Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2024 – 01:15 pm BST

PDB ID	:	8ONK
Title	:	Human insulin in complex with the analytical antibody S1 Fab and the analytical antibody HUI-001 Fab
Authors	:	Johansson, E.
Deposited on	:	2023-04-03
Resolution	:	3.40 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:

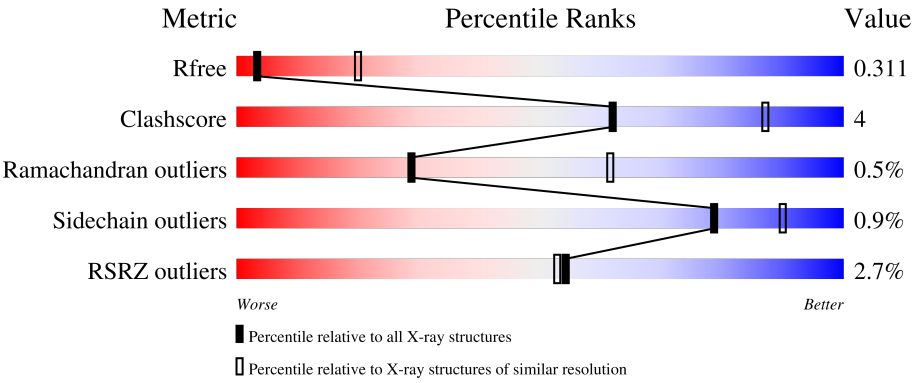
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	C	223	3% 88% 8% ·
1	H	223	% 85% 11% ·
2	E	213	2% 84% 15% ·
2	L	213	% 85% 13% ••
3	D	21	86% 14%

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Mol	Chain	Length	Quality of chain
3	I	21	67% 33%
4	A	30	13% 93% 7%
4	B	30	3% 90% 7%
5	F	215	% 88% 11%
5	J	215	5% 88% 11%
6	G	220	% 85% 13%
6	K	220	5% 86% 12%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13887 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 Heavy chain of analytical antibody S1 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	214	Total	C	N	O	S	0	0	0
			1649	1042	277	324	6			
1	C	215	Total	C	N	O	S	0	0	0
			1653	1044	278	325	6			

- Molecule 2 is a protein called Light chain of analytical antibody S1 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	0	0
			1622	1011	270	332	9			
2	E	211	Total	C	N	O	S	0	0	0
			1622	1011	270	332	9			

- Molecule 3 is a protein called Insulin A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
3	D	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			

- Molecule 4 is a protein called Insulin B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	28	Total	C	N	O	S	0	0	0
			225	148	37	38	2			
4	A	28	Total	C	N	O	S	0	0	0
			225	148	37	38	2			

- Molecule 5 is a protein called Light chain of analytical antibody HUI-001 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	215	Total	C	N	O	S	0	0	0
			1652	1027	278	338	9			
5	J	214	Total	C	N	O	S	0	0	0
			1645	1024	277	336	8			

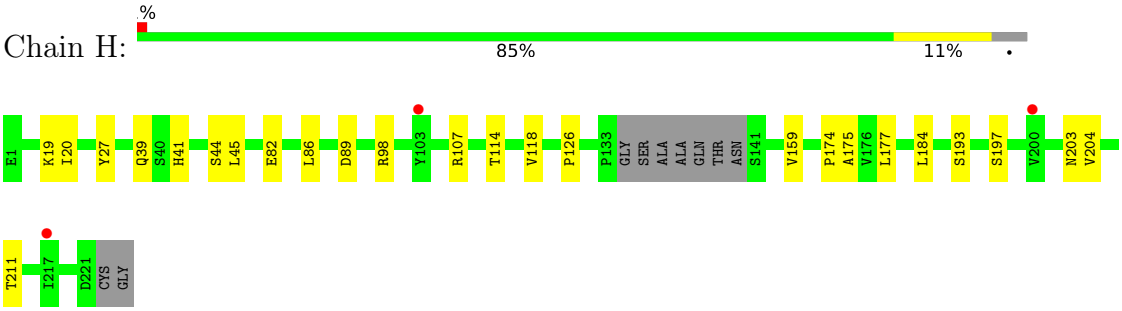
- Molecule 6 is a protein called Heavy chain of analytical antibody HUI-001 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	217	Total	C	N	O	S	0	0	0
			1634	1039	269	319	7			
6	K	217	Total	C	N	O	S	0	0	0
			1634	1039	269	319	7			

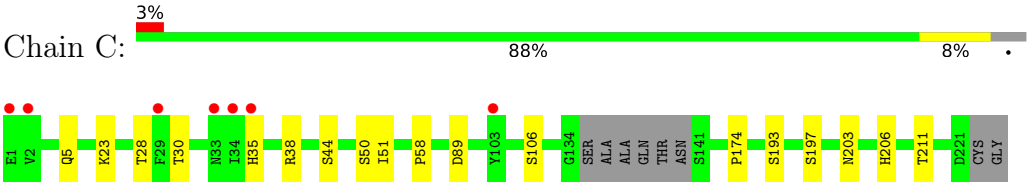
3 Residue-property plots (i)

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.

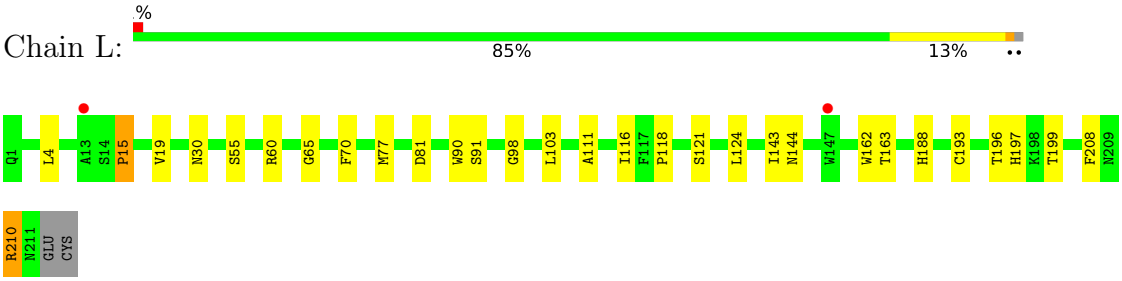
• Molecule 1: Heavy chain of analytical antibody S1 Fab



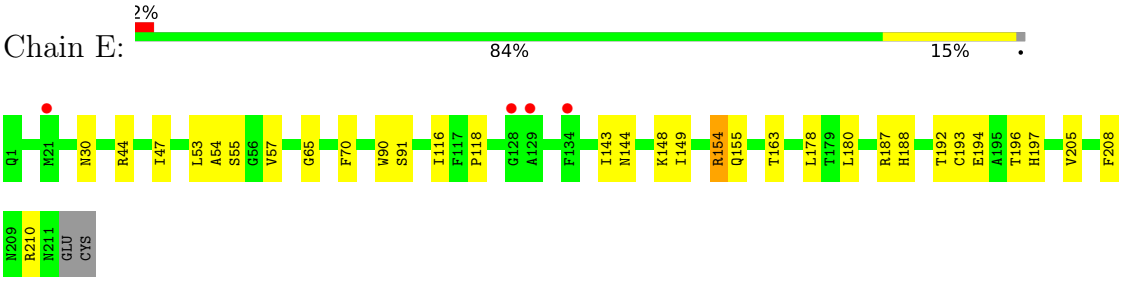
• Molecule 1: Heavy chain of analytical antibody S1 Fab



• Molecule 2: Light chain of analytical antibody S1 Fab

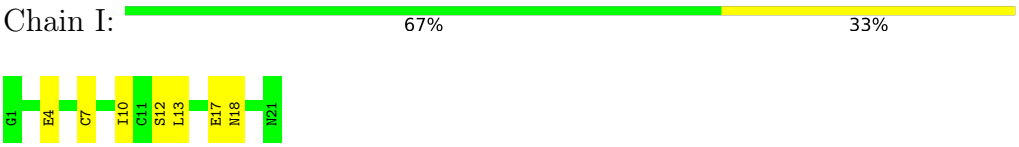


• Molecule 2: Light chain of analytical antibody S1 Fab



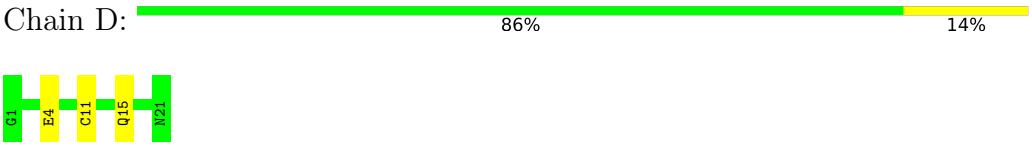
• Molecule 3: Insulin A chain

Chain I:



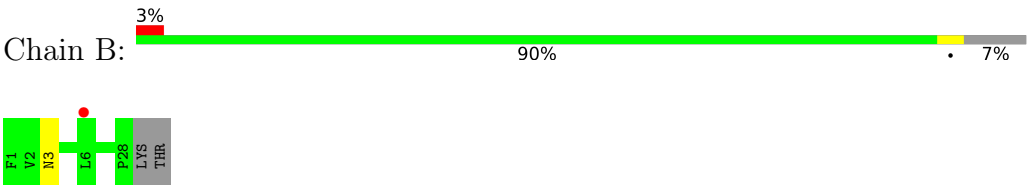
• Molecule 3: Insulin A chain

Chain D:



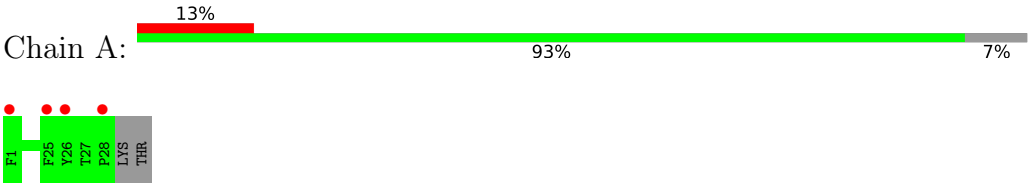
• Molecule 4: Insulin B chain

Chain B:



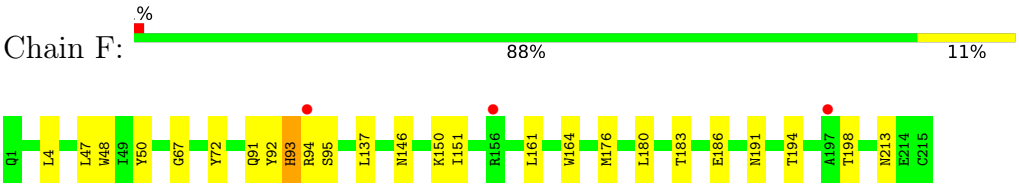
• Molecule 4: Insulin B chain

Chain A:



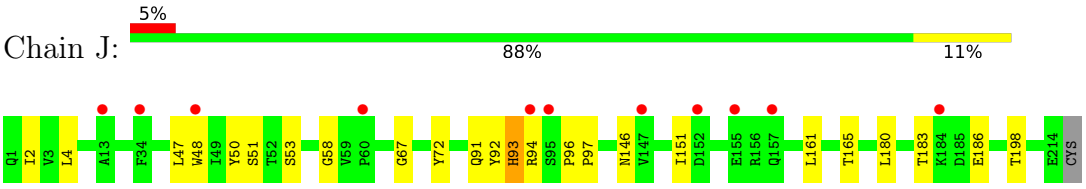
• Molecule 5: Light chain of analytical antibody HUI-001 Fab

Chain F:



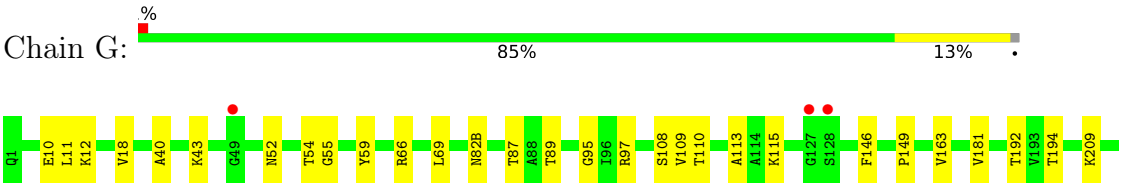
• Molecule 5: Light chain of analytical antibody HUI-001 Fab

Chain J:

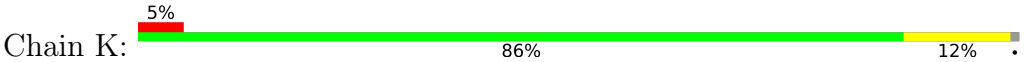


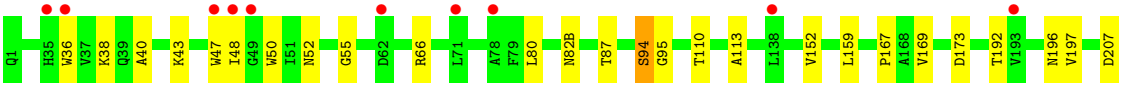
• Molecule 6: Heavy chain of analytical antibody HUI-001 Fab

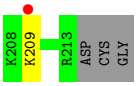
Chain G:



• Molecule 6: Heavy chain of analytical antibody HUI-001 Fab







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	278.90Å 52.33Å 179.50Å 90.00° 101.14° 90.00°	Depositor
Resolution (Å)	45.61 – 3.40 48.86 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.61-3.40) 99.2 (48.86-3.40)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.258 , 0.311 0.260 , 0.311	Depositor DCC
R_{free} test set	1776 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	90.3	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13887	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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	C	0.24	0/1698	0.46	0/2317
1	H	0.24	0/1694	0.46	0/2312
2	E	0.24	0/1660	0.47	0/2257
2	L	0.24	0/1660	0.46	0/2257
3	D	0.22	0/164	0.37	0/220
3	I	0.22	0/164	0.43	0/220
4	A	0.24	0/232	0.45	0/314
4	B	0.23	0/232	0.45	0/314
5	F	0.24	0/1693	0.47	0/2300
5	J	0.24	0/1686	0.46	0/2292
6	G	0.24	0/1679	0.45	0/2296
6	K	0.24	0/1679	0.45	0/2296
All	All	0.24	0/14241	0.46	0/19395

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	C	1653	0	1609	10	0
1	H	1649	0	1606	17	0
2	E	1622	0	1551	22	0
2	L	1622	0	1551	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	163	0	149	2	0
3	I	163	0	149	4	0
4	A	225	0	212	0	0
4	B	225	0	212	5	0
5	F	1652	0	1572	17	0
5	J	1645	0	1567	15	0
6	G	1634	0	1604	16	0
6	K	1634	0	1604	17	0
All	All	13887	0	13386	121	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 4.

All (121) 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)
4:B:3:ASN:ND2	5:F:93:HIS:O	2.23	0.71
1:H:39:GLN:NE2	1:H:44:SER:O	2.25	0.70
3:I:18:ASN:HB3	6:G:54:THR:HG21	1.78	0.65
2:E:65:GLY:HA3	2:E:70:PHE:HA	1.81	0.62
6:G:163:VAL:HG22	6:G:181:VAL:HG12	1.82	0.62
6:G:11:LEU:HD21	6:G:146:PHE:HE1	1.64	0.61
5:J:67:GLY:HA3	5:J:72:TYR:HA	1.82	0.61
2:E:144:ASN:HB3	2:E:196:THR:HB	1.83	0.60
5:J:146:ASN:HB3	5:J:198:THR:HB	1.85	0.59
6:K:40:ALA:HB3	6:K:43:LYS:HB2	1.86	0.58
2:E:188:HIS:O	2:E:210:ARG:NH1	2.37	0.58
5:J:165:THR:HG22	6:K:167:PRO:HD3	1.86	0.58
6:G:40:ALA:HB3	6:G:43:LYS:HB2	1.86	0.57
1:H:175:ALA:HB2	1:H:184:LEU:HD23	1.87	0.56
5:J:183:THR:HG23	5:J:186:GLU:H	1.71	0.55
5:F:67:GLY:HA3	5:F:72:TYR:HA	1.89	0.55
6:K:152:VAL:HG22	6:K:197:VAL:HG23	1.89	0.55
2:L:19:VAL:HG11	2:L:103:LEU:HD11	1.87	0.55
2:L:188:HIS:O	2:L:210:ARG:NH1	2.33	0.54
5:F:183:THR:HG23	5:F:186:GLU:H	1.73	0.53
5:F:47:LEU:HD21	5:F:50:TYR:HB3	1.90	0.53
1:H:159:VAL:HG22	1:H:204:VAL:HG12	1.90	0.53
5:F:191:ASN:ND2	5:F:213:ASN:OD1	2.41	0.53
5:J:91:GLN:HE21	5:J:97:PRO:HA	1.73	0.53
2:E:30:ASN:H	2:E:91:SER:HB2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:149:ILE:HD11	2:E:178:LEU:HD21	1.92	0.52
2:L:30:ASN:H	2:L:91:SER:HB2	1.74	0.52
6:K:94:SER:OG	6:K:95:GLY:N	2.36	0.51
2:L:65:GLY:HA3	2:L:70:PHE:HA	1.93	0.51
5:F:4:LEU:HD21	5:F:91:GLN:HG2	1.92	0.51
6:G:12:LYS:HG3	6:G:18:VAL:HB	1.91	0.51
5:J:4:LEU:HD21	5:J:91:GLN:HG2	1.93	0.51
5:F:151:ILE:HD11	5:F:180:LEU:HD21	1.92	0.50
2:E:154:ARG:HD3	2:E:178:LEU:HD11	1.94	0.50
2:L:15:PRO:HA	2:L:77:MET:HG3	1.94	0.49
6:G:87:THR:HG23	6:G:110:THR:HA	1.93	0.49
2:E:194:GLU:HG2	2:E:205:VAL:HG22	1.94	0.49
3:D:11:CYS:HA	6:K:50:TRP:HZ2	1.77	0.49
6:K:87:THR:HG23	6:K:110:THR:HA	1.93	0.49
5:J:161:LEU:HD22	6:K:169:VAL:HG11	1.94	0.49
1:H:193:SER:O	1:H:197:SER:OG	2.28	0.48
1:C:106:SER:HB2	2:E:54:ALA:HA	1.95	0.48
6:G:52:ASN:O	6:G:55:GLY:N	2.45	0.48
2:L:144:ASN:ND2	2:E:144:ASN:HD21	2.12	0.48
2:E:148:LYS:HB2	2:E:192:THR:HB	1.96	0.48
1:H:41:HIS:CD2	1:H:44:SER:HB3	2.48	0.48
5:F:93:HIS:HB3	5:F:94:ARG:H	1.48	0.48
1:H:89:ASP:O	2:E:187:ARG:NH2	2.47	0.47
6:G:194:THR:HG22	6:G:209:LYS:HA	1.96	0.47
1:H:86:LEU:HB3	1:H:118:VAL:HG21	1.97	0.47
2:L:60:ARG:NE	2:L:81:ASP:OD2	2.47	0.47
1:C:193:SER:O	1:C:197:SER:OG	2.25	0.47
1:H:20:ILE:HD12	1:H:114:THR:HG21	1.97	0.47
1:C:35:HIS:ND1	1:C:50:SER:OG	2.40	0.46
1:H:19:LYS:HA	1:H:82:GLU:HA	1.97	0.46
2:L:121:SER:HA	2:L:124:LEU:HD12	1.98	0.46
6:K:66:ARG:NH1	6:K:82(B):ASN:O	2.49	0.46
2:L:162:TRP:HH2	2:E:155:GLN:HG3	1.79	0.46
2:E:143:ILE:HG13	2:E:197:HIS:HD2	1.79	0.46
6:G:89:THR:HA	6:G:108:SER:HA	1.98	0.46
6:K:38:LYS:HB3	6:K:48:ILE:HD11	1.97	0.46
5:F:146:ASN:HB3	5:F:198:THR:HB	1.98	0.46
6:G:11:LEU:HD21	6:G:146:PHE:CE1	2.50	0.46
6:K:52:ASN:O	6:K:55:GLY:N	2.49	0.46
1:H:174:PRO:HD3	2:L:163:THR:HG22	1.97	0.45
5:F:150:LYS:HB2	5:F:194:THR:OG1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:116:ILE:HD12	2:E:193:CYS:HB2	1.99	0.44
5:J:93:HIS:HB3	5:J:94:ARG:H	1.62	0.44
2:L:144:ASN:HB3	2:L:196:THR:HB	1.99	0.44
2:E:53:LEU:HD23	2:E:54:ALA:O	2.17	0.44
4:B:3:ASN:HD22	5:F:95:SER:N	2.16	0.44
1:C:38:ARG:NH2	1:C:89:ASP:O	2.51	0.44
6:G:192:THR:HB	6:G:209:LYS:HE3	2.00	0.44
6:K:196:ASN:ND2	6:K:207:ASP:OD1	2.39	0.44
4:B:3:ASN:ND2	5:F:95:SER:N	2.66	0.44
3:I:4:GLU:HG3	3:I:7:CYS:HB3	1.99	0.43
3:I:10:ILE:HG21	4:B:3:ASN:OD1	2.17	0.43
5:J:96:PRO:HB3	6:K:47:TRP:CZ3	2.53	0.43
5:J:151:ILE:HD11	5:J:180:LEU:HD21	2.00	0.43
5:F:50:TYR:OH	6:G:97:ARG:NH2	2.51	0.43
6:G:59:TYR:HE1	6:G:69:LEU:HG	1.84	0.43
1:H:45:LEU:HD23	1:H:45:LEU:HA	1.83	0.43
1:H:177:LEU:HD12	1:H:177:LEU:HA	1.89	0.43
1:C:5:GLN:O	1:C:23:LYS:N	2.49	0.43
6:K:192:THR:HB	6:K:209:LYS:HE3	2.00	0.43
3:I:13:LEU:O	3:I:17:GLU:HG3	2.18	0.43
1:C:28:THR:HG22	1:C:30:THR:HG22	2.01	0.43
2:L:143:ILE:HG13	2:L:197:HIS:HD2	1.83	0.42
6:K:159:LEU:HD23	6:K:159:LEU:HA	1.92	0.42
5:F:161:LEU:HD23	5:F:161:LEU:HA	1.91	0.42
5:J:47:LEU:HD11	5:J:50:TYR:HB3	2.00	0.42
1:H:41:HIS:NE2	1:H:44:SER:HB3	2.34	0.42
2:L:116:ILE:HD12	2:L:193:CYS:HB2	2.01	0.42
2:E:154:ARG:HH11	2:E:180:LEU:HD11	1.85	0.42
4:B:3:ASN:HD22	5:F:94:ARG:C	2.23	0.42
5:F:137:LEU:HB2	5:F:176:MET:HG3	2.00	0.42
2:L:118:PRO:HB3	2:L:208:PHE:CE2	2.55	0.42
6:G:66:ARG:NH1	6:G:82(B):ASN:O	2.53	0.42
6:K:36:TRP:CE3	6:K:80:LEU:HD12	2.55	0.42
1:H:107:ARG:HB2	2:L:55:SER:OG	2.19	0.42
2:E:118:PRO:HB3	2:E:208:PHE:CE2	2.55	0.42
3:D:15:GLN:NE2	6:K:52:ASN:HB2	2.35	0.42
2:E:44:ARG:HH21	2:E:57:VAL:HG12	1.84	0.42
1:H:126:PRO:HD2	1:H:211:THR:HG21	2.01	0.41
5:J:97:PRO:HG2	6:K:47:TRP:CG	2.55	0.41
2:E:47:ILE:HD13	2:E:53:LEU:HA	2.02	0.41
2:L:162:TRP:CH2	2:E:155:GLN:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:91:GLN:NE2	5:J:97:PRO:HA	2.35	0.41
2:L:4:LEU:HB2	2:L:98:GLY:HA2	2.03	0.41
1:C:174:PRO:HD3	2:E:163:THR:HG22	2.01	0.41
5:F:164:TRP:CD1	5:F:176:MET:HB3	2.55	0.41
2:L:111:ALA:HA	2:L:199:THR:HG21	2.03	0.41
1:H:175:ALA:HA	1:H:184:LEU:HB3	2.02	0.41
1:C:206:HIS:HB3	1:C:211:THR:HB	2.03	0.41
5:J:2:ILE:O	5:J:2:ILE:HG13	2.20	0.40
1:H:27:TYR:CE2	1:H:98:ARG:HD2	2.56	0.40
1:C:51:ILE:HA	1:C:58:PRO:HA	2.03	0.40
1:C:106:SER:O	2:E:55:SER:N	2.41	0.40
6:G:10:GLU:HB2	6:G:109:VAL:HG12	2.03	0.40
6:G:115:LYS:HD2	6:G:115:LYS:HA	1.88	0.40
5:J:51:SER:O	5:J:53:SER:N	2.49	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	C	211/223 (95%)	202 (96%)	9 (4%)	0	100	100
1	H	210/223 (94%)	200 (95%)	10 (5%)	0	100	100
2	E	209/213 (98%)	200 (96%)	9 (4%)	0	100	100
2	L	209/213 (98%)	200 (96%)	8 (4%)	1 (0%)	29	61
3	D	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
3	I	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
4	A	26/30 (87%)	23 (88%)	3 (12%)	0	100	100
4	B	26/30 (87%)	23 (88%)	3 (12%)	0	100	100
5	F	213/215 (99%)	202 (95%)	10 (5%)	1 (0%)	29	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	J	212/215 (99%)	199 (94%)	11 (5%)	2 (1%)	17 49
6	G	215/220 (98%)	195 (91%)	17 (8%)	3 (1%)	11 37
6	K	215/220 (98%)	195 (91%)	18 (8%)	2 (1%)	17 49
All	All	1784/1844 (97%)	1674 (94%)	101 (6%)	9 (0%)	29 61

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	95	GLY
6	K	113	ALA
5	F	93	HIS
6	G	113	ALA
5	J	58	GLY
5	J	93	HIS
6	K	94	SER
2	L	15	PRO
6	G	149	PRO

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	C	190/195 (97%)	188 (99%)	2 (1%)	73 86
1	H	190/195 (97%)	189 (100%)	1 (0%)	88 94
2	E	186/188 (99%)	184 (99%)	2 (1%)	73 86
2	L	186/188 (99%)	184 (99%)	2 (1%)	73 86
3	D	20/20 (100%)	19 (95%)	1 (5%)	24 54
3	I	20/20 (100%)	19 (95%)	1 (5%)	24 54
4	A	24/26 (92%)	24 (100%)	0	100 100
4	B	24/26 (92%)	24 (100%)	0	100 100
5	F	189/189 (100%)	187 (99%)	2 (1%)	73 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	J	188/189 (100%)	186 (99%)	2 (1%)	73 86
6	G	183/185 (99%)	183 (100%)	0	100 100
6	K	183/185 (99%)	182 (100%)	1 (0%)	88 94
All	All	1583/1606 (99%)	1569 (99%)	14 (1%)	78 90

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	203	ASN
2	L	90	TRP
2	L	210	ARG
3	I	12	SER
1	C	44	SER
1	C	203	ASN
2	E	90	TRP
2	E	154	ARG
3	D	4	GLU
5	F	48	TRP
5	F	92	TYR
5	J	48	TRP
5	J	92	TYR
6	K	173	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	3	ASN
1	C	171	HIS
5	J	91	GLN
6	K	171	GLN

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	C	215/223 (96%)	0.24	7 (3%) 46 45	83, 126, 156, 183	0
1	H	214/223 (95%)	0.02	3 (1%) 75 74	60, 99, 136, 161	0
2	E	211/213 (99%)	0.15	4 (1%) 66 65	82, 115, 141, 158	0
2	L	211/213 (99%)	0.17	2 (0%) 84 83	65, 105, 128, 147	0
3	D	21/21 (100%)	0.02	0 100 100	115, 134, 154, 156	0
3	I	21/21 (100%)	-0.33	0 100 100	60, 82, 130, 136	0
4	A	28/30 (93%)	0.60	4 (14%) 2 3	106, 136, 165, 170	0
4	B	28/30 (93%)	0.31	1 (3%) 42 42	68, 98, 133, 147	0
5	F	215/215 (100%)	-0.03	3 (1%) 75 74	59, 88, 112, 140	0
5	J	214/215 (99%)	0.40	11 (5%) 28 28	101, 145, 176, 197	0
6	G	217/220 (98%)	-0.06	3 (1%) 75 74	60, 85, 121, 172	0
6	K	217/220 (98%)	0.31	11 (5%) 28 28	80, 126, 161, 204	0
All	All	1812/1844 (98%)	0.15	49 (2%) 54 53	59, 112, 158, 204	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	103	TYR	5.5
6	K	49	GLY	5.1
5	J	94	ARG	4.9
2	E	129	ALA	4.2
4	A	1	PHE	3.9
1	C	1	GLU	3.9
5	J	155	GLU	3.8
5	J	95	SER	3.8
4	A	26	TYR	3.7
5	J	34	PHE	3.7
1	C	2	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
6	K	47	TRP	3.2
6	G	128	SER	3.1
2	E	134	PHE	3.0
6	G	127	GLY	2.9
5	J	184	LYS	2.8
2	E	21	MET	2.8
1	C	34	ILE	2.8
1	C	35	HIS	2.8
6	G	49	GLY	2.8
6	K	193	VAL	2.8
5	J	157	GLN	2.6
2	L	13	ALA	2.6
1	H	217	ILE	2.6
4	A	28	PRO	2.6
6	K	36	TRP	2.5
6	K	138	LEU	2.5
5	J	147	VAL	2.5
1	H	103	TYR	2.5
6	K	35	HIS	2.5
5	J	152	ASP	2.5
5	F	197	ALA	2.4
2	L	147	TRP	2.4
6	K	48	ILE	2.4
5	F	156	ARG	2.3
4	A	25	PHE	2.3
6	K	78	ALA	2.3
5	J	60	PRO	2.3
5	F	94	ARG	2.2
5	J	48	TRP	2.2
6	K	209	LYS	2.2
1	C	29	PHE	2.2
6	K	71	LEU	2.1
2	E	128	GLY	2.1
1	C	33	ASN	2.1
4	B	6	LEU	2.0
6	K	62	ASP	2.0
5	J	13	ALA	2.0
1	H	200	VAL	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.