Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2022 – 06:08 pm GMT

PDB ID	:	7NFA
Title	:	The structure of the humanised A33 Fab C226S variant, an immunotherapy candidate for colorectal cancer
Authors	:	Tang, J.; Zhang, C.; Dalby, P.; Kozielski, F.
Deposited on	:	2021-02-05
Resolution	:	2.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

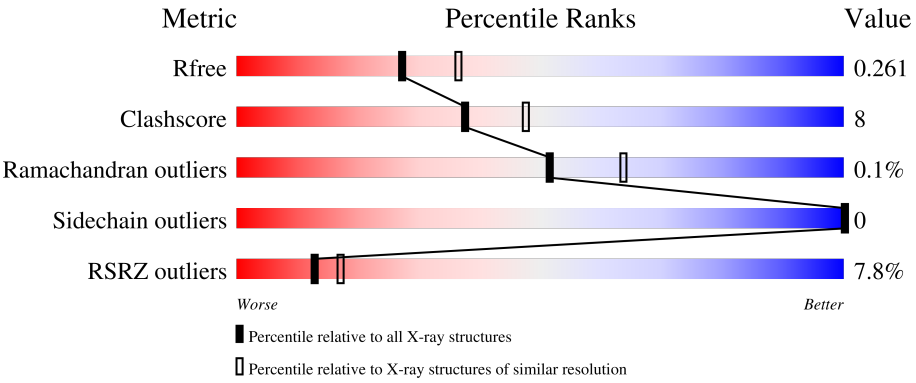
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.26
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 2.30 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	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	214	6% 86% 13%
1	B	214	9% 83% 16%
2	C	228	7% 76% 16% 7%
2	D	228	8% 75% 18% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6612 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 A33 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1612	1013	274	320	5			
1	B	213	Total	C	N	O	S	0	0	0
			1626	1019	276	326	5			

- Molecule 2 is a protein called A33 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	211	Total	C	N	O	S	0	0	0
			1564	994	255	309	6			
2	D	211	Total	C	N	O	S	0	1	0
			1563	994	256	307	6			

- Molecule 3 is water.

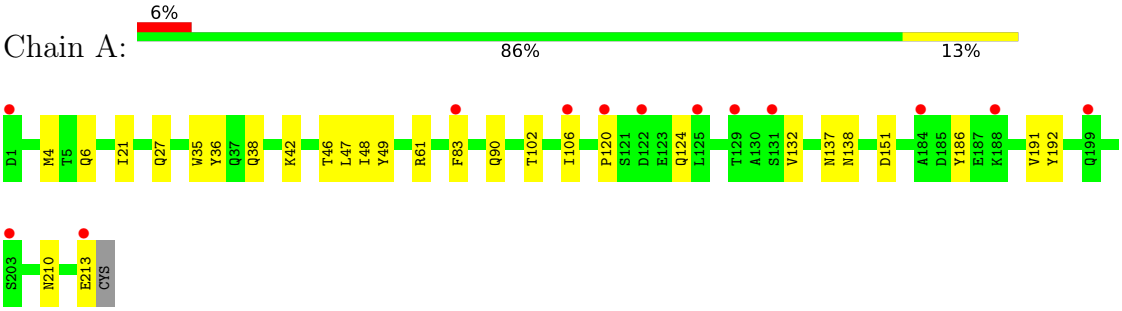
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total	O	0	0
			54	54		
3	C	77	Total	O	0	0
			77	77		
3	B	44	Total	O	0	0
			44	44		
3	D	72	Total	O	0	0
			72	72		

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.

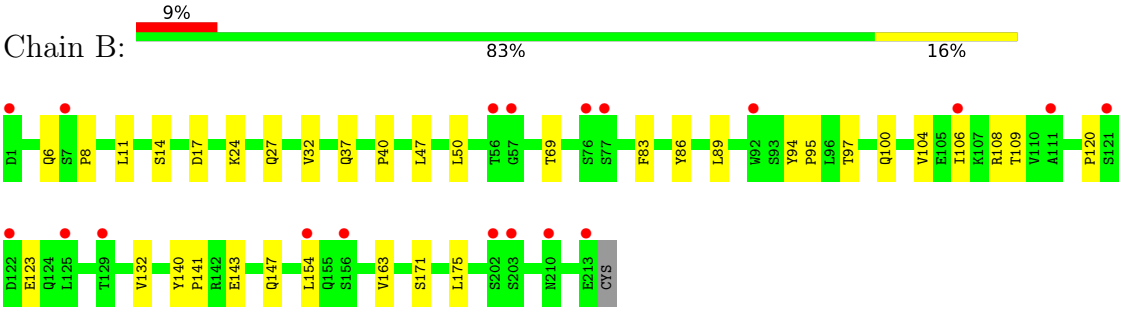
• Molecule 1: A33 Fab light chain

Chain A:



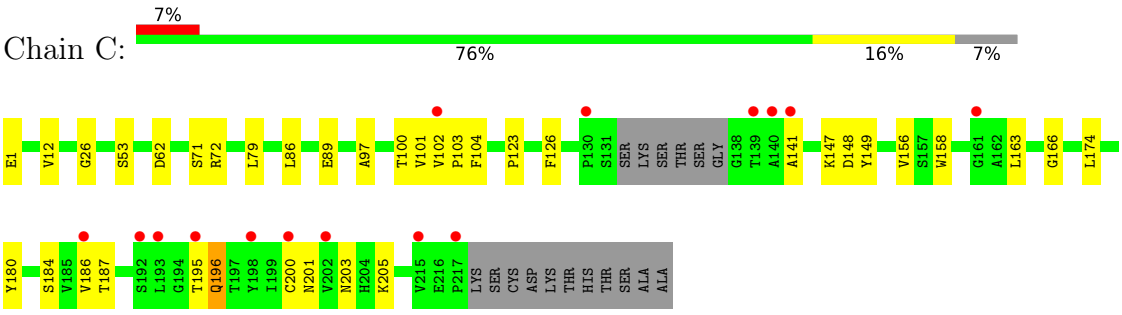
• Molecule 1: A33 Fab light chain

Chain B:



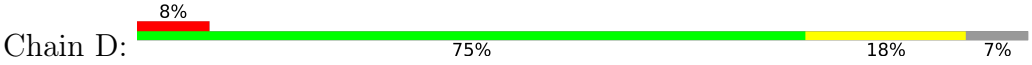
• Molecule 2: A33 Fab heavy chain

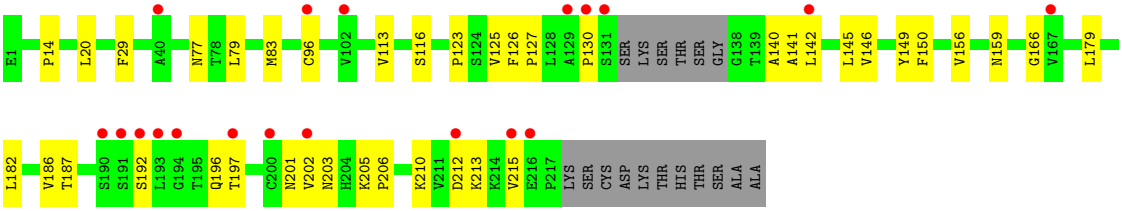
Chain C:



• Molecule 2: A33 Fab heavy chain

Chain D:




E1 P14 L20 F29 A40 N77 T78 L79 M83 C96 V102 V113 S116 P123 S124 V125 F126 P127 L128 A129 P130 S131 SER LYS SER THR SER GLY G138 T139 A140 A141 L142 L145 V146 Y149 F150 V156 N159 G166 V167 L179
L182 V186 T187 S190 S191 S192 L193 G194 T195 Q196 T197 C200 N201 V202 N203 H204 K205 P206 K210 V211 D212 K213 K214 V215 E216 P217 LYS SER CYS ASP LYS THR HIS THR SER ALA ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	37.67Å 69.73Å 89.85Å 99.71° 101.43° 105.66°	Depositor
Resolution (Å)	59.02 – 2.30 85.59 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.9 (59.02-2.30) 94.0 (85.59-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.43 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.193 , 0.260 0.193 , 0.261	Depositor DCC
R_{free} test set	1713 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.036 for h,-h-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6612	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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

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	0.55	0/1649	0.70	1/2247 (0.0%)
1	B	0.52	0/1663	0.73	0/2265
2	C	0.61	0/1603	0.78	0/2191
2	D	0.60	0/1602	0.78	0/2190
All	All	0.57	0/6517	0.74	1/8893 (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	47	LEU	CA-CB-CG	5.52	127.99	115.30

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	1612	0	1551	20	0
1	B	1626	0	1563	24	0
2	C	1564	0	1526	29	0
2	D	1563	0	1524	28	0
3	A	54	0	0	2	0
3	B	44	0	0	1	0
3	C	77	0	0	1	0
3	D	72	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6612	0	6164	97	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.

All (97) 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)
2:C:163:LEU:HD21	2:C:186:VAL:HG21	1.62	0.81
2:D:166:GLY:O	2:D:186:VAL:HA	1.81	0.79
2:C:100:THR:HG22	2:C:101:VAL:H	1.49	0.77
2:C:203:ASN:HD21	2:C:205:LYS:HE3	1.51	0.75
1:B:83:PHE:CD2	1:B:106:ILE:HD13	2.24	0.71
1:A:137:ASN:OD1	1:A:138:ASN:ND2	2.25	0.69
2:D:156:VAL:HG22	2:D:202:VAL:HG12	1.72	0.69
1:A:6:GLN:HE21	1:A:102:THR:HG23	1.58	0.68
2:C:100:THR:HG22	2:C:101:VAL:N	2.15	0.61
1:A:21:ILE:HG23	1:A:102:THR:HG21	1.85	0.59
2:C:89:GLU:OE1	3:C:301:HOH:O	2.16	0.59
2:C:195:THR:O	2:C:196:GLN:HB2	2.03	0.59
2:C:158:TRP:CH2	2:C:200:CYS:HB3	2.38	0.59
1:B:147:GLN:OE1	1:B:154:LEU:HD11	2.03	0.58
1:A:186:TYR:O	1:A:192:TYR:OH	2.22	0.58
1:A:151:ASP:HA	1:A:191:VAL:HG12	1.87	0.57
1:A:38:GLN:NE2	1:A:42:LYS:O	2.33	0.56
2:C:1:GLU:OE1	2:C:26:GLY:HA2	2.05	0.56
1:B:108:ARG:HG3	1:B:108:ARG:HH21	1.69	0.56
1:B:83:PHE:CE2	1:B:106:ILE:HD13	2.41	0.56
2:D:130:PRO:HD3	2:D:142:LEU:HB3	1.87	0.55
2:C:156:VAL:HA	2:C:201:ASN:O	2.07	0.55
1:A:83:PHE:CE2	1:A:106:ILE:HG12	2.42	0.55
2:C:97:ALA:HB1	2:C:104:PHE:HA	1.89	0.54
1:B:14:SER:HB2	1:B:17:ASP:OD2	2.07	0.54
1:B:108:ARG:HD2	1:B:171:SER:HB2	1.89	0.54
1:B:6:GLN:NE2	1:B:86:TYR:O	2.40	0.53
2:D:83:MET:HE1	2:D:113:VAL:HG21	1.90	0.53
3:A:315:HOH:O	2:C:100:THR:HG21	2.09	0.53
2:C:158:TRP:CZ3	2:C:200:CYS:HB3	2.44	0.53
1:B:37:GLN:HB2	1:B:47:LEU:HD11	1.90	0.53
1:B:163:VAL:HG22	1:B:175:LEU:HD12	1.91	0.53
1:A:83:PHE:CD2	1:A:106:ILE:HG12	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:196:GLN:NE2	3:D:301:HOH:O	2.42	0.52
1:B:108:ARG:NH2	1:B:109:THR:O	2.42	0.52
2:D:201:ASN:ND2	2:D:212:ASP:OD2	2.36	0.51
2:D:123:PRO:HB3	2:D:149:TYR:HB3	1.92	0.51
2:C:12:VAL:HG11	2:C:86:LEU:HD13	1.93	0.51
2:D:159:ASN:ND2	2:D:197:THR:O	2.38	0.50
1:A:124:GLN:HG3	2:C:126:PHE:CE2	2.46	0.50
1:B:6:GLN:HB3	1:B:100:GLN:HE21	1.77	0.50
1:B:8:PRO:HG2	1:B:11:LEU:HD23	1.92	0.50
1:A:49:TYR:HB3	2:C:102:VAL:HB	1.94	0.49
2:D:146:VAL:HG23	2:D:146:VAL:O	2.13	0.49
1:B:24:LYS:HG3	1:B:69:THR:O	2.13	0.48
2:C:102:VAL:HG22	2:C:103:PRO:O	2.13	0.48
1:A:36:TYR:CE2	1:A:46:THR:HG23	2.49	0.48
2:D:127:PRO:HD3	2:D:213:LYS:HZ3	1.79	0.48
2:D:192:SER:HB2	2:D:196:GLN:HG2	1.97	0.47
1:B:120:PRO:HD3	1:B:132:VAL:HG22	1.97	0.47
2:D:203:ASN:OD1	2:D:210:LYS:HE2	2.15	0.47
2:C:123:PRO:HB3	2:C:149:TYR:HB3	1.96	0.46
2:D:203:ASN:ND2	2:D:205:LYS:HE3	2.30	0.46
2:C:147:LYS:HG2	2:C:148:ASP:OD2	2.16	0.46
1:A:137:ASN:CG	1:A:138:ASN:HD22	2.19	0.46
1:B:89:LEU:HD12	1:B:97:THR:O	2.16	0.46
2:D:140:ALA:O	2:D:187:THR:HA	2.16	0.46
1:B:140:TYR:CD1	1:B:141:PRO:HA	2.51	0.46
2:D:20:LEU:HD11	2:D:83:MET:HE1	1.97	0.45
1:A:35:TRP:HB2	1:A:48:ILE:HB	1.97	0.45
2:D:29:PHE:CD2	2:D:77:ASN:HA	2.52	0.45
1:A:27:GLN:HB3	3:A:307:HOH:O	2.17	0.45
2:C:100:THR:CG2	2:C:101:VAL:H	2.19	0.45
1:A:6:GLN:NE2	1:A:102:THR:HG23	2.29	0.45
1:A:210:ASN:ND2	1:A:213:GLU:OE2	2.48	0.45
2:C:62:ASP:N	2:C:62:ASP:OD1	2.49	0.45
2:D:213:LYS:HD2	2:D:213:LYS:HA	1.68	0.45
1:A:4:MET:SD	1:A:90:GLN:HB3	2.57	0.45
1:A:120:PRO:HD3	1:A:132:VAL:HG22	1.98	0.44
1:B:32:VAL:HA	1:B:50:LEU:HD23	1.99	0.44
2:D:150:PHE:HB2	2:D:179:LEU:HD23	2.00	0.44
2:C:156:VAL:HG21	2:C:184:SER:HB2	1.99	0.44
1:B:83:PHE:CD1	1:B:104:VAL:HG12	2.53	0.43
2:C:53:SER:HA	2:C:72:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:PRO:HA	3:B:340:HOH:O	2.18	0.43
2:C:141:ALA:HB2	2:C:187:THR:HG22	2.01	0.43
2:C:166:GLY:O	2:C:186:VAL:HG23	2.18	0.43
2:C:1:GLU:OE1	2:C:26:GLY:CA	2.67	0.43
1:B:140:TYR:CG	1:B:141:PRO:HA	2.54	0.43
2:D:126:PHE:CD2	2:D:145:LEU:HD23	2.54	0.43
2:D:125:VAL:HG21	2:D:202:VAL:HG21	2.01	0.42
1:B:123:GLU:OE1	2:D:213:LYS:NZ	2.36	0.42
2:D:146:VAL:CG2	2:D:182:LEU:HG	2.50	0.42
2:D:205:LYS:HB2	2:D:206:PRO:HD3	2.02	0.42
1:A:49:TYR:CB	2:C:102:VAL:HB	2.49	0.42
1:B:94:TYR:HA	1:B:95:PRO:C	2.40	0.42
1:A:61:ARG:HG2	1:A:61:ARG:HH11	1.84	0.42
2:C:71:SER:O	2:C:79:LEU:HD12	2.20	0.41
2:D:141:ALA:HB2	2:D:187:THR:HG22	2.02	0.41
1:B:143:GLU:CD	1:B:143:GLU:H	2.22	0.41
2:D:79:LEU:HD23	2:D:96:CYS:HB2	2.01	0.41
2:C:86:LEU:HD23	2:C:86:LEU:HA	1.81	0.41
2:D:142:LEU:HD13	2:D:215:VAL:HG21	2.03	0.41
2:D:14:PRO:HD3	2:D:116:SER:C	2.41	0.40
2:C:174:LEU:HD13	2:C:180:TYR:CZ	2.57	0.40
1:B:27:GLN:O	1:B:69:THR:HG22	2.21	0.40
2:D:196:GLN:OE1	2:D:196:GLN:HA	2.21	0.40

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	211/214 (99%)	199 (94%)	12 (6%)	0	100	100
1	B	211/214 (99%)	198 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	207/228 (91%)	199 (96%)	7 (3%)	1 (0%)	29 35
2	D	208/228 (91%)	202 (97%)	6 (3%)	0	100 100
All	All	837/884 (95%)	798 (95%)	38 (4%)	1 (0%)	51 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	196	GLN

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	180/189 (95%)	180 (100%)	0	100 100
1	B	183/189 (97%)	183 (100%)	0	100 100
2	C	175/190 (92%)	175 (100%)	0	100 100
2	D	174/190 (92%)	174 (100%)	0	100 100
All	All	712/758 (94%)	712 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
2	C	168	HIS
2	C	175	GLN
1	B	100	GLN
2	D	175	GLN

5.3.3 RNA (i)

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

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	213/214 (99%)	0.75	13 (6%) 21 27	20, 35, 53, 63	0
1	B	213/214 (99%)	0.85	19 (8%) 9 13	23, 39, 56, 68	0
2	C	211/228 (92%)	0.67	15 (7%) 16 21	16, 29, 49, 66	0
2	D	211/228 (92%)	0.74	19 (9%) 9 12	15, 31, 54, 70	0
All	All	848/884 (95%)	0.75	66 (7%) 13 17	15, 34, 53, 70	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	197	THR	5.1
1	B	57	GLY	4.7
1	B	1	ASP	4.2
1	B	203	SER	4.1
1	A	129	THR	3.7
1	B	125	LEU	3.7
1	A	83	PHE	3.7
2	C	217	PRO	3.5
2	D	130	PRO	3.5
2	C	139	THR	3.4
1	B	7	SER	3.4
1	A	120	PRO	3.4
2	D	190	SER	3.4
2	C	141	ALA	3.4
2	D	193	LEU	3.3
1	B	202	SER	3.3
1	B	92	TRP	3.3
1	B	156	SER	3.2
2	C	102	VAL	3.1
1	B	76	SER	3.1
1	A	203	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	213	GLU	3.1
2	C	192	SER	3.0
1	B	129	THR	3.0
1	B	106	ILE	2.9
1	B	154	LEU	2.9
1	A	1	ASP	2.9
2	D	215	VAL	2.8
2	D	200	CYS	2.8
2	C	195	THR	2.8
2	D	216	GLU	2.7
2	D	167	VAL	2.7
1	B	121	SER	2.6
1	B	56	THR	2.6
1	A	122	ASP	2.6
2	C	200	CYS	2.6
1	B	210	ASN	2.6
2	C	161	GLY	2.5
2	D	202	VAL	2.5
2	C	215	VAL	2.4
1	A	131	SER	2.4
1	A	199	GLN	2.4
2	C	202	VAL	2.4
2	C	193	LEU	2.3
1	B	77	SER	2.3
2	D	192	SER	2.3
1	A	106	ILE	2.3
1	A	184	ALA	2.3
2	D	96	CYS	2.3
1	A	125	LEU	2.2
2	D	142	LEU	2.2
2	C	198	TYR	2.2
2	D	129	ALA	2.2
2	D	191	SER	2.2
2	D	212	ASP	2.1
2	C	140	ALA	2.1
1	A	213	GLU	2.1
1	B	122	ASP	2.1
2	C	130	PRO	2.1
2	C	186	VAL	2.1
1	B	111	ALA	2.1
2	D	40	ALA	2.0
2	D	102	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	188	LYS	2.0
2	D	194	GLY	2.0
2	D	131	SER	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.