



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:49 pm BST

PDB ID : 3FRT
Title : The structure of human CHMP3 (residues 8 - 222).
Authors : Schubert, H.L.; McCullough, J.; Hill, C.P.; Sundquist, W.I.
Deposited on : 2009-01-08
Resolution : 4.00 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 : 2.11
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) : 2.11

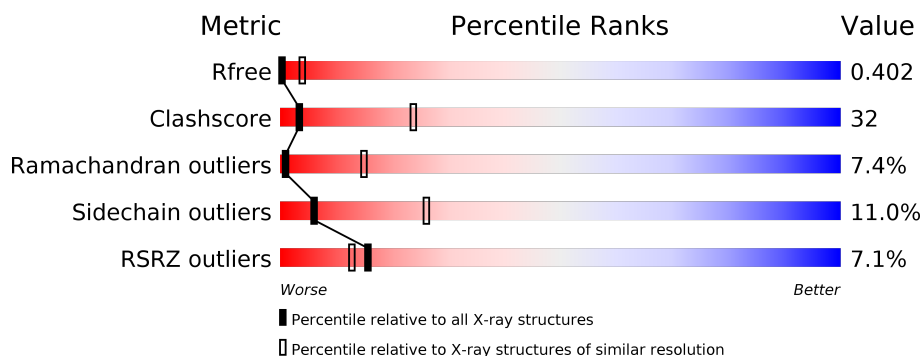
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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 on 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 $\leq 5\%$. 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	218	<div> <div>4%</div> <div>29% 29% 5% . 35%</div> </div>
1	B	218	<div> <div>5%</div> <div>32% 28% . . 35%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2270 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 Charged multivesicular body protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1133	709	203	208	13			
1	B	142	Total	C	N	O	S	0	0	0
			1137	711	204	209	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLY	-	EXPRESSION TAG	UNP Q9Y3E7
A	6	HIS	-	EXPRESSION TAG	UNP Q9Y3E7
A	7	MET	-	EXPRESSION TAG	UNP Q9Y3E7
B	5	GLY	-	EXPRESSION TAG	UNP Q9Y3E7
B	6	HIS	-	EXPRESSION TAG	UNP Q9Y3E7
B	7	MET	-	EXPRESSION TAG	UNP Q9Y3E7

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

Chain A:

Sequence logo for Chain A. The y-axis represents information content in bits. The x-axis shows positions 1 to 100. A color scale at the top indicates conservation levels: 4% (red), 29% (green), 29% (yellow), 5% (orange), and 35% (grey).

Position	Amino Acid
1	GLY
2	HIS
3	MET
4	GLN
5	GLU
6	LYS
7	PRO
8	P12
9	K13
10	E14
11	E18
12	W19
13	S20
14	L21
15	K22
16	T23
17	R24
18	M27
19	R28
20	V29
21	V30
22	D31
23	R32
24	Q33
25	E40
26	K43
27	V44
28	K45
29	R46
30	S47
31	V48
32	K54
33	G55
34	Q56
35	K57
36	D58
37	V59
38	C60
39	I61
40	V62
41	L63
42	A64
43	K65
44	E66
45	M67
46	I68
47	R69
48	V74
49	L77
50	S80
51	M84
52	N85
53	L88
54	M89
55	G90
56	M91
57	K92
58	N93
59	Q94
60	W97
61	L96
62	ARG
63	VAL
64	ALA
65	GLY
66	S103
67	L104
68	Q105
69	K106
70	S107
71	T108
72	E109
73	V110
74	M111
75	M114
76	L117
77	V118
78	R119
79	I120
80	P121
81	E122
82	I123
83	Q124
84	A125
85	T126
86	M127
87	L130
88	S131
89	K132
90	E133
91	M134
92	M135
93	K136
94	I139
95	I140
96	GLU
97	MET
98	GLU
99	LEU
100	GLU

Chain B:

5% 32% 28% 35%

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.47Å 131.51Å 48.51Å 90.00° 108.06° 90.00°	Depositor
Resolution (Å)	30.00 – 4.00 37.76 – 3.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-4.00) 78.5 (37.76-3.99)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 3.99Å)	Xtriage
Refinement program		Depositor
R, R_{free}	0.383 , 0.436 0.402 , 0.402	Depositor DCC
R_{free} test set	126 reflections (4.27%)	wwPDB-VP
Wilson B-factor (Å ²)	135.4	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 10.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	2270	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.74	3/1137 (0.3%)	0.68	0/1504
1	B	0.74	1/1141 (0.1%)	0.68	0/1509
All	All	0.74	4/2278 (0.2%)	0.68	0/3013

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	MET	CG-SD	5.64	1.95	1.81
1	B	157	MET	CG-SD	5.61	1.95	1.81
1	A	157	MET	CG-SD	5.60	1.95	1.81
1	A	134	MET	CG-SD	5.23	1.94	1.81

There are no bond angle outliers.

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	1133	0	1222	87	0
1	B	1137	0	1225	81	0
All	All	2270	0	2447	153	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 32.

All (153) 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:59:VAL:HG22	1:B:62:VAL:CG1	1.83	1.08
1:A:33:GLN:HE22	1:A:122:GLU:HG2	1.16	1.07
1:B:33:GLN:HE22	1:B:122:GLU:HG2	1.16	1.06
1:A:33:GLN:NE2	1:A:122:GLU:HG2	1.74	1.03
1:B:33:GLN:NE2	1:B:122:GLU:HG2	1.74	1.02
1:A:139:ILE:HD13	1:A:139:ILE:H	1.27	0.99
1:A:59:VAL:HG22	1:B:62:VAL:HG12	1.45	0.97
1:B:139:ILE:HD13	1:B:139:ILE:H	1.27	0.97
1:A:58:ASP:O	1:A:62:VAL:HG23	1.67	0.95
1:B:165:ILE:HD12	1:B:166:ASP:N	1.82	0.94
1:A:165:ILE:HD12	1:A:166:ASP:N	1.82	0.93
1:B:165:ILE:HD12	1:B:166:ASP:H	1.34	0.93
1:B:58:ASP:O	1:B:62:VAL:HG23	1.67	0.92
1:B:27:MET:HG2	1:B:84:MET:SD	2.11	0.91
1:B:33:GLN:HE22	1:B:122:GLU:CG	1.84	0.91
1:A:40:GLU:CD	1:B:54:LYS:HE3	1.90	0.90
1:A:33:GLN:HE22	1:A:122:GLU:CG	1.84	0.90
1:A:165:ILE:HD12	1:A:166:ASP:H	1.34	0.85
1:A:40:GLU:OE2	1:B:54:LYS:HE3	1.76	0.85
1:B:27:MET:CG	1:B:84:MET:SD	2.66	0.84
1:A:59:VAL:HG22	1:B:62:VAL:HG11	1.65	0.79
1:B:139:ILE:CD1	1:B:139:ILE:H	1.98	0.77
1:A:59:VAL:CG2	1:B:62:VAL:CG1	2.63	0.77
1:A:63:LEU:HD21	1:B:59:VAL:HG11	1.67	0.76
1:A:48:VAL:HG11	1:A:172:ILE:HD11	1.68	0.74
1:A:59:VAL:CG2	1:B:62:VAL:HG12	2.17	0.73
1:B:48:VAL:HG11	1:B:172:ILE:HD11	1.68	0.73
1:B:139:ILE:N	1:B:139:ILE:HD13	2.03	0.72
1:A:139:ILE:N	1:A:139:ILE:HD13	2.03	0.72
1:A:157:MET:HG3	1:A:159:GLU:HB2	1.71	0.71
1:B:29:VAL:O	1:B:33:GLN:HG3	1.90	0.71
1:A:29:VAL:O	1:A:33:GLN:HG3	1.90	0.71
1:B:157:MET:HG3	1:B:159:GLU:HB2	1.71	0.70
1:A:139:ILE:CD1	1:A:139:ILE:H	1.98	0.67
1:B:111:MET:SD	1:B:140:ILE:HB	2.35	0.66
1:A:63:LEU:O	1:A:66:GLU:HB3	1.95	0.66
1:A:66:GLU:OE1	1:B:56:GLN:HG2	1.96	0.66
1:B:157:MET:CG	1:B:159:GLU:HB2	2.27	0.65
1:B:63:LEU:O	1:B:66:GLU:HB3	1.95	0.65
1:A:157:MET:CG	1:A:159:GLU:HB2	2.26	0.65
1:B:27:MET:HG3	1:B:84:MET:SD	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:MET:SD	1:B:140:ILE:HD13	2.37	0.64
1:B:107:SER:H	1:B:139:ILE:HG22	1.63	0.64
1:A:107:SER:H	1:A:139:ILE:HG22	1.63	0.64
1:A:22:LYS:HD2	1:A:130:LEU:HD21	1.80	0.63
1:B:22:LYS:HD2	1:B:130:LEU:HD21	1.81	0.63
1:A:59:VAL:CG2	1:B:62:VAL:HG11	2.28	0.62
1:B:65:LYS:O	1:B:68:ILE:HG12	2.00	0.62
1:A:27:MET:HG2	1:A:84:MET:SD	2.40	0.62
1:B:134:MET:HB3	1:B:139:ILE:HG12	1.80	0.62
1:A:65:LYS:O	1:A:68:ILE:HG12	2.00	0.62
1:B:106:LYS:HA	1:B:139:ILE:HA	1.83	0.61
1:A:106:LYS:HA	1:A:139:ILE:HA	1.83	0.60
1:A:68:ILE:HG13	1:A:69:ARG:N	2.17	0.59
1:B:94:GLN:HA	1:B:94:GLN:NE2	2.17	0.59
1:A:169:LEU:O	1:A:172:ILE:HG12	2.03	0.59
1:A:56:GLN:HB3	1:A:59:VAL:HG23	1.84	0.59
1:A:164:GLU:HG3	1:A:167:ARG:NH1	2.18	0.59
1:B:169:LEU:O	1:B:172:ILE:HG12	2.03	0.59
1:A:94:GLN:HA	1:A:94:GLN:NE2	2.17	0.58
1:B:61:ILE:O	1:B:64:ALA:HB3	2.04	0.58
1:B:68:ILE:HG13	1:B:69:ARG:N	2.17	0.58
1:B:164:GLU:HG3	1:B:167:ARG:NH1	2.18	0.58
1:B:56:GLN:HB3	1:B:59:VAL:HG23	1.84	0.58
1:A:160:GLU:HB3	1:A:163:MET:CE	2.34	0.58
1:A:111:MET:SD	1:A:140:ILE:HB	2.43	0.58
1:B:160:GLU:HB3	1:B:163:MET:CE	2.34	0.58
1:A:111:MET:SD	1:A:140:ILE:HD13	2.45	0.57
1:A:61:ILE:O	1:A:64:ALA:HB3	2.04	0.57
1:A:24:ARG:O	1:A:27:MET:HB2	2.04	0.56
1:B:33:GLN:HE22	1:B:122:GLU:CD	2.09	0.56
1:A:33:GLN:HE22	1:A:122:GLU:CD	2.09	0.56
1:B:74:VAL:O	1:B:77:LEU:HB2	2.06	0.55
1:A:74:VAL:O	1:A:77:LEU:HB2	2.06	0.54
1:A:134:MET:HB3	1:A:139:ILE:HG12	1.90	0.54
1:A:157:MET:HA	1:A:157:MET:CE	2.38	0.53
1:B:157:MET:CE	1:B:157:MET:HA	2.38	0.53
1:B:126:THR:O	1:B:127:MET:C	2.46	0.53
1:A:126:THR:O	1:A:127:MET:C	2.46	0.53
1:B:106:LYS:O	1:B:106:LYS:HG3	2.09	0.53
1:A:106:LYS:O	1:A:106:LYS:HG3	2.09	0.52
1:B:90:GLY:HA3	1:B:110:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ILE:HD13	1:A:123:ILE:HD11	1.92	0.52
1:B:140:ILE:HD12	1:B:140:ILE:H	1.75	0.52
1:A:62:VAL:HG11	1:B:58:ASP:HB2	1.91	0.52
1:B:120:ILE:O	1:B:124:GLN:N	2.38	0.51
1:A:66:GLU:OE1	1:B:56:GLN:CG	2.58	0.51
1:A:120:ILE:O	1:A:124:GLN:N	2.38	0.51
1:A:90:GLY:HA3	1:A:110:VAL:HG11	1.92	0.51
1:A:54:LYS:HE2	1:A:56:GLN:NE2	2.25	0.51
1:A:80:SER:OG	1:A:120:ILE:HG12	2.11	0.51
1:B:120:ILE:HD13	1:B:123:ILE:HD11	1.92	0.51
1:B:80:SER:OG	1:B:120:ILE:HG12	2.11	0.51
1:B:68:ILE:CG1	1:B:69:ARG:N	2.74	0.50
1:A:40:GLU:OE2	1:B:54:LYS:CE	2.54	0.50
1:A:140:ILE:HD12	1:A:140:ILE:H	1.75	0.50
1:A:90:GLY:HA3	1:A:110:VAL:CG1	2.42	0.50
1:B:90:GLY:HA3	1:B:110:VAL:CG1	2.42	0.50
1:A:68:ILE:CG1	1:A:69:ARG:N	2.74	0.49
1:B:157:MET:HG3	1:B:159:GLU:H	1.77	0.49
1:B:160:GLU:HB3	1:B:163:MET:HE1	1.93	0.49
1:A:160:GLU:HB3	1:A:163:MET:HE2	1.95	0.48
1:A:44:VAL:O	1:A:48:VAL:HG23	2.13	0.48
1:B:44:VAL:O	1:B:48:VAL:HG23	2.13	0.48
1:A:157:MET:HG3	1:A:159:GLU:H	1.77	0.48
1:A:159:GLU:O	1:A:162:GLU:HG2	2.13	0.48
1:B:159:GLU:O	1:B:162:GLU:HG2	2.13	0.48
1:A:160:GLU:HB3	1:A:163:MET:HE1	1.95	0.48
1:A:30:VAL:HG21	1:A:84:MET:HE1	1.96	0.48
1:B:88:LEU:O	1:B:91:MET:HB2	2.13	0.48
1:A:43:LYS:HG2	1:A:46:ARG:HH22	1.78	0.47
1:A:48:VAL:HG11	1:A:172:ILE:CD1	2.42	0.47
1:A:88:LEU:O	1:A:91:MET:HB2	2.13	0.47
1:A:85:ASN:O	1:A:89:MET:HG2	2.14	0.47
1:A:43:LYS:HG2	1:A:46:ARG:NH2	2.30	0.47
1:A:63:LEU:CD2	1:B:59:VAL:HG11	2.43	0.47
1:A:107:SER:O	1:A:109:GLU:N	2.49	0.46
1:B:160:GLU:HB3	1:B:163:MET:HE2	1.96	0.46
1:A:117:LEU:O	1:A:120:ILE:HD12	2.16	0.46
1:B:30:VAL:HG21	1:B:84:MET:HE1	1.97	0.46
1:B:117:LEU:O	1:B:120:ILE:HD12	2.16	0.46
1:B:107:SER:O	1:B:109:GLU:N	2.49	0.46
1:A:89:MET:O	1:A:92:LYS:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLU:OE2	1:B:109:GLU:HA	2.16	0.45
1:A:27:MET:CG	1:A:84:MET:SD	3.04	0.45
1:B:117:LEU:HA	1:B:117:LEU:HD12	1.79	0.45
1:B:107:SER:N	1:B:139:ILE:HG22	2.30	0.45
1:B:48:VAL:HG11	1:B:172:ILE:CD1	2.42	0.45
1:A:165:ILE:CD1	1:A:166:ASP:H	2.17	0.45
1:A:107:SER:N	1:A:139:ILE:HG22	2.30	0.44
1:B:33:GLN:NE2	1:B:122:GLU:OE2	2.50	0.44
1:A:132:LYS:HE3	1:A:132:LYS:HB2	1.84	0.44
1:A:62:VAL:CG1	1:B:58:ASP:HB2	2.48	0.44
1:A:33:GLN:NE2	1:A:122:GLU:OE2	2.49	0.43
1:B:18:GLU:O	1:B:21:LEU:HB2	2.19	0.43
1:A:77:LEU:O	1:A:80:SER:HB2	2.19	0.43
1:B:122:GLU:OE1	1:B:122:GLU:N	2.27	0.43
1:B:77:LEU:O	1:B:80:SER:HB2	2.19	0.42
1:A:94:GLN:CA	1:A:94:GLN:NE2	2.81	0.42
1:A:18:GLU:O	1:A:21:LEU:HB2	2.19	0.42
1:B:165:ILE:CD1	1:B:166:ASP:H	2.18	0.42
1:A:19:TRP:O	1:A:20:SER:C	2.59	0.42
1:A:121:PRO:HA	1:A:124:GLN:OE1	2.20	0.42
1:B:118:VAL:HG12	1:B:127:MET:HB3	2.03	0.41
1:B:85:ASN:O	1:B:89:MET:HG2	2.20	0.41
1:A:88:LEU:HA	1:A:88:LEU:HD12	1.88	0.41
1:A:77:LEU:HA	1:A:77:LEU:HD23	1.86	0.41
1:B:19:TRP:O	1:B:20:SER:C	2.59	0.41
1:B:121:PRO:HA	1:B:124:GLN:OE1	2.20	0.40
1:B:68:ILE:CG1	1:B:69:ARG:H	2.35	0.40
1:A:106:LYS:O	1:A:108:THR:N	2.55	0.40
1:A:118:VAL:HG12	1:A:127:MET:HB3	2.03	0.40
1:A:168:ILE:O	1:A:169:LEU:C	2.60	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	135/218 (62%)	112 (83%)	13 (10%)	10 (7%)	1	15
1	B	136/218 (62%)	113 (83%)	13 (10%)	10 (7%)	1	15
All	All	271/436 (62%)	225 (83%)	26 (10%)	20 (7%)	1	15

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	SER
1	A	136	LYS
1	B	107	SER
1	B	136	LYS
1	A	118	VAL
1	A	125	ALA
1	A	171	GLU
1	B	118	VAL
1	B	125	ALA
1	B	171	GLU
1	A	108	THR
1	B	108	THR
1	A	127	MET
1	B	127	MET
1	A	121	PRO
1	A	139	ILE
1	B	121	PRO
1	B	139	ILE
1	A	97	VAL
1	B	97	VAL

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	127/188 (68%)	113 (89%)	14 (11%)	6	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	127/188 (68%)	113 (89%)	14 (11%)	6	26
All	All	254/376 (68%)	226 (89%)	28 (11%)	6	26

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	32	ARG
1	A	105	GLN
1	A	108	THR
1	A	114	MET
1	A	117	LEU
1	A	124	GLN
1	A	127	MET
1	A	139	ILE
1	A	140	ILE
1	A	157	MET
1	A	159	GLU
1	A	166	ASP
1	A	168	ILE
1	B	14	GLU
1	B	32	ARG
1	B	105	GLN
1	B	108	THR
1	B	114	MET
1	B	117	LEU
1	B	124	GLN
1	B	127	MET
1	B	139	ILE
1	B	140	ILE
1	B	157	MET
1	B	159	GLU
1	B	166	ASP
1	B	168	ILE

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

Mol	Chain	Res	Type
1	A	33	GLN
1	A	94	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	141/218 (64%)	0.15	9 (6%) 19 15	34, 58, 81, 89	0
1	B	142/218 (65%)	0.20	11 (7%) 13 11	34, 59, 82, 90	0
All	All	283/436 (64%)	0.17	20 (7%) 16 13	34, 59, 82, 90	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	120	ILE	4.0
1	A	122	GLU	3.8
1	A	172	ILE	3.7
1	A	12	PRO	3.6
1	A	120	ILE	3.6
1	B	12	PRO	3.5
1	A	123	ILE	3.2
1	B	123	ILE	3.1
1	A	54	LYS	2.8
1	A	103	SER	2.8
1	B	169	LEU	2.7
1	B	122	GLU	2.6
1	B	104	LEU	2.6
1	B	127	MET	2.6
1	A	104	LEU	2.4
1	B	157	MET	2.4
1	B	54	LYS	2.3
1	B	51	ALA	2.2
1	A	140	ILE	2.1
1	B	131	SER	2.1

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 carbohydrates 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.