WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:25 pm GMT

PDB ID	:	1M9F
Title	:	X-ray crystal structure of Cyclophilin A/HIV-1 CA N-terminal domain (1-146) M-type H87A,A88M Complex.
Authors	:	Howard, B.R.; Vajdos, F.F.; Li, S.; Sundquist, W.I.; Hill, C.P.
Deposited on	:	2002-07-28
Resolution	:	1.73 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
http://wwpdb.org/validation/2016/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:

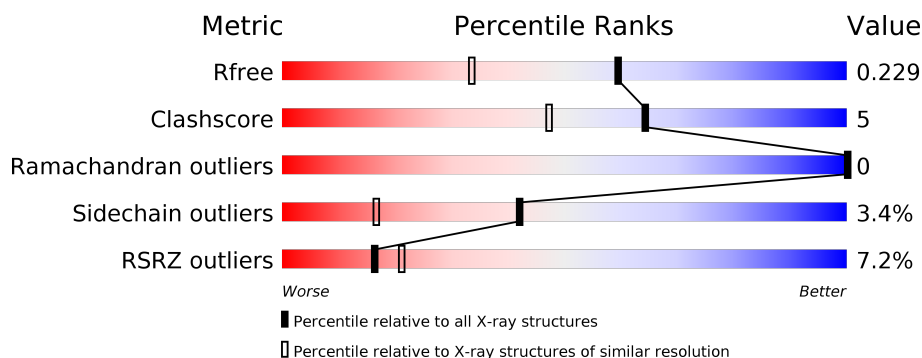|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 1.73 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		0.229
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		3.4%
RSRZ outliers		7.2%

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}	100719	2694 (1.76-1.72)
Clashscore	112137	2854 (1.76-1.72)
Ramachandran outliers	110173	2824 (1.76-1.72)
Sidechain outliers	110143	2824 (1.76-1.72)
RSRZ outliers	101464	2705 (1.76-1.72)

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. 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	165	3% / 87% / 11% ·
1	B	165	4% / 89% / 9% ··
2	C	146	6% / 81% / 15% ·
2	D	146	16% / 71% / 17% ·· 8%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 5284 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 Cyclophilin A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total 1266	C 802	N 218	O 237	S 9	0	0	0
1	B	164	Total 1258	C 797	N 217	O 236	S 8	0	0	0

- Molecule 2 is a protein called HIV-1 Capsid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	146	Total 1134	C 717	N 198	O 210	S 9	0	0	0
2	D	135	Total 1050	C 664	N 183	O 195	S 8	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	87	ALA	HIS	ENGINEERED	UNP Q72497
C	88	MET	ALA	ENGINEERED	UNP Q72497
C	120	HIS	ASN	SEE REMARK 999	UNP Q72497
D	87	ALA	HIS	ENGINEERED	UNP Q72497
D	88	MET	ALA	ENGINEERED	UNP Q72497
D	120	HIS	ASN	SEE REMARK 999	UNP Q72497

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	203	Total 203	O 203	0	0
3	B	133	Total 133	O 133	0	0
3	C	152	Total 152	O 152	0	0

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	88	Total 88	O 88	0	0

3 Residue-property plots ⓘ

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 (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.
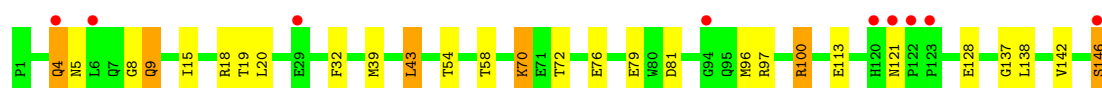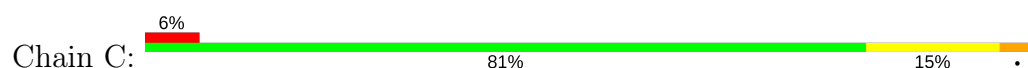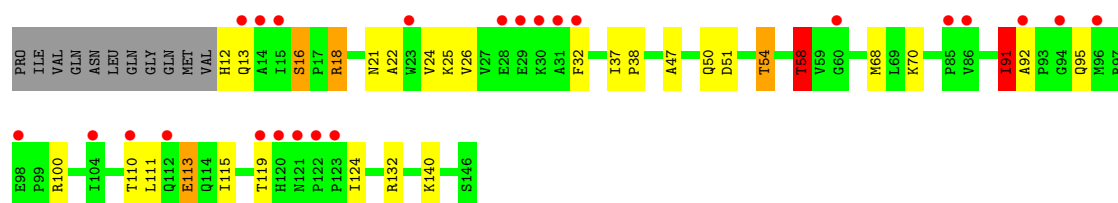
- Molecule 1: Cyclophilin A

Chain A:

- Molecule 1: Cyclophilin A

Chain B:

- Molecule 2: HIV-1 Capsid

Chain C:
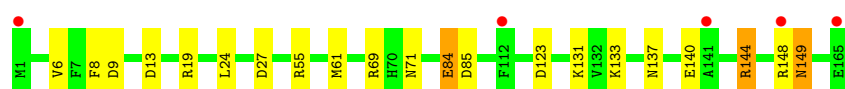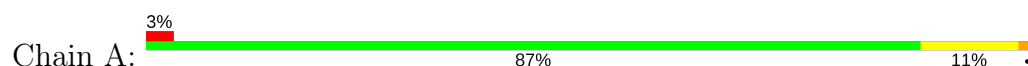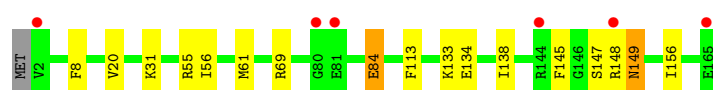
- Molecule 2: HIV-1 Capsid

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	38.51Å　110.94Å　67.93Å 90.00°　101.41°　90.00°	Depositor
Resolution (Å)	19.69　–　1.73 19.67　–　1.73	Depositor EDS
% Data completeness (in resolution range)	96.0 (19.69-1.73) 96.0 (19.67-1.73)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$<I/\sigma(I)>$ [1]	2.34 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.167　,　0.220 0.177　,　0.229	Depositor DCC
R_{free} test set	5627 reflections (11.20%)	DCC
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 62.0	EDS
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5284	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.88	0/1294	1.56	23/1733 (1.3%)
1	B	0.76	0/1286	1.43	9/1723 (0.5%)
2	C	0.79	0/1161	1.62	11/1578 (0.7%)
2	D	0.76	0/1076	1.47	11/1463 (0.8%)
All	All	0.80	0/4817	1.52	54/6497 (0.8%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	100	ARG	NE-CZ-NH1	25.20	132.90	120.30
2	C	100	ARG	NE-CZ-NH2	-17.30	111.65	120.30
2	D	18	ARG	NE-CZ-NH2	-14.38	113.11	120.30
1	B	55	ARG	NE-CZ-NH2	-11.07	114.76	120.30
1	A	144	ARG	NE-CZ-NH1	10.59	125.59	120.30
1	B	55	ARG	NE-CZ-NH1	8.99	124.80	120.30
2	C	100	ARG	CD-NE-CZ	8.98	136.17	123.60
1	A	55	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	A	85	ASP	CB-CG-OD2	8.65	126.09	118.30
2	D	18	ARG	NE-CZ-NH1	8.60	124.60	120.30
2	D	132	ARG	NE-CZ-NH2	-8.13	116.24	120.30
2	D	132	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	B	69	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	A	19	ARG	NE-CZ-NH2	-7.79	116.40	120.30
2	C	76	GLU	OE1-CD-OE2	-7.70	114.06	123.30
1	A	144	ARG	NE-CZ-NH2	-7.55	116.53	120.30
2	C	70	LYS	CD-CE-NZ	7.20	128.26	111.70
1	A	8	PHE	CB-CG-CD1	6.85	125.60	120.80
1	A	13	ASP	CB-CG-OD1	6.66	124.29	118.30
1	A	9	ASP	CB-CG-OD1	6.52	124.17	118.30
1	A	84	GLU	OE1-CD-OE2	-6.38	115.64	123.30
1	A	55	ARG	NE-CZ-NH1	6.27	123.43	120.30
2	D	12	HIS	N-CA-C	6.23	127.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	69	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	27	ASP	CB-CG-OD1	6.16	123.84	118.30
1	B	8	PHE	CB-CG-CD2	-6.13	116.51	120.80
1	B	113	PHE	CB-CG-CD2	6.03	125.02	120.80
2	D	91	ILE	CG1-CB-CG2	-5.97	98.27	111.40
2	C	18	ARG	NE-CZ-NH1	-5.96	117.32	120.30
2	D	16	SER	CB-CA-C	-5.94	98.81	110.10
2	D	58	THR	N-CA-CB	-5.94	99.01	110.30
1	A	84	GLU	CG-CD-OE1	5.82	129.94	118.30
1	B	55	ARG	CD-NE-CZ	5.72	131.61	123.60
1	A	148	ARG	NE-CZ-NH1	5.70	123.15	120.30
2	C	79	GLU	CG-CD-OE1	-5.66	106.99	118.30
2	C	146	SER	CA-C-O	5.66	131.97	120.10
2	C	39	MET	CG-SD-CE	5.62	109.20	100.20
1	A	71	ASN	N-CA-CB	-5.57	100.58	110.60
1	A	9	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	133	LYS	CA-CB-CG	5.41	125.30	113.40
1	A	6	VAL	CA-CB-CG2	-5.40	102.81	110.90
2	C	43	LEU	CB-CG-CD1	5.38	120.15	111.00
1	A	69	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	6	VAL	CG1-CB-CG2	5.30	119.38	110.90
2	D	100	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	B	8	PHE	CB-CG-CD1	5.22	124.45	120.80
1	A	123	ASP	CB-CG-OD1	5.17	122.95	118.30
2	D	32	PHE	CB-CA-C	5.15	120.70	110.40
1	B	148	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	148	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	140	GLU	OE1-CD-OE2	-5.08	117.20	123.30
2	D	54	THR	OG1-CB-CG2	-5.07	98.33	110.00
1	A	24	LEU	CB-CG-CD2	-5.06	102.39	111.00
2	C	81	ASP	CB-CG-OD1	5.03	122.82	118.30

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	1266	0	1237	5	0
1	B	1258	0	1225	9	0
2	C	1134	0	1137	16	0
2	D	1050	0	1045	15	0
3	A	203	0	0	3	0
3	B	133	0	0	1	0
3	C	152	0	0	5	0
3	D	88	0	0	3	0
All	All	5284	0	4644	45	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 5.

All (45) 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:70:LYS:HD2	3:C:246:HOH:O	1.79	0.80
1:B:56:ILE:CD1	1:B:156:ILE:HD12	2.24	0.68
2:D:91:ILE:O	3:D:176:HOH:O	2.13	0.67
2:C:32:PHE:O	2:C:142:VAL:HG12	1.98	0.62
2:C:128:GLU:HG2	3:C:209:HOH:O	2.00	0.60
2:C:4:GLN:HE21	2:C:8:GLY:HA2	1.65	0.60
2:C:4:GLN:NE2	2:C:8:GLY:HA2	2.17	0.59
2:D:50:GLN:HE22	2:D:111:LEU:HD22	1.68	0.58
2:C:5:ASN:OD1	2:C:9:GLN:HG2	2.05	0.57
1:B:31:LYS:NZ	1:B:84:GLU:OE1	2.39	0.56
1:B:149:ASN:H	1:B:149:ASN:HD22	1.54	0.54
2:C:138:LEU:O	2:C:142:VAL:HG13	2.08	0.53
2:D:21:ASN:HD21	2:D:25:LYS:HE3	1.73	0.53
2:C:15:ILE:HD13	2:C:20:LEU:HD21	1.90	0.52
2:D:70:LYS:NZ	3:D:232:HOH:O	2.37	0.52
2:D:91:ILE:HG23	3:D:176:HOH:O	2.10	0.51
1:B:20:VAL:HG22	1:B:138:ILE:HB	1.93	0.51
1:B:147:SER:OG	1:B:149:ASN:ND2	2.44	0.51
1:B:133:LYS:NZ	1:B:134:GLU:OE2	2.44	0.50
2:D:47:ALA:HB1	2:D:51:ASP:HB2	1.94	0.50
1:B:56:ILE:HD12	1:B:156:ILE:HD12	1.94	0.48
2:D:110:THR:OG1	2:D:113:GLU:HB2	2.13	0.48
1:A:137:ASN:ND2	3:A:233:HOH:O	2.42	0.48
1:A:144:ARG:NH1	3:A:220:HOH:O	2.46	0.47
2:D:50:GLN:O	2:D:54:THR:HG23	2.13	0.47
1:B:84:GLU:OE1	3:B:237:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:100:ARG:HD3	3:C:192:HOH:O	2.14	0.47
2:C:5:ASN:HD21	2:C:9:GLN:HE21	1.62	0.47
2:C:97:ARG:HD3	3:C:198:HOH:O	2.15	0.46
2:D:37:ILE:HB	2:D:38:PRO:HD3	1.97	0.46
1:A:144:ARG:NH2	3:A:337:HOH:O	2.49	0.46
2:C:72:THR:HG21	2:C:137:GLY:HA2	1.97	0.45
1:B:145:PHE:HB2	1:B:156:ILE:HD11	1.99	0.45
1:A:149:ASN:HD22	1:A:149:ASN:C	2.20	0.45
2:C:70:LYS:CD	3:C:246:HOH:O	2.50	0.44
2:D:91:ILE:HD12	2:D:92:ALA:N	2.33	0.44
1:A:84:GLU:H	1:A:84:GLU:CD	2.21	0.43
2:D:68:MET:HB3	2:D:140:LYS:HD2	2.00	0.43
2:D:91:ILE:HD11	2:D:95:GLN:HB3	1.99	0.43
2:D:22:ALA:O	2:D:26:VAL:HG23	2.19	0.42
2:C:54:THR:O	2:C:58:THR:HG23	2.20	0.42
2:C:19:THR:HG23	2:C:43:LEU:HD22	2.02	0.41
2:D:24:VAL:HG22	2:D:58:THR:HG23	2.02	0.41
2:C:96:MET:HE3	2:C:113:GLU:HA	2.03	0.41
2:D:115:ILE:O	2:D:119:THR:HG23	2.20	0.41

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	163/165 (99%)	157 (96%)	6 (4%)	0	100	100
1	B	162/165 (98%)	157 (97%)	5 (3%)	0	100	100
2	C	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
2	D	133/146 (91%)	128 (96%)	5 (4%)	0	100	100
All	All	602/622 (97%)	584 (97%)	18 (3%)	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	133/133 (100%)	130 (98%)	3 (2%)	56	31
1	B	132/133 (99%)	129 (98%)	3 (2%)	56	31
2	C	123/123 (100%)	119 (97%)	4 (3%)	43	17
2	D	113/123 (92%)	106 (94%)	7 (6%)	21	4
All	All	501/512 (98%)	484 (97%)	17 (3%)	42	17

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	MET
1	A	131	LYS
1	A	149	ASN
1	B	61	MET
1	B	84	GLU
1	B	149	ASN
2	C	4	GLN
2	C	9	GLN
2	C	121	ASN
2	C	146	SER
2	D	13	GLN
2	D	16	SER
2	D	18	ARG
2	D	58	THR
2	D	91	ILE
2	D	113	GLU
2	D	124	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	149	ASN
1	B	149	ASN
2	C	4	GLN
2	C	9	GLN
2	C	50	GLN
2	C	74	ASN
2	D	21	ASN
2	D	50	GLN
2	D	74	ASN
2	D	84	HIS

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 carbohydrates 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, 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	165/165 (100%)	0.11	5 (3%)	51	58	11, 19, 32, 56	0
1	B	164/165 (99%)	0.26	6 (3%)	42	49	16, 26, 41, 56	0
2	C	146/146 (100%)	0.29	9 (6%)	21	27	15, 23, 42, 52	0
2	D	135/146 (92%)	0.86	24 (17%)	2	3	17, 31, 56, 79	0
All	All	610/622 (98%)	0.36	44 (7%)	16	21	11, 24, 44, 79	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	121	ASN	7.0
2	D	122	PRO	7.0
2	C	6	LEU	6.1
2	C	121	ASN	6.0
2	D	120	HIS	5.2
1	B	2	VAL	5.1
2	C	146	SER	4.7
2	D	119	THR	4.7
2	D	112	GLN	4.5
1	A	165	GLU	4.3
2	D	60	GLY	4.1
1	B	148	ARG	3.9
2	D	31	ALA	3.8
2	D	110	THR	3.8
2	D	15	ILE	3.6
2	D	29	GLU	3.6
1	B	144	ARG	3.5
2	D	30	LYS	3.5
2	D	14	ALA	3.4
2	D	28	GLU	3.4
2	D	123	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	C	4	GLN	3.3
1	B	165	GLU	3.3
2	C	123	PRO	3.2
2	D	13	GLN	3.1
1	A	148	ARG	2.9
2	D	85	PRO	2.9
1	A	1	MET	2.9
2	C	120	HIS	2.7
2	D	32	PHE	2.7
2	C	94	GLY	2.7
2	C	122	PRO	2.7
2	D	96	MET	2.4
1	B	81	GLU	2.4
2	D	92	ALA	2.3
2	D	94	GLY	2.3
2	D	104	ILE	2.3
2	D	23	TRP	2.2
1	A	112	PHE	2.2
1	A	141	ALA	2.2
2	D	86	VAL	2.2
2	C	29	GLU	2.1
1	B	80	GLY	2.1
2	D	98	GLU	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.