



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:58 PM UTC

PDB ID : 6XM2 / pdb_00006xm2
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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

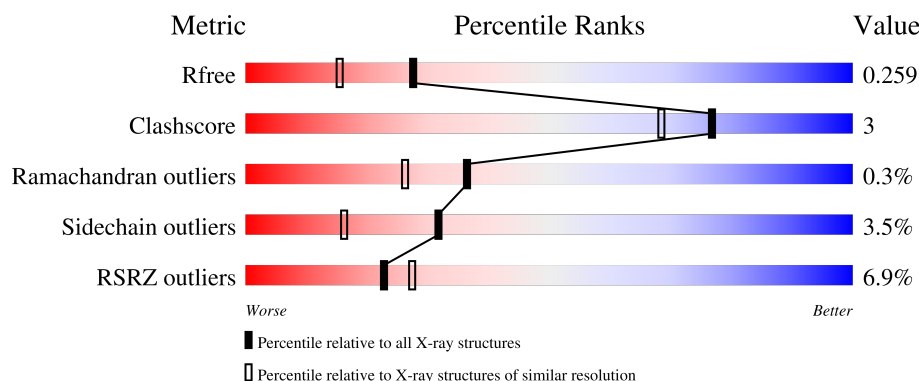
1 Overall quality at a glance

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}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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 $\leq 5\%$. 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	
1	C	219	
1	E	219	
1	G	219	
2	B	233	

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Mol	Chain	Length	Quality of chain
2	D	233	5% 82% 10% 7%
2	F	233	4% 89% 6% 5%
2	H	233	7% 83% 9% 7%
3	I	112	6% 86% 12%
3	J	112	12% 89% 5%
3	K	112	2% 84% 8%
3	L	112	8% 85% 11%

2 Entry composition

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			

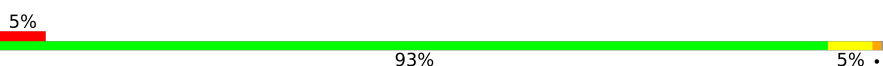
- Molecule 4 is water.

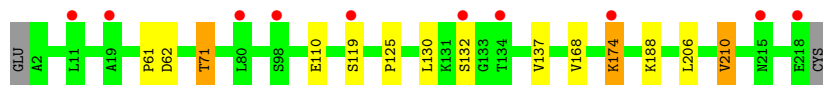
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total 57	O 57	0	0
4	B	60	Total 60	O 60	0	0
4	C	54	Total 54	O 54	0	0
4	D	47	Total 47	O 47	0	0
4	E	96	Total 96	O 96	0	0
4	F	120	Total 120	O 120	0	0
4	G	65	Total 65	O 65	0	0
4	H	48	Total 48	O 48	0	0
4	I	46	Total 46	O 46	0	0
4	J	44	Total 44	O 44	0	0
4	K	38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

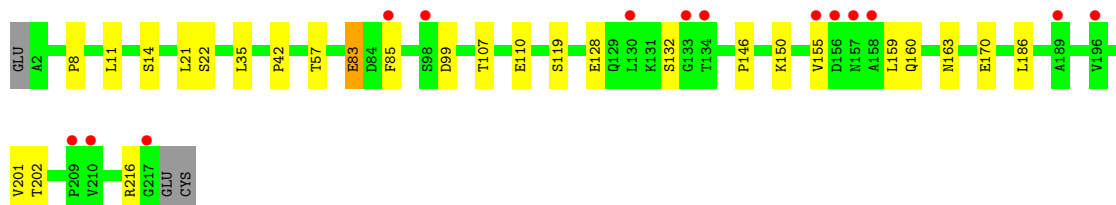
- Molecule 1: 4A11.v7 kappa light chain Fab (VL-CL) humanized

Chain A: 

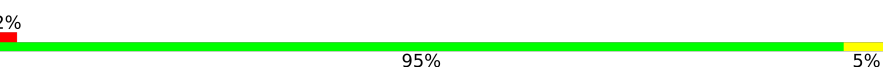


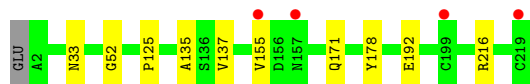
- Molecule 1: 4A11.v7 kappa light chain Fab (VL-CL) humanized

Chain C: 



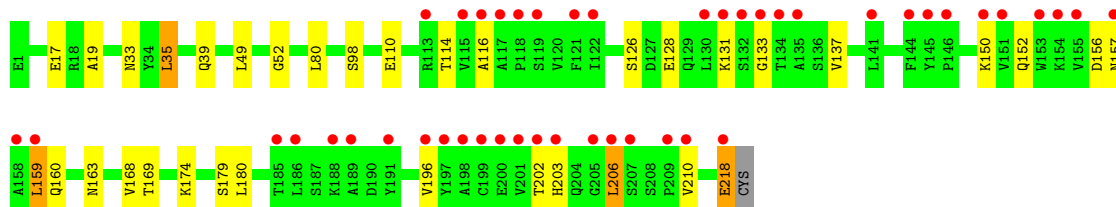
- Molecule 1: 4A11.v7 kappa light chain Fab (VL-CL) humanized

Chain E: 

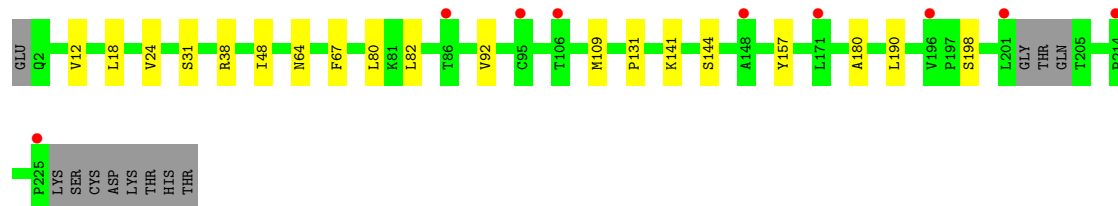
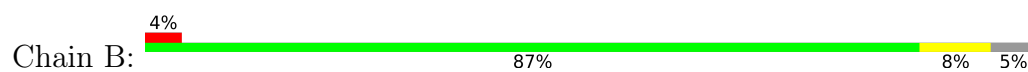


- Molecule 1: 4A11.v7 kappa light chain Fab (VL-CL) humanized

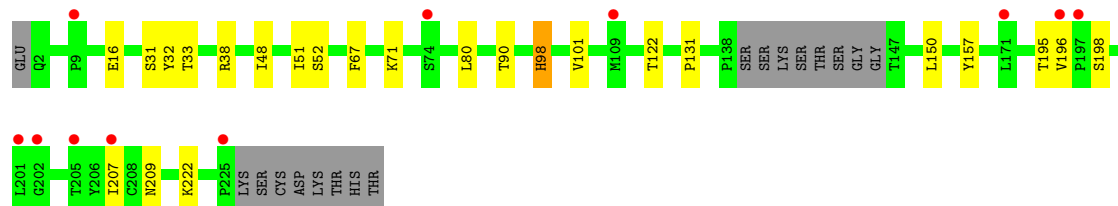
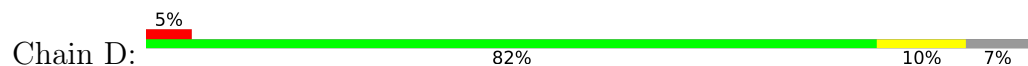
Chain G: 



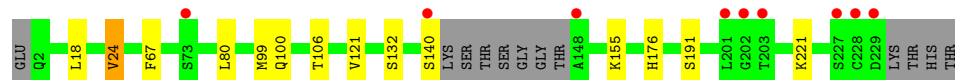
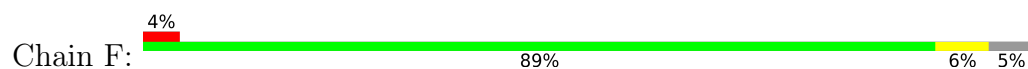
- Molecule 2: 4A11.v7 heavy chain Fab (VH-CH1) IgG1 humanized



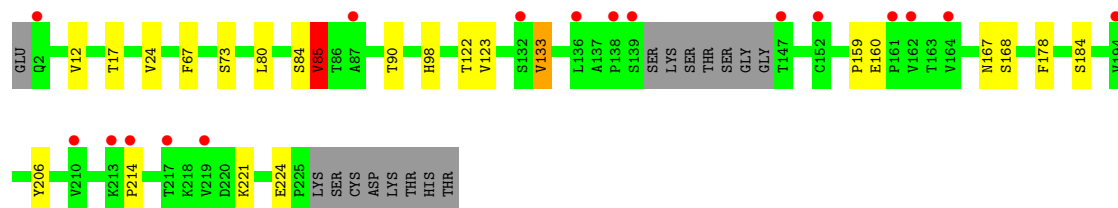
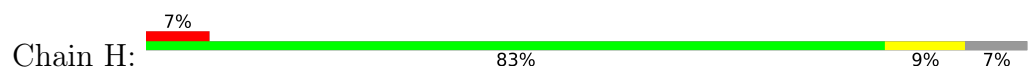
- Molecule 2: 4A11.v7 heavy chain Fab (VH-CH1) IgG1 humanized



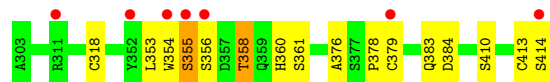
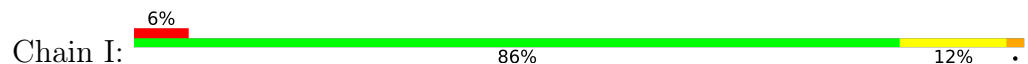
- Molecule 2: 4A11.v7 heavy chain Fab (VH-CH1) IgG1 humanized



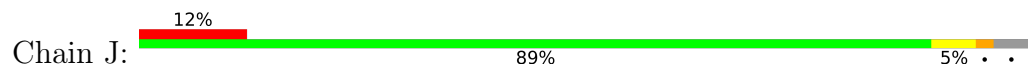
- Molecule 2: 4A11.v7 heavy chain Fab (VH-CH1) IgG1 humanized



- Molecule 3: Transforming growth factor beta-2

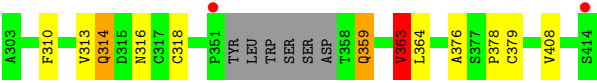
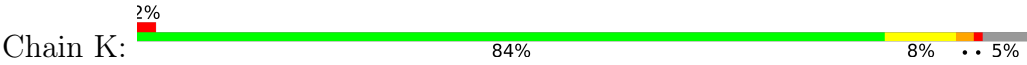


- Molecule 3: Transforming growth factor beta-2

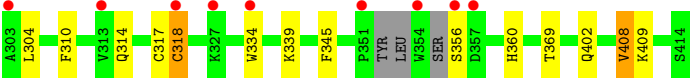
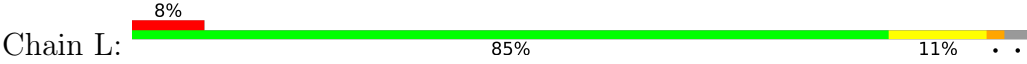




• Molecule 3: Transforming growth factor beta-2



• Molecule 3: Transforming growth factor beta-2



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 1.91Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.205 , 0.244 0.212 , 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)	0.33 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	A	0.80	0/1673	1.14	7/2275 (0.3%)
1	C	0.85	0/1673	1.12	6/2273 (0.3%)
1	E	0.89	0/1689	1.12	0/2295
1	G	0.82	0/1692	1.19	4/2298 (0.2%)
2	B	0.84	0/1656	1.12	3/2264 (0.1%)
2	D	0.79	0/1624	1.14	3/2224 (0.1%)
2	F	0.87	0/1662	1.12	1/2272 (0.0%)
2	H	0.86	0/1638	1.17	6/2240 (0.3%)
3	I	0.84	0/911	1.16	4/1238 (0.3%)
3	J	0.85	0/866	1.11	2/1176 (0.2%)
3	K	0.83	0/846	1.13	4/1149 (0.3%)
3	L	0.83	0/881	1.15	4/1194 (0.3%)
All	All	0.84	0/16811	1.14	44/22898 (0.2%)

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	318	CYS	CA-C-N	6.63	130.17	120.82
3	J	318	CYS	C-N-CA	6.63	130.17	120.82
3	L	356	SER	CA-C-N	6.61	129.43	120.44
3	L	356	SER	C-N-CA	6.61	129.43	120.44
1	A	61	PRO	CA-C-N	6.49	129.85	120.38
1	A	61	PRO	C-N-CA	6.49	129.85	120.38
1	A	132	SER	N-CA-C	6.32	119.47	111.69
3	K	363	VAL	N-CA-CB	6.23	119.92	110.58
2	H	84	SER	CA-C-N	6.18	128.84	120.63
2	H	84	SER	C-N-CA	6.18	128.84	120.63
3	K	378	PRO	CA-C-N	5.98	132.50	122.87
3	K	378	PRO	C-N-CA	5.98	132.50	122.87
2	B	198	SER	CA-C-N	5.98	128.57	120.38
2	B	198	SER	C-N-CA	5.98	128.57	120.38
2	D	98	HIS	N-CA-C	-5.85	101.63	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	310	PHE	CA-CB-CG	5.77	119.57	113.80
3	I	354	TRP	N-CA-C	5.71	117.70	110.33
2	H	85	VAL	N-CA-CB	-5.70	102.50	110.13
1	C	146	PRO	CA-C-N	5.69	128.22	120.54
1	C	146	PRO	C-N-CA	5.69	128.22	120.54
1	G	206	LEU	CA-C-N	5.65	127.86	120.28
1	G	206	LEU	C-N-CA	5.65	127.86	120.28
1	C	119	SER	N-CA-C	-5.59	100.07	108.96
2	H	184	SER	CA-C-N	5.58	128.31	120.28
2	H	184	SER	C-N-CA	5.58	128.31	120.28
1	A	119	SER	N-CA-C	-5.55	100.24	109.46
2	D	195	THR	CB-CA-C	5.51	119.11	110.19
1	G	35	LEU	CD1-CG-CD2	5.41	122.70	110.80
1	A	71	THR	CB-CA-C	5.39	116.11	109.16
2	B	92	VAL	N-CA-C	-5.35	100.87	108.58
1	A	62	ASP	CA-CB-CG	5.31	117.91	112.60
3	I	353	LEU	N-CA-C	5.30	118.91	112.23
1	C	201	VAL	N-CA-C	5.28	115.45	107.80
2	F	24	VAL	N-CA-CB	-5.26	101.48	111.21
3	L	408	VAL	N-CA-CB	5.21	117.31	111.21
1	A	71	THR	N-CA-CB	-5.19	103.58	111.15
2	H	178	PHE	N-CA-C	5.16	116.33	109.93
1	G	157	ASN	CA-CB-CG	5.14	117.74	112.60
3	I	354	TRP	CA-C-N	5.11	131.30	121.54
3	I	354	TRP	C-N-CA	5.11	131.30	121.54
2	D	32	TYR	N-CA-C	5.09	117.55	109.50
1	C	99	ASP	CA-C-N	5.03	127.02	120.28
1	C	99	ASP	C-N-CA	5.03	127.02	120.28
3	K	310	PHE	N-CA-C	5.00	116.73	111.28

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	18	0
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	7	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	92	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 (92) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:150:LYS:HB3	1:G:202:THR:HG1	1.61	0.65
1:G:19:ALA:CB	1:G:80:LEU:HD21	2.25	0.65
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
3:L:334:TRP:H	3:L:334:TRP:CD1	2.28	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
1:C:21:LEU:HD22	1:C:107:THR:HG21	1.94	0.49
3:J:314:GLN:HG2	3:J:315:ASP:N	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:207:ILE:HD12	2:D:209:ASN:HD21	1.79	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
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:F:99:MET:HE3	2:F:100:GLN:HE21	1.84	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%)	24	14
1	E	216/219 (99%)	210 (97%)	6 (3%)	0	100	100
1	G	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	14	5
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%)	14	5
3	J	103/112 (92%)	93 (90%)	9 (9%)	1 (1%)	12	4
3	K	102/112 (91%)	97 (95%)	5 (5%)	0	100	100
3	L	104/112 (93%)	98 (94%)	5 (5%)	1 (1%)	12	4
All	All	2139/2256 (95%)	2047 (96%)	86 (4%)	6 (0%)	36	26

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 ⓘ

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%)	45	32
1	C	183/188 (97%)	172 (94%)	11 (6%)	17	5
1	E	186/188 (99%)	185 (100%)	1 (0%)	81	80
1	G	186/188 (99%)	178 (96%)	8 (4%)	26	11
2	B	181/194 (93%)	178 (98%)	3 (2%)	53	41
2	D	176/194 (91%)	171 (97%)	5 (3%)	38	22
2	F	182/194 (94%)	176 (97%)	6 (3%)	33	17
2	H	179/194 (92%)	170 (95%)	9 (5%)	22	8
3	I	99/100 (99%)	96 (97%)	3 (3%)	36	20
3	J	93/100 (93%)	90 (97%)	3 (3%)	34	18
3	K	92/100 (92%)	86 (94%)	6 (6%)	15	4
3	L	95/100 (95%)	90 (95%)	5 (5%)	20	7
All	All	1835/1928 (95%)	1771 (96%)	64 (4%)	32	16

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	THR
1	A	110	GLU
1	A	174	LYS
1	A	210	VAL
2	B	24	VAL
2	B	64	ASN
2	B	109	MET
1	C	14	SER
1	C	22	SER
1	C	35	LEU
1	C	57	THR
1	C	83	GLU
1	C	110	GLU
1	C	128	GLU

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Mol	Chain	Res	Type
1	C	132	SER
1	C	155	VAL
1	C	159	LEU
1	C	186	LEU
2	D	16	GLU
2	D	98	HIS
2	D	150	LEU
2	D	196	VAL
2	D	198	SER
1	E	155	VAL
2	F	24	VAL
2	F	132	SER
2	F	140	SER
2	F	155	LYS
2	F	191	SER
2	F	221	LYS
1	G	35	LEU
1	G	98	SER
1	G	110	GLU
1	G	114	THR
1	G	126	SER
1	G	137	VAL
1	G	159	LEU
1	G	218	GLU
2	H	12	VAL
2	H	24	VAL
2	H	73	SER
2	H	85	VAL
2	H	98	HIS
2	H	133	VAL
2	H	160	GLU
2	H	168	SER
2	H	224	GLU
3	I	318	CYS
3	I	356	SER
3	I	358	THR
3	J	314	GLN
3	J	324	ILE
3	J	358	THR
3	K	314	GLN
3	K	318	CYS
3	K	359	GLN

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Mol	Chain	Res	Type
3	K	363	VAL
3	K	364	LEU
3	K	379	CYS
3	L	314	GLN
3	L	339	LYS
3	L	402	GLN
3	L	408	VAL
3	L	409	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	33	ASN
1	A	39	GLN
1	A	40	GLN
1	A	204	GLN
2	B	5	GLN
2	B	39	GLN
2	B	211	ASN
1	C	24	GLN
1	C	143	ASN
1	C	152	GLN
1	C	160	GLN
2	D	77	GLN
2	D	176	HIS
2	D	216	ASN
1	E	32	ASN
1	E	40	GLN
1	E	44	GLN
1	E	152	GLN
1	E	157	ASN
1	E	165	GLN
2	F	39	GLN
2	F	77	GLN
2	F	100	GLN
1	G	39	GLN
1	G	40	GLN
1	G	157	ASN
1	G	160	GLN
1	G	215	ASN
2	H	39	GLN

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Mol	Chain	Res	Type
2	H	167	ASN
2	H	183	GLN
2	H	216	ASN
3	I	360	HIS
3	J	314	GLN
3	J	342	ASN
3	K	312	ASN
3	K	314	GLN
3	K	336	HIS
3	K	342	ASN
3	K	383	GLN
3	K	405	ASN
3	L	336	HIS

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 oligosaccharides 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

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, 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(Å ²)	Q<0.9
1	A	217/219 (99%)	0.48	10 (4%) 37 42	27, 40, 58, 87	0
1	C	216/219 (98%)	0.81	14 (6%) 25 29	29, 42, 61, 82	0
1	E	218/219 (99%)	0.31	4 (1%) 67 74	22, 35, 53, 80	0
1	G	218/219 (99%)	1.01	45 (20%) 2 3	27, 44, 76, 97	0
2	B	221/233 (94%)	0.51	9 (4%) 41 46	24, 40, 57, 73	0
2	D	216/233 (92%)	0.64	11 (5%) 33 37	28, 43, 66, 88	0
2	F	221/233 (94%)	0.26	9 (4%) 41 46	22, 33, 54, 95	0
2	H	217/233 (93%)	0.68	17 (7%) 19 22	26, 42, 62, 78	0
3	I	112/112 (100%)	0.42	7 (6%) 26 30	23, 33, 59, 74	0
3	J	108/112 (96%)	0.77	14 (12%) 7 10	28, 39, 64, 80	0
3	K	106/112 (94%)	0.38	2 (1%) 66 73	25, 36, 52, 61	0
3	L	109/112 (97%)	0.64	9 (8%) 17 21	27, 39, 64, 82	0
All	All	2179/2256 (96%)	0.58	151 (6%) 23 27	22, 40, 62, 97	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	354	TRP	5.4
1	C	217	GLY	5.2
1	G	116	ALA	5.1
3	I	354	TRP	5.1
3	J	313	VAL	4.6
3	J	354	TRP	4.4
1	A	98	SER	4.3
1	G	210	VAL	4.1
2	D	201	LEU	4.1
1	E	219	CYS	4.1
1	G	206	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
3	I	414	SER	3.9
1	G	202	THR	3.9
3	L	318	CYS	3.9
3	L	356	SER	3.8
3	I	379	CYS	3.7
1	G	201	VAL	3.7
2	B	171	LEU	3.6
1	G	153	TRP	3.6
3	L	334	TRP	3.5
1	C	98	SER	3.5
1	G	191	TYR	3.4
1	G	158	ALA	3.4
3	J	349	ALA	3.3
3	J	397	THR	3.3
2	F	140	SER	3.3
1	G	154	LYS	3.3
1	G	199	CYS	3.3
1	G	196	VAL	3.2
3	L	303	ALA	3.2
2	D	225	PRO	3.2
1	C	189	ALA	3.2
2	F	148	ALA	3.2
1	G	207	SER	3.2
1	E	199	CYS	3.2
1	A	132	SER	3.1
1	G	134	THR	3.1
3	J	318	CYS	3.1
1	G	151	VAL	3.0
2	H	162	VAL	3.0
1	G	185	THR	3.0
2	F	202	GLY	2.9
1	C	85	PHE	2.9
3	L	351	PRO	2.9
2	F	73	SER	2.9
1	E	155	VAL	2.9
2	H	219	VAL	2.9
2	B	86	THR	2.9
3	J	303	ALA	2.9
1	G	205	GLY	2.9
1	G	157	ASN	2.8
2	B	201	LEU	2.8
1	G	145	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	139	SER	2.8
3	J	309	CYS	2.8
1	G	144	PHE	2.8
3	K	351	PRO	2.8
1	G	198	ALA	2.7
1	C	130	LEU	2.7
2	D	74	SER	2.7
3	I	355	SER	2.7
1	A	218	GLU	2.7
1	G	189	ALA	2.7
1	C	134	THR	2.7
2	D	196	VAL	2.7
1	G	135	ALA	2.6
3	J	351	PRO	2.6
1	G	133	GLY	2.6
1	G	197	TYR	2.6
2	F	203	THR	2.6
2	B	95	CYS	2.6
2	D	9	PRO	2.6
1	G	130	LEU	2.6
1	G	121	PHE	2.6
2	H	132	SER	2.6
1	G	209	PRO	2.5
3	I	352	TYR	2.5
1	G	150	LYS	2.5
1	C	210	VAL	2.5
3	L	313	VAL	2.5
1	G	159	LEU	2.5
2	D	207	ILE	2.5
1	G	155	VAL	2.5
1	A	11	LEU	2.5
1	C	156	ASP	2.5
1	C	196	VAL	2.5
2	H	164	VAL	2.5
1	G	118	PRO	2.5
1	C	158	ALA	2.4
3	J	357	ASP	2.4
2	H	194	VAL	2.4
1	G	141	LEU	2.4
2	D	109	MET	2.4
1	A	119	SER	2.4
2	D	171	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	106	THR	2.4
1	G	146	PRO	2.4
2	B	214	PRO	2.4
1	G	115	VAL	2.4
1	G	132	SER	2.4
1	A	174	LYS	2.4
2	H	2	GLN	2.3
3	L	357	ASP	2.3
2	B	225	PRO	2.3
2	H	138	PRO	2.3
2	F	201	LEU	2.3
1	C	157	ASN	2.3
3	J	310	PHE	2.3
2	B	148	ALA	2.3
2	H	161	PRO	2.3
2	D	202	GLY	2.3
1	C	155	VAL	2.3
2	H	147	THR	2.3
3	L	327	LYS	2.3
1	A	19	ALA	2.2
1	G	117	ALA	2.2
3	K	414	SER	2.2
1	C	133	GLY	2.2
1	C	209	PRO	2.2
2	F	229	ASP	2.2
3	I	356	SER	2.2
1	E	157	ASN	2.2
1	G	188	LYS	2.2
3	I	311	ARG	2.2
1	A	134	THR	2.2
2	H	217	THR	2.2
2	D	197	PRO	2.2
1	G	122	ILE	2.2
2	B	196	VAL	2.2
2	D	205	THR	2.2
2	F	228	CYS	2.2
1	G	186	LEU	2.2
2	H	136	LEU	2.2
1	G	218	GLU	2.1
3	J	308	TYR	2.1
2	H	210	VAL	2.1
1	G	119	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	131	LYS	2.1
1	G	113	ARG	2.1
1	G	203	HIS	2.1
2	H	152	CYS	2.1
3	J	350	CYS	2.1
2	H	87	ALA	2.1
2	H	213	LYS	2.1
1	A	215	ASN	2.1
2	H	214	PRO	2.1
3	J	307	ALA	2.1
1	A	80	LEU	2.0
1	G	200	GLU	2.0
2	F	227	SER	2.0
3	J	316	ASN	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 oligosaccharides 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.