Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:31 pm BST

PDB ID	:	6JYO
Title	:	GII.13/21 noroviruses recognize glycans with a terminal beta-galactose via an unconventional glycan binding site
Authors	:	Duan, Z.; Xin, C.
Deposited on	:	2019-04-27
Resolution	:	1.50 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 ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

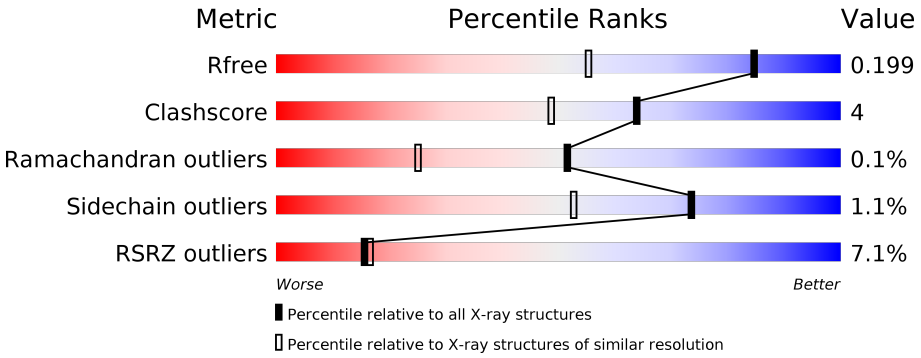
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 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 <=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	309	7% 90% 10%
1	B	309	6% 90% 9%
1	C	309	6% 95% 5%
1	D	309	8% 90% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11206 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 norovirus P domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	1	0
			2401	1525	410	460	6			
1	B	309	Total	C	N	O	S	0	0	0
			2396	1522	409	459	6			
1	C	309	Total	C	N	O	S	0	0	0
			2396	1522	409	459	6			
1	D	307	Total	C	N	O	S	0	0	0
			2381	1514	407	454	6			

- Molecule 2 is water.

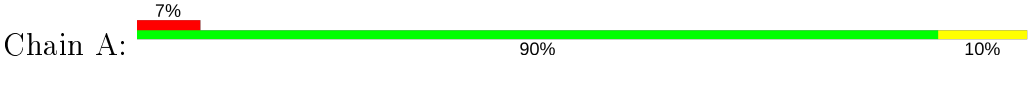
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	364	Total	O	0	0
			364	364		
2	B	449	Total	O	0	0
			449	449		
2	C	416	Total	O	0	0
			416	416		
2	D	403	Total	O	0	0
			403	403		

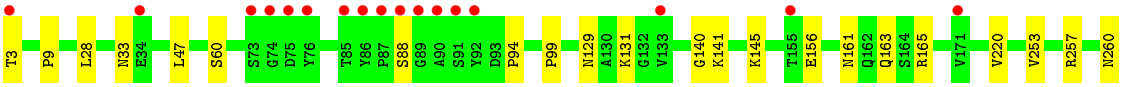
3 Residue-property plots (i)

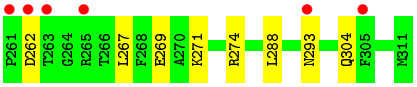
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: norovirus P domain protein

Chain A:

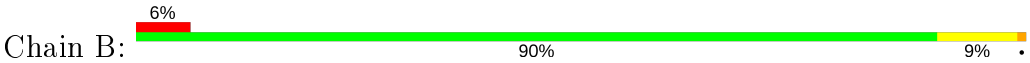


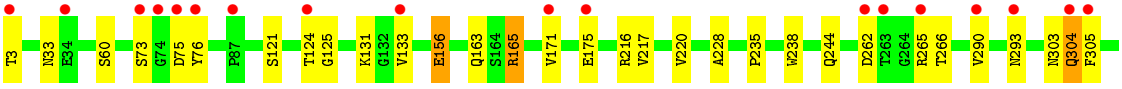




- Molecule 1: norovirus P domain protein

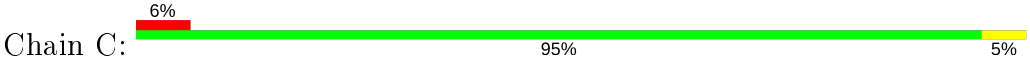
Chain B:

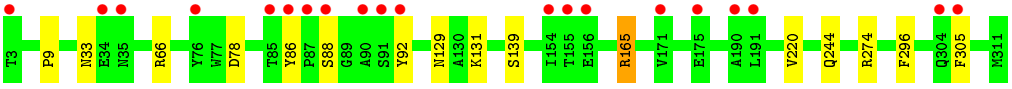




- Molecule 1: norovirus P domain protein

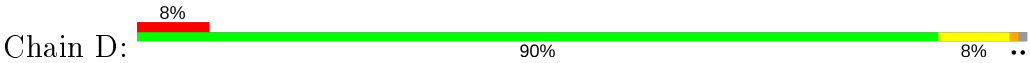
Chain C:





- Molecule 1: norovirus P domain protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	87.64Å 105.67Å 138.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.35 – 1.50 49.35 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.35-1.50) 98.9 (49.35-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.188 , 0.199 0.188 , 0.199	Depositor DCC
R_{free} test set	10095 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	14.1	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11206	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.6027e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.31	1/2471 (0.0%)	0.49	0/3383
1	B	0.31	1/2463 (0.0%)	0.58	2/3372 (0.1%)
1	C	0.31	0/2463	0.55	2/3372 (0.1%)
1	D	0.36	1/2447 (0.0%)	0.59	5/3348 (0.1%)
All	All	0.33	3/9844 (0.0%)	0.56	9/13475 (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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	156	GLU	CD-OE2	-9.73	1.15	1.25
1	A	156	GLU	CD-OE1	-6.80	1.18	1.25
1	B	156	GLU	CD-OE2	-5.79	1.19	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	165	ARG	NE-CZ-NH1	-12.22	114.19	120.30
1	B	165	ARG	NE-CZ-NH2	11.24	125.92	120.30
1	C	165	ARG	NE-CZ-NH1	-10.24	115.18	120.30
1	C	165	ARG	NE-CZ-NH2	9.01	124.80	120.30
1	D	165	ARG	NE-CZ-NH2	8.88	124.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	224	ARG	NE-CZ-NH1	-8.05	116.28	120.30
1	D	224	ARG	NE-CZ-NH2	6.86	123.73	120.30
1	D	68	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	D	165	ARG	NE-CZ-NH1	-5.52	117.54	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	33	ASN	Peptide
1	B	33	ASN	Peptide
1	C	33	ASN	Peptide
1	D	260	ASN	Peptide
1	D	33	ASN	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	2401	0	2315	20	1
1	B	2396	0	2309	25	0
1	C	2396	0	2309	13	0
1	D	2381	0	2297	27	1
2	A	364	0	0	10	0
2	B	449	0	0	13	3
2	C	416	0	0	7	2
2	D	403	0	0	13	6
All	All	11206	0	9230	79	9

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 4.

All (79) 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:165:ARG:NH1	2:D:401:HOH:O	1.84	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:ASN:OD1	2:D:402:HOH:O	1.85	0.93
1:B:165:ARG:NH1	2:B:401:HOH:O	2.00	0.93
1:B:3:THR:N	2:B:402:HOH:O	2.02	0.93
1:B:303:ASN:HA	2:B:585:HOH:O	1.69	0.91
1:D:87:PRO:O	2:D:403:HOH:O	1.90	0.88
1:B:60:SER:HB3	2:B:698:HOH:O	1.79	0.82
1:A:94:PRO:O	1:A:145:LYS:NZ	2.19	0.76
1:D:264:GLY:N	2:D:405:HOH:O	2.22	0.73
1:B:304:GLN:HG2	2:B:648:HOH:O	1.90	0.71
1:D:226:GLN:NE2	2:D:406:HOH:O	2.23	0.71
1:A:274:ARG:NH1	2:A:409:HOH:O	2.23	0.71
1:D:264:GLY:O	2:D:404:HOH:O	2.09	0.69
1:D:165:ARG:HD2	2:D:719:HOH:O	1.92	0.68
1:B:76:TYR:OH	2:B:403:HOH:O	2.07	0.66
1:B:244:GLN:HG2	2:B:685:HOH:O	1.95	0.66
1:B:175:GLU:H	1:B:175:GLU:CD	2.00	0.64
1:B:163:GLN:NE2	2:B:406:HOH:O	2.26	0.63
1:C:92:TYR:HA	2:C:406:HOH:O	1.98	0.63
1:D:93:ASP:OD2	1:D:95:THR:OG1	2.11	0.61
1:A:165:ARG:NH2	2:A:407:HOH:O	2.22	0.60
1:D:48:ASP:CG	1:D:274:ARG:HH22	2.05	0.59
2:B:566:HOH:O	1:D:60:SER:HB3	2.03	0.58
1:B:262:ASP:OD2	1:B:293:ASN:ND2	2.36	0.58
1:D:257:ARG:NH2	1:D:299:ASP:OD1	2.35	0.57
1:D:295:HIS:HB2	2:D:410:HOH:O	2.05	0.56
1:A:262:ASP:OD2	1:A:293:ASN:ND2	2.38	0.56
1:B:121:SER:HB3	1:D:224:ARG:CZ	2.37	0.55
1:D:257:ARG:HH22	1:D:299:ASP:HB2	1.70	0.55
1:B:73:SER:HB3	1:C:305:PHE:CZ	2.42	0.54
1:D:303:ASN:ND2	2:D:414:HOH:O	2.40	0.54
1:B:266:THR:OG1	2:B:404:HOH:O	2.10	0.54
1:D:257:ARG:HH22	1:D:299:ASP:CG	2.11	0.54
1:C:66:ARG:HG2	1:C:165:ARG:HG3	1.91	0.53
1:C:274:ARG:HD2	2:C:723:HOH:O	2.08	0.53
1:B:303:ASN:OD1	1:B:305:PHE:N	2.39	0.53
1:A:141:LYS:NZ	2:A:418:HOH:O	2.38	0.53
1:A:60:SER:O	2:A:404:HOH:O	2.19	0.53
1:D:141:LYS:NZ	2:D:416:HOH:O	2.42	0.52
1:D:260:ASN:O	1:D:261:PRO:O	2.28	0.51
1:D:257:ARG:HH22	1:D:299:ASP:CB	2.24	0.51
1:D:296:PHE:HB2	2:D:447:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:VAL:HG12	1:B:228:ALA:O	2.11	0.51
1:D:299:ASP:HA	2:D:420:HOH:O	2.10	0.51
1:A:304:GLN:HG2	2:A:406:HOH:O	2.11	0.50
1:A:129:ASN:HB3	1:C:220:VAL:HA	1.93	0.50
1:A:140:GLY:HA2	2:A:567:HOH:O	2.13	0.49
1:B:265:ARG:NE	1:B:265:ARG:HA	2.28	0.49
1:B:121:SER:H	1:D:224:ARG:NH2	2.10	0.49
1:C:9:PRO:HB3	2:C:636:HOH:O	2.13	0.48
1:B:220:VAL:HA	1:D:129:ASN:HB3	1.95	0.48
1:A:28:LEU:HB2	1:A:288:LEU:HB2	1.96	0.47
1:A:260:ASN:HB2	1:A:267:LEU:HD21	1.96	0.47
1:A:220:VAL:HA	1:C:129:ASN:HB3	1.97	0.47
1:A:88:SER:O	2:A:405:HOH:O	2.20	0.46
1:B:124:THR:HB	2:B:430:HOH:O	2.17	0.45
1:B:216:ARG:NH1	2:B:423:HOH:O	2.49	0.45
1:D:274:ARG:HH21	1:D:274:ARG:HG2	1.80	0.45
1:A:47:LEU:HG	1:A:274:ARG:HA	1.98	0.45
1:D:235:PRO:HG2	1:D:238:TRP:CD1	2.52	0.45
1:D:257:ARG:NH2	1:D:299:ASP:HB2	2.31	0.45
1:A:9:PRO:HB3	2:A:641:HOH:O	2.17	0.44
1:C:86:TYR:HE2	2:C:406:HOH:O	2.01	0.44
1:A:163:GLN:NE2	2:A:423:HOH:O	2.51	0.43
1:A:3:THR:HA	2:A:503:HOH:O	2.17	0.43
1:A:257:ARG:NH1	1:A:269:GLU:OE1	2.51	0.43
1:C:165:ARG:HG2	1:C:165:ARG:HH21	1.83	0.43
1:C:78:ASP:OD2	1:C:139:SER:OG	2.28	0.43
1:C:88:SER:CB	2:C:428:HOH:O	2.67	0.43
1:B:235:PRO:HG2	1:B:238:TRP:CD1	2.54	0.42
1:A:99:PRO:O	1:A:145:LYS:HD3	2.20	0.42
1:B:304:GLN:HG3	1:B:305:PHE:CD2	2.55	0.42
1:C:296:PHE:HB2	2:C:558:HOH:O	2.20	0.41
1:A:253:VAL:HG11	1:A:271:LYS:HG2	2.03	0.41
1:B:125:GLY:N	2:B:430:HOH:O	2.53	0.41
1:B:73:SER:C	1:B:75:ASP:H	2.24	0.41
1:C:244:GLN:HG2	2:C:628:HOH:O	2.21	0.40
1:D:293:ASN:CG	2:D:402:HOH:O	2.45	0.40
1:B:303:ASN:OD1	1:B:305:PHE:HB2	2.21	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:514:HOH:O	2:D:514:HOH:O[2_665]	1.35	0.85
2:B:834:HOH:O	2:B:841:HOH:O[4_455]	2.06	0.14
2:B:740:HOH:O	2:D:677:HOH:O[2_655]	2.12	0.08
2:B:809:HOH:O	2:B:810:HOH:O[4_455]	2.15	0.05
1:A:161[B]:ASN:ND2	1:D:252:ASP:OD2[1_455]	2.16	0.04
2:C:799:HOH:O	2:D:791:HOH:O[1_455]	2.17	0.03
2:D:535:HOH:O	2:D:725:HOH:O[2_655]	2.18	0.02
2:D:404:HOH:O	2:D:514:HOH:O[2_665]	2.19	0.01
2:C:495:HOH:O	2:D:708:HOH:O[2_665]	2.19	0.01

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	308/309 (100%)	298 (97%)	10 (3%)	0	100	100
1	B	307/309 (99%)	294 (96%)	12 (4%)	1 (0%)	41	18
1	C	307/309 (99%)	299 (97%)	8 (3%)	0	100	100
1	D	303/309 (98%)	288 (95%)	15 (5%)	0	100	100
All	All	1225/1236 (99%)	1179 (96%)	45 (4%)	1 (0%)	51	25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	156	GLU

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	264/263 (100%)	263 (100%)	1 (0%)	91 82
1	B	263/263 (100%)	258 (98%)	5 (2%)	57 27
1	C	263/263 (100%)	262 (100%)	1 (0%)	91 82
1	D	261/263 (99%)	256 (98%)	5 (2%)	57 27
All	All	1051/1052 (100%)	1039 (99%)	12 (1%)	73 53

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LYS
1	B	131	LYS
1	B	133	VAL
1	B	171	VAL
1	B	290	VAL
1	B	304	GLN
1	C	131	LYS
1	D	131	LYS
1	D	171	VAL
1	D	274	ARG
1	D	290	VAL
1	D	297	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	B	304	GLN
1	D	250	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

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, 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	309/309 (100%)	0.44	23 (7%)	14	15	9, 17, 42, 82	0
1	B	309/309 (100%)	0.26	18 (5%)	23	25	7, 14, 30, 63	0
1	C	309/309 (100%)	0.27	20 (6%)	18	20	8, 15, 30, 69	0
1	D	307/309 (99%)	0.37	26 (8%)	10	11	8, 17, 36, 65	0
All	All	1234/1236 (99%)	0.34	87 (7%)	16	17	7, 16, 36, 82	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	76	TYR	12.5
1	A	90	ALA	9.7
1	A	86	TYR	8.8
1	A	91	SER	8.6
1	B	305	PHE	8.1
1	C	191	LEU	7.9
1	A	89	GLY	7.6
1	C	305	PHE	7.3
1	B	76	TYR	6.7
1	A	87	PRO	6.4
1	A	76	TYR	6.1
1	C	155	THR	5.3
1	B	73	SER	5.2
1	D	3	THR	5.1
1	D	264	GLY	5.0
1	C	87	PRO	4.7
1	A	88	SER	4.5
1	D	87	PRO	4.5
1	A	305	PHE	4.5
1	B	304	GLN	4.4
1	A	262	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	74	GLY	4.2
1	A	73	SER	4.2
1	A	263	THR	4.1
1	C	86	TYR	4.1
1	D	86	TYR	4.0
1	D	261	PRO	3.9
1	A	92	TYR	3.8
1	B	263	THR	3.7
1	D	260	ASN	3.5
1	B	3	THR	3.5
1	D	305	PHE	3.4
1	D	293	ASN	3.4
1	C	154	ILE	3.3
1	D	250	GLN	3.3
1	B	124	THR	3.2
1	C	91	SER	3.2
1	A	85	THR	3.1
1	D	171	VAL	3.0
1	B	133	VAL	3.0
1	A	155	THR	3.0
1	B	265	ARG	3.0
1	D	10	ILE	2.9
1	D	267	LEU	2.8
1	C	35	ASN	2.8
1	C	175	GLU	2.8
1	D	259	VAL	2.8
1	A	261	PRO	2.7
1	A	133	VAL	2.6
1	D	85	THR	2.6
1	D	5	PRO	2.6
1	C	156	GLU	2.5
1	A	293	ASN	2.5
1	A	171	VAL	2.5
1	D	274	ARG	2.5
1	C	190	ALA	2.5
1	A	75	ASP	2.5
1	B	262	ASP	2.4
1	A	3	THR	2.4
1	D	265	ARG	2.4
1	D	301	TRP	2.4
1	B	175	GLU	2.4
1	D	90	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	3	THR	2.4
1	C	34	GLU	2.4
1	B	171	VAL	2.4
1	B	293	ASN	2.4
1	D	224	ARG	2.4
1	B	75	ASP	2.3
1	C	92	TYR	2.3
1	D	91	SER	2.3
1	D	289	VAL	2.3
1	A	34	GLU	2.3
1	B	34	GLU	2.3
1	D	191	LEU	2.3
1	B	290	VAL	2.3
1	C	304	GLN	2.2
1	D	290	VAL	2.2
1	D	252	ASP	2.2
1	C	171	VAL	2.2
1	A	265	ARG	2.2
1	B	87	PRO	2.2
1	C	90	ALA	2.1
1	C	85	THR	2.1
1	C	88	SER	2.1
1	D	34	GLU	2.1
1	A	74	GLY	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 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.