Full wwPDB X-ray Structure Validation Report ⓘ

Jan 14, 2024 – 08:14 am GMT

PDB ID	:	6ZH9
Title	:	Ternary complex CR3022 H11-H4 and RBD (SARS-CoV-2)
Authors	:	Naismith, J.H.; Mikolajek, H.; Le Bas, A.
Deposited on	:	2020-06-21
Resolution	:	3.31 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:

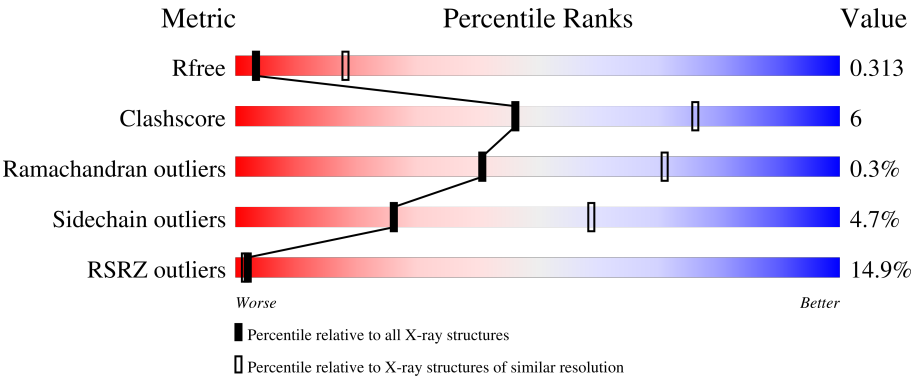
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.31 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	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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	HHH	216	16% 81% 18% ·
2	LLL	219	9% 76% 22% ·
3	EEE	197	16% 86% 12% ··
4	FFF	134	20% 87% 7% · ·

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5906 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 CR3022 heavy.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	HHH	216	1609	1023	261	317	8	0	1	0

- Molecule 2 is a protein called CR3022 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	LLL	219	1703	1070	282	347	4	0	0	0

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	EEE	195	1562	1003	258	293	8	0	4	0

- Molecule 4 is a protein called Nanobody H11-H4.

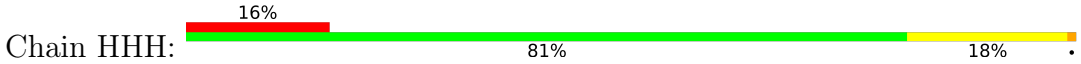
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	FFF	128	1032	654	176	194	8	0	5	0

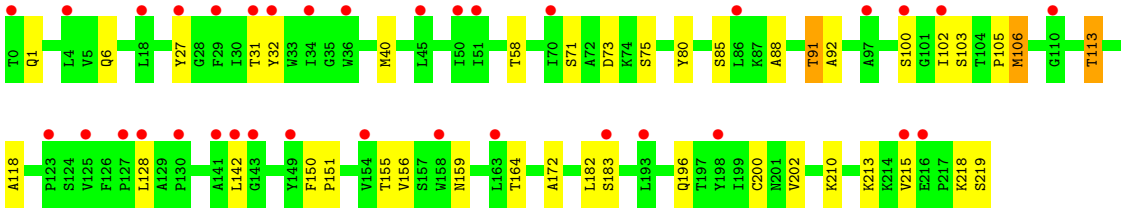
3 Residue-property plots (i)

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: CR3022 heavy

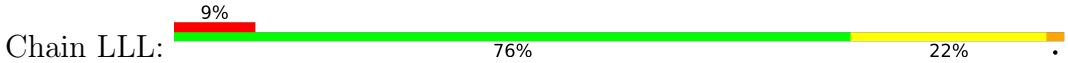
Chain HHH:

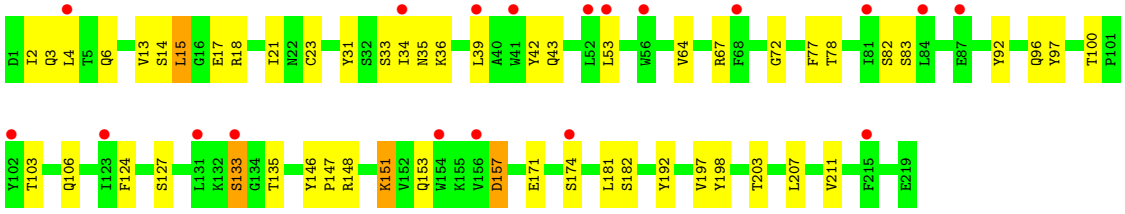




• Molecule 2: CR3022 Light chain

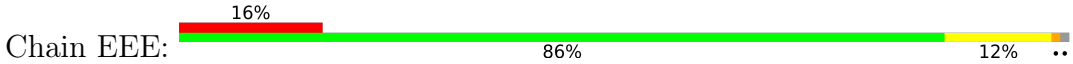
Chain LLL:

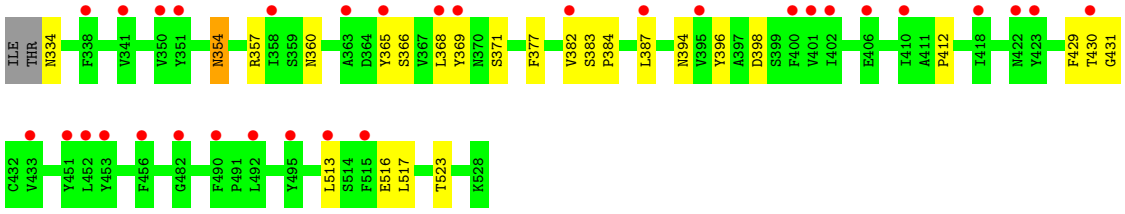




• Molecule 3: Spike glycoprotein

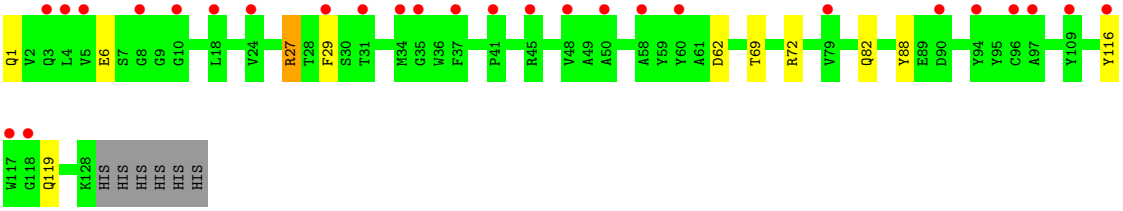
Chain EEE:





• Molecule 4: Nanobody H11-H4

Chain FFF:


Q1
V2
Q3
L4
V5
E6
S7
G8
G9
G10
L18
V24
R27
T28
F29
S30
T31
M34
G35
W36
F37
P41
R45
V48
A49
A50
A58
Y59
Y60
A61
D62
T69
R72
V79
Q82
Y88
E89
D90
Y94
Y95
C96
A97
Y109
Y116
W117
G118
Q119
K128
HIS
HIS
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HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	156.41Å 156.41Å 116.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.24 – 3.31 80.11 – 3.31	Depositor EDS
% Data completeness (in resolution range)	100.0 (80.24-3.31) 100.0 (80.11-3.31)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.261 , 0.305 0.266 , 0.313	Depositor DCC
R_{free} test set	1088 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	159.7	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 178.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	5906	wwPDB-VP
Average B, all atoms (Å^2)	199.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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	HHH	0.71	0/1654	0.89	0/2253
2	LLL	0.72	0/1741	0.94	0/2367
3	EEE	0.70	0/1618	0.94	0/2202
4	FFF	0.72	0/1066	0.86	0/1441
All	All	0.71	0/6079	0.91	0/8263

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

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	HHH	1609	0	1585	27	0
2	LLL	1703	0	1649	36	0
3	EEE	1562	0	1491	23	0
4	FFF	1032	0	995	4	0
All	All	5906	0	5720	73	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 (73) 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:LLL:96:GLN:HE21	2:LLL:103:THR:HG22	1.44	0.83
2:LLL:34:ILE:HG22	3:EEE:517:LEU:HB2	1.74	0.69
2:LLL:157:ASP:HA	2:LLL:197:VAL:HG22	1.78	0.66
2:LLL:133:SER:HB2	2:LLL:135:THR:HG22	1.78	0.66
1:HHH:128:LEU:HB3	2:LLL:124:PHE:CD1	2.32	0.65
1:HHH:88:ALA:O	1:HHH:91:THR:HG23	1.98	0.63
1:HHH:142:LEU:HD13	1:HHH:215:VAL:HG21	1.81	0.63
2:LLL:34:ILE:HG22	3:EEE:517:LEU:CB	2.30	0.61
2:LLL:2:ILE:O	2:LLL:103:THR:HG21	2.02	0.59
2:LLL:33:SER:HB3	3:EEE:430[B]:THR:HG21	1.85	0.58
2:LLL:6:GLN:O	2:LLL:106:GLN:NE2	2.37	0.57
4:FFF:69:THR:HB	4:FFF:82:GLN:HB3	1.86	0.56
1:HHH:31:THR:CG2	3:EEE:384:PRO:HG2	2.37	0.56
1:HHH:31:THR:HG21	3:EEE:384:PRO:HG2	1.87	0.56
2:LLL:13:VAL:HG13	2:LLL:17:GLU:HB2	1.90	0.54
3:EEE:366:SER:HA	3:EEE:369:TYR:CE2	2.43	0.54
1:HHH:32:TYR:HA	1:HHH:100:SER:HA	1.89	0.53
1:HHH:103:SER:HA	2:LLL:97:TYR:O	2.09	0.53
4:FFF:6:GLU:OE1	4:FFF:119:GLN:OE1	2.27	0.53
2:LLL:151:LYS:HG3	2:LLL:203:THR:HB	1.89	0.52
3:EEE:360:ASN:HA	3:EEE:523:THR:OG1	2.10	0.51
2:LLL:53:LEU:HA	2:LLL:64:VAL:HG21	1.91	0.51
3:EEE:368:LEU:O	3:EEE:371:SER:HB3	2.09	0.51
2:LLL:34:ILE:O	2:LLL:36:LYS:N	2.44	0.51
1:HHH:156:VAL:HB	1:HHH:202:VAL:HG12	1.94	0.50
2:LLL:192:TYR:O	2:LLL:198:TYR:OH	2.28	0.50
1:HHH:159:ASN:ND2	1:HHH:196:GLN:HE21	2.11	0.49
2:LLL:31:TYR:CD2	3:EEE:430[B]:THR:HG22	2.47	0.49
1:HHH:31:THR:CG2	1:HHH:100:SER:HB2	2.44	0.48
2:LLL:31:TYR:CE2	3:EEE:430[B]:THR:HG22	2.48	0.47
2:LLL:43:GLN:HB2	2:LLL:53:LEU:HD11	1.97	0.47
3:EEE:365:TYR:CE2	3:EEE:387:LEU:HB3	2.51	0.46
1:HHH:31:THR:HG22	1:HHH:100:SER:HB2	1.96	0.46
2:LLL:67:ARG:HB2	2:LLL:82:SER:O	2.16	0.46
2:LLL:207:LEU:HD13	2:LLL:211:VAL:HG12	1.97	0.46
1:HHH:1:GLN:OE1	3:EEE:369:TYR:HE1	1.99	0.46
3:EEE:412:PRO:HG3	3:EEE:429:PHE:HB3	1.97	0.45
1:HHH:6:GLN:NE2	1:HHH:113:THR:HG23	2.31	0.45
1:HHH:102:ILE:HD11	2:LLL:100:THR:CG2	2.47	0.45
1:HHH:155:THR:O	1:HHH:202:VAL:HA	2.17	0.45
1:HHH:71:SER:OG	1:HHH:80:TYR:HB2	2.17	0.45
1:HHH:105:PRO:HG3	2:LLL:97:TYR:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HHH:6:GLN:HB3	1:HHH:113:THR:CG2	2.48	0.44
2:LLL:72:GLY:HA3	2:LLL:77:PHE:HA	1.99	0.44
3:EEE:334:ASN:N	3:EEE:334:ASN:OD1	2.51	0.44
3:EEE:431:GLY:HA3	3:EEE:513:LEU:O	2.18	0.44
2:LLL:39:LEU:HD13	2:LLL:77:PHE:CD2	2.54	0.43
2:LLL:33:SER:CB	3:EEE:430[B]:THR:HG21	2.48	0.43
2:LLL:42:TYR:O	2:LLL:92:TYR:HA	2.18	0.43
1:HHH:172:ALA:HA	1:HHH:182:LEU:HB3	2.00	0.43
1:HHH:172:ALA:HB2	1:HHH:182:LEU:HD23	2.00	0.43
3:EEE:357:ARG:HG3	3:EEE:396:TYR:CE1	2.54	0.42
2:LLL:151:LYS:NZ	2:LLL:153:GLN:HG3	2.34	0.42
1:HHH:40:MET:HG2	1:HHH:92:ALA:HB2	2.02	0.42
1:HHH:73:ASP:OD1	1:HHH:75:SER:OG	2.36	0.42
4:FFF:1:GLN:HA	4:FFF:116:TYR:CZ	2.55	0.42
2:LLL:21:ILE:O	2:LLL:78:THR:HA	2.20	0.42
1:HHH:106:MET:HG3	2:LLL:42:TYR:OH	2.20	0.41
3:EEE:354:ASN:O	3:EEE:398:ASP:HA	2.20	0.41
1:HHH:118:ALA:HB3	1:HHH:150:PHE:CE1	2.55	0.41
3:EEE:360:ASN:CA	3:EEE:523:THR:OG1	2.69	0.41
1:HHH:102:ILE:HD11	2:LLL:100:THR:HG21	2.03	0.41
2:LLL:146:TYR:CG	2:LLL:147:PRO:HA	2.55	0.41
3:EEE:382:VAL:HG21	3:EEE:387:LEU:HD21	2.02	0.41
3:EEE:394:ASN:O	3:EEE:516:GLU:HB3	2.21	0.41
1:HHH:1:GLN:NE2	1:HHH:27:TYR:O	2.54	0.41
2:LLL:181:LEU:HD23	2:LLL:182:SER:N	2.36	0.41
2:LLL:33:SER:CB	3:EEE:430[B]:THR:CG2	2.99	0.40
4:FFF:27:ARG:HG2	4:FFF:29:PHE:CZ	2.56	0.40
1:HHH:150:PHE:HA	1:HHH:151:PRO:HA	1.87	0.40
2:LLL:4:LEU:HD23	2:LLL:23:CYS:SG	2.62	0.40
2:LLL:31:TYR:HD2	3:EEE:430[B]:THR:CG2	2.35	0.40
2:LLL:83:SER:O	2:LLL:83:SER:OG	2.35	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	HHH	213/216 (99%)	199 (93%)	14 (7%)	0	100 100
2	LLL	217/219 (99%)	204 (94%)	11 (5%)	2 (1%)	17 49
3	EEE	197/197 (100%)	189 (96%)	8 (4%)	0	100 100
4	FFF	131/134 (98%)	130 (99%)	1 (1%)	0	100 100
All	All	758/766 (99%)	722 (95%)	34 (4%)	2 (0%)	41 71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	LLL	35	ASN
2	LLL	15	LEU

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	HHH	182/181 (101%)	170 (93%)	12 (7%)	16 47
2	LLL	194/194 (100%)	183 (94%)	11 (6%)	20 52
3	EEE	172/170 (101%)	169 (98%)	3 (2%)	60 79
4	FFF	107/108 (99%)	103 (96%)	4 (4%)	34 64
All	All	655/653 (100%)	625 (95%)	30 (5%)	26 60

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	HHH	58	THR
1	HHH	85	SER
1	HHH	91	THR
1	HHH	106	MET
1	HHH	113	THR
1	HHH	164	THR

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Mol	Chain	Res	Type
1	HHH	183	SER
1	HHH	200	CYS
1	HHH	210	LYS
1	HHH	213	LYS
1	HHH	218	LYS
1	HHH	219	SER
2	LLL	3	GLN
2	LLL	14	SER
2	LLL	15	LEU
2	LLL	18	ARG
2	LLL	127	SER
2	LLL	133	SER
2	LLL	148	ARG
2	LLL	151	LYS
2	LLL	157	ASP
2	LLL	171	GLU
2	LLL	174	SER
3	EEE	354	ASN
3	EEE	377	PHE
3	EEE	383	SER
4	FFF	27	ARG
4	FFF	62	ASP
4	FFF	72	ARG
4	FFF	88	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	HHH	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	HHH	132:SER	C	137:GLY	N	3.83

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	HHH	216/216 (100%)	0.99	35 (16%) 1 1	136, 194, 241, 279	0
2	LLL	219/219 (100%)	0.71	19 (8%) 10 10	120, 176, 223, 254	0
3	EEE	195/197 (98%)	0.81	32 (16%) 1 1	132, 180, 240, 281	0
4	FFF	128/134 (95%)	1.03	27 (21%) 1 0	203, 275, 331, 352	0
All	All	758/766 (98%)	0.87	113 (14%) 2 1	120, 191, 292, 352	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	FFF	109	TYR	8.5
1	HHH	142	LEU	7.4
4	FFF	8	GLY	6.7
4	FFF	35	GLY	6.1
4	FFF	118	GLY	5.9
4	FFF	34[A]	MET	5.8
1	HHH	215	VAL	5.3
4	FFF	24	VAL	5.2
1	HHH	86	LEU	4.8
2	LLL	123	ILE	4.7
4	FFF	117	TRP	4.6
4	FFF	50	ALA	4.3
1	HHH	193	LEU	4.2
3	EEE	382	VAL	4.1
3	EEE	482	GLY	3.9
3	EEE	423	TYR	3.9
4	FFF	3	GLN	3.8
3	EEE	490	PHE	3.7
3	EEE	400	PHE	3.6
1	HHH	51	ILE	3.6
4	FFF	41	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
3	EEE	430[A]	THR	3.6
1	HHH	141	ALA	3.5
1	HHH	29	PHE	3.5
3	EEE	495	TYR	3.5
3	EEE	365	TYR	3.4
3	EEE	410	ILE	3.4
3	EEE	338	PHE	3.4
1	HHH	163	LEU	3.4
4	FFF	31	THR	3.3
3	EEE	422	ASN	3.2
1	HHH	130	PRO	3.2
3	EEE	387	LEU	3.2
4	FFF	10	GLY	3.2
3	EEE	358	ILE	3.1
4	FFF	116	TYR	3.1
1	HHH	50	ILE	3.1
4	FFF	79	VAL	3.1
1	HHH	158	TRP	3.1
3	EEE	341	VAL	3.0
1	HHH	70	ILE	3.0
4	FFF	4	LEU	3.0
1	HHH	125	VAL	3.0
3	EEE	453	TYR	3.0
4	FFF	29	PHE	3.0
1	HHH	198	TYR	2.9
1	HHH	128	LEU	2.9
1	HHH	149	TYR	2.8
1	HHH	97	ALA	2.8
4	FFF	48	VAL	2.7
2	LLL	174	SER	2.7
3	EEE	395	VAL	2.7
1	HHH	102	ILE	2.7
4	FFF	45	ARG	2.6
2	LLL	81	ILE	2.6
3	EEE	406	GLU	2.6
1	HHH	34	ILE	2.6
3	EEE	401	VAL	2.6
2	LLL	154	TRP	2.6
1	HHH	123	PRO	2.5
3	EEE	515	PHE	2.5
1	HHH	32	TYR	2.5
3	EEE	369	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	HHH	183	SER	2.5
1	HHH	36	TRP	2.5
3	EEE	513	LEU	2.5
2	LLL	53	LEU	2.5
4	FFF	37	PHE	2.5
4	FFF	94	TYR	2.5
1	HHH	127	PRO	2.4
3	EEE	351	TYR	2.4
3	EEE	350	VAL	2.4
3	EEE	492	LEU	2.4
1	HHH	31	THR	2.4
2	LLL	102	TYR	2.4
1	HHH	0	THR	2.4
1	HHH	143	GLY	2.4
3	EEE	402	ILE	2.4
2	LLL	52	LEU	2.3
4	FFF	96[A]	CYS	2.3
2	LLL	87	GLU	2.3
1	HHH	100	SER	2.3
1	HHH	154	VAL	2.3
2	LLL	39	LEU	2.3
4	FFF	58	ALA	2.3
4	FFF	97	ALA	2.3
2	LLL	41	TRP	2.3
3	EEE	452	LEU	2.3
3	EEE	368	LEU	2.2
1	HHH	18	LEU	2.2
2	LLL	84	LEU	2.2
2	LLL	133	SER	2.2
4	FFF	90	ASP	2.2
1	HHH	27	TYR	2.2
2	LLL	4	LEU	2.2
1	HHH	4	LEU	2.1
3	EEE	363	ALA	2.1
1	HHH	110	GLY	2.1
2	LLL	131	LEU	2.1
1	HHH	216	GLU	2.1
2	LLL	156	VAL	2.1
3	EEE	418	ILE	2.1
2	LLL	215	PHE	2.1
4	FFF	18	LEU	2.1
2	LLL	68	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
3	EEE	433	VAL	2.1
4	FFF	5	VAL	2.1
2	LLL	34	ILE	2.0
3	EEE	456	PHE	2.0
2	LLL	56	TRP	2.0
3	EEE	451	TYR	2.0
1	HHH	45	LEU	2.0
4	FFF	60	TYR	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.