Full wwPDB X-ray Structure Validation Report

May 22, 2020 – 06:15 am BST

PDB ID	:	3V6F
Title	:	Crystal Structure of an anti-HBV e-antigen monoclonal Fab fragment (e6), unbound
Authors	:	Dimattia, M.A.; Watts, N.R.; Stahl, S.J.; Grimes, J.M.; Steven, A.C.; Stuart, D.I.; Wingfield, P.T.
Deposited on	:	2011-12-19
Resolution	:	2.52 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 following versions of software and data (see references ①) were used in the production of this report:

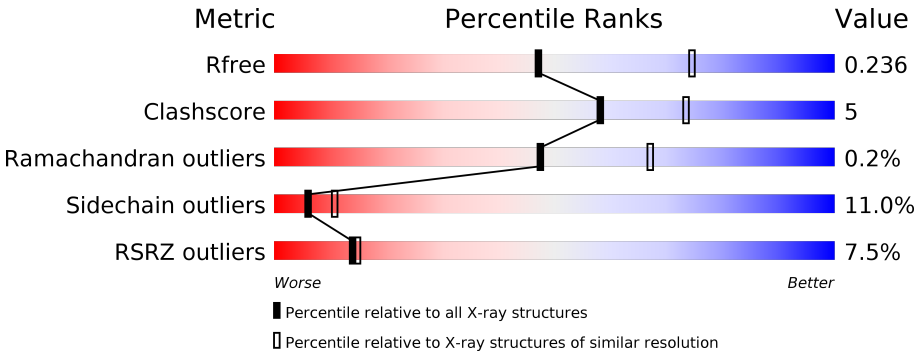
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.52 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 on 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	224	10%, 77%, 18%
1	C	224	6%, 78%, 15%, 5%
1	E	224	4%, 75%, 17%, 5%
1	H	224	6%, 76%, 17%
2	B	219	14%, 85%, 12%
2	D	219	8%, 82%, 15%

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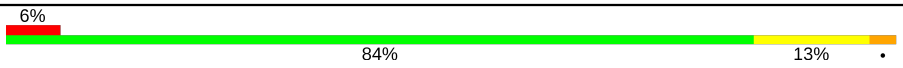
Mol	Chain	Length	Quality of chain
2	F	219	
2	L	219	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13731 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 Fab e6 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1630	1027	262	332	9			
1	C	212	Total	C	N	O	S	0	0	0
			1596	1008	256	323	9			
1	E	212	Total	C	N	O	S	0	0	0
			1596	1008	256	323	9			
1	H	215	Total	C	N	O	S	0	0	0
			1612	1016	259	328	9			

- Molecule 2 is a protein called Fab e6 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	0	0
			1707	1066	284	348	9			
2	D	219	Total	C	N	O	S	0	0	0
			1707	1066	284	348	9			
2	F	219	Total	C	N	O	S	0	0	0
			1707	1066	284	348	9			
2	L	219	Total	C	N	O	S	0	0	0
			1707	1066	284	348	9			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	40	Total	O	0	0
			40	40		
3	B	51	Total	O	0	0
			51	51		
3	C	48	Total	O	0	0
			48	48		
3	D	44	Total	O	0	0
			44	44		

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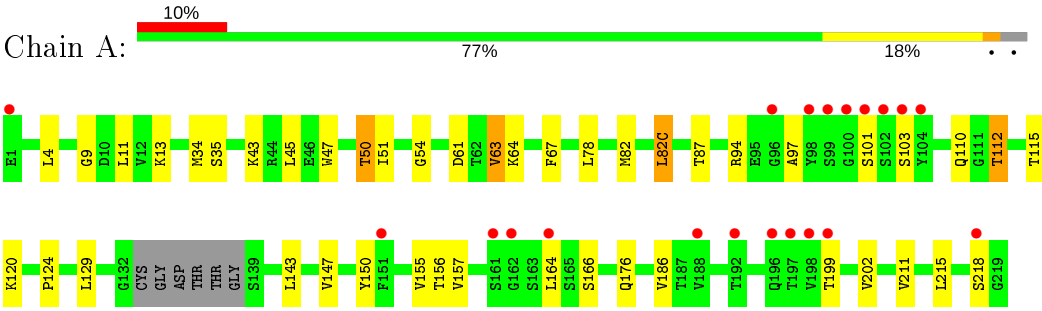
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	60	Total O 60 60	0	0
3	F	51	Total O 51 51	0	0
3	H	88	Total O 88 88	0	0
3	L	87	Total O 87 87	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

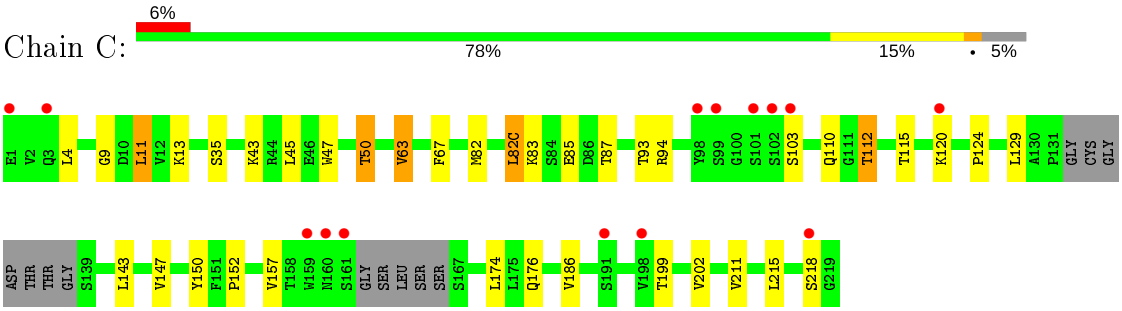
- Molecule 1: Fab e6 Heavy Chain

Chain A:



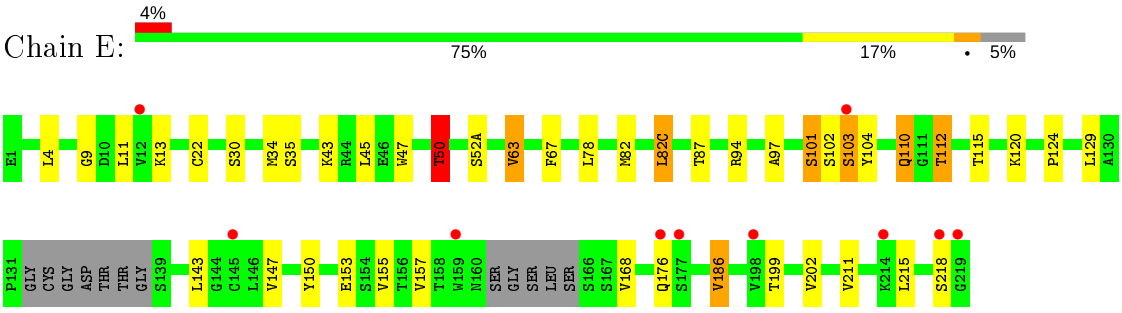
- Molecule 1: Fab e6 Heavy Chain

Chain C:



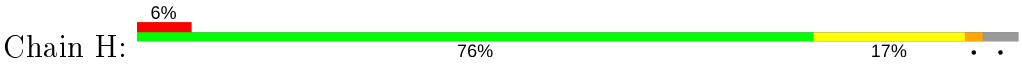
- Molecule 1: Fab e6 Heavy Chain

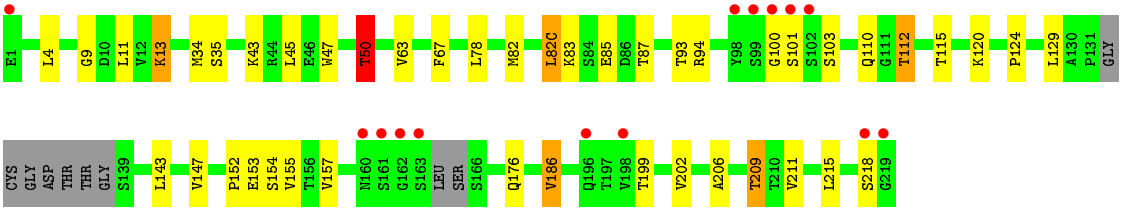
Chain E:



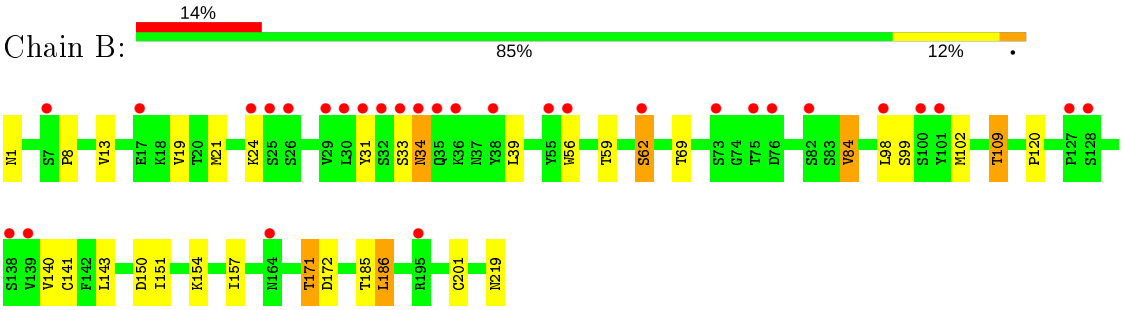
- Molecule 1: Fab e6 Heavy Chain

Chain H:

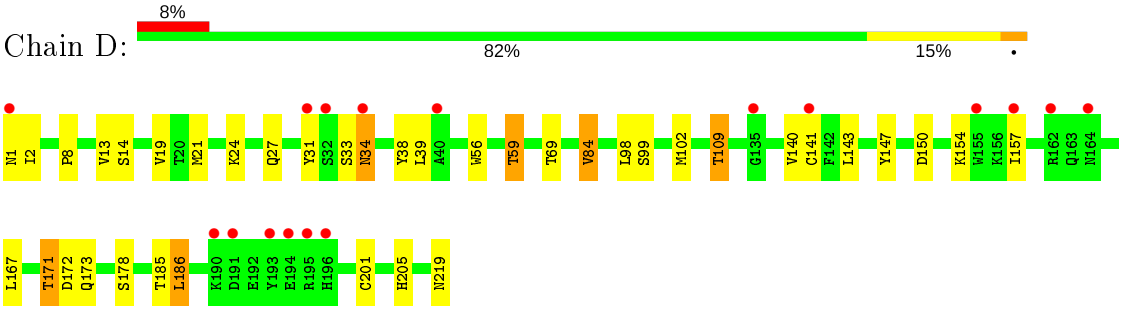




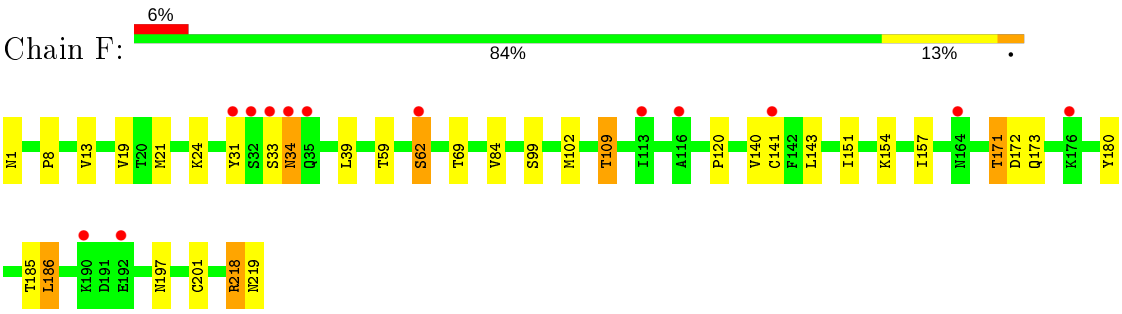
• Molecule 2: Fab e6 Light Chain



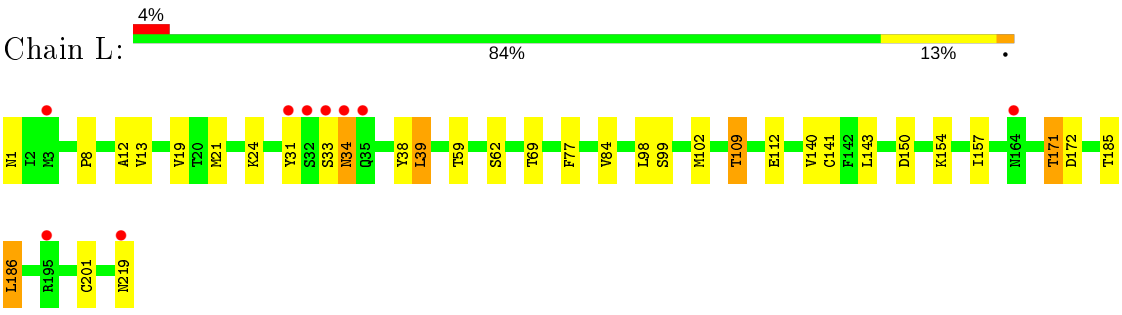
• Molecule 2: Fab e6 Light Chain



• Molecule 2: Fab e6 Light Chain



• Molecule 2: Fab e6 Light Chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	124.12Å 68.24Å 236.64Å 90.00° 96.27° 90.00°	Depositor
Resolution (Å)	31.06 – 2.52 31.06 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.3 (31.06-2.52) 99.5 (31.06-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.179 , 0.220 0.195 , 0.236	Depositor DCC
R_{free} test set	3376 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	47.5	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 63.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13731	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.51	0/1672	0.78	0/2281
1	C	0.50	0/1637	0.75	0/2233
1	E	0.54	0/1637	0.78	1/2233 (0.0%)
1	H	0.57	0/1653	0.79	1/2254 (0.0%)
2	B	0.49	0/1746	0.76	0/2369
2	D	0.48	0/1746	0.75	0/2369
2	F	0.49	0/1746	0.75	0/2369
2	L	0.53	0/1746	0.78	0/2369
All	All	0.51	0/13583	0.77	2/18477 (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})
1	H	50	THR	N-CA-CB	5.27	120.32	110.30
1	E	50	THR	N-CA-CB	5.11	120.01	110.30

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	1630	0	1576	17	0
1	C	1596	0	1543	16	0
1	E	1596	0	1543	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1612	0	1556	21	0
2	B	1707	0	1637	11	0
2	D	1707	0	1637	19	0
2	F	1707	0	1637	12	0
2	L	1707	0	1637	19	0
3	A	40	0	0	0	0
3	B	51	0	0	0	0
3	C	48	0	0	0	0
3	D	44	0	0	0	0
3	E	60	0	0	1	0
3	F	51	0	0	0	0
3	H	88	0	0	1	0
3	L	87	0	0	0	0
All	All	13731	0	12766	125	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 5.

All (125) 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:A:47:TRP:HE1	1:A:50:THR:HG22	1.26	1.01
1:E:47:TRP:HE1	1:E:50:THR:HG22	1.25	0.99
1:H:47:TRP:HE1	1:H:50:THR:HG22	1.31	0.92
1:H:103:SER:HB2	2:L:38:TYR:HE1	1.41	0.84
1:A:47:TRP:NE1	1:A:50:THR:HG22	1.97	0.79
1:E:47:TRP:HE1	1:E:50:THR:CG2	1.94	0.77
1:C:103:SER:HB2	2:D:38:TYR:HE1	1.51	0.76
1:H:13:LYS:HE2	3:H:309:HOH:O	1.84	0.75
1:E:47:TRP:NE1	1:E:50:THR:HG22	2.05	0.68
1:H:47:TRP:NE1	1:H:50:THR:HG22	2.08	0.67
1:C:63:VAL:HG13	1:C:67:PHE:HB2	1.76	0.67
2:L:19:VAL:HG21	2:L:84:VAL:HG21	1.77	0.67
1:A:63:VAL:HG13	1:A:67:PHE:HB2	1.79	0.64
1:H:47:TRP:CZ3	2:L:102:MET:HG2	2.34	0.62
1:A:34:MET:HB3	1:A:78:LEU:HD22	1.83	0.61
1:H:47:TRP:HZ3	2:L:102:MET:HG2	1.66	0.61
2:L:8:PRO:O	2:L:109:THR:HB	2.01	0.61
2:F:8:PRO:O	2:F:109:THR:HB	2.02	0.60
2:B:8:PRO:O	2:B:109:THR:HB	2.01	0.60
2:D:8:PRO:O	2:D:109:THR:HB	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:13:VAL:HG11	2:F:19:VAL:HG22	1.84	0.60
2:L:13:VAL:HG11	2:L:19:VAL:HG22	1.84	0.59
1:H:103:SER:HB2	2:L:38:TYR:CE1	2.30	0.59
2:B:157:ILE:HD11	2:B:186:LEU:HD11	1.85	0.59
1:C:47:TRP:CZ2	1:C:50:THR:HG22	2.38	0.58
1:E:47:TRP:NE1	1:E:50:THR:CG2	2.64	0.58
1:E:82:MET:HE2	1:E:82(C):LEU:HD11	1.85	0.58
2:F:157:ILE:HD11	2:F:186:LEU:HD11	1.86	0.58
2:L:157:ILE:HD11	2:L:186:LEU:HD11	1.86	0.57
2:D:157:ILE:HD11	2:D:186:LEU:HD11	1.86	0.57
2:L:19:VAL:HG23	2:L:84:VAL:HG23	1.86	0.57
1:H:82:MET:HE2	1:H:82(C):LEU:HD11	1.86	0.56
1:E:47:TRP:HZ3	2:F:102:MET:HG2	1.70	0.56
2:L:19:VAL:CG2	2:L:84:VAL:HG21	2.36	0.55
1:C:82:MET:HE2	1:C:82(C):LEU:HD11	1.87	0.55
1:E:63:VAL:HG13	1:E:67:PHE:HB2	1.88	0.55
2:F:173:GLN:HG3	2:F:180:TYR:CZ	2.42	0.55
1:A:124:PRO:HB3	1:A:150:TYR:HB3	1.88	0.54
2:D:13:VAL:HG11	2:D:19:VAL:HG22	1.90	0.54
1:H:63:VAL:HG13	1:H:67:PHE:HB2	1.89	0.54
1:A:47:TRP:HZ3	2:B:102:MET:HG2	1.72	0.53
1:H:124:PRO:HD2	1:H:209:THR:HG21	1.90	0.53
1:C:124:PRO:HB3	1:C:150:TYR:HB3	1.91	0.52
2:B:13:VAL:HG11	2:B:19:VAL:HG22	1.92	0.52
2:L:19:VAL:CG2	2:L:84:VAL:CG2	2.88	0.51
2:D:2:ILE:HG12	2:D:27:GLN:HG2	1.92	0.51
1:A:143:LEU:HB3	1:A:215:LEU:HD22	1.93	0.51
2:D:13:VAL:HG21	2:D:19:VAL:HG22	1.93	0.50
2:F:31:TYR:HB3	2:F:34:ASN:HB2	1.93	0.50
2:B:31:TYR:HB3	2:B:34:ASN:HB2	1.93	0.50
2:D:19:VAL:HG21	2:D:84:VAL:HG21	1.93	0.50
2:D:31:TYR:HB3	2:D:34:ASN:HB2	1.93	0.50
1:C:47:TRP:CZ3	2:D:102:MET:HG2	2.46	0.49
1:H:143:LEU:HB3	1:H:215:LEU:HD22	1.94	0.49
1:E:168:VAL:HG22	1:E:186:VAL:CG1	2.43	0.49
2:L:12:ALA:HB2	2:L:112:GLU:HG3	1.93	0.49
1:E:47:TRP:CZ3	2:F:102:MET:HG2	2.49	0.48
1:H:152:PRO:HD2	1:H:206:ALA:CB	2.44	0.47
2:L:19:VAL:HG23	2:L:84:VAL:CG2	2.44	0.47
1:C:143:LEU:HB3	1:C:215:LEU:HD22	1.95	0.47
1:C:47:TRP:HZ3	2:D:102:MET:HG2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:VAL:HG22	1:A:202:VAL:HG22	1.96	0.47
1:A:35:SER:OG	1:A:50:THR:HB	2.15	0.47
2:L:31:TYR:HB3	2:L:34:ASN:HB2	1.96	0.47
1:C:174:LEU:HD12	2:D:167:LEU:HD13	1.97	0.47
1:H:87:THR:HG23	1:H:115:THR:HA	1.97	0.47
1:E:143:LEU:HB3	1:E:215:LEU:HD22	1.96	0.46
1:A:87:THR:HG23	1:A:115:THR:HA	1.97	0.46
2:D:171:THR:HG23	2:D:172:ASP:O	2.14	0.46
1:C:47:TRP:HZ2	1:C:50:THR:HG22	1.79	0.46
2:D:56:TRP:HB2	2:D:59:THR:HG23	1.98	0.46
2:F:171:THR:HG23	2:F:172:ASP:O	2.16	0.46
1:H:34:MET:HB3	1:H:78:LEU:HD22	1.97	0.46
2:F:197:ASN:HA	2:F:218:ARG:HD3	1.97	0.45
1:E:168:VAL:HG22	1:E:186:VAL:HG12	1.98	0.45
1:E:157:VAL:HG22	1:E:202:VAL:HG22	1.98	0.45
1:E:30:SER:O	1:E:52(A):SER:HB2	2.17	0.45
2:F:140:VAL:HG22	2:F:185:THR:HG23	1.98	0.45
1:A:103:SER:O	2:B:56:TRP:NE1	2.50	0.45
1:E:97:ALA:HB1	1:E:101:SER:O	2.16	0.45
1:C:11:LEU:HG	1:C:152:PRO:HG3	1.97	0.45
1:C:157:VAL:HG22	1:C:202:VAL:HG22	1.98	0.45
1:E:102:SER:O	1:E:103:SER:HB3	2.17	0.45
1:A:9:GLY:H	1:A:112:THR:HG21	1.81	0.45
1:C:87:THR:HG23	1:C:115:THR:HA	1.99	0.45
1:E:110:GLN:HG3	3:E:315:HOH:O	2.17	0.45
1:E:87:THR:HG23	1:E:115:THR:HA	1.98	0.45
1:H:35:SER:HB2	1:H:93:THR:OG1	2.16	0.45
1:A:97:ALA:HB1	1:A:101:SER:O	2.17	0.44
2:B:171:THR:HG23	2:B:172:ASP:O	2.17	0.44
2:B:19:VAL:HG21	2:B:84:VAL:HG21	1.98	0.44
1:E:102:SER:O	1:E:103:SER:CB	2.65	0.44
1:C:9:GLY:H	1:C:112:THR:HG21	1.82	0.44
1:H:9:GLY:H	1:H:112:THR:HG21	1.83	0.44
2:L:39:LEU:HD13	2:L:77:PHE:CD2	2.54	0.43
2:D:147:TYR:O	2:D:205:HIS:HE1	2.02	0.43
2:F:120:PRO:HG3	2:F:151:ILE:HD11	2.00	0.43
1:H:157:VAL:HG22	1:H:202:VAL:HG22	2.00	0.43
1:E:9:GLY:H	1:E:112:THR:HG21	1.83	0.42
2:B:140:VAL:HG22	2:B:185:THR:HG23	2.02	0.42
2:D:140:VAL:HG22	2:D:185:THR:HG23	2.01	0.42
1:H:100:GLY:HA2	1:H:101:SER:HA	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:173:GLN:NE2	2:D:178:SER:HB3	2.35	0.42
2:L:19:VAL:HG21	2:L:84:VAL:CG2	2.48	0.42
1:A:103:SER:HB2	2:B:56:TRP:HE1	1.85	0.42
2:L:171:THR:HG23	2:L:172:ASP:O	2.20	0.42
2:F:13:VAL:HG21	2:F:19:VAL:HG22	2.02	0.41
2:L:140:VAL:HG22	2:L:185:THR:HG23	2.02	0.41
1:C:83:LYS:HG3	1:C:85:GLU:HG2	2.02	0.41
1:E:143:LEU:HB2	1:E:186:VAL:HG23	2.02	0.41
1:A:61:ASP:HA	1:A:64:LYS:HD3	2.03	0.41
1:H:143:LEU:HB2	1:H:186:VAL:HG23	2.02	0.41
1:A:82:MET:HE2	1:A:82(C):LEU:HD11	2.02	0.41
2:L:31:TYR:HB2	2:L:38:TYR:HE2	1.86	0.41
1:E:124:PRO:HB3	1:E:150:TYR:HB3	2.02	0.41
2:B:120:PRO:HG3	2:B:151:ILE:HD11	2.03	0.41
1:E:34:MET:HB3	1:E:78:LEU:HD22	2.02	0.41
2:D:13:VAL:HG11	2:D:19:VAL:CG2	2.51	0.40
1:H:83:LYS:HG3	1:H:85:GLU:HG2	2.03	0.40
1:C:35:SER:OG	1:C:50:THR:HB	2.21	0.40
2:D:19:VAL:CG2	2:D:84:VAL:HG21	2.51	0.40
1:E:22:CYS:HB3	1:E:78:LEU:HB3	2.03	0.40
1:H:153:GLU:HA	1:H:154:SER:HA	1.86	0.40
2:D:2:ILE:HG12	2:D:27:GLN:CG	2.51	0.40
1:A:51:ILE:CG1	1:A:54:GLY:HA2	2.52	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	214/224 (96%)	207 (97%)	7 (3%)	0	100	100
1	C	206/224 (92%)	201 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	206/224 (92%)	201 (98%)	3 (2%)	2 (1%)	15 27
1	H	209/224 (93%)	204 (98%)	5 (2%)	0	100 100
2	B	217/219 (99%)	207 (95%)	9 (4%)	1 (0%)	29 47
2	D	217/219 (99%)	210 (97%)	7 (3%)	0	100 100
2	F	217/219 (99%)	211 (97%)	5 (2%)	1 (0%)	29 47
2	L	217/219 (99%)	209 (96%)	8 (4%)	0	100 100
All	All	1703/1772 (96%)	1650 (97%)	49 (3%)	4 (0%)	47 67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	103	SER
1	E	101	SER
2	B	62	SER
2	F	62	SER

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	188/192 (98%)	165 (88%)	23 (12%)	5 8
1	C	184/192 (96%)	164 (89%)	20 (11%)	6 11
1	E	184/192 (96%)	161 (88%)	23 (12%)	4 8
1	H	186/192 (97%)	166 (89%)	20 (11%)	6 11
2	B	196/196 (100%)	175 (89%)	21 (11%)	6 12
2	D	196/196 (100%)	175 (89%)	21 (11%)	6 12
2	F	196/196 (100%)	176 (90%)	20 (10%)	7 13
2	L	196/196 (100%)	176 (90%)	20 (10%)	7 13
All	All	1526/1552 (98%)	1358 (89%)	168 (11%)	6 11

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	11	LEU
1	A	13	LYS
1	A	43	LYS
1	A	45	LEU
1	A	50	THR
1	A	63	VAL
1	A	82(C)	LEU
1	A	94	ARG
1	A	110	GLN
1	A	112	THR
1	A	120	LYS
1	A	129	LEU
1	A	147	VAL
1	A	155	VAL
1	A	156	THR
1	A	164	LEU
1	A	166	SER
1	A	176	GLN
1	A	186	VAL
1	A	199	THR
1	A	211	VAL
1	A	218	SER
2	B	1	ASN
2	B	21	MET
2	B	24	LYS
2	B	33	SER
2	B	34	ASN
2	B	39	LEU
2	B	59	THR
2	B	62	SER
2	B	69	THR
2	B	84	VAL
2	B	98	LEU
2	B	99	SER
2	B	109	THR
2	B	141	CYS
2	B	143	LEU
2	B	150	ASP
2	B	154	LYS
2	B	171	THR
2	B	186	LEU
2	B	201	CYS

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Mol	Chain	Res	Type
2	B	219	ASN
1	C	4	LEU
1	C	11	LEU
1	C	13	LYS
1	C	43	LYS
1	C	45	LEU
1	C	50	THR
1	C	63	VAL
1	C	82(C)	LEU
1	C	93	THR
1	C	94	ARG
1	C	110	GLN
1	C	112	THR
1	C	120	LYS
1	C	129	LEU
1	C	147	VAL
1	C	176	GLN
1	C	186	VAL
1	C	199	THR
1	C	211	VAL
1	C	218	SER
2	D	1	ASN
2	D	14	SER
2	D	21	MET
2	D	24	LYS
2	D	33	SER
2	D	34	ASN
2	D	39	LEU
2	D	59	THR
2	D	69	THR
2	D	84	VAL
2	D	98	LEU
2	D	99	SER
2	D	109	THR
2	D	141	CYS
2	D	143	LEU
2	D	150	ASP
2	D	154	LYS
2	D	171	THR
2	D	186	LEU
2	D	201	CYS
2	D	219	ASN

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Mol	Chain	Res	Type
1	E	4	LEU
1	E	11	LEU
1	E	13	LYS
1	E	35	SER
1	E	43	LYS
1	E	45	LEU
1	E	50	THR
1	E	63	VAL
1	E	82(C)	LEU
1	E	94	ARG
1	E	104	TYR
1	E	110	GLN
1	E	112	THR
1	E	120	LYS
1	E	129	LEU
1	E	147	VAL
1	E	153	GLU
1	E	155	VAL
1	E	176	GLN
1	E	186	VAL
1	E	199	THR
1	E	211	VAL
1	E	218	SER
2	F	1	ASN
2	F	21	MET
2	F	24	LYS
2	F	33	SER
2	F	34	ASN
2	F	39	LEU
2	F	59	THR
2	F	62	SER
2	F	69	THR
2	F	84	VAL
2	F	99	SER
2	F	109	THR
2	F	141	CYS
2	F	143	LEU
2	F	154	LYS
2	F	171	THR
2	F	186	LEU
2	F	201	CYS
2	F	218	ARG

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Mol	Chain	Res	Type
2	F	219	ASN
1	H	4	LEU
1	H	11	LEU
1	H	13	LYS
1	H	43	LYS
1	H	45	LEU
1	H	50	THR
1	H	82(C)	LEU
1	H	94	ARG
1	H	110	GLN
1	H	112	THR
1	H	120	LYS
1	H	129	LEU
1	H	147	VAL
1	H	155	VAL
1	H	176	GLN
1	H	186	VAL
1	H	199	THR
1	H	209	THR
1	H	211	VAL
1	H	218	SER
2	L	1	ASN
2	L	21	MET
2	L	24	LYS
2	L	33	SER
2	L	34	ASN
2	L	39	LEU
2	L	59	THR
2	L	62	SER
2	L	69	THR
2	L	98	LEU
2	L	99	SER
2	L	109	THR
2	L	141	CYS
2	L	143	LEU
2	L	150	ASP
2	L	154	LYS
2	L	171	THR
2	L	186	LEU
2	L	201	CYS
2	L	219	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
2	D	217	ASN
2	D	219	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	218/224 (97%)	0.44	23 (10%) 6 6	40, 58, 102, 139	0
1	C	212/224 (94%)	0.28	14 (6%) 18 19	38, 60, 101, 137	0
1	E	212/224 (94%)	0.20	10 (4%) 31 34	30, 53, 99, 146	0
1	H	215/224 (95%)	0.09	14 (6%) 18 20	30, 44, 85, 135	0
2	B	219/219 (100%)	0.54	30 (13%) 3 3	38, 65, 103, 153	0
2	D	219/219 (100%)	0.42	17 (7%) 13 13	37, 69, 121, 132	0
2	F	219/219 (100%)	0.30	13 (5%) 22 23	32, 62, 106, 122	0
2	L	219/219 (100%)	-0.01	9 (4%) 37 41	27, 49, 91, 114	0
All	All	1733/1772 (97%)	0.28	130 (7%) 14 15	27, 58, 105, 153	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	100	GLY	7.1
2	F	164	ASN	6.5
1	C	101	SER	5.6
2	B	32	SER	5.5
1	H	163	SER	4.9
2	D	32	SER	4.8
1	A	102	SER	4.8
2	D	191	ASP	4.7
1	H	101	SER	4.6
1	C	102	SER	4.4
2	D	164	ASN	4.4
2	B	33	SER	4.4
2	D	1	ASN	4.3
2	F	33	SER	4.3
1	A	161	SER	4.3
2	B	31	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	198	VAL	4.2
1	A	104	TYR	4.2
1	A	188	VAL	4.1
2	B	164	ASN	4.1
1	H	161	SER	4.1
1	A	103	SER	4.0
2	L	164	ASN	4.0
2	D	31	TYR	4.0
2	D	195	ARG	3.9
1	A	196	GLN	3.9
1	H	162	GLY	3.9
2	F	32	SER	3.8
1	C	98	TYR	3.7
1	E	198	VAL	3.6
2	F	31	TYR	3.5
1	A	198	VAL	3.5
2	L	32	SER	3.5
2	F	176	LYS	3.4
1	C	120	LYS	3.3
2	L	195	ARG	3.2
2	B	34	ASN	3.1
1	A	98	TYR	3.1
1	C	160	ASN	3.1
2	B	138	SER	3.1
2	D	162	ARG	3.0
2	D	135	GLY	3.0
1	A	1	GLU	3.0
1	E	103	SER	2.9
2	B	100	SER	2.8
1	H	160	ASN	2.8
1	H	218	SER	2.8
2	L	33	SER	2.8
1	E	159	TRP	2.8
2	D	193	TYR	2.8
2	B	73	SER	2.8
2	B	24	LYS	2.8
1	A	119	ALA	2.7
2	B	82	SER	2.7
1	E	176	GLN	2.7
2	B	38	TYR	2.7
1	C	161	SER	2.7
1	C	218	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	40	ALA	2.7
1	H	102	SER	2.6
2	B	30	LEU	2.6
1	A	162	GLY	2.6
2	F	116	ALA	2.6
2	B	17	GLU	2.6
2	B	62	SER	2.6
1	A	164	LEU	2.6
1	H	99	SER	2.6
2	B	101	TYR	2.6
2	D	157	ILE	2.5
2	B	195	ARG	2.5
2	F	190	LYS	2.5
1	H	98	TYR	2.5
1	E	214	LYS	2.5
1	E	219	GLY	2.5
1	A	192	THR	2.5
2	B	56	TRP	2.5
2	F	192	GLU	2.5
2	D	190	LYS	2.5
2	L	31	TYR	2.4
2	D	196	HIS	2.4
1	C	103	SER	2.4
2	L	34	ASN	2.4
2	B	75	THR	2.4
1	A	118	SER	2.4
1	E	177	SER	2.4
2	B	26	SER	2.4
2	F	141	CYS	2.3
1	C	1	GLU	2.3
2	F	113	ILE	2.3
2	B	139	VAL	2.3
1	E	145	CYS	2.3
2	F	62	SER	2.3
2	B	98	LEU	2.3
2	D	141	CYS	2.3
2	D	194	GLU	2.3
2	D	34	ASN	2.3
1	A	100	GLY	2.3
2	B	127	PRO	2.3
1	H	198	VAL	2.3
1	A	199	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	117	SER	2.2
2	L	3	MET	2.2
1	H	219	GLY	2.2
2	B	76	ASP	2.2
2	B	55	TYR	2.2
1	A	218	SER	2.2
1	C	99	SER	2.2
2	F	34	ASN	2.2
1	C	191	SER	2.2
2	L	219	ASN	2.2
1	A	96	GLY	2.2
2	B	128	SER	2.2
2	L	35	GLN	2.2
1	A	197	THR	2.2
2	B	29	VAL	2.1
1	A	99	SER	2.1
2	D	155	TRP	2.1
2	F	35	GLN	2.1
1	E	218	SER	2.1
1	A	151	PHE	2.1
2	B	25	SER	2.1
1	C	159	TRP	2.1
1	H	196	GLN	2.1
1	A	101	SER	2.1
2	B	7	SER	2.1
1	E	12	VAL	2.0
1	H	1	GLU	2.0
2	B	35	GLN	2.0
2	B	36	LYS	2.0
1	C	3	GLN	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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.