:SER:HB3	1.98	0.64
1:C:54:ARG:HG2	1:C:57:ASP:OD2	1.99	0.63
1:A:201:TRP:CD2	1:A:212:PRO:HG3	2.34	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:ARG:NE	1:C:202:ALA:O	2.32	0.62
1:C:101:GLU:H	1:C:101:GLU:CD	1.98	0.62
1:C:193:SER:OG	1:C:219:ASN:HB2	2.02	0.60
1:D:80:VAL:HG21	1:D:143:LEU:HD21	1.82	0.60
1:B:170:ASP:O	1:B:173:VAL:HG12	2.02	0.59
1:A:64:VAL:CG1	1:A:68:THR:HB	2.33	0.59
1:C:162:LEU:O	1:C:166:MET:HG2	2.02	0.59
1:B:116:LEU:HD22	1:B:212:PRO:HB2	1.85	0.59
1:D:170:ASP:O	1:D:173:VAL:HG12	2.02	0.59
1:C:57:ASP:OD1	1:C:60:ARG:NH2	2.38	0.57
1:C:222:VAL:O	1:D:222:VAL:CG1	2.52	0.57
1:A:129:TRP:HA	1:A:132:THR:HG22	1.87	0.56
1:D:223:LEU:O	1:D:226:PHE:N	2.39	0.56
1:C:193:SER:OG	1:C:219:ASN:CB	2.54	0.56
1:A:149:GLU:HG3	1:B:145:LYS:CD	2.35	0.56
1:B:172:ASN:O	1:B:175:VAL:HG12	2.06	0.56
1:A:108:LEU:O	1:A:112:VAL:HG23	2.06	0.55
1:B:165:ARG:HB2	2:B:301:HOH:O	2.05	0.55
1:B:210:ARG:CG	1:B:211:SER:H	2.20	0.55
1:B:91:TRP:HB2	1:B:115:THR:HG21	1.90	0.54
1:B:124:ALA:N	1:B:125:PRO:CD	2.71	0.54
1:B:108:LEU:O	1:B:112:VAL:HG23	2.08	0.53
1:A:172:ASN:O	1:A:175:VAL:HG12	2.08	0.52
1:B:92:VAL:CG2	1:B:154:THR:HG23	2.39	0.52
1:C:170:ASP:HB2	1:C:173:VAL:HB	1.91	0.52
1:C:102:LEU:HD22	1:C:106:GLU:CB	2.40	0.52
1:A:57:ASP:N	1:A:57:ASP:OD1	2.42	0.51
1:C:108:LEU:O	1:C:112:VAL:HG23	2.11	0.51
1:D:220:LEU:HD23	1:D:220:LEU:O	2.10	0.51
1:B:123:SER:C	1:B:125:PRO:HD2	2.32	0.49
1:A:64:VAL:HG12	1:A:68:THR:HB	1.94	0.49
1:D:162:LEU:O	1:D:166:MET:HG2	2.13	0.49
1:A:145:LYS:HG2	1:B:149:GLU:HG3	1.95	0.49
1:B:51:ARG:NH2	1:C:214:GLU:OE2	2.45	0.49
1:B:167:SER:O	1:B:173:VAL:CG1	2.61	0.49
1:C:69:PHE:C	1:C:69:PHE:CD1	2.86	0.49
1:C:91:TRP:HB2	1:C:115:THR:HG21	1.94	0.48
1:C:32:GLU:O	1:C:36:GLU:HG3	2.13	0.48
1:A:32:GLU:O	1:A:36:GLU:HG3	2.13	0.48
1:C:46:VAL:HG21	1:C:129:TRP:CZ3	2.49	0.47
1:A:156:ARG:O	1:A:160:GLN:HG3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:ARG:NH1	1:C:32:GLU:OE1	2.48	0.46
1:A:86:LEU:O	1:A:90:ARG:HD2	2.15	0.46
1:D:131:ARG:HG2	1:D:201:TRP:CZ3	2.50	0.46
1:B:69:PHE:C	1:B:69:PHE:CD1	2.89	0.46
1:B:102:LEU:HD22	1:B:106:GLU:HB3	1.98	0.46
1:D:167:SER:O	1:D:173:VAL:CG1	2.62	0.46
1:A:28:ARG:O	1:A:32:GLU:N	2.44	0.45
1:B:210:ARG:CG	1:B:211:SER:N	2.80	0.45
1:D:69:PHE:CD1	1:D:69:PHE:C	2.89	0.45
1:A:145:LYS:CG	1:B:149:GLU:HG3	2.47	0.44
1:A:149:GLU:HG3	1:B:145:LYS:CG	2.48	0.44
1:B:151:CYS:O	1:B:154:THR:HB	2.18	0.44
1:B:109:GLU:HB3	1:B:113:ARG:NH2	2.32	0.44
1:A:115:THR:OG1	1:A:116:LEU:N	2.51	0.43
1:A:81:ALA:N	1:A:82:PRO:CD	2.81	0.43
1:D:151:CYS:O	1:D:154:THR:HB	2.18	0.43
1:A:126:SER:O	1:A:129:TRP:HE3	2.01	0.43
1:C:135:ARG:CZ	1:C:202:ALA:O	2.68	0.42
1:D:218:LEU:O	1:D:221:GLU:HB2	2.20	0.42
1:C:81:ALA:N	1:C:82:PRO:CD	2.83	0.42
1:A:69:PHE:CD1	1:A:69:PHE:C	2.93	0.42
1:A:50:LEU:HD13	1:A:136:LEU:HD22	2.00	0.41
1:C:100:ALA:N	1:C:101:GLU:OE2	2.53	0.41
1:A:64:VAL:HG12	1:A:65:ALA:N	2.34	0.41
1:A:50:LEU:HD11	1:A:136:LEU:HD13	2.02	0.41
1:D:162:LEU:O	1:D:166:MET:CG	2.68	0.41
1:D:182:ARG:HG3	1:D:226:PHE:HZ	1.86	0.41
1:D:90:ARG:CG	1:D:91:TRP:N	2.83	0.41
1:D:77:GLU:O	1:D:80:VAL:HG22	2.21	0.40
1:A:102:LEU:HD22	1:A:106:GLU:HB3	2.04	0.40
1:B:80:VAL:O	1:B:80:VAL:HG12	2.21	0.40
1:D:110:ARG:O	1:D:113:ARG:CB	2.70	0.40
1:D:131:ARG:HG3	1:D:201:TRP:CH2	2.51	0.40
1:D:220:LEU:HG	1:D:223:LEU:HD23	2.04	0.40

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	184/216 (85%)	184 (100%)	0	0	100	100
1	B	187/216 (87%)	187 (100%)	0	0	100	100
1	C	193/216 (89%)	190 (98%)	3 (2%)	0	100	100
1	D	172/216 (80%)	171 (99%)	1 (1%)	0	100	100
All	All	736/864 (85%)	732 (100%)	4 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	112/156 (72%)	110 (98%)	2 (2%)	59	83
1	B	121/156 (78%)	120 (99%)	1 (1%)	81	93
1	C	118/156 (76%)	113 (96%)	5 (4%)	30	58
1	D	84/156 (54%)	81 (96%)	3 (4%)	35	64
All	All	435/624 (70%)	424 (98%)	11 (2%)	47	76

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ARG
1	A	160	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	171	ASP
1	C	67	ARG
1	C	166	MET
1	C	171	ASP
1	C	193	SER
1	C	220	LEU
1	D	129	TRP
1	D	139	SER
1	D	166	MET

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 ⓘ

There are no ligands in this entry.

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 (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	190/216 (87%)	0.20	7 (3%)	41	41	47, 79, 118, 144	0
1	B	193/216 (89%)	0.12	2 (1%)	82	83	38, 71, 115, 138	0
1	C	197/216 (91%)	0.16	8 (4%)	37	36	52, 81, 133, 168	0
1	D	178/216 (82%)	0.44	14 (7%)	12	10	57, 90, 156, 176	0
All	All	758/864 (87%)	0.23	31 (4%)	37	36	38, 79, 134, 176	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	95	VAL	5.1
1	C	174	ALA	4.3
1	A	204	SER	4.0
1	D	164	ALA	3.9
1	D	168	GLY	3.7
1	D	107	ALA	3.2
1	C	177	LEU	3.2
1	D	98	ALA	3.2
1	D	127	TRP	3.0
1	A	136	LEU	3.0
1	A	213	LEU	3.0
1	C	172	ASN	2.9
1	A	26	THR	2.8
1	C	170	ASP	2.8
1	C	183	LEU	2.8
1	D	174	ALA	2.6
1	D	108	LEU	2.4
1	A	37	ILE	2.4
1	A	212	PRO	2.4
1	D	129	TRP	2.3
1	A	50	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	169	GLY	2.2
1	D	74	ALA	2.2
1	C	137	ALA	2.2
1	C	123	SER	2.2
1	D	111	ALA	2.2
1	D	169	GLY	2.1
1	B	174	ALA	2.1
1	D	163	ALA	2.1
1	D	173	VAL	2.1
1	C	163	ALA	2.1

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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.