Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2024 – 11:37 AM EST

PDB ID	:	3L8I
Title	:	Crystal structure of CCM3, a cerebral cavernous malformation protein critical for vascular integrity
Authors	:	Li, X.; Zhang, R.; Zhang, H.; He, Y.; Ji, W.; Min, W.; Boggon, T.J.
Deposited on	:	2009-12-31
Resolution	:	2.50 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 (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:

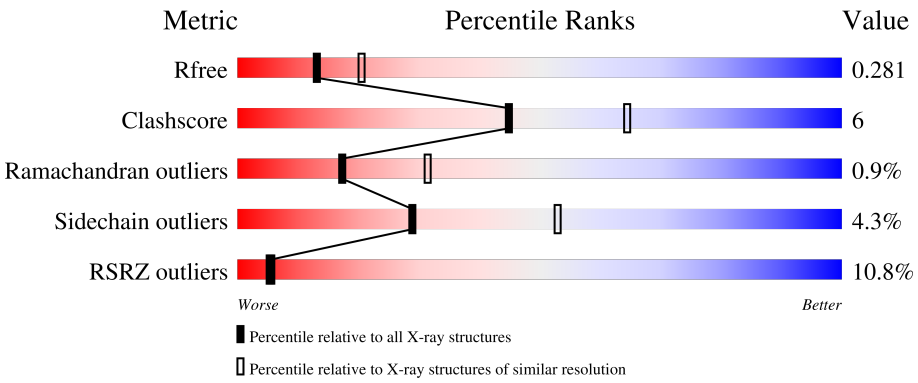
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	7%; 77%; 15%; • 7%
1	B	214	7%; 74%; 18%; • 6%
1	C	214	14%; 82%; 17%; •
1	D	214	13%; 79%; 14%; • 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6725 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 Programmed cell death protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	198	1618	1034	274	304	6	0	0	0
1	B	201	1643	1047	278	312	6	0	0	0
1	C	212	1734	1101	295	328	10	0	0	0
1	D	203	1660	1058	281	314	7	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9BUL8
A	0	HIS	-	expression tag	UNP Q9BUL8
B	-1	GLY	-	expression tag	UNP Q9BUL8
B	0	HIS	-	expression tag	UNP Q9BUL8
C	-1	GLY	-	expression tag	UNP Q9BUL8
C	0	HIS	-	expression tag	UNP Q9BUL8
D	-1	GLY	-	expression tag	UNP Q9BUL8
D	0	HIS	-	expression tag	UNP Q9BUL8

- Molecule 2 is water.

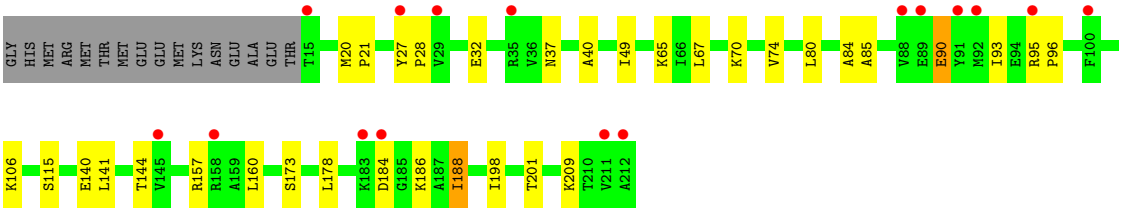
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	21	21	21	0	0
2	B	10	10	10	0	0
2	C	23	23	23	0	0
2	D	16	16	16	0	0

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.

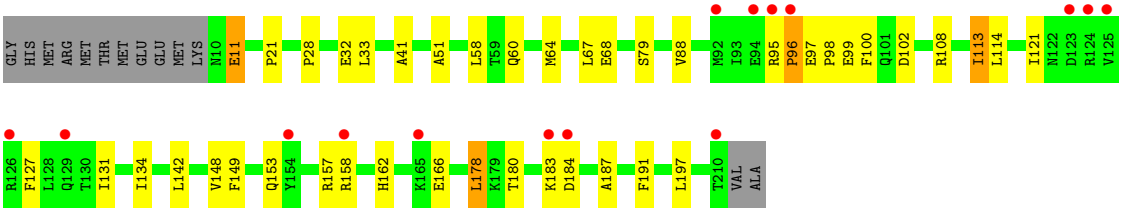
• Molecule 1: Programmed cell death protein 10

Chain A:



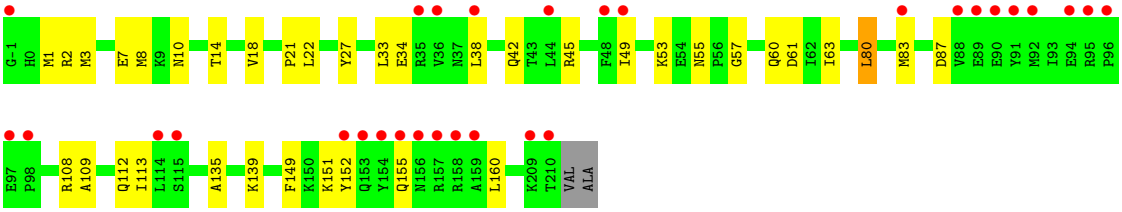
• Molecule 1: Programmed cell death protein 10

Chain B:



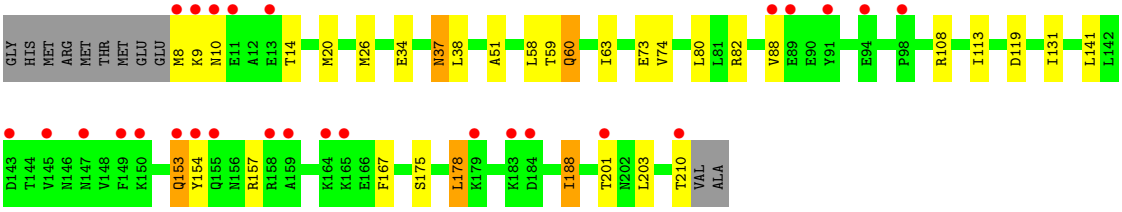
• Molecule 1: Programmed cell death protein 10

Chain C:



• Molecule 1: Programmed cell death protein 10

Chain D:


GLY
HIS
MET
ARG
MET
THR
MET
GLU
GLU
M8
K9
N10
E11
A12
E13
T14
M20
M26
E34
N37
L38
A51
L58
T59
Q60
I63
E73
V74
L80
L81
R82
V88
E89
E90
Y91
E94
P98
R108
I113
D119
I131
L141
L142
D143
T144
V145
N146
N147
V148
F149
K150
Q153
Y154
Q155
N156
R157
R158
A159
K164
K165
E166
F167
S175
L178
K179
K183
D184
I188
T201
N202
L203
T210
VAL
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.08Å 116.01Å 123.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 25.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (25.00-2.50) 99.0 (25.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.229 , 0.288 0.222 , 0.281	Depositor DCC
R_{free} test set	1601 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	61.7	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6725	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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 (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	0.44	0/1643	0.54	0/2210
1	B	0.43	0/1668	0.53	0/2245
1	C	0.42	0/1760	0.54	0/2364
1	D	0.44	0/1685	0.56	0/2266
All	All	0.43	0/6756	0.54	0/9085

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 (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	1618	0	1662	23	0
1	B	1643	0	1678	26	0
1	C	1734	0	1772	25	0
1	D	1660	0	1700	20	0
2	A	21	0	0	0	0
2	B	10	0	0	0	0
2	C	23	0	0	0	0
2	D	16	0	0	0	0
All	All	6725	0	6812	87	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 6.

All (87) 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:D:88:VAL:HG22	1:D:108:ARG:HG3	1.55	0.88
1:C:10:ASN:O	1:C:14:THR:HG23	1.77	0.84
1:C:1:MET:HG3	1:C:34:GLU:HG3	1.67	0.75
1:C:3:MET:HG2	1:C:8:MET:HG3	1.70	0.73
1:C:33:LEU:HD11	1:D:58:LEU:HD11	1.72	0.71
1:D:74:VAL:HG22	1:D:188:ILE:HG13	1.73	0.70
1:A:141:LEU:O	1:A:144:THR:HG22	1.92	0.69
1:C:80:LEU:HA	1:C:83:MET:HE2	1.74	0.68
1:A:37:ASN:HD22	1:A:40:ALA:H	1.42	0.68
1:D:10:ASN:O	1:D:14:THR:HG22	1.99	0.63
1:B:113:ILE:HD12	1:B:134:ILE:HG13	1.82	0.61
1:C:109:ALA:O	1:C:113:ILE:HG12	1.99	0.61
1:A:27:TYR:OH	1:A:49:ILE:HD11	2.01	0.61
1:C:1:MET:HE3	1:C:42:GLN:HA	1.84	0.60
1:C:2:ARG:H	1:C:42:GLN:HE22	1.48	0.60
1:D:82:ARG:NH2	1:D:119:ASP:OD1	2.38	0.57
1:B:114:LEU:HD11	1:B:197:LEU:HD23	1.88	0.56
1:B:127:PHE:O	1:B:131:ILE:HG12	2.06	0.56
1:B:21:PRO:HG3	1:B:60:GLN:HE21	1.71	0.55
1:D:26:MET:SD	1:D:63:ILE:HD11	2.46	0.55
1:B:64:MET:O	1:B:68:GLU:HG3	2.07	0.55
1:A:37:ASN:ND2	1:A:40:ALA:H	2.06	0.54
1:C:63:ILE:HG21	1:D:73:GLU:HG3	1.90	0.54
1:D:74:VAL:HG13	1:D:188:ILE:HG12	1.88	0.53
1:A:85:ALA:HB2	1:A:115:SER:CB	2.39	0.53
1:A:74:VAL:HG22	1:A:188:ILE:HG23	1.91	0.52
1:A:74:VAL:HG22	1:A:188:ILE:CG2	2.40	0.52
1:D:88:VAL:HG13	1:D:108:ARG:HD2	1.92	0.52
1:A:84:ALA:HB1	1:A:198:ILE:HG21	1.91	0.52
1:D:74:VAL:HG22	1:D:188:ILE:CG1	2.40	0.52
1:C:3:MET:HG3	1:C:7:GLU:HB2	1.91	0.51
1:C:21:PRO:HG2	1:C:60:GLN:HE21	1.76	0.51
1:B:33:LEU:HG	1:B:41:ALA:HB2	1.93	0.51
1:C:135:ALA:O	1:C:139:LYS:HG3	2.10	0.51
1:B:149:PHE:O	1:B:153:GLN:HB2	2.11	0.51
1:C:1:MET:HE2	1:C:45:ARG:CZ	2.41	0.51
1:A:90:GLU:O	1:A:209:LYS:NZ	2.44	0.50
1:B:99:GLU:HB3	1:B:148:VAL:HG22	1.93	0.50
1:C:14:THR:HG21	1:C:53:LYS:HA	1.92	0.50
1:A:32:GLU:HA	1:C:8:MET:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ARG:HA	1:A:160:LEU:HD23	1.96	0.47
1:C:1:MET:HE1	1:C:45:ARG:CB	2.44	0.47
1:C:45:ARG:O	1:C:49:ILE:HG12	2.14	0.47
1:A:65:LYS:HE2	1:B:32:GLU:OE2	2.15	0.47
1:C:18:VAL:HG23	1:D:80:LEU:HD21	1.96	0.47
1:B:162:HIS:O	1:B:166:GLU:HG2	2.15	0.46
1:D:60:GLN:HE21	1:D:60:GLN:HA	1.81	0.46
1:D:153:GLN:HA	1:D:153:GLN:HE21	1.81	0.46
1:C:55:ASN:ND2	1:D:37:ASN:OD1	2.49	0.45
1:B:60:GLN:HE21	1:B:60:GLN:HA	1.82	0.44
1:D:175:SER:HA	1:D:178:LEU:HD22	2.00	0.44
1:A:95:ARG:HA	1:A:96:PRO:HD3	1.78	0.44
1:B:60:GLN:HA	1:B:60:GLN:NE2	2.33	0.44
1:A:106:LYS:HD2	1:A:140:GLU:HB3	2.00	0.44
1:C:27:TYR:OH	1:C:49:ILE:HD11	2.18	0.43
1:B:131:ILE:HD12	1:B:178:LEU:HG	2.00	0.43
1:C:1:MET:HE2	1:C:45:ARG:NE	2.33	0.43
1:D:51:ALA:HB1	1:D:58:LEU:HD23	1.99	0.43
1:A:67:LEU:HD23	1:B:67:LEU:HD23	2.01	0.43
1:B:11:GLU:H	1:B:11:GLU:CD	2.22	0.43
1:B:28:PRO:O	1:B:32:GLU:HG3	2.18	0.43
1:B:88:VAL:CG1	1:B:108:ARG:HG2	2.49	0.43
1:B:97:GLU:HG2	1:B:100:PHE:HD2	1.83	0.42
1:A:27:TYR:OH	1:A:49:ILE:CD1	2.67	0.42
1:C:14:THR:CG2	1:C:53:LYS:HA	2.48	0.42
1:D:8:MET:HG2	1:D:9:LYS:H	1.84	0.42
1:A:93:ILE:HG22	1:A:95:ARG:HG2	2.02	0.42
1:C:3:MET:HG3	1:C:7:GLU:CB	2.50	0.42
1:A:27:TYR:HB2	1:A:28:PRO:HD3	2.02	0.42
1:A:70:LYS:O	1:A:74:VAL:HG23	2.20	0.42
1:A:184:ASP:HB3	1:A:186:LYS:HG3	2.02	0.42
1:B:95:ARG:HA	1:B:96:PRO:HD3	1.90	0.42
1:B:153:GLN:OE1	1:B:157:ARG:HG3	2.20	0.41
1:C:108:ARG:O	1:C:112:GLN:HB2	2.19	0.41
1:B:51:ALA:HB1	1:B:58:LEU:CD2	2.50	0.41
1:A:95:ARG:HG2	1:A:95:ARG:H	1.59	0.41
1:D:59:THR:O	1:D:63:ILE:HG12	2.20	0.41
1:D:141:LEU:HD23	1:D:167:PHE:CZ	2.56	0.41
1:A:20:MET:N	1:A:21:PRO:CD	2.83	0.41
1:B:51:ALA:HB1	1:B:58:LEU:HD23	2.03	0.41
1:B:187:ALA:HB1	1:B:191:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ILE:HD12	1:A:93:ILE:H	1.86	0.41
1:C:18:VAL:HG22	1:C:57:GLY:HA2	2.01	0.41
1:B:97:GLU:HB2	1:B:98:PRO:HD2	2.03	0.41
1:D:34:GLU:HG3	1:D:38:LEU:HD12	2.03	0.40
1:B:88:VAL:HG13	1:B:108:ARG:HG2	2.02	0.40
1:B:180:THR:O	1:B:184:ASP:HB2	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	196/214 (92%)	189 (96%)	6 (3%)	1 (0%)	29	48
1	B	199/214 (93%)	189 (95%)	8 (4%)	2 (1%)	15	28
1	C	210/214 (98%)	197 (94%)	10 (5%)	3 (1%)	11	20
1	D	201/214 (94%)	195 (97%)	5 (2%)	1 (0%)	29	48
All	All	806/856 (94%)	770 (96%)	29 (4%)	7 (1%)	17	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	96	PRO
1	C	152	TYR
1	D	157	ARG
1	A	90	GLU
1	B	158	ARG
1	C	87	ASP
1	C	155	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	180/194 (93%)	175 (97%)	5 (3%)	43	70
1	B	183/194 (94%)	175 (96%)	8 (4%)	28	52
1	C	193/194 (100%)	186 (96%)	7 (4%)	35	61
1	D	185/194 (95%)	173 (94%)	12 (6%)	17	33
All	All	741/776 (96%)	709 (96%)	32 (4%)	29	53

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LEU
1	A	173	SER
1	A	178	LEU
1	A	188	ILE
1	A	201	THR
1	B	11	GLU
1	B	79	SER
1	B	102	ASP
1	B	113	ILE
1	B	121	ILE
1	B	142	LEU
1	B	178	LEU
1	B	183	LYS
1	C	22	LEU
1	C	38	LEU
1	C	61	ASP
1	C	80	LEU
1	C	149	PHE
1	C	151	LYS
1	C	160	LEU
1	D	20	MET
1	D	37	ASN
1	D	60	GLN
1	D	113	ILE

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Mol	Chain	Res	Type
1	D	131	ILE
1	D	153	GLN
1	D	154	TYR
1	D	178	LEU
1	D	188	ILE
1	D	201	THR
1	D	203	LEU
1	D	210	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	60	GLN
1	A	147	ASN
1	B	55	ASN
1	B	60	GLN
1	B	75	ASN
1	B	129	GLN
1	B	146	ASN
1	C	42	GLN
1	C	55	ASN
1	C	60	GLN
1	C	153	GLN
1	D	37	ASN
1	D	60	GLN
1	D	146	ASN
1	D	153	GLN
1	D	189	ASN
1	D	195	ASN

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)

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 (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	198/214 (92%)	0.40	16 (8%)	12	12	38, 68, 107, 127	0
1	B	201/214 (93%)	0.50	15 (7%)	14	14	37, 77, 142, 191	0
1	C	212/214 (99%)	0.74	30 (14%)	2	2	39, 69, 168, 205	0
1	D	203/214 (94%)	0.71	27 (13%)	3	2	37, 75, 141, 164	0
All	All	814/856 (95%)	0.59	88 (10%)	5	5	37, 71, 141, 205	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	156	ASN	11.2
1	C	96	PRO	6.8
1	A	15	THR	6.2
1	C	91	TYR	6.2
1	C	210	THR	6.1
1	B	96	PRO	5.7
1	B	154	TYR	5.6
1	B	94	GLU	5.1
1	C	89	GLU	5.0
1	D	88	VAL	4.9
1	C	88	VAL	4.7
1	D	210	THR	4.5
1	C	154	TYR	4.5
1	A	88	VAL	4.4
1	D	9	LYS	4.4
1	B	158	ARG	4.4
1	B	183	LYS	4.3
1	C	155	GLN	4.1
1	A	212	ALA	4.0
1	C	209	LYS	4.0
1	D	98	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	89	GLU	3.7
1	C	98	PRO	3.6
1	C	159	ALA	3.6
1	D	158	ARG	3.4
1	B	123	ASP	3.4
1	C	157	ARG	3.3
1	D	150	LYS	3.3
1	B	129	GLN	3.3
1	B	92	MET	3.2
1	C	35	ARG	3.2
1	A	211	VAL	3.2
1	A	100	PHE	3.2
1	D	89	GLU	3.2
1	D	13	GLU	3.1
1	D	183	LYS	3.1
1	D	8	MET	3.0
1	B	210	THR	3.0
1	A	95	ARG	3.0
1	D	11	GLU	3.0
1	D	94	GLU	3.0
1	D	155	GLN	3.0
1	D	147	ASN	2.9
1	D	184	ASP	2.9
1	C	92	MET	2.9
1	B	124	ARG	2.9
1	D	143	ASP	2.9
1	D	149	PHE	2.9
1	C	97	GLU	2.8
1	D	10	ASN	2.8
1	A	35	ARG	2.8
1	D	153	GLN	2.8
1	C	90	GLU	2.8
1	C	94	GLU	2.6
1	D	154	TYR	2.6
1	C	44	LEU	2.6
1	A	158	ARG	2.6
1	C	152	TYR	2.6
1	D	91	TYR	2.6
1	B	125	VAL	2.5
1	C	95	ARG	2.5
1	A	92	MET	2.5
1	C	115	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	126	ARG	2.4
1	A	27	TYR	2.4
1	C	48	PHE	2.4
1	A	183	LYS	2.3
1	C	49	ILE	2.3
1	D	164	LYS	2.3
1	B	95	ARG	2.3
1	B	165	LYS	2.3
1	C	153	GLN	2.3
1	D	165	LYS	2.2
1	A	145	VAL	2.2
1	D	145	VAL	2.2
1	C	36	VAL	2.2
1	D	201	THR	2.2
1	A	91	TYR	2.1
1	A	184	ASP	2.1
1	D	179	LYS	2.1
1	C	-1	GLY	2.1
1	A	29	VAL	2.1
1	B	184	ASP	2.1
1	C	114	LEU	2.1
1	D	159	ALA	2.0
1	C	38	LEU	2.0
1	C	158	ARG	2.0
1	C	83	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.