Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 09:38 AM EDT

PDB ID	:	5XAJ
Title	:	Structural mimicry of the dengue virus envelope glycoprotein revealed by the crystallographic study of an idiotype-anti-idiotype Fab complex.
Authors	:	Wong, Y.H.; Goh, B.C.; Lescar, J.
Deposited on	:	2017-03-13
Resolution	:	2.50 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 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:

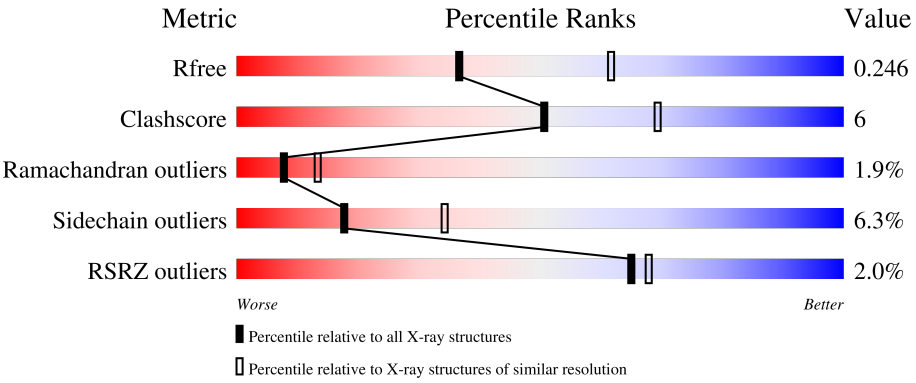
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	227	4% 82% 15%
1	H	227	4% 85% 13%
2	B	214	84% 12%
2	L	214	% 82% 16%
3	C	214	2% 88% 11%

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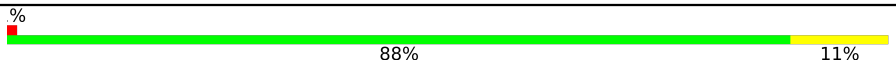
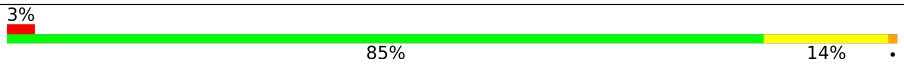
Mol	Chain	Length	Quality of chain
3	D	214	
4	E	215	
5	F	218	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14313 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 FabHM14c10 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1678	1067	280	323	8			
1	H	227	Total	C	N	O	S	0	0	0
			1688	1073	282	325	8			

- Molecule 2 is a protein called FabHM14c10 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1646	1031	281	328	6			
2	L	214	Total	C	N	O	S	0	0	0
			1649	1032	281	330	6			

- Molecule 3 is a protein called Fab E1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1613	1008	272	327	6			
3	D	213	Total	C	N	O	S	0	0	0
			1603	1002	270	326	5			

- Molecule 4 is a protein called Fab E1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	215	Total	C	N	O	S	0	0	0
			1578	998	258	316	6			

- Molecule 5 is a protein called Fab E1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	213	Total	C	N	O	S	0	0	0
			1565	991	256	311	7			

- Molecule 6 is water.

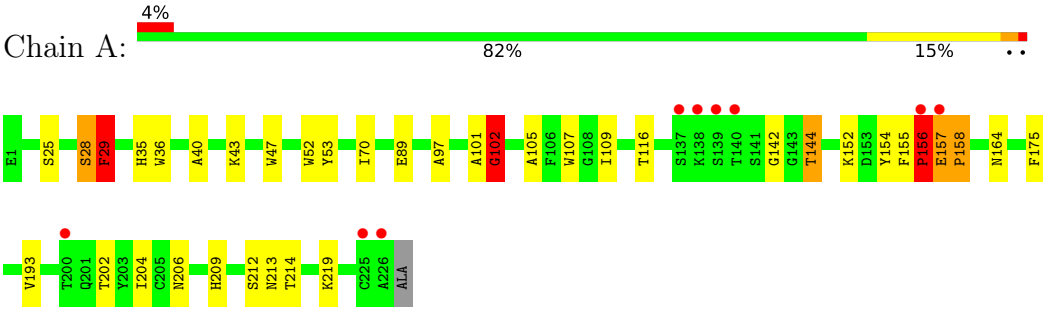
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	171	Total O 171 171	0	0
6	B	190	Total O 190 190	0	0
6	C	124	Total O 124 124	0	0
6	D	151	Total O 151 151	0	0
6	E	158	Total O 158 158	0	0
6	F	157	Total O 157 157	0	0
6	H	184	Total O 184 184	0	0
6	L	158	Total O 158 158	0	0

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.

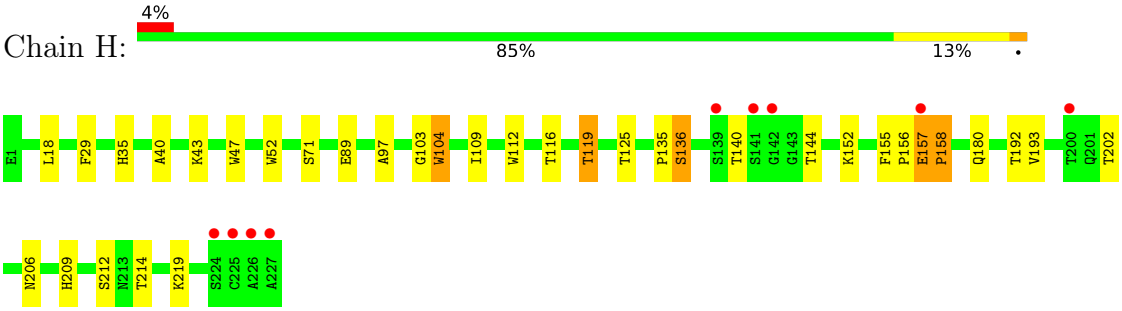
• Molecule 1: FabHM14c10 heavy chain

Chain A:



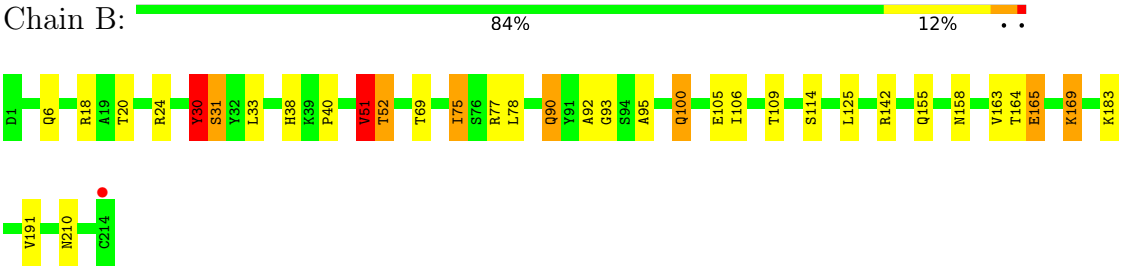
• Molecule 1: FabHM14c10 heavy chain

Chain H:



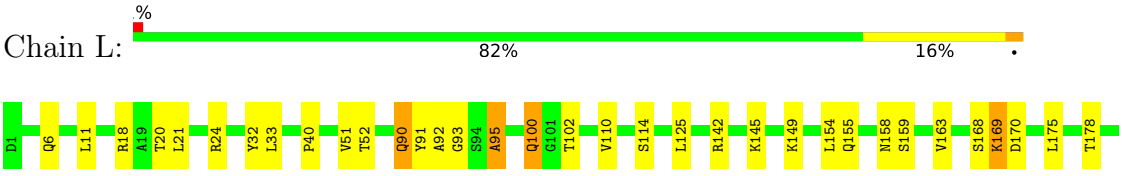
• Molecule 2: FabHM14c10 light chain

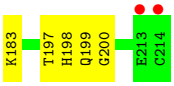
Chain B:



• Molecule 2: FabHM14c10 light chain

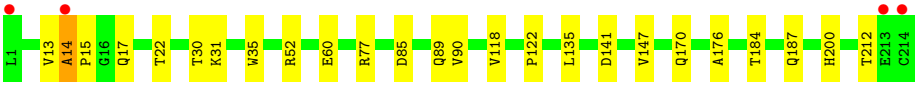
Chain L:





• Molecule 3: Fab E1 light chain

Chain C:

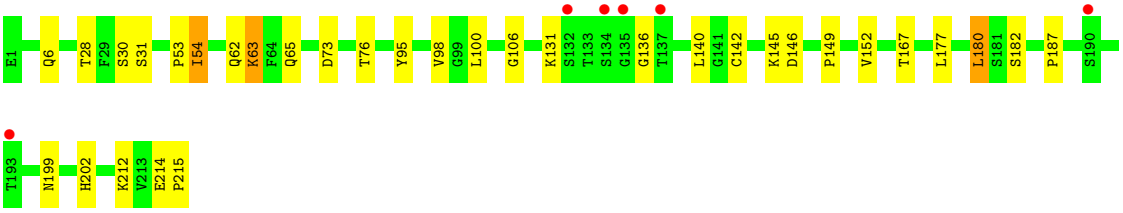


• Molecule 3: Fab E1 light chain

Chain D:

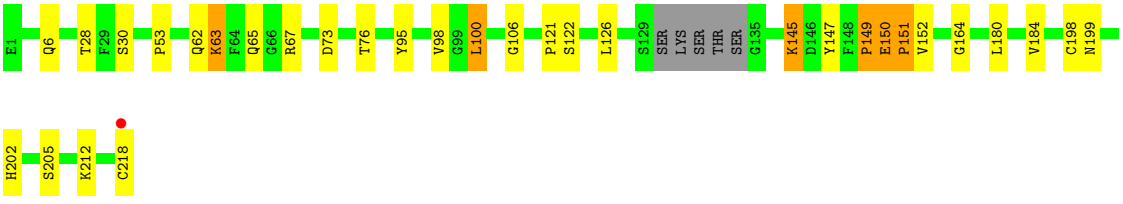
• Molecule 4: Fab E1 heavy chain

Chain E:



• Molecule 5: Fab E1 heavy chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	116.30Å 47.59Å 220.76Å 90.00° 93.43° 90.00°	Depositor
Resolution (Å)	46.93 – 2.50 46.93 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.93-2.50) 99.7 (46.93-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.185 , 0.239 0.190 , 0.246	Depositor DCC
R_{free} test set	4183 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 56.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14313	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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	0.53	0/1722	0.83	3/2344 (0.1%)
1	H	0.52	0/1732	0.80	1/2356 (0.0%)
2	B	0.55	0/1683	0.82	2/2284 (0.1%)
2	L	0.49	0/1686	0.77	1/2288 (0.0%)
3	C	0.49	0/1654	0.73	0/2261
3	D	0.49	0/1644	0.71	0/2249
4	E	0.49	0/1615	0.75	1/2204 (0.0%)
5	F	0.49	0/1601	0.74	0/2183
All	All	0.51	0/13337	0.77	8/18169 (0.0%)

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	156	PRO	C-N-CA	7.69	140.93	121.70
1	A	102	GLY	N-CA-C	6.35	128.97	113.10
1	A	53	TYR	C-N-CA	6.09	136.94	121.70
1	H	29	PHE	CB-CA-C	-6.07	98.25	110.40
2	L	170	ASP	C-N-CA	-5.29	108.48	121.70
4	E	140	LEU	N-CA-CB	-5.13	100.13	110.40
2	B	52	THR	N-CA-CB	-5.09	100.63	110.30
2	B	165	GLU	N-CA-CB	5.00	119.60	110.60

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	1678	0	1633	34	0
1	H	1688	0	1653	19	0
2	B	1646	0	1593	19	0
2	L	1649	0	1596	23	0
3	C	1613	0	1551	15	0
3	D	1603	0	1535	10	0
4	E	1578	0	1558	21	0
5	F	1565	0	1545	19	0
6	A	171	0	0	0	0
6	B	190	0	0	2	0
6	C	124	0	0	0	0
6	D	151	0	0	2	0
6	E	158	0	0	0	0
6	F	157	0	0	0	0
6	H	184	0	0	2	0
6	L	158	0	0	0	0
All	All	14313	0	12664	146	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 (146) 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:A:156:PRO:HB3	1:A:209:HIS:CE1	1.67	1.29
1:A:157:GLU:HB2	1:A:158:PRO:HD3	1.16	1.16
5:F:150:GLU:HB3	5:F:151:PRO:HD3	1.18	1.10
1:H:157:GLU:HB3	1:H:158:PRO:HD3	1.13	1.09
1:A:156:PRO:CB	1:A:209:HIS:HE1	1.74	1.00
2:B:6:GLN:H	2:B:100:GLN:HE22	0.96	0.95
1:A:156:PRO:HB3	1:A:209:HIS:HE1	0.81	0.95
2:L:6:GLN:H	2:L:100:GLN:HE22	0.96	0.94
2:L:21:LEU:HD22	2:L:102:THR:HG21	1.49	0.94
5:F:150:GLU:HB3	5:F:151:PRO:CD	1.98	0.94
1:H:157:GLU:HB3	1:H:158:PRO:CD	1.98	0.93
1:H:119:THR:HG21	6:H:347:HOH:O	1.68	0.93
1:H:157:GLU:CB	1:H:158:PRO:HD3	2.00	0.91
5:F:150:GLU:CB	5:F:151:PRO:HD3	2.00	0.90
1:A:157:GLU:HB2	1:A:158:PRO:CD	2.03	0.86
1:H:35:HIS:HD2	1:H:47:TRP:HE1	1.21	0.85
4:E:136:GLY:HA2	4:E:187:PRO:HA	1.61	0.83
1:A:35:HIS:HD2	1:A:47:TRP:HE1	1.22	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:TRP:HH2	4:E:54:ILE:CD1	1.90	0.83
2:L:6:GLN:H	2:L:100:GLN:NE2	1.77	0.82
5:F:150:GLU:CB	5:F:151:PRO:CD	2.57	0.82
5:F:152:VAL:HG22	5:F:180:LEU:HD21	1.61	0.81
3:C:14:ALA:HB1	3:C:15:PRO:CA	2.11	0.80
2:B:6:GLN:H	2:B:100:GLN:NE2	1.78	0.80
1:A:157:GLU:CB	1:A:158:PRO:HD3	2.08	0.79
3:C:170:GLN:HE21	3:C:176:ALA:HB2	1.48	0.78
3:D:170:GLN:HE21	3:D:176:ALA:HB2	1.50	0.77
3:C:14:ALA:HB1	3:C:15:PRO:HA	1.67	0.76
5:F:149:PRO:HG2	5:F:150:GLU:HG3	1.69	0.75
2:B:6:GLN:N	2:B:100:GLN:HE22	1.81	0.72
2:L:6:GLN:N	2:L:100:GLN:HE22	1.81	0.70
3:C:14:ALA:HB1	3:C:15:PRO:C	2.13	0.69
2:B:155:GLN:HE21	2:B:158:ASN:HD21	1.41	0.69
2:L:155:GLN:HE21	2:L:158:ASN:HD21	1.40	0.68
3:D:89:GLN:HE22	5:F:100:LEU:HD21	1.60	0.67
4:E:6:GLN:HE21	4:E:106:GLY:HA3	1.60	0.67
2:L:21:LEU:HD22	2:L:102:THR:CG2	2.25	0.66
5:F:6:GLN:HE21	5:F:106:GLY:HA3	1.59	0.65
3:D:211:PRO:HD3	6:D:374:HOH:O	1.97	0.64
1:A:107:TRP:HH2	4:E:54:ILE:HD11	1.62	0.64
1:A:152:LYS:HE2	1:A:180:GLN:HE22	1.63	0.64
2:B:31:SER:HA	2:B:51:VAL:HG12	1.80	0.64
4:E:214:GLU:HG3	4:E:215:PRO:HD2	1.78	0.63
3:C:89:GLN:HE22	4:E:100:LEU:HD21	1.63	0.62
1:H:152:LYS:HE2	1:H:180:GLN:HE22	1.63	0.62
1:H:209:HIS:HD2	1:H:212:SER:OG	1.83	0.62
1:H:119:THR:CG2	6:H:347:HOH:O	2.37	0.61
1:A:164:ASN:ND2	1:A:204:ILE:H	1.99	0.60
4:E:149:PRO:O	4:E:202:HIS:HE1	1.83	0.60
1:A:47:TRP:CZ3	2:B:95:ALA:HA	2.37	0.59
1:H:47:TRP:CZ3	2:L:95:ALA:HA	2.38	0.59
1:A:107:TRP:CH2	4:E:54:ILE:CD1	2.79	0.59
2:L:21:LEU:CD2	2:L:102:THR:HG21	2.29	0.58
1:A:212:SER:OG	1:A:214:THR:HG22	2.04	0.58
1:H:35:HIS:CD2	1:H:47:TRP:HE1	2.12	0.58
1:H:97:ALA:HB1	1:H:109:ILE:CG2	2.34	0.58
1:H:157:GLU:CB	1:H:158:PRO:CD	2.73	0.57
2:L:90:GLN:NE2	2:L:93:GLY:H	2.02	0.57
2:L:198:HIS:CD2	2:L:200:GLY:H	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:GLN:NE2	2:B:93:GLY:H	2.03	0.57
1:A:97:ALA:HB1	1:A:109:ILE:CG2	2.35	0.57
1:H:212:SER:OG	1:H:214:THR:HG22	2.04	0.56
2:B:38:HIS:HD2	6:B:326:HOH:O	1.88	0.56
1:A:209:HIS:HD2	1:A:212:SER:OG	1.86	0.56
1:A:107:TRP:CH2	4:E:54:ILE:HD13	2.40	0.56
1:A:101:ALA:O	1:A:105:ALA:O	2.25	0.54
1:A:154:TYR:CD2	1:A:156:PRO:HG3	2.41	0.54
2:L:90:GLN:HE21	2:L:92:ALA:H	1.56	0.54
2:B:90:GLN:HE21	2:B:92:ALA:N	2.06	0.54
1:A:164:ASN:HD21	1:A:204:ILE:H	1.54	0.54
1:A:154:TYR:HD2	1:A:156:PRO:HG3	1.73	0.53
5:F:6:GLN:HE22	5:F:95:TYR:HA	1.73	0.53
4:E:30:SER:O	4:E:54:ILE:HG13	2.08	0.53
2:L:149:LYS:HG2	2:L:154:LEU:HD22	1.91	0.53
3:D:141:ASP:H	3:D:170:GLN:HE22	1.57	0.52
4:E:6:GLN:HE22	4:E:95:TYR:HA	1.74	0.52
1:A:107:TRP:HH2	4:E:54:ILE:HD13	1.71	0.52
3:C:184:THR:HG23	3:C:187:GLN:H	1.74	0.52
5:F:121:PRO:HB3	5:F:147:TYR:HB3	1.92	0.52
3:C:14:ALA:CB	3:C:15:PRO:CA	2.86	0.51
4:E:167:THR:HA	4:E:182:SER:HA	1.92	0.51
3:D:189:LYS:HG2	6:D:444:HOH:O	2.11	0.51
2:L:90:GLN:HE21	2:L:92:ALA:N	2.09	0.51
3:C:147:VAL:HG12	3:C:200:HIS:HB2	1.92	0.51
5:F:202:HIS:HD2	5:F:205:SER:OG	1.94	0.51
2:B:90:GLN:HE21	2:B:92:ALA:H	1.59	0.50
3:C:141:ASP:H	3:C:170:GLN:HE22	1.58	0.50
1:A:156:PRO:CB	1:A:209:HIS:CE1	2.63	0.50
3:C:14:ALA:CB	3:C:15:PRO:HA	2.39	0.50
2:B:125:LEU:O	2:B:183:LYS:HD2	2.12	0.50
2:L:32:TYR:HB3	2:L:91:TYR:HB2	1.93	0.49
1:A:28:SER:O	1:A:29:PHE:HB2	2.11	0.49
2:L:125:LEU:O	2:L:183:LYS:HD2	2.12	0.49
2:L:11:LEU:HD22	2:L:21:LEU:HD23	1.95	0.49
3:C:14:ALA:HB2	3:C:17:GLN:HB2	1.95	0.48
4:E:30:SER:HA	4:E:53:PRO:HB2	1.96	0.48
5:F:164:GLY:O	5:F:184:VAL:HA	2.14	0.48
1:A:156:PRO:HG2	1:A:157:GLU:O	2.13	0.47
5:F:30:SER:HA	5:F:53:PRO:HB2	1.97	0.47
1:A:36:TRP:HD1	1:A:70:ILE:HD12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLY:HA3	1:A:107:TRP:CD2	2.49	0.47
4:E:146:ASP:HB3	4:E:177:LEU:HD13	1.97	0.47
1:A:156:PRO:HB2	1:A:157:GLU:H	1.30	0.47
2:L:163:VAL:HG22	2:L:175:LEU:HD23	1.95	0.47
2:L:163:VAL:HG22	2:L:175:LEU:CD2	2.45	0.47
3:D:147:VAL:HG12	3:D:200:HIS:HB2	1.97	0.47
2:B:106:ILE:HD13	6:B:313:HOH:O	2.14	0.46
2:L:145:LYS:HB3	2:L:197:THR:HB	1.97	0.46
3:C:184:THR:CG2	3:C:187:GLN:H	2.29	0.46
5:F:152:VAL:CG2	5:F:180:LEU:HD21	2.41	0.46
1:A:35:HIS:CD2	1:A:47:TRP:HE1	2.13	0.45
3:C:89:GLN:HE22	4:E:100:LEU:CD2	2.29	0.45
1:A:155:PHE:HA	1:A:156:PRO:HD3	1.64	0.45
2:B:75:ILE:HG12	2:B:78:LEU:HD23	1.99	0.45
1:H:104:TRP:CD1	1:H:104:TRP:C	2.90	0.45
1:H:202:THR:HG23	1:H:219:LYS:HE3	1.99	0.45
2:B:30:TYR:O	2:B:31:SER:CB	2.63	0.45
3:D:122:PRO:HA	3:D:135:LEU:HD23	1.98	0.44
3:C:122:PRO:HA	3:C:135:LEU:HD23	1.98	0.44
4:E:62:GLN:O	4:E:63:LYS:HB2	2.17	0.44
2:B:100:GLN:NE2	2:B:100:GLN:H	2.15	0.44
4:E:73:ASP:HB3	4:E:76:THR:HG22	1.99	0.44
5:F:150:GLU:HB2	5:F:151:PRO:CD	2.46	0.44
4:E:180:LEU:C	4:E:180:LEU:HD23	2.38	0.44
2:B:169:LYS:H	2:B:169:LYS:HG3	1.69	0.44
1:H:135:PRO:O	1:H:136:SER:CB	2.65	0.44
2:L:169:LYS:H	2:L:169:LYS:HG3	1.63	0.44
2:L:100:GLN:NE2	2:L:100:GLN:H	2.15	0.43
5:F:73:ASP:HB3	5:F:76:THR:HG22	2.00	0.43
5:F:62:GLN:O	5:F:63:LYS:HB2	2.19	0.43
2:B:142:ARG:NH1	2:B:163:VAL:HG21	2.34	0.43
4:E:31:SER:HA	4:E:54:ILE:HD11	2.01	0.43
3:D:127:GLU:OE2	5:F:145:LYS:HE2	2.19	0.42
3:D:89:GLN:HE22	5:F:100:LEU:CD2	2.29	0.42
1:H:40:ALA:HB3	1:H:43:LYS:HD2	2.00	0.42
1:A:202:THR:HG23	1:A:219:LYS:HE3	2.01	0.42
1:A:40:ALA:HB3	1:A:43:LYS:HD2	2.03	0.41
2:L:110:VAL:HG21	2:L:199:GLN:NE2	2.35	0.41
1:A:102:GLY:HA2	4:E:31:SER:HB2	2.02	0.41
1:A:175:PHE:CE1	2:B:164:THR:HG23	2.55	0.41
1:H:209:HIS:CD2	1:H:212:SER:OG	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:125:THR:HA	1:H:156:PRO:HD3	2.02	0.41
2:B:191:VAL:HG22	2:B:210:ASN:HD22	1.86	0.40
3:D:46:LEU:HD21	3:D:49:TYR:HB3	2.02	0.40
3:C:184:THR:HG22	3:C:187:GLN:HG3	2.04	0.40
2:L:159:SER:HA	2:L:178:THR:O	2.22	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	224/227 (99%)	206 (92%)	10 (4%)	8 (4%)	3 4
1	H	225/227 (99%)	207 (92%)	12 (5%)	6 (3%)	5 7
2	B	212/214 (99%)	204 (96%)	4 (2%)	4 (2%)	8 13
2	L	212/214 (99%)	205 (97%)	4 (2%)	3 (1%)	11 20
3	C	212/214 (99%)	201 (95%)	9 (4%)	2 (1%)	17 31
3	D	211/214 (99%)	203 (96%)	4 (2%)	4 (2%)	8 13
4	E	213/215 (99%)	208 (98%)	4 (2%)	1 (0%)	29 48
5	F	209/218 (96%)	202 (97%)	3 (1%)	4 (2%)	8 13
All	All	1718/1743 (99%)	1636 (95%)	50 (3%)	32 (2%)	8 13

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	29	PHE
1	A	102	GLY
1	A	144	THR
1	A	156	PRO

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Mol	Chain	Res	Type
1	A	157	GLU
1	A	158	PRO
2	B	165	GLU
5	F	149	PRO
5	F	150	GLU
1	H	136	SER
1	H	157	GLU
1	A	142	GLY
3	C	14	ALA
3	D	15	PRO
4	E	63	LYS
5	F	63	LYS
1	H	103	GLY
3	C	118	VAL
3	D	118	VAL
1	H	155	PHE
1	H	158	PRO
3	D	16	GLY
5	F	151	PRO
1	H	140	THR
2	B	30	TYR
2	B	51	VAL
3	D	154	ASP
2	L	95	ALA
2	L	40	PRO
2	B	40	PRO
2	L	51	VAL

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	183/185 (99%)	173 (94%)	10 (6%)	21 41
1	H	185/185 (100%)	173 (94%)	12 (6%)	17 33
2	B	184/185 (100%)	167 (91%)	17 (9%)	9 18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	L	185/185 (100%)	174 (94%)	11 (6%)	19 37
3	C	181/181 (100%)	170 (94%)	11 (6%)	18 36
3	D	179/181 (99%)	171 (96%)	8 (4%)	27 51
4	E	178/178 (100%)	167 (94%)	11 (6%)	18 35
5	F	176/181 (97%)	164 (93%)	12 (7%)	16 30
All	All	1451/1461 (99%)	1359 (94%)	92 (6%)	18 34

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	29	PHE
1	A	52	TRP
1	A	89	GLU
1	A	116	THR
1	A	144	THR
1	A	188	SER
1	A	193	VAL
1	A	206	ASN
1	A	213	ASN
2	B	18	ARG
2	B	20	THR
2	B	24	ARG
2	B	30	TYR
2	B	31	SER
2	B	33	LEU
2	B	51	VAL
2	B	52	THR
2	B	69	THR
2	B	75	ILE
2	B	77	ARG
2	B	90	GLN
2	B	100	GLN
2	B	105	GLU
2	B	109	THR
2	B	114	SER
2	B	169	LYS
3	C	13	VAL
3	C	22	THR
3	C	30	THR

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Mol	Chain	Res	Type
3	C	31	LYS
3	C	35	TRP
3	C	52	ARG
3	C	60	GLU
3	C	77	ARG
3	C	85	ASP
3	C	90	VAL
3	C	212	THR
3	D	15	PRO
3	D	30	THR
3	D	31	LYS
3	D	52	ARG
3	D	60	GLU
3	D	85	ASP
3	D	90	VAL
3	D	212	THR
4	E	28	THR
4	E	54	ILE
4	E	65	GLN
4	E	98	VAL
4	E	131	LYS
4	E	142	CYS
4	E	145	LYS
4	E	152	VAL
4	E	180	LEU
4	E	199	ASN
4	E	212	LYS
5	F	28	THR
5	F	65	GLN
5	F	67	ARG
5	F	98	VAL
5	F	100	LEU
5	F	122	SER
5	F	126	LEU
5	F	145	LYS
5	F	198	CYS
5	F	199	ASN
5	F	212	LYS
5	F	218	CYS
1	H	18	LEU
1	H	52	TRP
1	H	71	SER

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Mol	Chain	Res	Type
1	H	89	GLU
1	H	104	TRP
1	H	112	TRP
1	H	116	THR
1	H	119	THR
1	H	144	THR
1	H	192	THR
1	H	193	VAL
1	H	206	ASN
2	L	18	ARG
2	L	20	THR
2	L	24	ARG
2	L	33	LEU
2	L	52	THR
2	L	90	GLN
2	L	100	GLN
2	L	114	SER
2	L	142	ARG
2	L	168	SER
2	L	169	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	164	ASN
1	A	180	GLN
1	A	209	HIS
2	B	38	HIS
2	B	90	GLN
2	B	100	GLN
2	B	155	GLN
2	B	210	ASN
3	C	37	GLN
3	C	42	GLN
3	C	89	GLN
3	C	170	GLN
3	D	37	GLN
3	D	42	GLN
3	D	89	GLN
3	D	170	GLN
3	D	173	ASN

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Mol	Chain	Res	Type
4	E	6	GLN
4	E	202	HIS
5	F	6	GLN
5	F	202	HIS
1	H	35	HIS
1	H	39	GLN
1	H	180	GLN
1	H	209	HIS
2	L	37	GLN
2	L	90	GLN
2	L	100	GLN
2	L	155	GLN
2	L	198	HIS
2	L	199	GLN

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 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	226/227 (99%)	-0.28	9 (3%)	38	41	15, 31, 76, 117	0
1	H	227/227 (100%)	-0.26	9 (3%)	38	41	16, 29, 62, 121	0
2	B	214/214 (100%)	-0.57	1 (0%)	91	91	13, 26, 49, 99	0
2	L	214/214 (100%)	-0.51	2 (0%)	84	86	17, 33, 54, 117	0
3	C	214/214 (100%)	-0.23	4 (1%)	66	69	20, 39, 67, 130	0
3	D	213/214 (99%)	-0.34	3 (1%)	75	77	20, 36, 62, 127	0
4	E	215/215 (100%)	-0.37	6 (2%)	53	56	17, 32, 75, 104	0
5	F	213/218 (97%)	-0.42	1 (0%)	91	91	19, 36, 67, 113	0
All	All	1736/1743 (99%)	-0.37	35 (2%)	65	68	13, 33, 66, 130	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	214	CYS	8.5
1	H	227	ALA	7.2
3	C	1	LEU	7.0
3	D	1	LEU	5.9
1	H	226	ALA	5.9
1	A	137	SER	5.8
1	A	140	THR	4.9
3	D	213	GLU	4.7
1	A	226	ALA	4.6
1	H	225	CYS	4.3
4	E	135	GLY	4.1
1	A	225	CYS	4.0
5	F	218	CYS	3.9
4	E	134	SER	3.9
1	H	224	SER	3.6
1	H	141	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	139	SER	3.1
1	A	139	SER	2.9
4	E	132	SER	2.8
3	C	213	GLU	2.7
3	D	212	THR	2.7
4	E	137	THR	2.6
4	E	193	THR	2.6
1	H	142	GLY	2.6
2	B	214	CYS	2.5
1	A	157	GLU	2.4
1	H	157	GLU	2.4
1	A	200	THR	2.4
2	L	213	GLU	2.3
3	C	14	ALA	2.3
1	A	156	PRO	2.3
1	H	200	THR	2.2
1	A	138	LYS	2.2
4	E	190	SER	2.1
2	L	214	CYS	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 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.