Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 07:16 am BST

PDB ID	:	3BKY
Title	:	Crystal Structure of Chimeric Antibody C2H7 Fab in complex with a CD20 Peptide
Authors	:	Du, J.; Zhong, C.; Ding, J.
Deposited on	:	2007-12-07
Resolution	:	2.61 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 following versions of software and data (see references (i)) 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 2.61 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		0.244
Clashscore		13
Ramachandran outliers		1.6%
Sidechain outliers		10.5%
RSRZ outliers		14.3%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
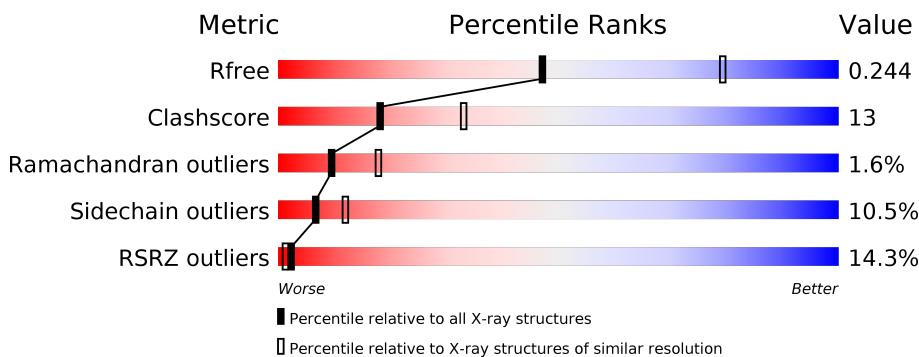
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	H	226	22% / 72% 20% 7%
2	L	213	2% / 75% 22% •
3	P	25	44% / 44% 16% 8% 32%
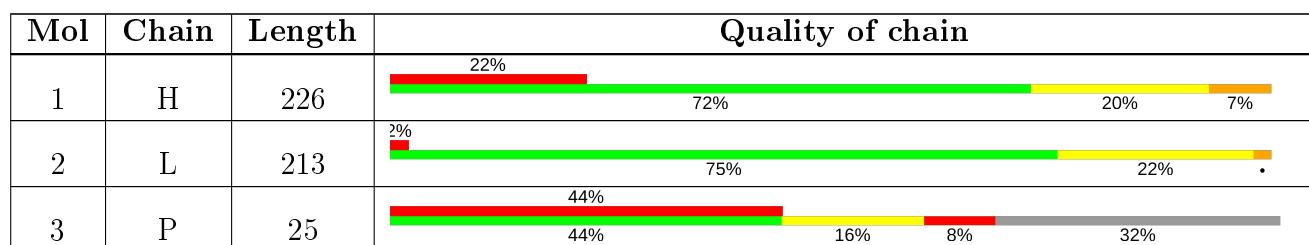
2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3573 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 the Fab fragment of chimeric 2H7, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	226	Total	C	N	O	S	0	0	0
			1703	1079	278	338	8			

- Molecule 2 is a protein called the Fab fragment of chimeric 2H7, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1626	1020	273	326	7			

- Molecule 3 is a protein called B-lymphocyte antigen CD20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	17	Total	C	N	O	S	0	0	0
			127	75	21	29	2			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	49	Total	O	0	0
			49	49		
4	L	67	Total	O	0	0
			67	67		
4	P	1	Total	O	0	0
			1	1		

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: the Fab fragment of chimeric 2H7, heavy chain
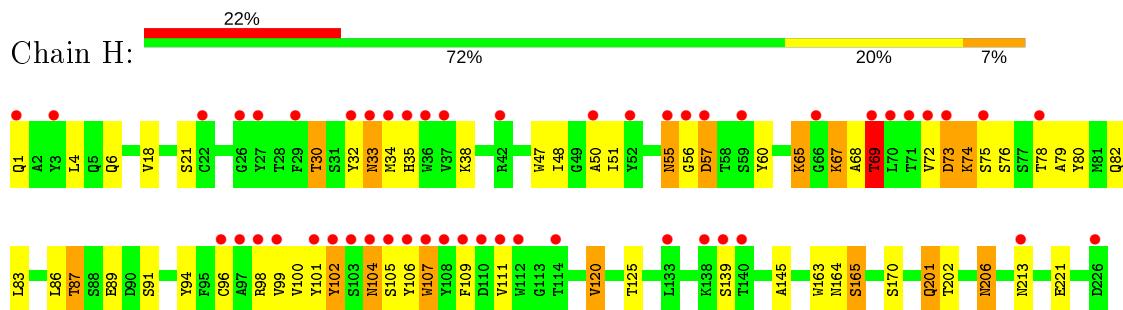
- Molecule 2: the Fab fragment of chimeric 2H7, light chain
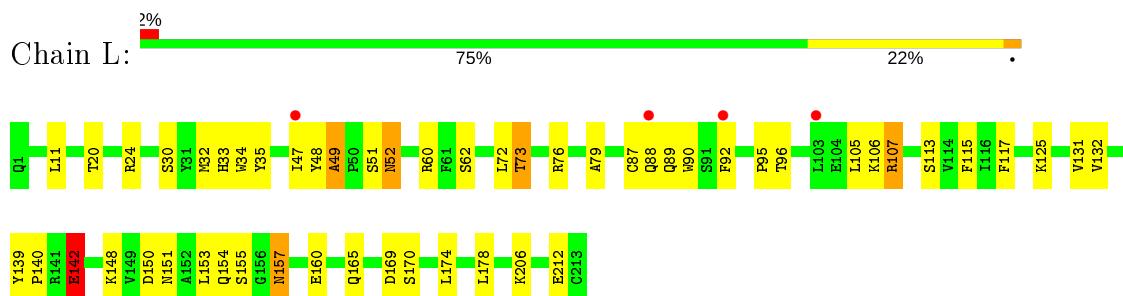
- Molecule 3: B-lymphocyte antigen CD20
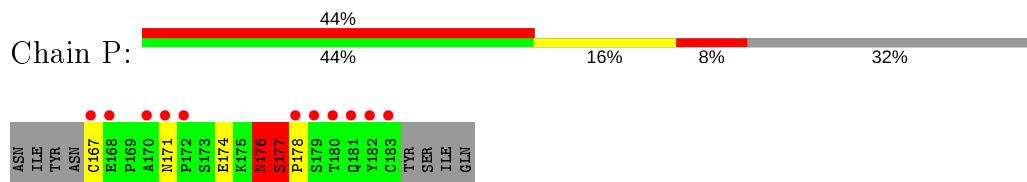
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	96.49Å 96.49Å 107.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.61 20.03 – 2.61	Depositor EDS
% Data completeness (in resolution range)	97.7 (20.00-2.61) 97.7 (20.03-2.61)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	4.37 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.234 , 0.301 0.243 , 0.244	Depositor DCC
R_{free} test set	781 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	49.3	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 35.6	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	0.90	EDS
Total number of atoms	3573	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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 (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	H	0.61	2/1748 (0.1%)	0.60	0/2384
2	L	0.49	0/1667	0.58	0/2268
3	P	1.44	1/130 (0.8%)	0.50	0/177
All	All	0.61	3/3545 (0.1%)	0.59	0/4829

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	69	THR	CB-OG1	15.05	1.73	1.43
3	P	177	SER	CB-OG	13.59	1.59	1.42
1	H	69	THR	CB-CG2	6.21	1.72	1.52

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	H	1703	0	1653	52	0
2	L	1626	0	1572	43	0
3	P	127	0	109	5	0
4	H	49	0	0	5	0
4	L	67	0	0	4	1
4	P	1	0	0	0	0
All	All	3573	0	3334	91	1

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 13.

All (91) 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:H:69:THR:OG1	1:H:69:THR:CB	1.73	1.36
1:H:33:ASN:H	1:H:33:ASN:HD22	1.04	1.01
1:H:33:ASN:N	1:H:33:ASN:HD22	1.62	0.95
1:H:106:TYR:HD1	2:L:33:HIS:HE2	1.11	0.94
2:L:79:ALA:HA	2:L:105:LEU:CD1	2.06	0.84
2:L:157:ASN:H	2:L:157:ASN:HD22	1.24	0.83
2:L:107:ARG:HD2	4:L:277:HOH:O	1.78	0.81
1:H:33:ASN:H	1:H:33:ASN:ND2	1.80	0.79
2:L:107:ARG:HG2	2:L:170:SER:HB2	1.69	0.75
1:H:35:HIS:CD2	1:H:47:TRP:HE1	2.06	0.74
2:L:169:ASP:HB2	4:L:277:HOH:O	1.88	0.73
1:H:106:TYR:HD1	2:L:33:HIS:NE2	1.86	0.72
3:P:177:SER:N	3:P:178:PRO:HD3	2.06	0.70
1:H:35:HIS:HD2	1:H:47:TRP:HE1	1.41	0.69
2:L:60:ARG:HD2	2:L:76:ARG:O	1.97	0.65
2:L:131:VAL:HG13	2:L:178:LEU:HB3	1.78	0.64
1:H:101:TYR:HA	1:H:107:TRP:HA	1.79	0.63
1:H:38:LYS:HB2	1:H:48:ILE:HD11	1.79	0.63
2:L:157:ASN:N	2:L:157:ASN:HD22	1.93	0.62
2:L:49:ALA:O	2:L:51:SER:N	2.33	0.61
1:H:65:LYS:HA	1:H:65:LYS:HZ3	1.64	0.61
1:H:57:ASP:HA	4:H:251:HOH:O	2.00	0.61
2:L:79:ALA:HA	2:L:105:LEU:HD12	1.81	0.61
3:P:177:SER:H	3:P:178:PRO:HD3	1.65	0.60
2:L:79:ALA:HA	2:L:105:LEU:HD11	1.82	0.59
1:H:164:ASN:O	1:H:165:SER:HB2	2.01	0.59
1:H:32:TYR:O	4:H:272:HOH:O	2.17	0.59
1:H:34:MET:CE	1:H:96:CYS:HB2	2.33	0.59
2:L:157:ASN:H	2:L:157:ASN:ND2	2.00	0.58
1:H:74:LYS:O	1:H:76:SER:N	2.33	0.58
2:L:47:ILE:CD1	2:L:72:LEU:HD13	2.35	0.57
1:H:106:TYR:CE1	2:L:90:TRP:HB2	2.39	0.57
1:H:33:ASN:N	1:H:33:ASN:ND2	2.36	0.56
2:L:34:TRP:HB2	2:L:47:ILE:HB	1.89	0.55
1:H:164:ASN:O	1:H:165:SER:CB	2.56	0.54
1:H:67:LYS:O	1:H:83:LEU:HA	2.08	0.53
1:H:86:LEU:HB3	1:H:120:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:107:TRP:CE3	1:H:107:TRP:N	2.76	0.53
2:L:32:MET:HE3	2:L:88:GLN:O	2.08	0.53
1:H:139:SER:HA	2:L:115:PHE:HD2	1.74	0.53
2:L:150:ASP:O	2:L:151:ASN:HB2	2.07	0.53
2:L:105:LEU:H	2:L:165:GLN:HE22	1.56	0.52
2:L:47:ILE:HD11	2:L:72:LEU:HD13	1.92	0.52
2:L:89:GLN:NE2	2:L:95:PRO:HA	2.25	0.52
2:L:148:LYS:HG2	2:L:153:LEU:HD23	1.92	0.52
2:L:52:ASN:HD22	2:L:52:ASN:N	2.07	0.52
1:H:30:THR:O	4:H:272:HOH:O	2.19	0.52
1:H:34:MET:HE1	1:H:96:CYS:HB2	1.91	0.51
2:L:48:TYR:O	2:L:52:ASN:HB2	2.12	0.50
2:L:33:HIS:O	2:L:87:CYS:HA	2.12	0.50
1:H:35:HIS:HD2	1:H:47:TRP:NE1	2.08	0.49
2:L:212:GLU:HB3	4:L:238:HOH:O	2.13	0.48
1:H:201:GLN:HE21	1:H:202:THR:N	2.11	0.48
1:H:60:TYR:HB3	1:H:65:LYS:HZ2	1.79	0.47
1:H:139:SER:HA	2:L:115:PHE:CD2	2.49	0.47
1:H:34:MET:O	1:H:50:ALA:HA	2.13	0.47
1:H:55:ASN:HD22	1:H:56:GLY:N	2.12	0.47
1:H:30:THR:C	4:H:272:HOH:O	2.53	0.47
2:L:154:GLN:HB3	2:L:157:ASN:HD21	1.80	0.47
1:H:73:ASP:OD2	1:H:80:TYR:CE1	2.69	0.46
2:L:32:MET:HE3	2:L:88:GLN:C	2.36	0.46
1:H:33:ASN:OD1	3:P:171:ASN:HB3	2.15	0.46
1:H:91:SER:OG	1:H:120:VAL:HG23	2.16	0.46
1:H:73:ASP:OD2	4:H:274:HOH:O	2.21	0.45
2:L:72:LEU:HD12	2:L:73:THR:N	2.30	0.45
2:L:139:TYR:CG	2:L:140:PRO:HA	2.51	0.45
3:P:177:SER:N	3:P:178:PRO:CD	2.78	0.45
1:H:165:SER:N	1:H:206:ASN:HD21	2.15	0.45
1:H:73:ASP:HB2	1:H:78:THR:HG23	1.99	0.45
2:L:174:LEU:HD23	2:L:174:LEU:C	2.37	0.45
1:H:60:TYR:CE1	1:H:68:ALA:O	2.70	0.45
1:H:107:TRP:NE1	2:L:90:TRP:HB3	2.32	0.44
2:L:20:THR:HG23	2:L:73:THR:HB	2.00	0.44
2:L:33:HIS:ND1	2:L:48:TYR:HA	2.33	0.44
1:H:6:GLN:NE2	1:H:94:TYR:O	2.50	0.44
1:H:104:ASN:HB3	2:L:48:TYR:HE1	1.83	0.43
2:L:142:GLU:CD	2:L:142:GLU:H	2.21	0.43
1:H:51:ILE:HA	1:H:57:ASP:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:139:SER:O	1:H:145:ALA:HA	2.19	0.42
1:H:100:VAL:C	1:H:102:TYR:H	2.23	0.42
1:H:33:ASN:O	1:H:99:VAL:HG22	2.20	0.42
2:L:160:GLU:HG3	4:L:236:HOH:O	2.19	0.42
1:H:87:THR:C	1:H:89:GLU:H	2.23	0.42
2:L:89:GLN:HE21	2:L:96:THR:H	1.68	0.41
3:P:176:ASN:HA	3:P:176:ASN:HD22	1.67	0.41
1:H:72:VAL:HG22	1:H:79:ALA:HA	2.01	0.41
2:L:117:PHE:HB2	2:L:132:VAL:HG22	2.02	0.41
1:H:109:PHE:HD2	2:L:35:TYR:OH	2.02	0.41
1:H:18:VAL:O	1:H:82:GLN:HA	2.20	0.41
1:H:163:TRP:C	1:H:165:SER:H	2.25	0.40
1:H:98:ARG:HH11	1:H:111:VAL:HG22	1.87	0.40

All (1) 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)
4:L:245:HOH:O	4:L:248:HOH:O[3_445]	2.09	0.11

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	H	224/226 (99%)	199 (89%)	22 (10%)	3 (1%)	12	23
2	L	211/213 (99%)	201 (95%)	8 (4%)	2 (1%)	17	33
3	P	15/25 (60%)	12 (80%)	1 (7%)	2 (13%)	0	0
All	All	450/464 (97%)	412 (92%)	31 (7%)	7 (2%)	9	18

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	75	SER
1	H	165	SER
3	P	176	ASN
1	H	105	SER
2	L	49	ALA
2	L	142	GLU
3	P	177	SER

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	H	192/192 (100%)	169 (88%)	23 (12%)	5	8
2	L	184/184 (100%)	169 (92%)	15 (8%)	11	21
3	P	16/24 (67%)	13 (81%)	3 (19%)	1	2
All	All	392/400 (98%)	351 (90%)	41 (10%)	7	12

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	GLN
1	H	4	LEU
1	H	21	SER
1	H	30	THR
1	H	33	ASN
1	H	55	ASN
1	H	57	ASP
1	H	65	LYS
1	H	67	LYS
1	H	69	THR
1	H	73	ASP
1	H	74	LYS
1	H	87	THR
1	H	102	TYR
1	H	104	ASN
1	H	107	TRP

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Mol	Chain	Res	Type
1	H	120	VAL
1	H	125	THR
1	H	170	SER
1	H	201	GLN
1	H	206	ASN
1	H	213	ASN
1	H	221	GLU
2	L	11	LEU
2	L	24	ARG
2	L	30	SER
2	L	52	ASN
2	L	62	SER
2	L	73	THR
2	L	92	PHE
2	L	106	LYS
2	L	107	ARG
2	L	113	SER
2	L	125	LYS
2	L	142	GLU
2	L	155	SER
2	L	157	ASN
2	L	206	LYS
3	P	167	CYS
3	P	174	GLU
3	P	176	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	33	ASN
1	H	35	HIS
1	H	55	ASN
1	H	180	GLN
1	H	201	GLN
1	H	206	ASN
1	H	208	ASN
1	H	213	ASN
2	L	36	GLN
2	L	52	ASN
2	L	137	ASN
2	L	157	ASN
2	L	165	GLN

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Mol	Chain	Res	Type
2	L	198	GLN
3	P	176	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 carbohydrates 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(Å²)	Q<0.9
1	H	226/226 (100%)	1.01	50 (22%)	0	0	27, 47, 75, 95	0
2	L	213/213 (100%)	0.12	4 (1%)	66	62	26, 38, 56, 64	0
3	P	17/25 (68%)	2.65	11 (64%)	0	0	73, 87, 105, 106	0
All	All	456/464 (98%)	0.66	65 (14%)	2	1	26, 43, 78, 106	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	182	TYR	7.5
1	H	34	MET	7.1
1	H	36	TRP	5.8
1	H	101	TYR	5.0
1	H	73	ASP	4.8
1	H	109	PHE	4.8
3	P	171	ASN	4.6
1	H	112	TRP	4.6
1	H	27	TYR	4.6
1	H	104	ASN	4.5
1	H	22	CYS	4.3
1	H	107	TRP	4.2
1	H	35	HIS	3.9
1	H	103	SER	3.8
1	H	66	GLY	3.8
3	P	170	ALA	3.8
1	H	69	THR	3.8
1	H	139	SER	3.8
1	H	33	ASN	3.7
3	P	167	CYS	3.6
1	H	71	THR	3.5
1	H	70	LEU	3.5
1	H	140	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	138	LYS	3.3
1	H	57	ASP	3.3
1	H	78	THR	3.2
1	H	3	TYR	3.1
1	H	52	TYR	3.1
1	H	226	ASP	3.0
1	H	50	ALA	3.0
1	H	37	VAL	2.9
1	H	97	ALA	2.9
1	H	99	VAL	2.9
1	H	213	ASN	2.8
3	P	180	THR	2.8
1	H	42	ARG	2.7
2	L	92	PHE	2.7
1	H	1	GLN	2.7
1	H	105	SER	2.7
1	H	108	TYR	2.7
3	P	181	GLN	2.7
1	H	55	ASN	2.6
1	H	59	SER	2.6
1	H	102	TYR	2.6
3	P	168	GLU	2.5
1	H	75	SER	2.5
1	H	111	VAL	2.4
2	L	47	ILE	2.4
1	H	72	VAL	2.4
1	H	114	THR	2.4
2	L	103	LEU	2.4
1	H	56	GLY	2.4
1	H	98	ARG	2.4
3	P	178	PRO	2.3
3	P	179	SER	2.3
1	H	106	TYR	2.3
1	H	26	GLY	2.3
1	H	133	LEU	2.2
3	P	172	PRO	2.2
1	H	96	CYS	2.1
1	H	110	ASP	2.1
3	P	183	CYS	2.1
2	L	88	GLN	2.1
1	H	32	TYR	2.0
1	H	29	PHE	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.