Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 05:54 PM EDT

PDB ID	:	5MP1
Title	:	Crystal structure of DC8E8 Fab in the complex with a 14-mer tau peptide at pH 7.5
Authors	:	Skrabana, R.; Novak, M.; Cehlar, O.; Kontsekova, E.
Deposited on	:	2016-12-15
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

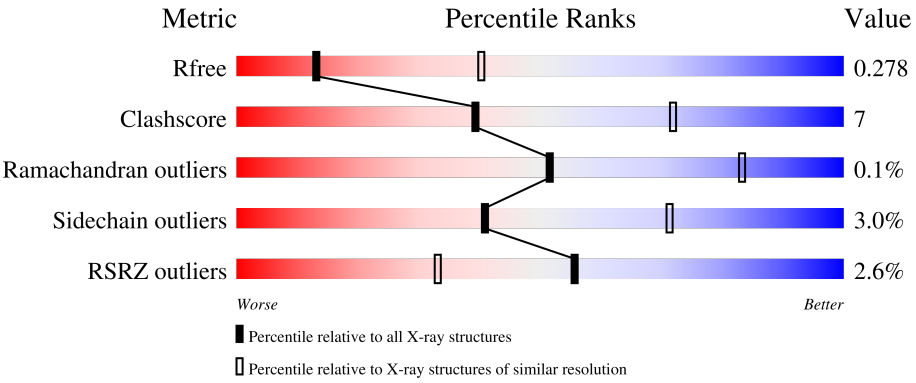
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	221	2% 80% 15%
1	F	221	3% 83% 13%
1	H	221	3% 84% 13%
1	J	221	3% 83% 13%
2	D	218	4% 83% 16%

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Mol	Chain	Length	Quality of chain
2	G	218	2% 87% 12%
2	K	218	4% 87% 12%
2	L	218	3% 89% 11%
3	A	14	29% 21% 50%
3	B	14	36% 14% 50%
3	E	14	7% 14% 36% 50%
3	I	14	7% 50% 50%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13383 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 antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	215	Total	C	N	O	S	0	0	0
			1633	1039	262	324	8			
1	C	214	Total	C	N	O	S	0	0	0
			1625	1035	261	321	8			
1	F	215	Total	C	N	O	S	0	0	0
			1633	1039	262	324	8			
1	J	214	Total	C	N	O	S	0	0	0
			1616	1030	257	321	8			

- Molecule 2 is a protein called antibody Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	218	Total	C	N	O	S	0	0	0
			1678	1047	284	340	7			
2	D	218	Total	C	N	O	S	0	0	0
			1682	1049	284	342	7			
2	G	218	Total	C	N	O	S	0	0	0
			1675	1043	282	343	7			
2	K	218	Total	C	N	O	S	0	0	0
			1673	1043	282	341	7			

- Molecule 3 is a protein called Microtubule-associated protein tau.

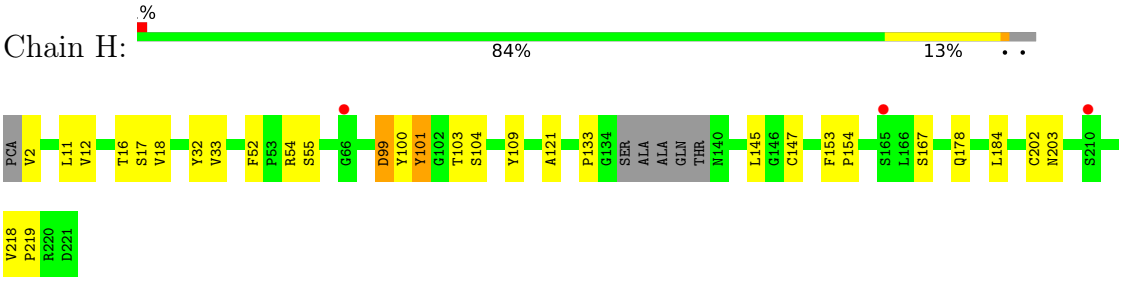
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	7	Total	C	N	O	0	0	0
			42	25	9	8			
3	B	7	Total	C	N	O	0	0	0
			42	25	9	8			
3	E	7	Total	C	N	O	0	0	0
			42	25	9	8			
3	I	7	Total	C	N	O	0	0	0
			42	25	9	8			

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.

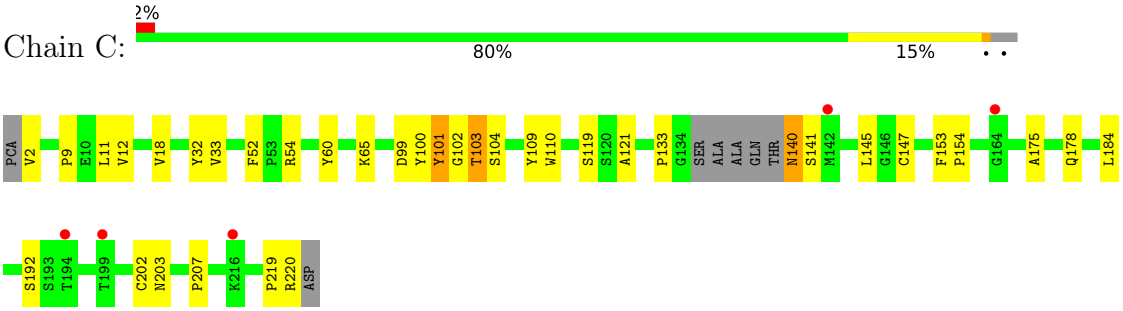
• Molecule 1: antibody Fab heavy chain

Chain H:



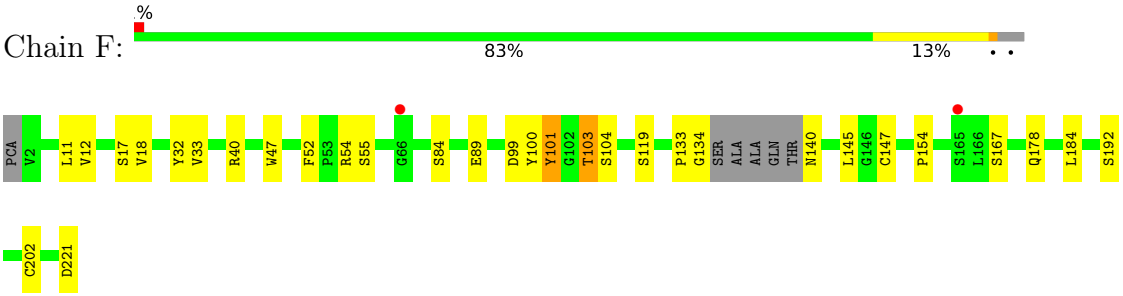
• Molecule 1: antibody Fab heavy chain

Chain C:



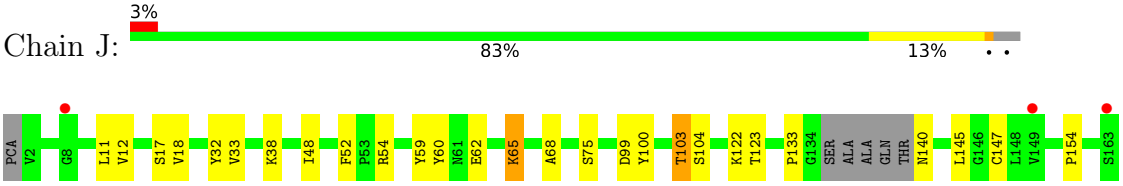
• Molecule 1: antibody Fab heavy chain

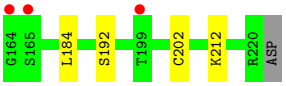
Chain F:



• Molecule 1: antibody Fab heavy chain

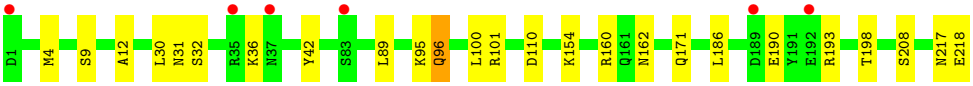
Chain J:





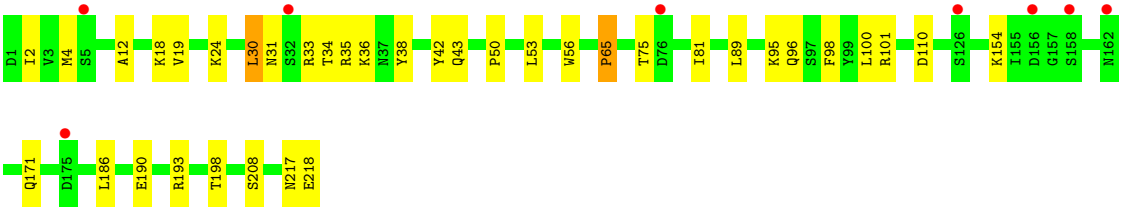
• Molecule 2: antibody Fab light chain

Chain L:



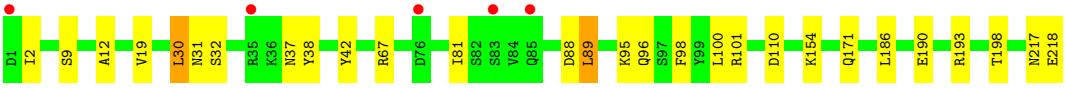
• Molecule 2: antibody Fab light chain

Chain D:



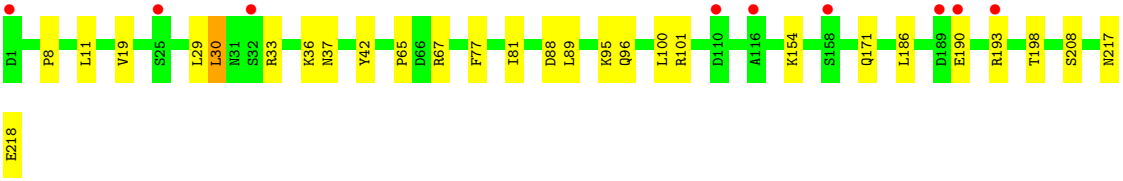
• Molecule 2: antibody Fab light chain

Chain G:



• Molecule 2: antibody Fab light chain

Chain K:

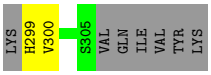


• Molecule 3: Microtubule-associated protein tau

Chain A:

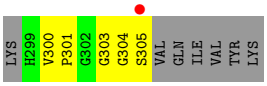
• Molecule 3: Microtubule-associated protein tau

Chain B:



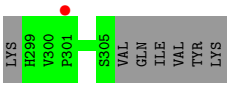
• Molecule 3: Microtubule-associated protein tau

Chain E:



• Molecule 3: Microtubule-associated protein tau

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.37Å 82.37Å 89.80Å 88.12° 84.78° 89.93°	Depositor
Resolution (Å)	39.83 – 3.10 39.83 – 3.01	Depositor EDS
% Data completeness (in resolution range)	71.8 (39.83-3.10) 89.3 (39.83-3.01)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.222 , 0.268 0.238 , 0.278	Depositor DCC
R_{free} test set	1561 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	46.7	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 38.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.011 for -h,k,-l	Xtriage
Reported twinning fraction	0.882 for H, K, L 0.118 for -H, K, -L	Depositor
Outliers	0 of 30453 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	13383	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.54% 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	0.58	0/1669	0.71	0/2279
1	F	0.57	0/1677	0.72	0/2290
1	H	0.59	0/1677	0.71	0/2290
1	J	0.54	0/1660	0.70	0/2269
2	D	0.55	0/1718	0.73	0/2330
2	G	0.55	0/1711	0.78	2/2323 (0.1%)
2	K	0.51	0/1709	0.73	0/2318
2	L	0.55	0/1714	0.72	0/2325
3	A	0.48	0/43	0.60	0/57
3	B	0.76	0/43	0.67	0/57
3	E	0.42	0/43	0.64	0/57
3	I	0.53	0/43	0.58	0/57
All	All	0.55	0/13707	0.73	2/18652 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	89	LEU	CB-CG-CD1	-6.54	99.88	111.00
2	G	37	ASN	N-CA-C	-5.38	96.46	111.00

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	1625	0	1584	41	0
1	F	1633	0	1588	19	0
1	H	1633	0	1588	21	0
1	J	1616	0	1564	19	0
2	D	1682	0	1613	28	0
2	G	1675	0	1594	20	0
2	K	1673	0	1596	29	0
2	L	1678	0	1609	19	0
3	A	42	0	36	2	0
3	B	42	0	36	4	0
3	E	42	0	36	5	0
3	I	42	0	36	0	0
All	All	13383	0	12880	193	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 7.

All (193) 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)
2:K:29:LEU:HD21	2:K:96:GLN:NE2	1.55	1.21
2:K:29:LEU:HD21	2:K:96:GLN:HE22	1.06	1.14
1:C:141:SER:O	1:C:192:SER:CB	1.98	1.10
2:K:30:LEU:HD23	2:K:36:LYS:O	1.53	1.07
1:C:32:TYR:CE2	1:C:100:TYR:HD1	1.74	1.04
1:C:141:SER:O	1:C:192:SER:HB2	1.58	1.04
2:K:29:LEU:CD2	2:K:96:GLN:HE22	1.72	1.02
1:C:32:TYR:CE2	1:C:100:TYR:CD1	2.49	0.99
2:D:4:MET:SD	2:D:96:GLN:NE2	2.37	0.97
1:C:101:TYR:OH	3:B:300:VAL:HG22	1.63	0.97
2:L:160:ARG:CZ	2:L:162:ASN:HB2	1.94	0.97
2:K:29:LEU:CD2	2:K:96:GLN:NE2	2.27	0.95
1:F:52:PHE:CE2	1:F:54:ARG:HB3	2.13	0.84
2:K:30:LEU:CD2	2:K:36:LYS:O	2.24	0.84
2:K:29:LEU:HD22	2:K:96:GLN:OE1	1.76	0.84
1:J:52:PHE:CE2	1:J:54:ARG:HB3	2.12	0.84
1:H:52:PHE:CE2	1:H:54:ARG:HB3	2.13	0.83
1:C:52:PHE:CE2	1:C:54:ARG:HB3	2.15	0.81
1:H:218:VAL:CG2	1:H:219:PRO:HD2	2.12	0.79
1:C:32:TYR:HE2	1:C:100:TYR:CD1	2.00	0.78
1:C:101:TYR:CZ	3:B:300:VAL:HG22	2.19	0.77
1:C:101:TYR:HD1	1:C:101:TYR:C	1.89	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ALA:HA	1:C:184:LEU:HB3	1.69	0.75
1:C:101:TYR:C	1:C:101:TYR:CD1	2.60	0.74
1:C:141:SER:O	1:C:192:SER:N	2.18	0.74
1:H:218:VAL:HG23	1:H:219:PRO:HD2	1.70	0.73
1:H:133:PRO:HD3	1:H:145:LEU:HD23	1.73	0.71
1:F:134:GLY:HA2	1:F:221:ASP:OD1	1.91	0.70
2:G:89:LEU:HD11	2:G:171:GLN:HB3	1.74	0.69
2:L:160:ARG:NH2	2:L:162:ASN:HB2	2.07	0.69
1:C:141:SER:O	1:C:192:SER:HB3	1.89	0.69
2:D:89:LEU:HD11	2:D:171:GLN:HB3	1.74	0.69
2:G:2:ILE:HG21	2:G:96:GLN:OE1	1.93	0.68
1:H:103:THR:OG1	1:H:104:SER:N	2.28	0.67
2:L:89:LEU:HD11	2:L:171:GLN:HB3	1.78	0.66
2:L:160:ARG:NH2	2:L:162:ASN:CB	2.59	0.65
2:L:186:LEU:HD23	2:L:190:GLU:HG3	1.77	0.65
2:D:2:ILE:HB	2:D:96:GLN:OE1	1.96	0.65
1:J:60:TYR:HE2	1:J:68:ALA:O	1.79	0.65
1:C:175:ALA:HB2	1:C:184:LEU:HD23	1.78	0.65
2:D:2:ILE:HG22	2:D:96:GLN:HE22	1.61	0.64
1:H:55:SER:HB2	2:D:65:PRO:HB3	1.79	0.64
2:K:29:LEU:HD12	2:K:77:PHE:CE2	2.33	0.63
2:K:89:LEU:HD11	2:K:171:GLN:HB3	1.81	0.63
2:L:160:ARG:NE	2:L:162:ASN:HB2	2.14	0.63
1:H:11:LEU:O	1:J:122:LYS:HD2	1.98	0.62
2:L:31:ASN:OD1	2:L:32:SER:N	2.32	0.62
1:C:32:TYR:CE2	1:C:100:TYR:CE1	2.87	0.62
1:F:55:SER:HB2	2:K:65:PRO:HB3	1.82	0.62
2:K:29:LEU:CD2	2:K:96:GLN:CD	2.68	0.61
2:K:30:LEU:HD21	2:K:36:LYS:N	2.16	0.61
2:K:29:LEU:HD22	2:K:96:GLN:CD	2.21	0.60
2:K:186:LEU:HD23	2:K:190:GLU:HG3	1.82	0.60
1:J:32:TYR:CE2	1:J:100:TYR:HD1	2.19	0.60
2:D:186:LEU:HD23	2:D:190:GLU:HG3	1.82	0.60
1:J:103:THR:OG1	1:J:104:SER:N	2.32	0.60
1:J:59:TYR:C	1:J:60:TYR:HD1	2.05	0.60
1:F:103:THR:OG1	1:F:104:SER:N	2.35	0.60
1:C:103:THR:OG1	1:C:104:SER:N	2.34	0.59
1:H:11:LEU:HB2	1:H:154:PRO:HG3	1.83	0.59
1:C:133:PRO:HD3	1:C:145:LEU:HD23	1.83	0.59
1:C:141:SER:O	1:C:192:SER:CA	2.50	0.59
1:F:32:TYR:CE2	1:F:100:TYR:HD1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:218:VAL:HG22	1:H:219:PRO:HD2	1.85	0.58
1:C:101:TYR:HH	3:B:300:VAL:HG22	1.67	0.58
2:G:100:LEU:O	2:G:101:ARG:HD3	2.02	0.58
1:F:12:VAL:HG11	1:F:18:VAL:HB	1.84	0.58
1:F:52:PHE:CZ	1:F:54:ARG:HB3	2.39	0.58
2:K:29:LEU:HB2	2:K:37:ASN:OD1	2.02	0.58
2:D:190:GLU:OE1	2:D:193:ARG:NH2	2.37	0.57
1:J:12:VAL:HG11	1:J:18:VAL:HB	1.87	0.57
2:L:190:GLU:OE1	2:L:193:ARG:NH2	2.38	0.57
1:H:100:TYR:HE1	1:H:103:THR:HG1	1.46	0.57
2:D:100:LEU:O	2:D:101:ARG:HD3	2.05	0.57
2:L:42:TYR:CE1	2:L:95:LYS:HE3	2.40	0.56
2:G:186:LEU:HD23	2:G:190:GLU:HG3	1.86	0.56
1:H:12:VAL:HG11	1:H:18:VAL:HB	1.86	0.56
1:F:32:TYR:CE2	1:F:100:TYR:CD1	2.94	0.56
2:D:30:LEU:O	2:D:98:PHE:HE2	1.88	0.56
1:H:2:VAL:HG11	1:H:109:TYR:CZ	2.40	0.56
1:F:140:ASN:O	1:F:192:SER:HB2	2.05	0.55
2:K:29:LEU:HD12	2:K:77:PHE:CZ	2.40	0.55
1:J:32:TYR:CE2	1:J:100:TYR:CD1	2.95	0.55
2:K:190:GLU:OE1	2:K:193:ARG:NH2	2.40	0.54
1:C:140:ASN:N	1:C:140:ASN:OD1	2.38	0.54
2:D:42:TYR:CE2	2:D:95:LYS:HE3	2.43	0.54
1:H:99:ASP:OD1	1:H:99:ASP:C	2.46	0.54
2:G:30:LEU:HG	2:G:31:ASN:N	2.21	0.54
2:G:89:LEU:HD11	2:G:171:GLN:CB	2.37	0.54
1:F:133:PRO:O	1:F:221:ASP:OD1	2.25	0.53
1:C:52:PHE:HB2	3:B:299:HIS:CE1	2.43	0.53
1:F:33:VAL:HG22	1:F:99:ASP:HB3	1.90	0.53
2:K:100:LEU:O	2:K:101:ARG:HD3	2.08	0.53
1:F:133:PRO:HD3	1:F:145:LEU:HD23	1.91	0.53
1:J:133:PRO:HD3	1:J:145:LEU:HD23	1.90	0.52
1:H:100:TYR:CE1	1:H:103:THR:OG1	2.56	0.52
2:D:89:LEU:HD11	2:D:171:GLN:CB	2.40	0.52
2:G:98:PHE:O	3:E:304:GLY:N	2.35	0.52
1:C:12:VAL:HG11	1:C:18:VAL:HB	1.91	0.52
1:H:218:VAL:CG2	1:H:219:PRO:CD	2.85	0.52
3:E:300:VAL:HB	3:E:301:PRO:CD	2.39	0.52
2:D:33:ARG:CB	2:D:38:TYR:OH	2.58	0.51
1:H:16:THR:HG21	1:J:123:THR:O	2.10	0.51
2:D:30:LEU:O	2:D:98:PHE:CE2	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:59:TYR:C	1:J:60:TYR:CD1	2.84	0.51
1:J:33:VAL:CG2	1:J:99:ASP:HB3	2.41	0.51
1:C:33:VAL:CG2	1:C:99:ASP:HB3	2.41	0.50
2:G:190:GLU:OE1	2:G:193:ARG:NH2	2.45	0.50
2:D:12:ALA:HA	2:D:110:ASP:O	2.12	0.50
2:L:89:LEU:HD11	2:L:171:GLN:CB	2.42	0.49
2:D:33:ARG:O	2:D:34:THR:CB	2.57	0.49
1:F:33:VAL:CG2	1:F:99:ASP:HB3	2.41	0.49
2:G:42:TYR:CE1	2:G:95:LYS:HE3	2.48	0.49
2:D:19:VAL:HG12	2:D:81:ILE:HB	1.95	0.49
1:H:32:TYR:HE2	1:H:100:TYR:CD2	2.31	0.49
1:J:52:PHE:CZ	1:J:54:ARG:HB3	2.48	0.48
2:D:24:LYS:HG3	2:D:75:THR:O	2.14	0.48
1:C:32:TYR:CZ	1:C:100:TYR:CE1	3.02	0.48
1:H:121:ALA:HB3	1:H:153:PHE:CE2	2.49	0.48
2:G:19:VAL:HG12	2:G:81:ILE:HB	1.96	0.48
2:K:33:ARG:CB	2:K:36:LYS:CB	2.92	0.48
2:K:42:TYR:CE1	2:K:95:LYS:HE3	2.49	0.48
2:D:2:ILE:HG22	2:D:96:GLN:NE2	2.27	0.47
2:G:38:TYR:CD2	3:E:303:GLY:HA3	2.49	0.47
3:A:300:VAL:HG21	3:A:305:SER:HB2	1.97	0.47
1:C:11:LEU:HB2	1:C:154:PRO:HG3	1.97	0.47
1:F:134:GLY:CA	1:F:221:ASP:OD1	2.61	0.47
1:C:32:TYR:CZ	1:C:100:TYR:HE1	2.32	0.47
2:G:89:LEU:HD11	2:G:171:GLN:CG	2.45	0.47
2:K:19:VAL:HG12	2:K:81:ILE:HB	1.97	0.47
2:D:154:LYS:HB2	2:D:198:THR:HB	1.97	0.47
1:C:32:TYR:CD2	1:C:100:TYR:HD1	2.28	0.47
2:G:31:ASN:OD1	2:G:32:SER:N	2.47	0.46
1:J:11:LEU:HB2	1:J:154:PRO:HG3	1.96	0.46
2:L:100:LEU:O	2:L:101:ARG:HD3	2.14	0.46
1:J:140:ASN:O	1:J:192:SER:HB2	2.16	0.46
2:D:36:LYS:HG2	2:D:56:TRP:NE1	2.31	0.46
2:K:89:LEU:HD11	2:K:171:GLN:CB	2.44	0.46
2:G:154:LYS:HB2	2:G:198:THR:HB	1.97	0.46
2:L:154:LYS:HB2	2:L:198:THR:HB	1.97	0.46
1:F:11:LEU:HB2	1:F:154:PRO:HG3	1.98	0.45
2:K:154:LYS:HB2	2:K:198:THR:HB	1.99	0.45
1:C:33:VAL:HG22	1:C:99:ASP:HB3	1.98	0.45
2:G:217:ASN:HB2	2:G:218:GLU:OE1	2.16	0.45
2:L:12:ALA:HA	2:L:110:ASP:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:36:LYS:HD3	2:L:36:LYS:HA	1.66	0.45
2:D:217:ASN:HB2	2:D:218:GLU:OE1	2.17	0.45
2:K:217:ASN:HB2	2:K:218:GLU:OE1	2.17	0.45
1:J:33:VAL:HG22	1:J:99:ASP:HB3	1.98	0.44
2:D:30:LEU:HD13	2:D:31:ASN:N	2.32	0.44
2:K:67:ARG:NH2	2:K:88:ASP:OD1	2.46	0.44
2:K:89:LEU:HD11	2:K:171:GLN:CG	2.47	0.44
1:C:2:VAL:HG11	1:C:109:TYR:CZ	2.53	0.44
1:C:121:ALA:HB3	1:C:153:PHE:CE2	2.52	0.44
1:H:101:TYR:CD1	1:H:101:TYR:C	2.91	0.43
1:C:33:VAL:HG12	1:C:52:PHE:HD1	1.84	0.43
2:D:2:ILE:CG2	2:D:96:GLN:NE2	2.80	0.43
3:E:303:GLY:C	3:E:305:SER:H	2.21	0.43
2:K:8:PRO:HG3	2:K:11:LEU:HD13	2.01	0.43
2:D:43:GLN:HB2	2:D:53:LEU:HD11	2.00	0.43
1:F:40:ARG:NH1	1:F:89:GLU:O	2.51	0.43
2:G:12:ALA:HA	2:G:110:ASP:O	2.19	0.43
2:G:98:PHE:CE1	3:E:304:GLY:HA2	2.54	0.43
1:J:38:LYS:HB2	1:J:48:ILE:HD11	2.00	0.43
1:J:60:TYR:HB2	1:J:65:LYS:HD3	2.01	0.43
1:C:133:PRO:HD3	1:C:145:LEU:CD2	2.48	0.42
2:G:2:ILE:HD13	2:G:96:GLN:NE2	2.34	0.42
3:A:300:VAL:HB	3:A:301:PRO:CD	2.50	0.42
1:F:140:ASN:O	1:F:192:SER:CB	2.67	0.42
1:C:219:PRO:O	1:C:220:ARG:CB	2.67	0.42
1:C:101:TYR:CD1	1:C:102:GLY:N	2.87	0.41
2:D:89:LEU:HD11	2:D:171:GLN:CG	2.50	0.41
2:D:34:THR:C	2:D:36:LYS:H	2.24	0.41
2:L:160:ARG:CZ	2:L:162:ASN:CB	2.82	0.41
2:K:96:GLN:O	2:K:101:ARG:HA	2.20	0.41
1:H:218:VAL:HG22	1:H:219:PRO:CD	2.50	0.41
1:C:119:SER:HG	1:C:153:PHE:HZ	1.67	0.41
2:K:30:LEU:HD23	2:K:30:LEU:HA	1.87	0.41
2:L:160:ARG:NH2	2:L:162:ASN:HD22	2.19	0.41
1:C:9:PRO:HD2	1:C:207:PRO:CB	2.51	0.41
1:F:47:TRP:CD2	2:G:101:ARG:HB2	2.56	0.41
2:L:89:LEU:HD11	2:L:171:GLN:CG	2.51	0.41
1:C:110:TRP:CZ3	2:D:50:PRO:HG2	2.55	0.41
1:F:101:TYR:CD1	1:F:101:TYR:C	2.93	0.41
2:L:4:MET:SD	2:L:96:GLN:HB2	2.61	0.41
1:C:60:TYR:HB2	1:C:65:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:VAL:HG13	1:C:101:TYR:CB	2.51	0.40
2:D:18:LYS:HD3	1:J:75:SER:O	2.21	0.40
2:L:217:ASN:HB2	2:L:218:GLU:OE1	2.22	0.40
1:C:33:VAL:HG13	1:C:101:TYR:HB3	2.03	0.40
1:H:33:VAL:HG13	1:H:101:TYR:CB	2.51	0.40
1:C:101:TYR:HD1	1:C:102:GLY:N	2.18	0.40
2:G:67:ARG:NH2	2:G:88:ASP:OD1	2.45	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	210/221 (95%)	201 (96%)	9 (4%)	0	100	100
1	F	211/221 (96%)	198 (94%)	13 (6%)	0	100	100
1	H	211/221 (96%)	202 (96%)	9 (4%)	0	100	100
1	J	210/221 (95%)	202 (96%)	8 (4%)	0	100	100
2	D	216/218 (99%)	206 (95%)	9 (4%)	1 (0%)	29	64
2	G	216/218 (99%)	207 (96%)	9 (4%)	0	100	100
2	K	216/218 (99%)	207 (96%)	9 (4%)	0	100	100
2	L	216/218 (99%)	209 (97%)	7 (3%)	0	100	100
3	A	5/14 (36%)	5 (100%)	0	0	100	100
3	B	5/14 (36%)	4 (80%)	1 (20%)	0	100	100
3	E	5/14 (36%)	4 (80%)	1 (20%)	0	100	100
3	I	5/14 (36%)	5 (100%)	0	0	100	100
All	All	1726/1812 (95%)	1650 (96%)	75 (4%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	35	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	C	186/190 (98%)	179 (96%)	7 (4%)	33	66
1	F	187/190 (98%)	177 (95%)	10 (5%)	22	54
1	H	187/190 (98%)	178 (95%)	9 (5%)	25	58
1	J	184/190 (97%)	176 (96%)	8 (4%)	29	62
2	D	190/194 (98%)	187 (98%)	3 (2%)	62	84
2	G	189/194 (97%)	187 (99%)	2 (1%)	73	89
2	K	188/194 (97%)	186 (99%)	2 (1%)	73	89
2	L	189/194 (97%)	185 (98%)	4 (2%)	53	79
3	A	4/11 (36%)	4 (100%)	0	100	100
3	B	4/11 (36%)	4 (100%)	0	100	100
3	E	4/11 (36%)	4 (100%)	0	100	100
3	I	4/11 (36%)	4 (100%)	0	100	100
All	All	1516/1580 (96%)	1471 (97%)	45 (3%)	41	71

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	17	SER
1	H	99	ASP
1	H	101	TYR
1	H	147	CYS
1	H	167	SER
1	H	178	GLN
1	H	184	LEU
1	H	202	CYS
1	H	203	ASN
2	L	9	SER

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Mol	Chain	Res	Type
2	L	30	LEU
2	L	96	GLN
2	L	208	SER
1	C	101	TYR
1	C	103	THR
1	C	140	ASN
1	C	147	CYS
1	C	178	GLN
1	C	202	CYS
1	C	203	ASN
2	D	30	LEU
2	D	65	PRO
2	D	208	SER
1	F	17	SER
1	F	84	SER
1	F	101	TYR
1	F	103	THR
1	F	119	SER
1	F	147	CYS
1	F	167	SER
1	F	178	GLN
1	F	184	LEU
1	F	202	CYS
2	G	9	SER
2	G	30	LEU
1	J	17	SER
1	J	62	GLU
1	J	65	LYS
1	J	103	THR
1	J	147	CYS
1	J	184	LEU
1	J	202	CYS
1	J	212	LYS
2	K	30	LEU
2	K	208	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	140	ASN
2	G	37	ASN
1	J	61	ASN

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	C	214/221 (96%)	0.18	5 (2%) 60 39	17, 34, 57, 84	0
1	F	215/221 (97%)	0.10	2 (0%) 84 69	22, 37, 56, 79	0
1	H	215/221 (97%)	0.03	3 (1%) 75 56	17, 34, 58, 71	0
1	J	214/221 (96%)	0.22	6 (2%) 53 30	24, 42, 61, 68	0
2	D	218/218 (100%)	0.39	8 (3%) 41 21	17, 45, 80, 102	0
2	G	218/218 (100%)	0.32	5 (2%) 60 39	23, 43, 73, 82	0
2	K	218/218 (100%)	0.45	9 (4%) 37 18	25, 51, 79, 102	0
2	L	218/218 (100%)	0.18	6 (2%) 53 30	16, 38, 73, 92	0
3	A	7/14 (50%)	0.46	0 100 100	29, 31, 40, 43	7 (100%)
3	B	7/14 (50%)	0.10	0 100 100	31, 35, 46, 47	0
3	E	7/14 (50%)	1.40	1 (14%) 2 1	23, 31, 42, 43	7 (100%)
3	I	7/14 (50%)	1.23	1 (14%) 2 1	37, 42, 54, 56	7 (100%)
All	All	1758/1812 (97%)	0.24	46 (2%) 56 33	16, 40, 71, 102	21 (1%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	165	SER	4.4
1	C	194	THR	3.6
2	L	35	ARG	3.5
1	F	165	SER	3.2
1	J	8	GLY	3.0
2	K	116	ALA	3.0
2	K	32	SER	3.0
2	D	175	ASP	2.9
2	G	35	ARG	2.8
2	K	110	ASP	2.8
2	G	83	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	199	THR	2.8
2	K	25	SER	2.7
3	E	305	SER	2.7
2	K	1	ASP	2.7
2	L	189	ASP	2.6
2	K	158	SER	2.6
2	L	37	ASN	2.6
1	J	164	GLY	2.6
2	D	126	SER	2.6
1	C	164	GLY	2.6
1	J	163	SER	2.6
2	L	1	ASP	2.5
2	G	85	GLN	2.5
2	G	1	ASP	2.5
1	J	165	SER	2.4
2	D	158	SER	2.4
1	J	199	THR	2.4
2	K	189	ASP	2.4
2	L	83	SER	2.4
1	F	66	GLY	2.4
1	C	142	MET	2.3
2	D	162	ASN	2.3
2	D	156	ASP	2.3
2	K	190	GLU	2.3
2	K	193	ARG	2.2
1	H	210	SER	2.2
2	L	192	GLU	2.2
3	I	301	PRO	2.2
2	G	76	ASP	2.1
2	D	76	ASP	2.1
2	D	32	SER	2.1
1	C	216	LYS	2.1
1	H	66	GLY	2.0
2	D	5	SER	2.0
1	J	149	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.