Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 01:36 PM EDT

PDB ID	:	6XM2
Title	:	The structure of the 4A11.v7 antibody in complex with human TGFb2
Authors	:	Lupardus, P.J.; Yin, J.P.
Deposited on	:	2020-06-29
Resolution	:	1.91 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:

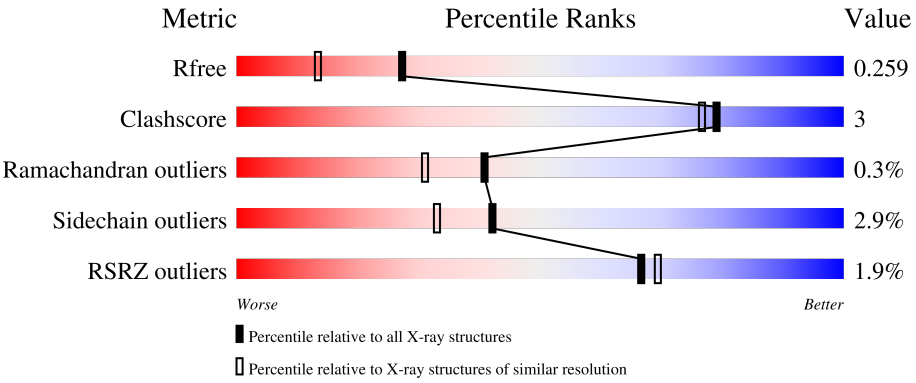
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	219	94% 5%
1	C	219	88% 10%
1	E	219	95%
1	G	219	8% 85% 14%
2	B	233	87% 8% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	233	2% 84% 9% 7%
2	F	233	89% 6% 5%
2	H	233	85% 7% 7%
3	I	112	3% 88% 10%
3	J	112	3% 90% 5%
3	K	112	86% 7% 5%
3	L	112	4% 90% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17117 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 4A11.v7 kappa light chain Fab (VL-CL) humanized.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1636	1024	272	336	4			
1	C	216	Total	C	N	O	S	0	0	0
			1636	1025	275	332	4			
1	E	218	Total	C	N	O	S	0	0	0
			1652	1032	276	339	5			
1	G	218	Total	C	N	O	S	0	0	0
			1655	1035	277	339	4			

- Molecule 2 is a protein called 4A11.v7 heavy chain Fab (VH-CH1) IgG1 humanized.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	221	Total	C	N	O	S	0	0	0
			1614	1024	265	319	6			
2	D	216	Total	C	N	O	S	0	0	0
			1582	1006	259	311	6			
2	F	221	Total	C	N	O	S	0	0	0
			1620	1027	266	320	7			
2	H	217	Total	C	N	O	S	0	0	0
			1596	1015	262	313	6			

- Molecule 3 is a protein called Transforming growth factor beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	112	Total	C	N	O	S	0	0	0
			887	563	149	165	10			
3	J	108	Total	C	N	O	S	0	0	0
			845	538	141	156	10			
3	K	106	Total	C	N	O	S	0	0	0
			826	524	138	154	10			
3	L	109	Total	C	N	O	S	0	0	0
			860	547	145	158	10			

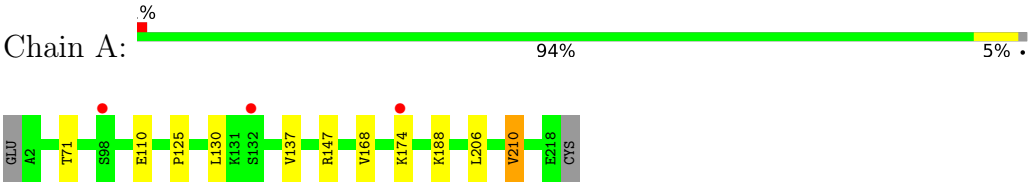
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	57	Total O 57 57	0	0
4	B	60	Total O 60 60	0	0
4	C	54	Total O 54 54	0	0
4	D	47	Total O 47 47	0	0
4	E	96	Total O 96 96	0	0
4	F	120	Total O 120 120	0	0
4	G	65	Total O 65 65	0	0
4	H	48	Total O 48 48	0	0
4	I	46	Total O 46 46	0	0
4	J	44	Total O 44 44	0	0
4	K	38	Total O 38 38	0	0
4	L	33	Total O 33 33	0	0

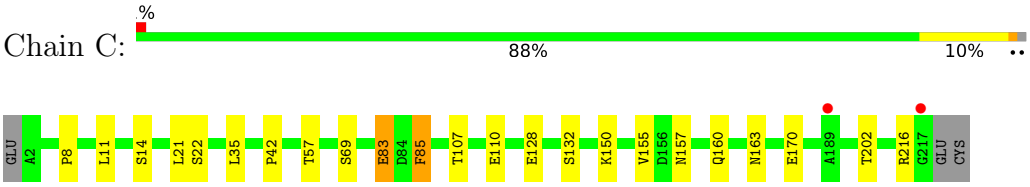
3 Residue-property plots (i)

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.

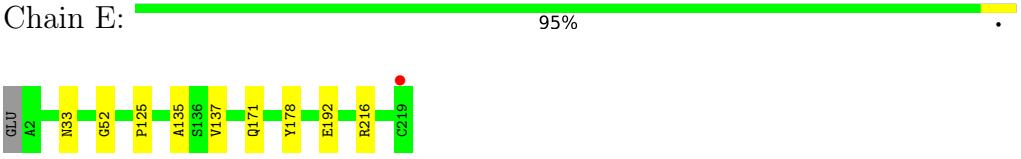
• Molecule 1: 4A11.v7 kappa light chain Fab (VL-CL) humanized



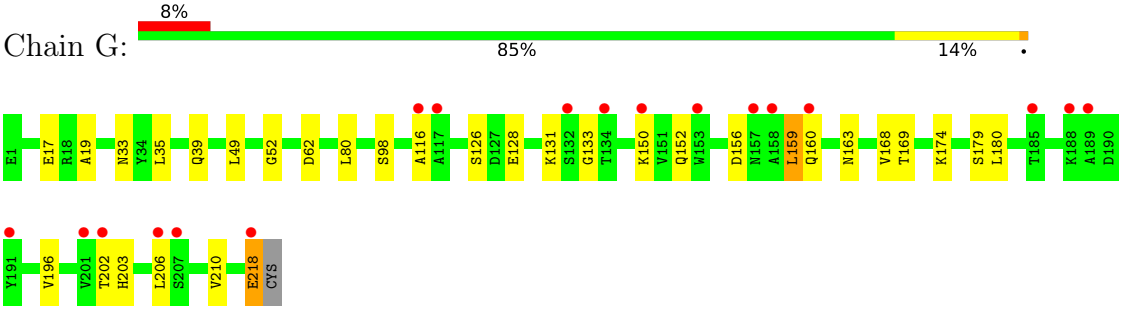
• Molecule 1: 4A11.v7 kappa light chain Fab (VL-CL) humanized



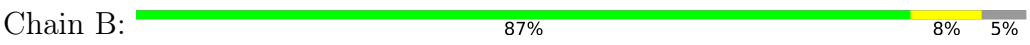
• Molecule 1: 4A11.v7 kappa light chain Fab (VL-CL) humanized

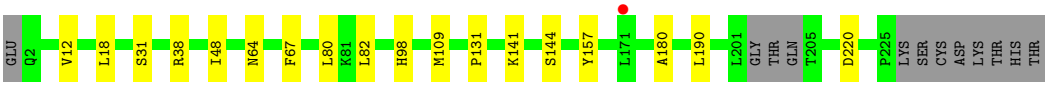


• Molecule 1: 4A11.v7 kappa light chain Fab (VL-CL) humanized



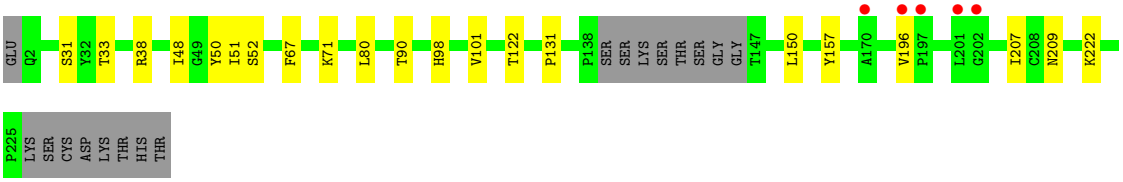
• Molecule 2: 4A11.v7 heavy chain Fab (VH-CH1) IgG1 humanized





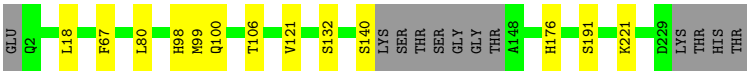
• Molecule 2: 4A11.v7 heavy chain Fab (VH-CH1) IgG1 humanized

Chain D:



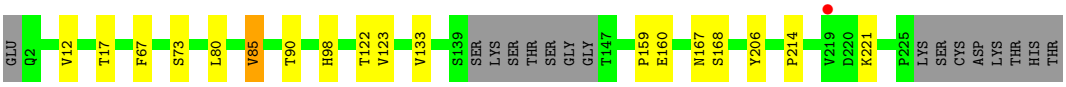
• Molecule 2: 4A11.v7 heavy chain Fab (VH-CH1) IgG1 humanized

Chain F:



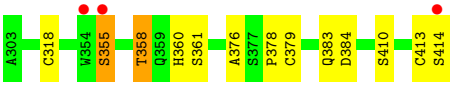
• Molecule 2: 4A11.v7 heavy chain Fab (VH-CH1) IgG1 humanized

Chain H:



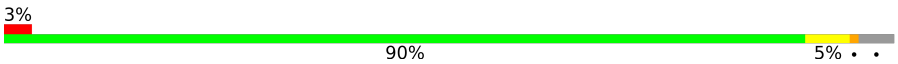
• Molecule 3: Transforming growth factor beta-2

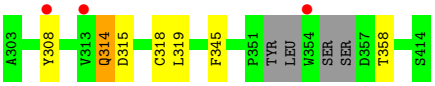
Chain I:



• Molecule 3: Transforming growth factor beta-2

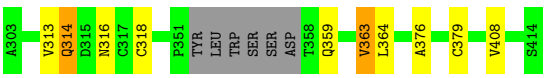
Chain J:





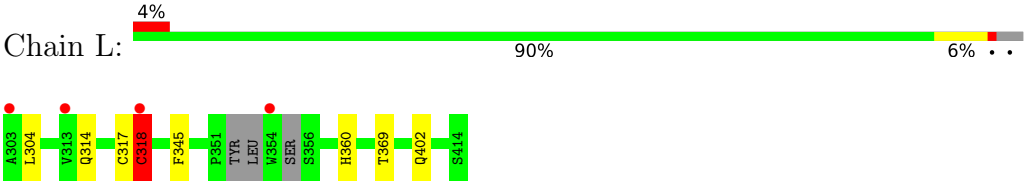
• Molecule 3: Transforming growth factor beta-2

Chain K:



• Molecule 3: Transforming growth factor beta-2

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	64.42Å 85.11Å 112.73Å 99.15° 99.51° 97.32°	Depositor
Resolution (Å)	82.97 – 1.91 82.97 – 1.91	Depositor EDS
% Data completeness (in resolution range)	90.5 (82.97-1.91) 90.5 (82.97-1.91)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 1.91Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.205 , 0.244 0.211 , 0.259	Depositor DCC
R_{free} test set	8036 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.4	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	0.96	EDS
Total number of atoms	17117	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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	0.48	0/1673	0.72	0/2275
1	C	0.50	0/1673	0.71	0/2273
1	E	0.55	0/1689	0.71	0/2295
1	G	0.50	0/1692	0.73	0/2298
2	B	0.51	0/1656	0.73	0/2264
2	D	0.47	0/1624	0.71	0/2224
2	F	0.54	0/1662	0.73	0/2272
2	H	0.51	0/1638	0.75	0/2240
3	I	0.52	0/911	0.71	0/1238
3	J	0.51	0/866	0.65	0/1176
3	K	0.51	0/846	0.68	0/1149
3	L	0.50	0/881	0.66	0/1194
All	All	0.51	0/16811	0.71	0/22898

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	A	1636	0	1560	5	0
1	C	1636	0	1573	7	0
1	E	1652	0	1580	5	0
1	G	1655	0	1591	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1614	0	1575	9	0
2	D	1582	0	1536	9	0
2	F	1620	0	1577	6	0
2	H	1596	0	1563	9	0
3	I	887	0	847	13	0
3	J	845	0	800	3	0
3	K	826	0	789	6	0
3	L	860	0	822	6	0
4	A	57	0	0	1	0
4	B	60	0	0	1	0
4	C	54	0	0	1	0
4	D	47	0	0	0	0
4	E	96	0	0	0	0
4	F	120	0	0	3	0
4	G	65	0	0	0	0
4	H	48	0	0	2	0
4	I	46	0	0	0	0
4	J	44	0	0	1	0
4	K	38	0	0	0	0
4	L	33	0	0	0	0
All	All	17117	0	15813	90	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 3.

All (90) 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:G:206:LEU:HD13	1:G:210:VAL:HG23	1.23	1.14
1:G:206:LEU:HD13	1:G:210:VAL:CG2	1.98	0.94
3:L:317:CYS:O	3:L:318:CYS:HB3	1.63	0.94
3:I:355:SER:HB2	3:I:413:CYS:H	1.41	0.85
1:G:19:ALA:HB2	1:G:80:LEU:HD21	1.58	0.84
2:B:67:PHE:HD2	2:B:80:LEU:HD11	1.53	0.74
2:H:67:PHE:HD2	2:H:80:LEU:HD11	1.54	0.71
3:I:358:THR:HG22	3:I:361:SER:H	1.56	0.71
3:L:304:LEU:HB3	3:L:318:CYS:HB2	1.75	0.69
3:K:314:GLN:HE22	3:K:316:ASN:HB2	1.59	0.67
1:G:150:LYS:HB3	1:G:202:THR:OG1	1.96	0.66
1:G:206:LEU:CD1	1:G:210:VAL:CG2	2.74	0.65
1:G:19:ALA:CB	1:G:80:LEU:HD21	2.25	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:LYS:HE3	2:B:144:SER:HB2	1.80	0.63
1:C:150:LYS:HB3	1:C:202:THR:HB	1.81	0.62
3:I:376:ALA:HB2	3:J:345:PHE:CD2	2.34	0.62
2:B:131:PRO:HB3	2:B:157:TYR:HB3	1.82	0.61
1:G:17:GLU:O	1:G:80:LEU:HD23	2.00	0.61
1:G:128:GLU:HA	1:G:131:LYS:HE2	1.83	0.61
1:C:160:GLN:HE21	1:C:163:ASN:HD21	1.49	0.58
2:D:38:ARG:HB3	2:D:48:ILE:HD11	1.86	0.58
2:H:133:VAL:HG22	2:H:221:LYS:HG3	1.86	0.58
1:G:169:THR:HG22	1:G:179:SER:H	1.69	0.57
2:F:67:PHE:HD1	2:F:80:LEU:HD11	1.68	0.57
1:A:206:LEU:HD13	1:A:210:VAL:HG13	1.88	0.55
2:B:67:PHE:CD2	2:B:80:LEU:HD11	2.39	0.55
1:E:192:GLU:HG2	1:E:216:ARG:NH1	2.22	0.54
2:H:159:PRO:HD2	2:H:214:PRO:HB2	1.90	0.54
3:I:383:GLN:HG3	3:I:410:SER:OG	2.07	0.54
1:A:130:LEU:O	1:A:188:LYS:HD3	2.07	0.54
2:H:17:THR:HG22	4:H:336:HOH:O	2.07	0.54
3:K:359:GLN:O	3:K:363:VAL:HG13	2.07	0.54
2:H:167:ASN:HD21	2:H:206:TYR:HA	1.74	0.53
3:K:408:VAL:HG23	3:L:360:HIS:CE1	2.43	0.53
2:F:18:LEU:CD1	4:F:374:HOH:O	2.56	0.53
1:E:171:GLN:HG3	1:E:178:TYR:CZ	2.44	0.52
1:A:168:VAL:HG21	4:A:356:HOH:O	2.09	0.52
2:F:106:THR:HG22	4:F:392:HOH:O	2.10	0.52
3:I:378:PRO:HA	3:I:414:SER:HB3	1.91	0.51
1:E:125:PRO:HD3	1:E:137:VAL:HG22	1.91	0.51
3:I:379:CYS:H	3:I:414:SER:CB	2.24	0.50
1:G:160:GLN:HE21	1:G:163:ASN:HD21	1.60	0.50
3:I:355:SER:CB	3:I:413:CYS:H	2.19	0.50
3:I:360:HIS:HD2	4:J:502:HOH:O	1.95	0.49
3:J:318:CYS:SG	3:J:319:LEU:N	2.85	0.49
3:J:314:GLN:HG2	3:J:315:ASP:N	2.28	0.49
1:C:21:LEU:HD22	1:C:107:THR:HG21	1.94	0.49
1:G:152:GLN:HB3	1:G:159:LEU:HD21	1.96	0.48
2:B:12:VAL:HG21	2:B:18:LEU:HD13	1.95	0.48
2:D:207:ILE:HD12	2:D:209:ASN:HD21	1.79	0.47
2:F:99:MET:HE2	2:F:100:GLN:HG2	1.96	0.47
1:C:42:PRO:HG2	1:C:170:GLU:HG2	1.96	0.47
2:D:51:ILE:HG12	2:D:71:LYS:HB2	1.97	0.47
1:E:33:ASN:O	1:E:52:GLY:HA2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:39:GLN:HB2	1:G:49:LEU:HD11	1.98	0.46
2:B:38:ARG:HB3	2:B:48:ILE:HD11	1.96	0.46
3:I:383:GLN:HG3	3:I:384:ASP:H	1.80	0.46
1:G:168:VAL:HG22	1:G:180:LEU:HD12	1.98	0.45
2:D:31:SER:HB3	2:D:101:VAL:HG12	1.98	0.45
2:D:131:PRO:HB3	2:D:157:TYR:HB3	1.99	0.45
4:B:302:HOH:O	3:L:369:THR:HG22	2.16	0.44
1:E:125:PRO:HG3	1:E:135:ALA:HB1	1.97	0.44
2:B:180:ALA:HA	2:B:190:LEU:HB3	1.98	0.44
1:C:85:PHE:CZ	1:C:170:GLU:HB3	2.52	0.44
1:A:125:PRO:HD3	1:A:137:VAL:HG22	2.00	0.43
2:D:90:THR:HG23	2:D:122:THR:HA	2.00	0.43
1:C:83:GLU:HG3	4:C:337:HOH:O	2.17	0.43
3:I:379:CYS:H	3:I:414:SER:HB2	1.82	0.43
1:C:8:PRO:HG3	1:C:11:LEU:HD13	2.01	0.43
2:D:67:PHE:HD2	2:D:80:LEU:HD11	1.84	0.43
2:F:18:LEU:HD13	2:F:121:VAL:HG11	2.00	0.42
2:H:85:VAL:HG13	2:H:123:VAL:CG1	2.50	0.42
2:D:207:ILE:HG22	2:D:222:LYS:HA	2.01	0.42
2:H:85:VAL:HG13	2:H:123:VAL:HG11	2.01	0.42
2:F:176:HIS:HD2	4:F:414:HOH:O	2.03	0.42
2:B:31:SER:OG	3:K:313:VAL:HG21	2.20	0.41
1:G:116:ALA:O	1:G:203:HIS:CE1	2.73	0.41
1:G:156:ASP:HA	1:G:196:VAL:HG13	2.01	0.41
2:H:17:THR:CG2	4:H:336:HOH:O	2.68	0.41
3:I:358:THR:CG2	3:I:361:SER:H	2.30	0.41
1:A:174:LYS:HD2	1:A:174:LYS:HA	1.81	0.41
2:D:33:THR:HG23	2:D:52:SER:HA	2.02	0.41
2:H:90:THR:HG23	2:H:122:THR:HA	2.03	0.41
2:B:18:LEU:HB3	2:B:82:LEU:HB3	2.03	0.41
1:G:218:GLU:H	1:G:218:GLU:HG3	1.54	0.41
3:I:355:SER:HB2	3:I:413:CYS:N	2.22	0.41
3:K:376:ALA:HB2	3:L:345:PHE:CD2	2.56	0.41
3:I:379:CYS:H	3:I:414:SER:HB3	1.85	0.40
1:G:33:ASN:O	1:G:52:GLY:HA2	2.22	0.40
3:K:408:VAL:HG23	3:L:360:HIS:NE2	2.36	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	215/219 (98%)	205 (95%)	10 (5%)	0	100 100
1	C	214/219 (98%)	201 (94%)	12 (6%)	1 (0%)	29 18
1	E	216/219 (99%)	210 (97%)	6 (3%)	0	100 100
1	G	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	17 7
2	B	217/233 (93%)	211 (97%)	6 (3%)	0	100 100
2	D	212/233 (91%)	207 (98%)	5 (2%)	0	100 100
2	F	217/233 (93%)	211 (97%)	6 (3%)	0	100 100
2	H	213/233 (91%)	208 (98%)	5 (2%)	0	100 100
3	I	110/112 (98%)	102 (93%)	7 (6%)	1 (1%)	17 7
3	J	103/112 (92%)	93 (90%)	9 (9%)	1 (1%)	15 6
3	K	102/112 (91%)	97 (95%)	5 (5%)	0	100 100
3	L	104/112 (93%)	98 (94%)	5 (5%)	1 (1%)	15 6
All	All	2139/2256 (95%)	2047 (96%)	86 (4%)	6 (0%)	41 31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	355	SER
3	J	308	TYR
3	L	318	CYS
1	G	133	GLY
1	G	174	LYS
1	C	216	ARG

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	183/188 (97%)	179 (98%)	4 (2%)	52 45
1	C	183/188 (97%)	171 (93%)	12 (7%)	16 7
1	E	186/188 (99%)	186 (100%)	0	100 100
1	G	186/188 (99%)	180 (97%)	6 (3%)	39 29
2	B	181/194 (93%)	177 (98%)	4 (2%)	52 45
2	D	176/194 (91%)	172 (98%)	4 (2%)	50 43
2	F	182/194 (94%)	177 (97%)	5 (3%)	44 36
2	H	179/194 (92%)	173 (97%)	6 (3%)	37 27
3	I	99/100 (99%)	97 (98%)	2 (2%)	55 49
3	J	93/100 (93%)	91 (98%)	2 (2%)	52 45
3	K	92/100 (92%)	87 (95%)	5 (5%)	22 12
3	L	95/100 (95%)	92 (97%)	3 (3%)	39 29
All	All	1835/1928 (95%)	1782 (97%)	53 (3%)	42 33

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	THR
1	A	110	GLU
1	A	147	ARG
1	A	210	VAL
2	B	64	ASN
2	B	98	HIS
2	B	109	MET
2	B	220	ASP
1	C	14	SER
1	C	22	SER
1	C	35	LEU
1	C	57	THR
1	C	69	SER
1	C	83	GLU
1	C	85	PHE
1	C	110	GLU
1	C	128	GLU
1	C	132	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	155	VAL
1	C	157	ASN
2	D	50	TYR
2	D	98	HIS
2	D	150	LEU
2	D	196	VAL
2	F	98	HIS
2	F	132	SER
2	F	140	SER
2	F	191	SER
2	F	221	LYS
1	G	35	LEU
1	G	62	ASP
1	G	98	SER
1	G	126	SER
1	G	159	LEU
1	G	218	GLU
2	H	12	VAL
2	H	73	SER
2	H	85	VAL
2	H	98	HIS
2	H	160	GLU
2	H	168	SER
3	I	318	CYS
3	I	358	THR
3	J	314	GLN
3	J	358	THR
3	K	314	GLN
3	K	318	CYS
3	K	363	VAL
3	K	364	LEU
3	K	379	CYS
3	L	314	GLN
3	L	318	CYS
3	L	402	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	142	ASN
1	C	160	GLN
1	C	215	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	24	GLN
1	E	152	GLN
2	F	100	GLN
1	G	44	GLN
1	G	143	ASN
1	G	160	GLN
2	H	167	ASN
2	H	183	GLN
3	I	360	HIS
3	K	312	ASN
3	K	314	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	217/219 (99%)	-0.04	3 (1%) 75 77	27, 40, 58, 87	0
1	C	216/219 (98%)	0.07	2 (0%) 84 85	29, 42, 61, 82	0
1	E	218/219 (99%)	-0.07	1 (0%) 91 92	22, 35, 53, 80	0
1	G	218/219 (99%)	0.41	18 (8%) 11 13	27, 44, 76, 97	0
2	B	221/233 (94%)	-0.16	1 (0%) 91 92	24, 40, 57, 73	0
2	D	216/233 (92%)	0.08	5 (2%) 60 63	28, 43, 66, 88	0
2	F	221/233 (94%)	-0.02	0 100 100	22, 33, 54, 95	0
2	H	217/233 (93%)	0.01	1 (0%) 91 92	26, 42, 62, 78	0
3	I	112/112 (100%)	0.02	3 (2%) 54 57	23, 33, 59, 74	0
3	J	108/112 (96%)	0.15	3 (2%) 53 56	28, 39, 64, 80	0
3	K	106/112 (94%)	-0.16	0 100 100	25, 36, 52, 61	0
3	L	109/112 (97%)	0.07	4 (3%) 41 44	27, 39, 64, 82	0
All	All	2179/2256 (96%)	0.03	41 (1%) 66 69	22, 40, 62, 97	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	354	TRP	4.7
1	G	207	SER	4.6
2	D	201	LEU	4.6
3	J	354	TRP	4.2
1	A	98	SER	4.1
1	G	157	ASN	4.0
1	G	206	LEU	4.0
3	J	313	VAL	3.8
3	L	313	VAL	3.8
1	G	189	ALA	3.8
3	L	318	CYS	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	I	354	TRP	3.6
1	G	117	ALA	3.5
1	G	202	THR	3.4
1	G	218	GLU	3.1
1	G	158	ALA	3.1
2	H	219	VAL	3.0
2	B	171	LEU	3.0
3	I	355	SER	3.0
2	D	170	ALA	2.8
1	G	150	LYS	2.8
1	G	132	SER	2.7
1	G	116	ALA	2.7
1	E	219	CYS	2.6
1	G	160	GLN	2.5
3	I	414	SER	2.3
1	G	191	TYR	2.3
1	G	134	THR	2.3
1	G	201	VAL	2.3
1	C	189	ALA	2.3
2	D	202	GLY	2.2
1	G	185	THR	2.2
3	J	308	TYR	2.2
1	A	132	SER	2.1
1	G	153	TRP	2.1
2	D	197	PRO	2.1
1	C	217	GLY	2.1
3	L	303	ALA	2.1
1	G	188	LYS	2.1
2	D	196	VAL	2.1
1	A	174	LYS	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.