Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 10:52 AM JST

PDB ID	:	7X8T
Title	:	Frizzled 10 CRD in complex with hB9L9.3 Fab
Authors	:	Ge, Q.; Wang, Q.
Deposited on	:	2022-03-14
Resolution	:	2.51 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:

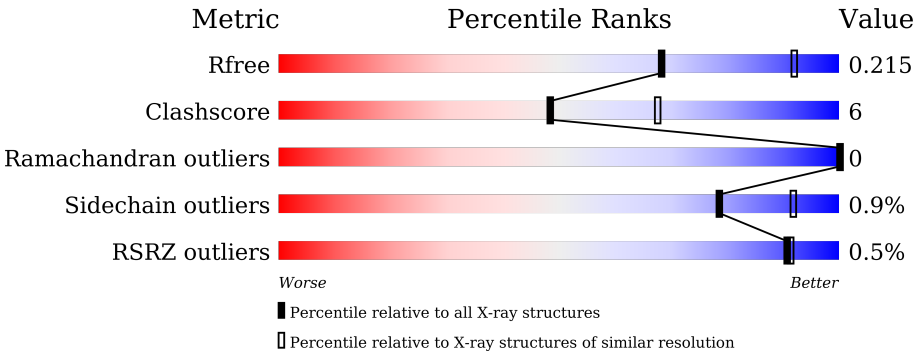
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.51 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	129	4% 81% 11% • 8%
1	D	129	2% 80% 12% • 8%
1	G	129	2% 78% 15% 8%
1	J	129	80% 12% 8%
2	B	212	89% 9% •
2	E	212	88% 10% •

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Mol	Chain	Length	Quality of chain
2	H	212	84% 14%
2	K	212	89% 9%
3	C	237	83% 10% 8%
3	F	237	81% 11% 8%
3	I	237	84% 8% 8%
3	L	237	78% 14% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17636 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 Frizzled-10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	119	Total	C	N	O	S	0	0	0
			954	602	165	169	18			
1	D	119	Total	C	N	O	S	0	0	0
			954	602	165	169	18			
1	G	119	Total	C	N	O	S	0	0	0
			954	602	165	169	18			
1	J	119	Total	C	N	O	S	0	0	0
			954	602	165	169	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	GLN	ASN	engineered mutation	UNP Q9ULW2
D	48	GLN	ASN	engineered mutation	UNP Q9ULW2
G	48	GLN	ASN	engineered mutation	UNP Q9ULW2
J	48	GLN	ASN	engineered mutation	UNP Q9ULW2

- Molecule 2 is a protein called Antibody hB9L9.3 Fab, Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	209	Total	C	N	O	S	0	0	0
			1553	971	257	321	4			
2	E	209	Total	C	N	O	S	0	0	0
			1553	971	257	321	4			
2	H	209	Total	C	N	O	S	0	0	0
			1553	971	257	321	4			
2	K	209	Total	C	N	O	S	0	0	0
			1553	971	257	321	4			

- Molecule 3 is a protein called Antibody hB9L9.3 Fab, Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	219	Total	C	N	O	S	0	0	0
			1616	1020	269	321	6			
3	F	219	Total	C	N	O	S	0	0	0
			1616	1020	269	321	6			
3	I	219	Total	C	N	O	S	0	0	0
			1616	1020	269	321	6			
3	L	219	Total	C	N	O	S	0	0	0
			1616	1020	269	321	6			

- Molecule 4 is water.

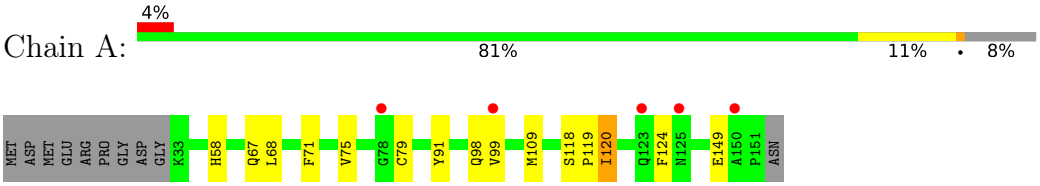
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	112	Total	O	0	0
			112	112		
4	C	142	Total	O	0	0
			142	142		
4	D	27	Total	O	0	0
			27	27		
4	E	101	Total	O	0	0
			101	101		
4	F	152	Total	O	0	0
			152	152		
4	G	35	Total	O	0	0
			35	35		
4	H	120	Total	O	0	0
			120	120		
4	I	133	Total	O	0	0
			133	133		
4	J	34	Total	O	0	0
			34	34		
4	K	121	Total	O	0	0
			121	121		
4	L	135	Total	O	0	0
			135	135		

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.

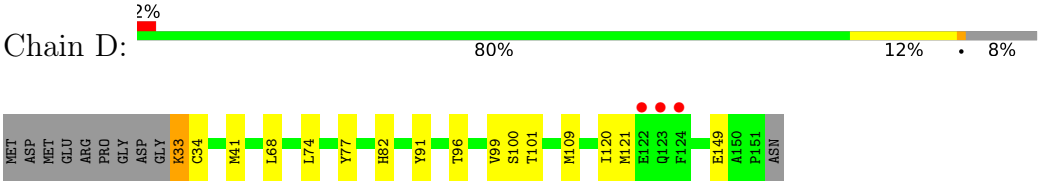
• Molecule 1: Frizzled-10

Chain A:



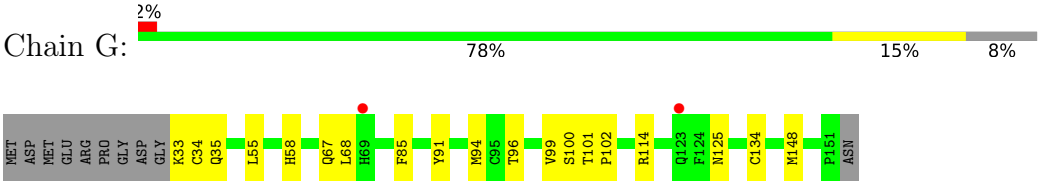
• Molecule 1: Frizzled-10

Chain D:



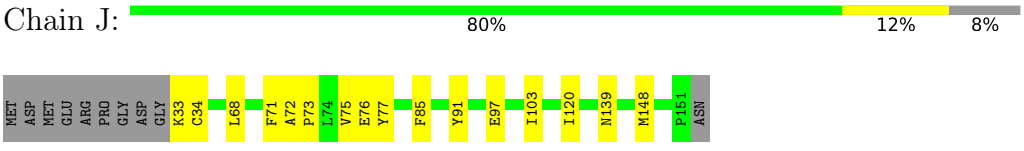
• Molecule 1: Frizzled-10

Chain G:



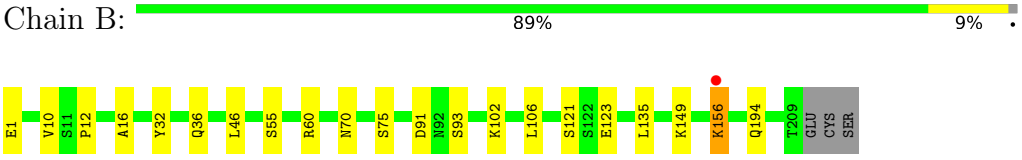
• Molecule 1: Frizzled-10

Chain J:



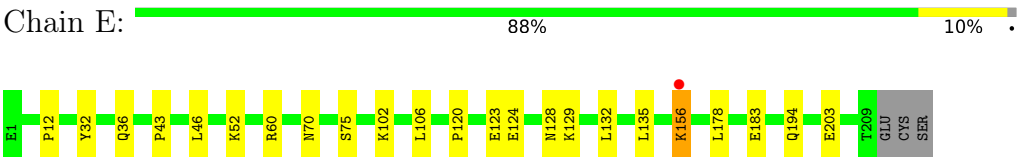
• Molecule 2: Antibody hB9L9.3 Fab, Light chain

Chain B:



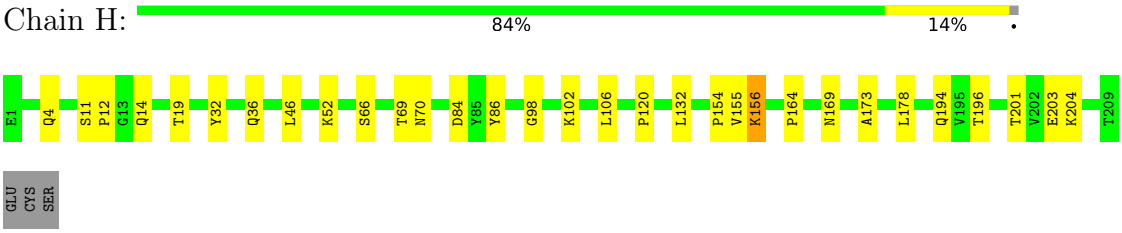
• Molecule 2: Antibody hB9L9.3 Fab, Light chain

Chain E:



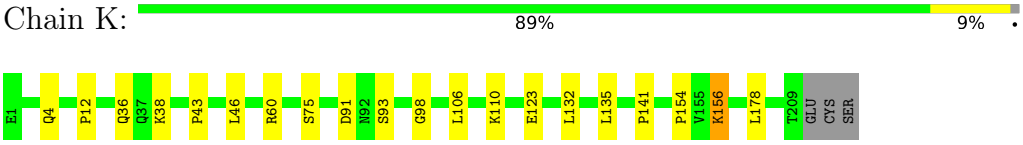
• Molecule 2: Antibody hB9L9.3 Fab, Light chain

Chain H:



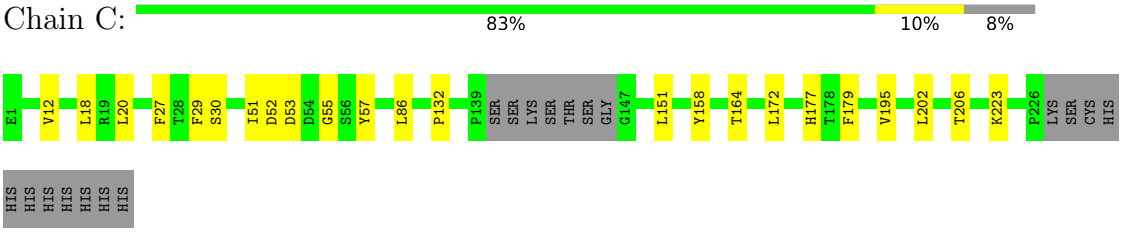
• Molecule 2: Antibody hB9L9.3 Fab, Light chain

Chain K:



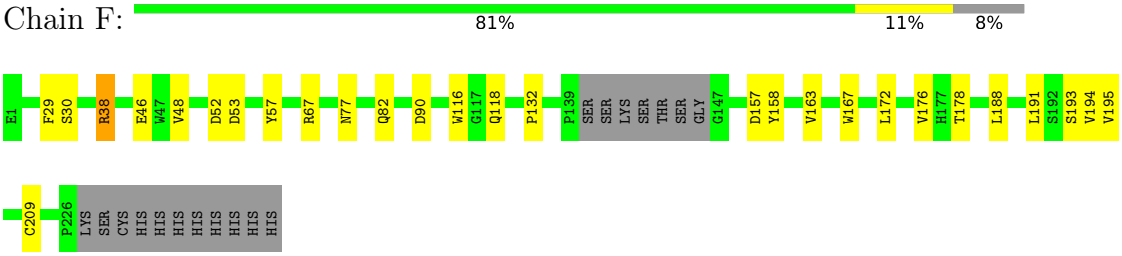
• Molecule 3: Antibody hB9L9.3 Fab, Heavy chain

Chain C:



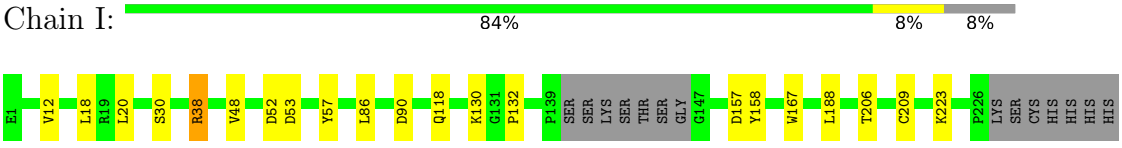
• Molecule 3: Antibody hB9L9.3 Fab, Heavy chain

Chain F:



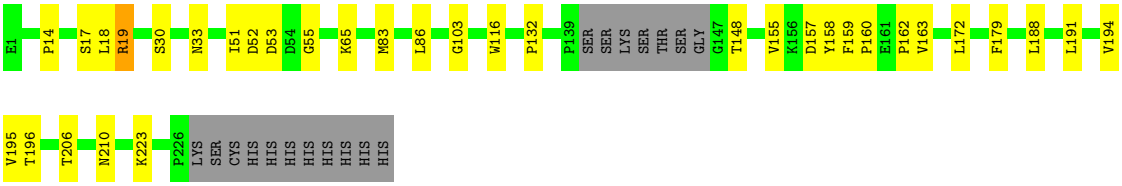
• Molecule 3: Antibody hB9L9.3 Fab, Heavy chain

Chain I:



• Molecule 3: Antibody hB9L9.3 Fab, Heavy chain

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	75.46Å 100.79Å 99.15Å 110.07° 89.94° 113.79°	Depositor
Resolution (Å)	46.06 – 2.51 48.83 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.1 (46.06-2.51) 98.2 (48.83-2.51)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.25 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.176 , 0.215 0.175 , 0.215	Depositor DCC
R_{free} test set	4123 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.000 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17636	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.9932e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.60	0/980	0.74	0/1325
1	D	0.55	0/980	0.69	0/1325
1	G	0.55	0/980	0.66	0/1325
1	J	0.57	0/980	0.74	0/1325
2	B	0.59	0/1593	0.71	0/2177
2	E	0.64	0/1593	0.71	0/2177
2	H	0.57	0/1593	0.69	0/2177
2	K	0.58	0/1593	0.69	0/2177
3	C	0.58	0/1655	0.70	0/2255
3	F	0.75	0/1655	0.77	0/2255
3	I	0.59	0/1655	0.73	0/2255
3	L	0.75	0/1655	0.77	0/2255
All	All	0.62	0/16912	0.72	0/23028

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	954	0	923	12	0
1	D	954	0	923	10	0
1	G	954	0	923	19	0
1	J	954	0	923	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1553	0	1486	15	0
2	E	1553	0	1486	21	0
2	H	1553	0	1486	23	0
2	K	1553	0	1486	15	0
3	C	1616	0	1561	14	0
3	F	1616	0	1561	19	0
3	I	1616	0	1561	16	0
3	L	1616	0	1561	32	0
4	A	32	0	0	0	0
4	B	112	0	0	1	0
4	C	142	0	0	1	0
4	D	27	0	0	1	0
4	E	101	0	0	2	0
4	F	152	0	0	2	0
4	G	35	0	0	2	0
4	H	120	0	0	1	0
4	I	133	0	0	2	0
4	J	34	0	0	1	0
4	K	121	0	0	2	0
4	L	135	0	0	0	0
All	All	17636	0	15880	195	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 (195) 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:96:THR:H	1:G:99:VAL:CG2	1.76	0.96
1:G:96:THR:H	1:G:99:VAL:HG22	1.27	0.96
1:A:120:ILE:HD11	1:A:124:PHE:CZ	2.06	0.91
1:G:96:THR:N	1:G:99:VAL:HG22	1.87	0.88
2:K:36:GLN:HB2	2:K:46:LEU:HD11	1.63	0.78
1:G:96:THR:N	1:G:99:VAL:CG2	2.44	0.78
1:D:96:THR:H	1:D:99:VAL:HG22	1.50	0.74
2:E:36:GLN:HB2	2:E:46:LEU:HD11	1.68	0.74
2:H:36:GLN:HB2	2:H:46:LEU:HD11	1.68	0.74
2:E:52:LYS:NZ	4:E:301:HOH:O	2.22	0.71
3:F:176:VAL:HG22	3:F:195:VAL:HG22	1.74	0.70
3:C:206:THR:HG23	3:C:223:LYS:HE3	1.75	0.69
3:L:33:ASN:HD21	3:L:103:GLY:H	1.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:206:THR:HG23	3:L:223:LYS:HE3	1.73	0.68
2:B:36:GLN:HB2	2:B:46:LEU:HD11	1.74	0.68
2:K:4:GLN:HE21	2:K:98:GLY:HA3	1.61	0.66
1:J:139:ASN:HB2	4:J:210:HOH:O	1.96	0.66
2:E:156:LYS:HD3	2:E:156:LYS:H	1.60	0.66
1:J:68:LEU:HG	1:J:91:TYR:CD2	2.30	0.66
1:J:71:PHE:O	1:J:75:VAL:HG23	1.96	0.66
3:L:148:THR:CG2	3:L:196:THR:HG23	2.26	0.66
3:L:148:THR:HG23	3:L:196:THR:HG23	1.78	0.66
1:A:120:ILE:HD11	1:A:124:PHE:CE2	2.31	0.65
2:E:123:GLU:HG3	4:E:384:HOH:O	1.95	0.65
2:B:55:SER:HB2	2:H:169:ASN:HB3	1.79	0.64
3:C:164:THR:HG22	4:C:315:HOH:O	1.96	0.64
3:F:118:GLN:NE2	4:F:302:HOH:O	2.31	0.64
3:I:38:ARG:HD2	3:I:48:VAL:HG22	1.78	0.63
2:H:154:PRO:HG2	2:H:156:LYS:HE2	1.79	0.63
3:I:38:ARG:NH2	3:I:90:ASP:OD1	2.32	0.63
3:I:130:LYS:NZ	4:I:301:HOH:O	2.31	0.62
2:E:129:LYS:HZ3	3:L:14:PRO:HB2	1.65	0.61
2:K:12:PRO:HD3	2:K:106:LEU:O	2.02	0.60
1:G:96:THR:OG1	1:G:99:VAL:HG13	2.01	0.60
2:H:196:THR:OG1	2:H:201:THR:HG22	2.02	0.59
3:L:18:LEU:HD12	3:L:18:LEU:O	2.03	0.59
2:K:154:PRO:HG2	2:K:156:LYS:NZ	2.17	0.59
2:H:14:GLN:HG3	3:L:19:ARG:HB2	1.85	0.59
3:F:38:ARG:HD3	3:F:46:GLU:OE1	2.03	0.59
3:F:30:SER:O	3:F:53:ASP:HB3	2.04	0.58
3:F:38:ARG:HD2	3:F:48:VAL:HG22	1.84	0.58
1:G:99:VAL:O	1:G:99:VAL:HG23	2.04	0.58
3:F:38:ARG:NH2	3:F:90:ASP:OD1	2.35	0.58
1:A:68:LEU:HG	1:A:91:TYR:CD2	2.39	0.57
3:F:132:PRO:HB3	3:F:158:TYR:HB3	1.86	0.57
2:E:156:LYS:H	2:E:156:LYS:CD	2.16	0.57
2:E:135:LEU:HD13	3:F:194:VAL:HG21	1.87	0.57
3:F:157:ASP:HB3	3:F:188:LEU:HD13	1.85	0.56
3:I:30:SER:O	3:I:53:ASP:HB3	2.05	0.56
2:B:123:GLU:OE1	2:B:123:GLU:N	2.21	0.56
2:E:128:ASN:O	2:E:129:LYS:HD2	2.07	0.55
3:I:38:ARG:NH2	3:I:90:ASP:HA	2.22	0.55
3:F:82:GLN:HB3	4:F:438:HOH:O	2.08	0.54
2:K:110:LYS:NZ	4:K:306:HOH:O	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:51:ILE:HD11	3:C:55:GLY:HA2	1.90	0.54
2:E:32:TYR:CD2	2:E:70:ASN:HB2	2.43	0.54
2:H:11:SER:OG	3:L:19:ARG:HG2	2.07	0.54
3:L:157:ASP:HB3	3:L:188:LEU:HD13	1.89	0.54
2:H:194:GLN:NE2	2:H:203:GLU:OE2	2.39	0.54
3:L:191:LEU:C	3:L:191:LEU:HD12	2.28	0.54
2:E:12:PRO:HD3	2:E:106:LEU:O	2.08	0.53
3:L:148:THR:HG23	3:L:196:THR:CG2	2.37	0.53
1:A:120:ILE:CD1	1:A:124:PHE:CZ	2.88	0.53
3:F:172:LEU:HD21	3:F:195:VAL:HG11	1.89	0.53
2:E:124:GLU:HG2	2:E:129:LYS:HB2	1.91	0.53
2:K:132:LEU:HD12	2:K:178:LEU:HD23	1.90	0.52
3:L:148:THR:CG2	3:L:196:THR:CG2	2.87	0.52
2:E:129:LYS:NZ	3:L:14:PRO:HB2	2.25	0.52
2:E:132:LEU:HD12	2:E:178:LEU:HD23	1.92	0.52
3:L:30:SER:O	3:L:53:ASP:HB3	2.09	0.52
3:L:132:PRO:HB3	3:L:158:TYR:HB3	1.91	0.52
2:E:120:PRO:HD3	2:E:132:LEU:CD2	2.40	0.52
3:L:33:ASN:HD22	3:L:52:ASP:HA	1.75	0.52
1:J:33:LYS:CG	1:J:34:CYS:H	2.23	0.51
2:K:154:PRO:HG2	2:K:156:LYS:HZ2	1.74	0.51
2:H:11:SER:O	2:H:14:GLN:HB2	2.11	0.51
3:I:52:ASP:OD1	3:I:57:TYR:N	2.42	0.51
1:J:72:ALA:O	1:J:76:GLU:HG2	2.11	0.51
2:E:120:PRO:HD3	2:E:132:LEU:HD23	1.93	0.51
2:H:4:GLN:HE22	2:H:86:TYR:HA	1.77	0.50
1:G:114:ARG:HD2	4:G:222:HOH:O	2.10	0.50
1:A:120:ILE:HG13	1:A:120:ILE:O	2.11	0.50
1:D:33:LYS:HD2	1:D:34:CYS:O	2.12	0.50
2:K:38:LYS:NZ	4:K:312:HOH:O	2.45	0.50
3:L:33:ASN:ND2	3:L:103:GLY:H	2.07	0.50
3:I:118:GLN:NE2	4:I:303:HOH:O	2.42	0.50
2:H:4:GLN:HE21	2:H:98:GLY:HA3	1.77	0.50
3:C:12:VAL:HG21	3:C:86:LEU:CD1	2.41	0.50
3:F:191:LEU:HD12	3:F:191:LEU:C	2.33	0.49
2:K:123:GLU:OE1	2:K:123:GLU:N	2.37	0.49
2:B:10:VAL:HG11	2:B:16:ALA:HB2	1.94	0.49
2:B:149:LYS:HE2	2:B:194:GLN:OE1	2.11	0.49
3:L:33:ASN:ND2	3:L:52:ASP:HA	2.26	0.49
3:F:178:THR:HA	3:F:193:SER:HA	1.94	0.49
1:A:118:SER:HB3	1:A:119:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:PRO:HD3	2:H:106:LEU:O	2.12	0.49
2:E:135:LEU:HD13	3:F:194:VAL:CG2	2.43	0.49
3:I:12:VAL:HG21	3:I:86:LEU:HD12	1.94	0.49
3:I:132:PRO:HB3	3:I:158:TYR:HB3	1.94	0.48
3:F:52:ASP:OD1	3:F:57:TYR:N	2.39	0.48
2:B:123:GLU:H	2:B:123:GLU:CD	2.07	0.48
3:C:30:SER:O	3:C:53:ASP:HB3	2.13	0.48
2:H:32:TYR:CD2	2:H:70:ASN:HB2	2.48	0.48
1:J:77:TYR:CE1	1:J:120:ILE:HG13	2.48	0.48
3:I:157:ASP:HB3	3:I:188:LEU:HD13	1.95	0.48
1:A:71:PHE:O	1:A:75:VAL:HG13	2.13	0.47
2:B:60:ARG:HB2	2:B:75:SER:O	2.14	0.47
1:D:77:TYR:CZ	1:D:120:ILE:HD13	2.50	0.47
2:B:91:ASP:HB3	2:B:93:SER:H	1.80	0.47
1:D:68:LEU:HG	1:D:91:TYR:CD2	2.50	0.47
3:L:172:LEU:HD21	3:L:195:VAL:HG21	1.97	0.47
3:C:132:PRO:HB3	3:C:158:TYR:HB3	1.95	0.47
2:E:43:PRO:HB2	3:F:116:TRP:CE2	2.50	0.47
1:G:125:ASN:O	1:G:125:ASN:ND2	2.48	0.47
2:K:110:LYS:HD3	2:K:141:PRO:HD3	1.97	0.47
2:H:19:THR:HG23	2:H:69:THR:HG23	1.96	0.47
2:B:121:SER:HB2	2:B:123:GLU:OE1	2.15	0.46
3:I:206:THR:HG23	3:I:223:LYS:HE3	1.97	0.46
3:C:12:VAL:HG21	3:C:86:LEU:HD13	1.96	0.46
2:E:194:GLN:NE2	2:E:203:GLU:OE2	2.45	0.46
3:L:33:ASN:HD21	3:L:103:GLY:N	2.10	0.46
1:A:109:MET:HE1	1:A:149:GLU:OE1	2.15	0.46
2:K:135:LEU:CD1	3:L:194:VAL:HG11	2.46	0.46
2:H:120:PRO:HD3	2:H:132:LEU:HD23	1.98	0.46
1:D:109:MET:HE3	1:D:149:GLU:HG2	1.98	0.46
2:E:183:GLU:H	2:E:183:GLU:CD	2.20	0.46
1:D:109:MET:CE	1:D:149:GLU:HG2	2.46	0.46
3:I:12:VAL:HG21	3:I:86:LEU:CD1	2.46	0.46
3:L:51:ILE:HD11	3:L:55:GLY:HA2	1.97	0.46
3:F:167:TRP:CH2	3:F:209:CYS:HB3	2.51	0.45
3:L:65:LYS:HB2	3:L:65:LYS:HE3	1.82	0.45
1:A:109:MET:CE	1:A:149:GLU:OE1	2.63	0.45
1:J:103:ILE:HG22	1:J:148:MET:HG3	1.98	0.45
2:H:66:SER:O	2:H:69:THR:HB	2.17	0.45
2:K:91:ASP:HB3	2:K:93:SER:H	1.82	0.45
1:G:96:THR:CA	1:G:99:VAL:HG22	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:72:ALA:N	1:J:73:PRO:CD	2.80	0.45
2:B:156:LYS:HD3	2:B:156:LYS:H	1.81	0.44
1:G:68:LEU:HG	1:G:91:TYR:CD2	2.52	0.44
2:K:60:ARG:HB2	2:K:75:SER:O	2.17	0.44
3:C:27:PHE:CE2	3:C:29:PHE:HA	2.52	0.44
1:J:72:ALA:HB3	1:J:73:PRO:HD3	1.99	0.44
2:B:32:TYR:CD2	2:B:70:ASN:HB2	2.52	0.44
3:L:18:LEU:HD12	3:L:18:LEU:C	2.37	0.44
3:C:202:LEU:HD23	3:C:202:LEU:HA	1.86	0.44
2:H:132:LEU:HD12	2:H:178:LEU:HD23	2.00	0.44
2:E:52:LYS:HB3	2:E:52:LYS:HE3	1.84	0.43
2:B:12:PRO:HD3	2:B:106:LEU:O	2.17	0.43
2:B:135:LEU:HB3	3:C:179:PHE:CZ	2.53	0.43
3:C:18:LEU:HD13	3:C:20:LEU:HG	2.00	0.43
3:L:18:LEU:HB3	3:L:86:LEU:HD11	1.99	0.43
3:C:52:ASP:OD1	3:C:57:TYR:N	2.42	0.43
1:G:58:HIS:NE2	1:G:67:GLN:HG3	2.33	0.43
3:I:18:LEU:HD13	3:I:20:LEU:HG	1.99	0.43
1:D:100:SER:OG	1:D:101:THR:HG23	2.18	0.43
2:E:60:ARG:HB2	2:E:75:SER:O	2.19	0.43
1:D:74:LEU:HD11	1:D:121:MET:HG2	1.99	0.43
2:H:52:LYS:HD2	4:H:351:HOH:O	2.19	0.43
1:D:82:HIS:HD2	4:D:227:HOH:O	2.01	0.42
1:D:96:THR:OG1	1:D:99:VAL:HG13	2.19	0.42
2:H:155:VAL:HG11	2:H:178:LEU:HD11	2.01	0.42
2:H:14:GLN:CG	3:L:19:ARG:HB2	2.48	0.42
1:A:79:CYS:HB3	1:A:120:ILE:HG21	2.01	0.42
1:G:94:MET:CE	1:G:99:VAL:HG11	2.49	0.42
1:J:97:GLU:CD	1:J:97:GLU:H	2.23	0.42
3:F:29:PHE:CD2	3:F:77:ASN:HA	2.54	0.42
3:L:18:LEU:HG	3:L:83:MET:HB3	2.01	0.42
1:A:98:GLN:HG2	1:A:99:VAL:HG23	2.02	0.42
3:C:172:LEU:HD21	3:C:195:VAL:HG21	2.01	0.42
3:I:38:ARG:HD2	3:I:48:VAL:CG2	2.46	0.42
1:J:33:LYS:HG3	1:J:34:CYS:H	1.84	0.42
1:G:114:ARG:NH1	1:G:134:CYS:SG	2.93	0.41
2:K:43:PRO:HB2	3:L:116:TRP:CE2	2.54	0.41
1:G:99:VAL:CG2	1:G:99:VAL:O	2.68	0.41
3:L:159:PHE:HA	3:L:160:PRO:HA	1.76	0.41
2:H:204:LYS:HA	2:H:204:LYS:HD3	1.84	0.41
2:K:135:LEU:HB3	3:L:179:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:34:CYS:O	1:G:35:GLN:NE2	2.53	0.41
3:I:167:TRP:CH2	3:I:209:CYS:HB3	2.56	0.41
2:H:84:ASP:OD1	2:H:102:LYS:HG2	2.20	0.41
1:A:58:HIS:NE2	1:A:67:GLN:HG3	2.35	0.41
2:H:164:PRO:HA	2:H:173:ALA:O	2.20	0.41
1:G:85:PHE:CZ	1:G:148:MET:HE3	2.56	0.41
3:C:151:LEU:HD12	3:C:151:LEU:C	2.41	0.41
2:H:120:PRO:HD3	2:H:132:LEU:CD2	2.50	0.41
1:G:114:ARG:CD	4:G:222:HOH:O	2.66	0.41
2:B:1:GLU:HB3	4:B:393:HOH:O	2.21	0.40
2:B:102:LYS:HA	2:B:102:LYS:HD2	1.93	0.40
1:G:55:LEU:HD21	1:G:102:PRO:HB2	2.03	0.40
3:I:86:LEU:HD23	3:I:86:LEU:HA	1.74	0.40
3:L:17:SER:HB3	3:L:19:ARG:HE	1.86	0.40
3:F:67:ARG:HH11	3:F:67:ARG:HD2	1.77	0.40
1:J:85:PHE:CZ	1:J:148:MET:HE3	2.56	0.40
3:L:155:VAL:HG11	3:L:163:VAL:HG11	2.02	0.40
1:G:33:LYS:HB3	1:G:34:CYS:H	1.66	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	117/129 (91%)	113 (97%)	4 (3%)	0	100	100
1	D	117/129 (91%)	112 (96%)	5 (4%)	0	100	100
1	G	117/129 (91%)	113 (97%)	4 (3%)	0	100	100
1	J	117/129 (91%)	112 (96%)	5 (4%)	0	100	100
2	B	207/212 (98%)	202 (98%)	5 (2%)	0	100	100
2	E	207/212 (98%)	201 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	207/212 (98%)	201 (97%)	6 (3%)	0	100	100
2	K	207/212 (98%)	202 (98%)	5 (2%)	0	100	100
3	C	215/237 (91%)	210 (98%)	5 (2%)	0	100	100
3	F	215/237 (91%)	209 (97%)	6 (3%)	0	100	100
3	I	215/237 (91%)	210 (98%)	5 (2%)	0	100	100
3	L	215/237 (91%)	209 (97%)	6 (3%)	0	100	100
All	All	2156/2312 (93%)	2094 (97%)	62 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	108/116 (93%)	107 (99%)	1 (1%)	78	92
1	D	108/116 (93%)	106 (98%)	2 (2%)	57	80
1	G	108/116 (93%)	106 (98%)	2 (2%)	57	80
1	J	108/116 (93%)	108 (100%)	0	100	100
2	B	171/174 (98%)	170 (99%)	1 (1%)	86	95
2	E	171/174 (98%)	169 (99%)	2 (1%)	71	88
2	H	171/174 (98%)	170 (99%)	1 (1%)	86	95
2	K	171/174 (98%)	170 (99%)	1 (1%)	86	95
3	C	176/193 (91%)	175 (99%)	1 (1%)	86	95
3	F	176/193 (91%)	174 (99%)	2 (1%)	73	89
3	I	176/193 (91%)	175 (99%)	1 (1%)	86	95
3	L	176/193 (91%)	173 (98%)	3 (2%)	60	82
All	All	1820/1932 (94%)	1803 (99%)	17 (1%)	78	92

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	ILE
2	B	156	LYS
3	C	177	HIS
1	D	33	LYS
1	D	41	MET
2	E	102	LYS
2	E	156	LYS
3	F	38	ARG
3	F	163	VAL
1	G	100	SER
1	G	101	THR
2	H	156	LYS
3	I	38	ARG
2	K	156	LYS
3	L	19	ARG
3	L	162	PRO
3	L	210	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	D	48	GLN
3	F	13	GLN
1	G	35	GLN
1	G	125	ASN
2	H	4	GLN
3	I	82	GLN
2	K	4	GLN
3	L	33	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	119/129 (92%)	-0.09	5 (4%) 36 39	30, 45, 79, 98	0
1	D	119/129 (92%)	-0.15	3 (2%) 57 61	28, 44, 76, 93	0
1	G	119/129 (92%)	-0.22	2 (1%) 70 72	28, 44, 78, 88	0
1	J	119/129 (92%)	-0.24	0 100 100	28, 44, 74, 88	0
2	B	209/212 (98%)	-0.44	1 (0%) 91 91	26, 36, 53, 81	0
2	E	209/212 (98%)	-0.43	1 (0%) 91 91	26, 35, 49, 67	0
2	H	209/212 (98%)	-0.44	0 100 100	25, 34, 49, 78	0
2	K	209/212 (98%)	-0.55	0 100 100	24, 33, 46, 67	0
3	C	219/237 (92%)	-0.58	0 100 100	25, 35, 51, 63	0
3	F	219/237 (92%)	-0.60	0 100 100	25, 32, 47, 59	0
3	I	219/237 (92%)	-0.54	0 100 100	24, 32, 47, 66	0
3	L	219/237 (92%)	-0.50	0 100 100	23, 31, 45, 56	0
All	All	2188/2312 (94%)	-0.44	12 (0%) 91 91	23, 35, 63, 98	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	125	ASN	3.0
1	D	123	GLN	2.8
1	A	123	GLN	2.7
1	A	78	GLY	2.6
1	D	124	PHE	2.3
2	E	156	LYS	2.3
1	G	123	GLN	2.3
2	B	156	LYS	2.2
1	D	122	GLU	2.1
1	A	150	ALA	2.0
1	A	99	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	69	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.