Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 09:04 PM EDT

PDB ID	:	2IKB
Title	:	Crystal Structure of a Protein of Unknown Function NMB1012 from Neisseria meningitidis
Authors	:	Zhang, R.; Li, H.; Bargassa, M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2006-10-02
Resolution	:	1.70 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:

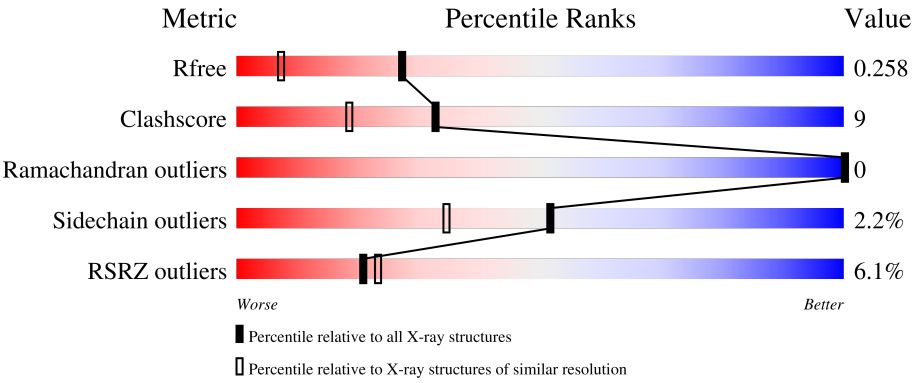
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.70 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	167	85% 12% • •
1	B	167	3% 82% 9% • 8%
1	C	167	6% 82% 13% • •
1	D	167	14% 79% 18% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5624 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 Hypothetical protein NMB1012.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	Se	0	0	0
			1285	809	239	231	1	5			
1	B	154	Total	C	N	O	S	Se	0	0	0
			1221	768	230	218	1	4			
1	C	162	Total	C	N	O	S	Se	0	0	0
			1276	803	237	230	1	5			
1	D	163	Total	C	N	O	S	Se	0	0	0
			1285	806	240	234	1	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q7DDI9
A	48	MSE	MET	MODIFIED RESIDUE	UNP Q7DDI9
A	51	MSE	MET	MODIFIED RESIDUE	UNP Q7DDI9
A	73	MSE	MET	MODIFIED RESIDUE	UNP Q7DDI9
A	96	MSE	MET	MODIFIED RESIDUE	UNP Q7DDI9
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q7DDI9
B	48	MSE	MET	MODIFIED RESIDUE	UNP Q7DDI9
B	51	MSE	MET	MODIFIED RESIDUE	UNP Q7DDI9
B	73	MSE	MET	MODIFIED RESIDUE	UNP Q7DDI9
B	96	MSE	MET	MODIFIED RESIDUE	UNP Q7DDI9
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q7DDI9
C	48	MSE	MET	MODIFIED RESIDUE	UNP Q7DDI9
C	51	MSE	MET	MODIFIED RESIDUE	UNP Q7DDI9
C	73	MSE	MET	MODIFIED RESIDUE	UNP Q7DDI9
C	96	MSE	MET	MODIFIED RESIDUE	UNP Q7DDI9
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q7DDI9
D	48	MSE	MET	MODIFIED RESIDUE	UNP Q7DDI9
D	51	MSE	MET	MODIFIED RESIDUE	UNP Q7DDI9
D	73	MSE	MET	MODIFIED RESIDUE	UNP Q7DDI9
D	96	MSE	MET	MODIFIED RESIDUE	UNP Q7DDI9

- Molecule 2 is water.

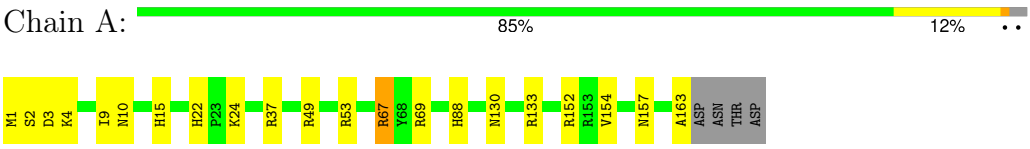
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	177	Total O 177 177	0	0
2	B	158	Total O 158 158	0	0
2	C	147	Total O 147 147	0	0
2	D	75	Total O 75 75	0	0

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.

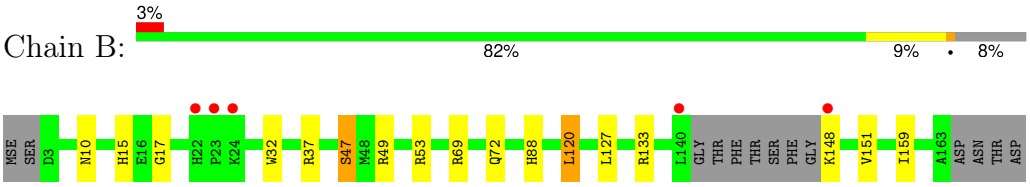
• Molecule 1: Hypothetical protein NMB1012

Chain A:



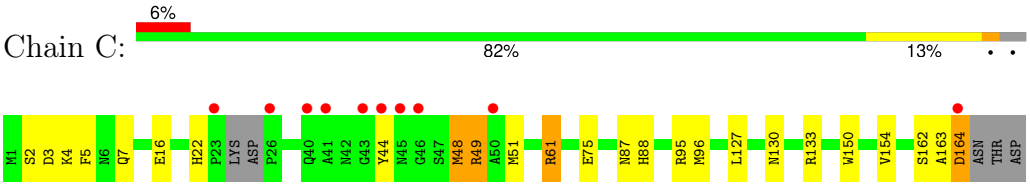
• Molecule 1: Hypothetical protein NMB1012

Chain B:



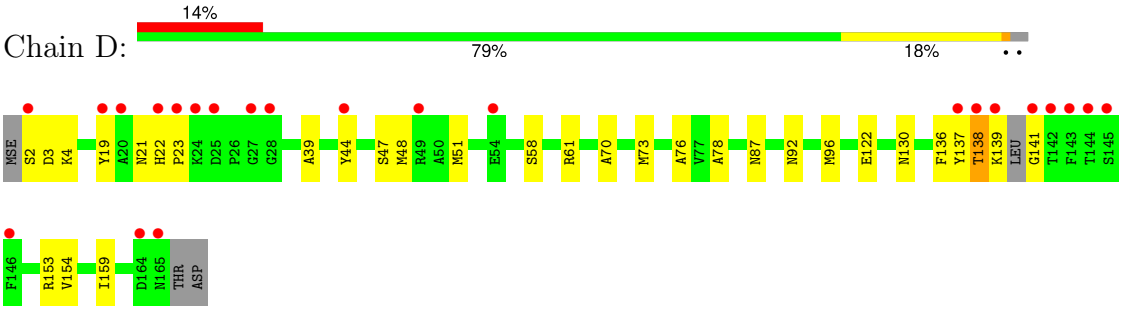
• Molecule 1: Hypothetical protein NMB1012

Chain C:



• Molecule 1: Hypothetical protein NMB1012

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	47.34Å 52.09Å 128.87Å 90.00° 90.68° 90.00°	Depositor
Resolution (Å)	38.38 – 1.70 38.36 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (38.38-1.70) 94.9 (38.36-1.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.195 , 0.247 0.209 , 0.258	Depositor DCC
R_{free} test set	3962 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	18.5	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 55.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5624	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.02% 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	0.83	0/1311	0.83	5/1762 (0.3%)
1	B	0.73	0/1244	0.77	1/1671 (0.1%)
1	C	0.83	0/1301	0.82	2/1747 (0.1%)
1	D	0.55	0/1310	0.65	0/1760
All	All	0.74	0/5166	0.77	8/6940 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	67	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	152	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	A	67	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	C	61	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	37	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	C	49	ARG	CG-CD-NE	-5.27	100.74	111.80
1	B	37	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	152	ARG	NE-CZ-NH2	-5.09	117.75	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	138	THR	Peptide

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	1285	0	1249	18	0
1	B	1221	0	1188	18	0
1	C	1276	0	1236	27	0
1	D	1285	0	1235	28	0
2	A	177	0	0	7	0
2	B	158	0	0	2	0
2	C	147	0	0	8	0
2	D	75	0	0	2	0
All	All	5624	0	4908	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 9.

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:C:48:MSE:CE	1:C:51:MSE:HE3	1.78	1.14
1:C:48:MSE:HE1	1:C:51:MSE:CE	1.82	1.09
1:C:48:MSE:SE	2:C:298:HOH:O	2.19	1.07
1:D:73:MSE:SE	2:D:169:HOH:O	2.23	1.04
1:C:48:MSE:CE	1:C:48:MSE:HA	1.92	0.98
1:C:48:MSE:HE1	1:C:51:MSE:HE3	0.97	0.96
1:C:75:GLU:HG2	2:C:266:HOH:O	1.70	0.90
1:D:70:ALA:CB	1:D:73:MSE:HE2	2.02	0.88
1:B:88:HIS:HE1	1:B:133:ARG:HE	1.23	0.84
1:A:88:HIS:HE1	1:A:133:ARG:HE	1.25	0.82
1:D:70:ALA:CA	1:D:73:MSE:HE2	2.10	0.81
1:D:70:ALA:HA	1:D:73:MSE:HE2	1.63	0.80
1:C:48:MSE:HA	1:C:48:MSE:HE3	1.66	0.76
1:B:69:ARG:CZ	1:B:72:GLN:HE21	1.98	0.76
1:B:127:LEU:HD22	2:B:323:HOH:O	1.86	0.76
1:C:48:MSE:HA	1:C:48:MSE:HE2	1.67	0.75
1:D:44:TYR:OH	1:D:47:SER:O	2.05	0.73
1:A:163:ALA:O	2:A:344:HOH:O	2.06	0.72
1:D:76:ALA:HB3	1:D:122:GLU:OE2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:ALA:HB1	1:D:73:MSE:HE2	1.71	0.70
1:B:159:ILE:HD11	1:D:159:ILE:HD12	1.75	0.69
1:A:22:HIS:HD2	1:A:24:LYS:H	1.39	0.68
1:D:73:MSE:HE3	1:D:78:ALA:HB2	1.76	0.66
1:B:69:ARG:CZ	1:B:72:GLN:NE2	2.59	0.66
1:A:4:LYS:HE3	2:A:261:HOH:O	1.97	0.63
1:C:44:TYR:CE2	1:C:48:MSE:HE3	2.33	0.63
1:B:88:HIS:CE1	1:B:133:ARG:HE	2.12	0.62
1:A:1:MSE:HE3	1:A:2:SER:HB3	1.81	0.62
1:B:159:ILE:HD12	1:D:159:ILE:CD1	2.31	0.61
1:D:130:ASN:HD22	1:D:154:VAL:HG13	1.65	0.60
1:B:159:ILE:CD1	1:D:159:ILE:HD12	2.31	0.60
1:C:130:ASN:HD22	1:C:154:VAL:HG13	1.68	0.59
1:D:70:ALA:HB1	1:D:73:MSE:CE	2.32	0.59
1:B:120:LEU:HD12	1:B:120:LEU:H	1.67	0.58
1:D:73:MSE:HE3	1:D:78:ALA:CB	2.32	0.58
1:A:22:HIS:CD2	1:A:24:LYS:H	2.19	0.58
1:C:4:LYS:CE	2:C:306:HOH:O	2.53	0.55
1:D:136:PHE:O	1:D:139:LYS:C	2.45	0.55
1:B:159:ILE:CD1	1:D:159:ILE:CD1	2.85	0.55
1:C:75:GLU:CG	2:C:266:HOH:O	2.39	0.54
1:A:10:ASN:ND2	1:A:53:ARG:HH22	2.06	0.53
1:A:88:HIS:CE1	1:A:133:ARG:HE	2.16	0.52
1:C:95:ARG:NH1	2:C:302:HOH:O	2.42	0.52
1:C:87:ASN:HD22	1:C:133:ARG:NH2	2.07	0.52
1:A:88:HIS:HD2	2:A:230:HOH:O	1.94	0.51
1:A:10:ASN:HD22	1:A:53:ARG:HH22	1.60	0.50
1:D:138:THR:N	1:D:139:LYS:C	2.66	0.49
1:C:127:LEU:C	1:C:127:LEU:HD23	2.33	0.49
1:D:141:GLY:N	2:D:237:HOH:O	2.46	0.49
1:A:15:HIS:HE1	2:A:259:HOH:O	1.95	0.49
1:B:148:LYS:HA	1:B:151:VAL:HG12	1.95	0.49
1:D:87:ASN:HD21	1:D:153:ARG:HH12	1.59	0.48
1:A:130:ASN:HD21	1:A:157:ASN:HD22	1.60	0.48
1:C:44:TYR:HE2	1:C:48:MSE:HE3	1.76	0.48
1:D:39:ALA:HB1	1:D:44:TYR:HB3	1.96	0.48
1:A:67:ARG:HD2	2:A:195:HOH:O	2.14	0.47
1:B:120:LEU:HD12	1:B:120:LEU:N	2.30	0.47
1:D:137:TYR:C	1:D:139:LYS:C	2.73	0.47
1:D:96:MSE:HE2	1:D:136:PHE:CG	2.50	0.47
1:C:16:GLU:HA	2:C:241:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MSE:HE2	1:A:3:ASP:CG	2.35	0.46
1:B:69:ARG:NH2	1:B:72:GLN:HE21	2.14	0.46
1:C:87:ASN:ND2	1:C:150:TRP:HE1	2.14	0.45
1:B:69:ARG:NH2	1:B:72:GLN:NE2	2.64	0.45
1:C:22:HIS:HE1	2:C:246:HOH:O	1.99	0.45
1:C:4:LYS:HE3	2:C:306:HOH:O	2.13	0.45
1:C:88:HIS:CG	1:C:96:MSE:HE1	2.52	0.44
1:C:127:LEU:HD12	1:C:162:SER:HA	2.00	0.44
1:A:15:HIS:HD2	2:A:276:HOH:O	2.00	0.44
1:C:163:ALA:O	1:C:164:ASP:CG	2.56	0.44
1:C:87:ASN:HD22	1:C:133:ARG:HH22	1.65	0.43
1:D:2:SER:OG	1:D:3:ASP:N	2.51	0.43
1:A:69:ARG:HD2	2:A:254:HOH:O	2.17	0.43
1:C:2:SER:HA	1:C:61:ARG:HH22	1.84	0.43
1:B:17:GLY:HA2	1:B:32:TRP:CE3	2.53	0.42
1:D:19:TYR:OH	1:D:21:ASN:ND2	2.52	0.42
1:B:15:HIS:HE1	2:B:274:HOH:O	2.03	0.42
1:A:130:ASN:HD22	1:A:154:VAL:HG13	1.84	0.41
1:B:47:SER:OG	1:B:49:ARG:HB2	2.20	0.41
1:C:164:ASP:OD1	1:C:164:ASP:C	2.58	0.41
1:D:92:ASN:HB3	1:D:96:MSE:HE3	2.02	0.41
1:D:22:HIS:HA	1:D:23:PRO:HD3	1.95	0.41
1:D:48:MSE:HE1	1:D:51:MSE:CE	2.51	0.41
1:D:73:MSE:CE	1:D:78:ALA:HA	2.50	0.41
1:A:9:ILE:HD12	1:A:9:ILE:HA	1.97	0.40
1:C:5:PHE:CE2	1:C:61:ARG:HB2	2.57	0.40
1:B:10:ASN:ND2	1:B:53:ARG:HH22	2.18	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	161/167 (96%)	159 (99%)	2 (1%)	0	100	100
1	B	150/167 (90%)	149 (99%)	1 (1%)	0	100	100
1	C	158/167 (95%)	154 (98%)	4 (2%)	0	100	100
1	D	159/167 (95%)	157 (99%)	2 (1%)	0	100	100
All	All	628/668 (94%)	619 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	128/127 (101%)	127 (99%)	1 (1%)	81	74
1	B	121/127 (95%)	119 (98%)	2 (2%)	60	46
1	C	127/127 (100%)	122 (96%)	5 (4%)	32	13
1	D	128/127 (101%)	125 (98%)	3 (2%)	50	33
All	All	504/508 (99%)	493 (98%)	11 (2%)	52	34

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

Mol	Chain	Res	Type
1	A	49	ARG
1	B	47	SER
1	B	120	LEU
1	C	3	ASP
1	C	7	GLN
1	C	48	MSE
1	C	49	ARG
1	C	164	ASP
1	D	4	LYS
1	D	58	SER
1	D	61	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	10	ASN
1	A	15	HIS
1	A	22	HIS
1	A	87	ASN
1	A	88	HIS
1	A	118	ASN
1	A	130	ASN
1	B	10	ASN
1	B	15	HIS
1	B	22	HIS
1	B	72	GLN
1	B	88	HIS
1	C	6	ASN
1	C	10	ASN
1	C	22	HIS
1	C	40	GLN
1	C	87	ASN
1	C	130	ASN
1	D	6	ASN
1	D	7	GLN
1	D	10	ASN
1	D	21	ASN
1	D	40	GLN
1	D	87	ASN
1	D	92	ASN
1	D	130	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

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	158/167 (94%)	0.03	0 100 100	13, 19, 31, 47	0
1	B	150/167 (89%)	0.14	5 (3%) 46 51	14, 23, 34, 45	0
1	C	157/167 (94%)	0.22	10 (6%) 19 21	13, 21, 39, 44	0
1	D	159/167 (95%)	0.81	23 (14%) 2 2	20, 30, 51, 56	0
All	All	624/668 (93%)	0.30	38 (6%) 21 23	13, 23, 44, 56	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	140	LEU	12.4
1	D	146	PHE	7.6
1	D	22	HIS	6.7
1	D	23	PRO	6.2
1	D	49	ARG	6.0
1	D	139	LYS	5.7
1	D	2	SER	5.1
1	D	144	THR	4.8
1	C	26	PRO	4.6
1	C	23	PRO	4.5
1	D	165	ASN	4.4
1	D	24	LYS	4.4
1	D	19	TYR	4.2
1	D	137	TYR	3.9
1	D	164	ASP	3.8
1	C	40	GLN	3.7
1	B	22	HIS	3.6
1	C	43	GLY	3.5
1	C	45	ASN	3.3
1	C	164	ASP	3.2
1	C	50	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	23	PRO	3.0
1	D	25	ASP	3.0
1	D	141	GLY	2.7
1	C	46	GLY	2.7
1	D	20	ALA	2.7
1	D	143	PHE	2.6
1	D	138	THR	2.4
1	D	142	THR	2.3
1	D	145	SER	2.3
1	D	44	TYR	2.2
1	D	27	GLY	2.2
1	B	148	LYS	2.1
1	D	54	GLU	2.1
1	C	44	TYR	2.1
1	C	41	ALA	2.1
1	D	28	GLY	2.1
1	B	24	LYS	2.0

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.