Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2024 – 04:35 pm BST

PDB ID	:	8C67
Title	:	Crystal structure of Ab25 Fab
Authors	:	Nyblom, M.; Izadi, A.; Tang, D.; Bahnan, W.; Happonen, L.; Malmstroem, J.; Shannon, O.; Malmstroem, L.; Nordenfelt, P.
Deposited on	:	2023-01-11
Resolution	:	1.88 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:

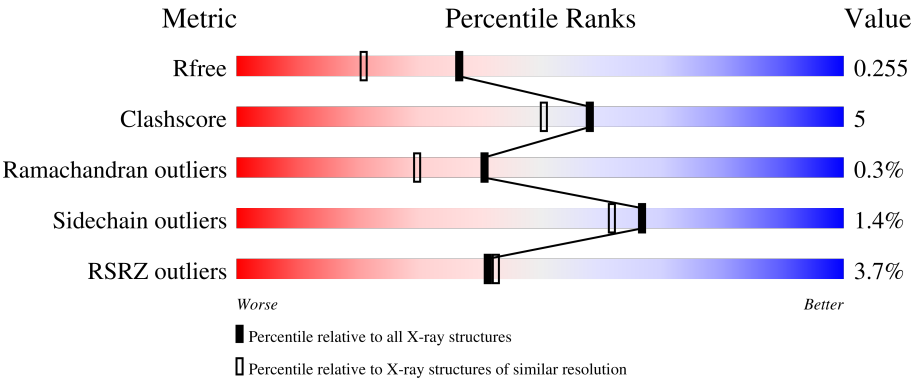
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 1.88 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	229	4% 87% 8%
1	C	229	3% 84% 11%
1	E	229	8% 81% 12% 6%
1	H	229	4% 86% 8% 5%
2	B	214	88% 11%

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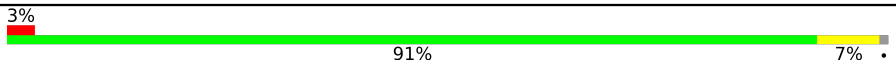
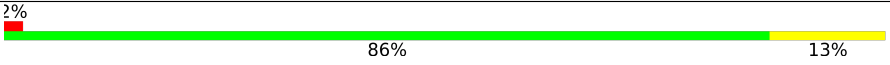
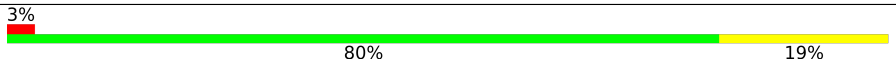
Mol	Chain	Length	Quality of chain
2	D	214	
2	F	214	
2	L	214	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14174 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 25 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	218	Total	C	N	O	S	0	0	0
			1672	1063	288	315	6			
1	A	221	Total	C	N	O	S	0	0	0
			1686	1069	290	321	6			
1	C	220	Total	C	N	O	S	0	0	0
			1682	1068	290	318	6			
1	E	215	Total	C	N	O	S	0	0	0
			1650	1048	284	312	6			

- Molecule 2 is a protein called antibody 25 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1637	1021	273	336	7			
2	B	213	Total	C	N	O	S	0	0	0
			1631	1018	272	335	6			
2	D	212	Total	C	N	O	S	0	0	0
			1622	1013	271	332	6			
2	F	213	Total	C	N	O	S	0	0	0
			1631	1018	272	335	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	114	Total	O	0	0
			114	114		
3	L	92	Total	O	0	0
			92	92		
3	A	142	Total	O	0	0
			142	142		
3	B	135	Total	O	0	0
			135	135		

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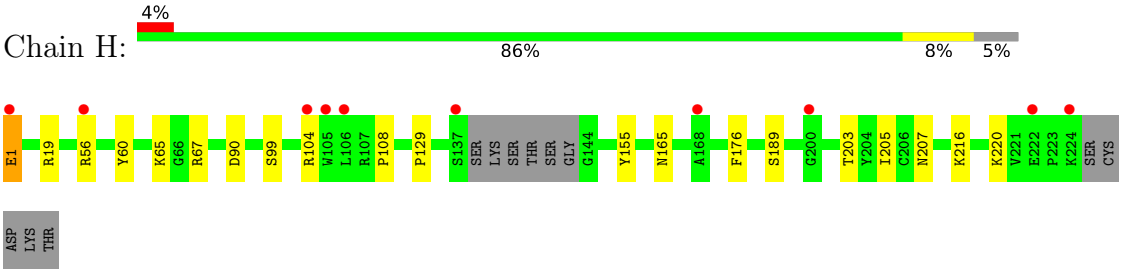
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	128	Total O 128 128	0	0
3	D	138	Total O 138 138	0	0
3	E	100	Total O 100 100	0	0
3	F	114	Total O 114 114	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

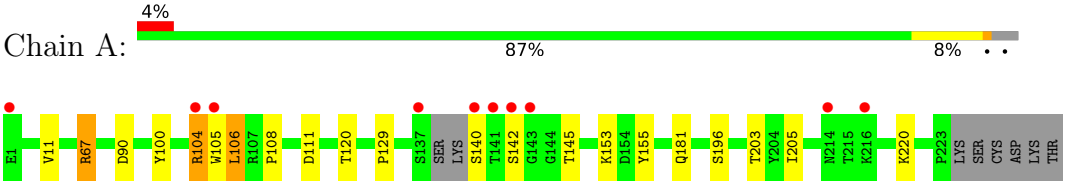
• Molecule 1: antibody 25 heavy chain

Chain H:



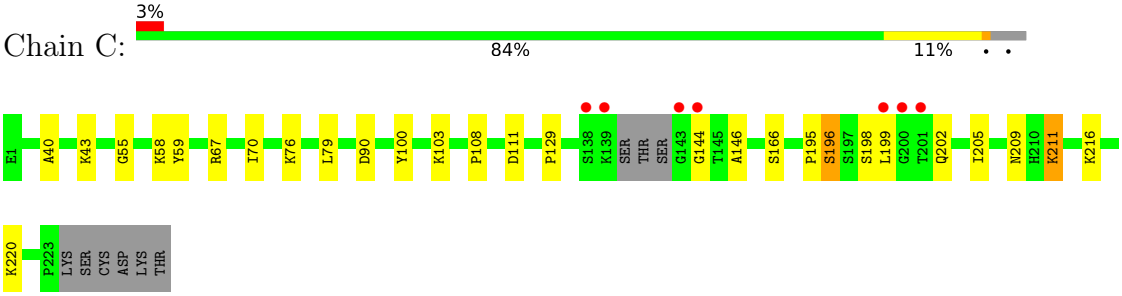
• Molecule 1: antibody 25 heavy chain

Chain A:



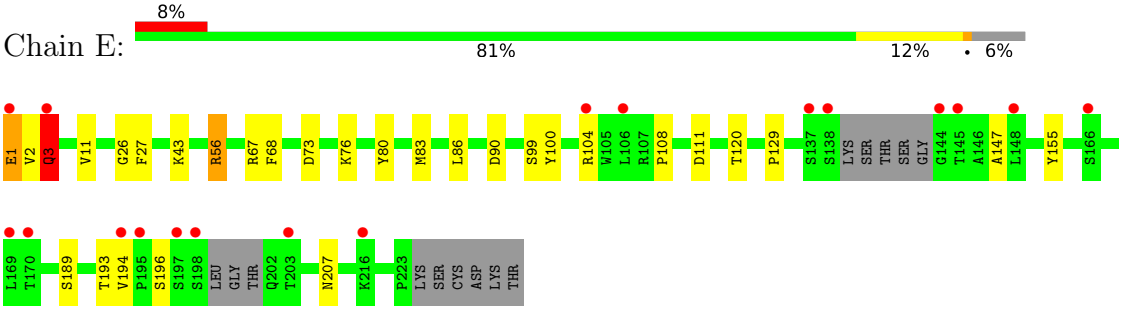
• Molecule 1: antibody 25 heavy chain

Chain C:



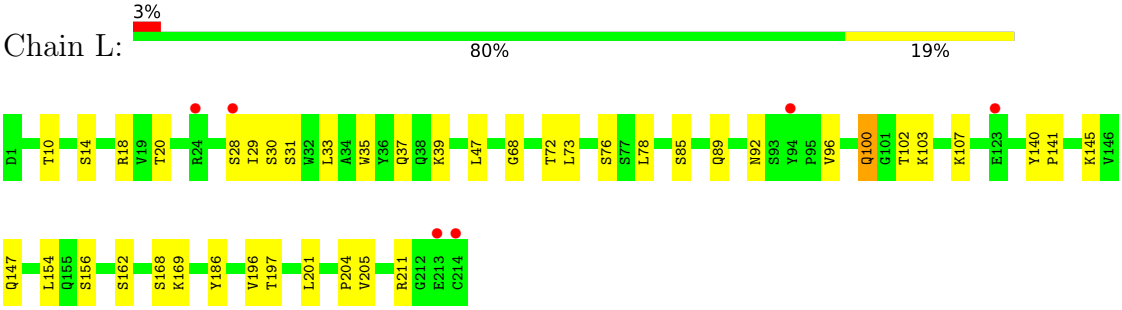
• Molecule 1: antibody 25 heavy chain

Chain E:



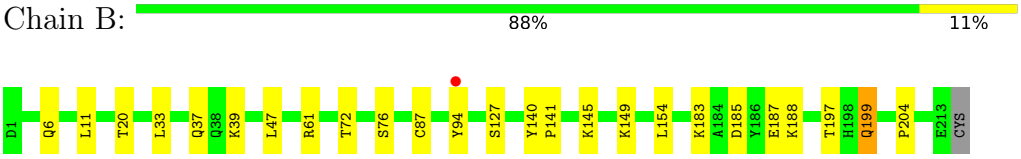
• Molecule 2: antibody 25 light chain

Chain L:



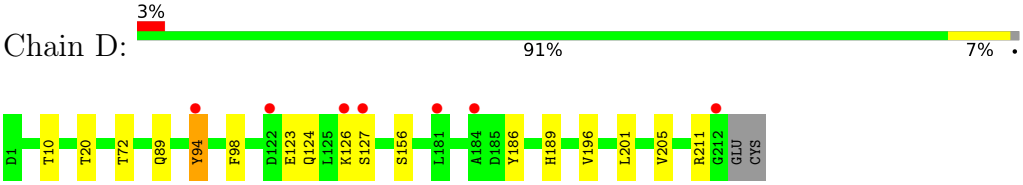
• Molecule 2: antibody 25 light chain

Chain B:



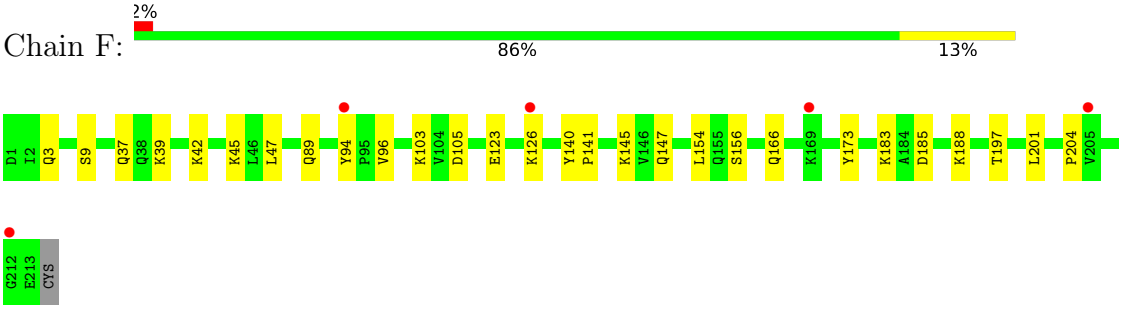
• Molecule 2: antibody 25 light chain

Chain D:



• Molecule 2: antibody 25 light chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.90Å 71.89Å 146.01Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	44.16 – 1.88 44.15 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.16-1.88) 99.2 (44.15-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.205 , 0.255 0.205 , 0.255	Depositor DCC
R_{free} test set	7361 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.916	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 33.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.194 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14174	wwPDB-VP
Average B, all atoms (Å^2)	39.0	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 32.98 % 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 8.6042e-04. 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	0.44	0/1731	0.70	3/2358 (0.1%)
1	C	0.39	0/1727	0.62	1/2351 (0.0%)
1	E	0.51	2/1694 (0.1%)	0.74	4/2306 (0.2%)
1	H	0.52	2/1717 (0.1%)	0.68	3/2338 (0.1%)
2	B	0.42	0/1666	0.61	2/2263 (0.1%)
2	D	0.40	0/1657	0.59	0/2251
2	F	0.39	0/1666	0.60	0/2263
2	L	0.44	0/1672	0.62	1/2271 (0.0%)
All	All	0.44	4/13530 (0.0%)	0.65	14/18401 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	1	GLU	CB-CG	10.62	1.72	1.52
1	E	1	GLU	CB-CG	7.32	1.66	1.52
1	H	1	GLU	CG-CD	6.73	1.62	1.51
1	E	43	LYS	CB-CG	-5.95	1.36	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	104	ARG	CB-CG-CD	-10.06	85.43	111.60
1	A	104	ARG	CG-CD-NE	8.31	129.26	111.80
1	E	56	ARG	CG-CD-NE	7.70	127.97	111.80
1	E	56	ARG	CD-NE-CZ	6.60	132.84	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	1	GLU	CA-CB-CG	6.25	127.16	113.40
1	E	1	GLU	CA-CB-CG	-6.18	99.80	113.40
2	L	100	GLN	CB-CA-C	-6.11	98.18	110.40
1	C	196	SER	CB-CA-C	6.08	121.66	110.10
1	E	3	GLN	CA-CB-CG	-5.99	100.22	113.40
1	H	104	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	H	56	ARG	CA-CB-CG	-5.72	100.81	113.40
1	A	67	ARG	NE-CZ-NH2	-5.62	117.49	120.30
2	B	127	SER	N-CA-CB	-5.30	102.55	110.50
2	B	11	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	56	ARG	Sidechain

5.2 Too-close contacts (i)

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	1686	0	1651	12	0
1	C	1682	0	1652	18	0
1	E	1650	0	1614	19	0
1	H	1672	0	1644	11	0
2	B	1631	0	1579	12	0
2	D	1622	0	1573	10	0
2	F	1631	0	1579	24	0
2	L	1637	0	1584	23	0
3	A	142	0	0	0	0
3	B	135	0	0	2	0
3	C	128	0	0	2	0
3	D	138	0	0	2	0
3	E	100	0	0	1	0
3	F	114	0	0	8	1
3	H	114	0	0	1	1
3	L	92	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14174	0	12876	125	1

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)
2:F:42:LYS:NZ	3:F:301:HOH:O	1.90	1.02
1:E:2:VAL:C	1:E:3:GLN:HG2	1.96	0.85
2:L:197:THR:HG22	2:L:204:PRO:HB3	1.66	0.76
2:B:199:GLN:NE2	3:B:301:HOH:O	2.16	0.75
1:H:1:GLU:N	3:H:301:HOH:O	2.05	0.74
2:F:147:GLN:OE1	3:F:302:HOH:O	2.04	0.74
1:C:196:SER:HA	1:C:199:LEU:HD12	1.69	0.73
2:F:147:GLN:HG2	2:F:154:LEU:HD11	1.75	0.68
2:L:28:SER:HB2	2:L:68:GLY:HA2	1.77	0.67
2:F:37:GLN:O	3:F:301:HOH:O	2.13	0.67
2:F:123:GLU:O	2:F:126:LYS:HB3	1.96	0.65
1:E:2:VAL:O	1:E:3:GLN:HG2	1.96	0.64
1:H:67:ARG:NH2	1:H:90:ASP:OD2	2.30	0.63
1:A:105:TRP:O	1:A:106:LEU:HB2	1.99	0.63
2:F:39:LYS:HB2	2:F:42:LYS:HG2	1.81	0.63
1:C:209:ASN:OD1	1:C:216:LYS:HG2	1.99	0.63
1:C:76:LYS:NZ	3:C:303:HOH:O	2.32	0.62
2:B:39:LYS:NZ	3:B:303:HOH:O	2.26	0.62
1:C:146:ALA:HB2	1:C:196:SER:HB3	1.82	0.61
1:C:67:ARG:NH2	1:C:90:ASP:OD2	2.29	0.61
2:D:124:GLN:O	2:D:127:SER:OG	2.10	0.60
2:F:145:LYS:HB3	2:F:197:THR:OG1	2.01	0.60
2:L:201:LEU:HD13	2:L:205:VAL:HG12	1.82	0.60
2:B:197:THR:HG22	2:B:204:PRO:HG3	1.85	0.59
2:F:45:LYS:NZ	3:F:305:HOH:O	2.36	0.58
1:E:100:TYR:CD2	1:E:111:ASP:HB3	2.39	0.56
1:C:59:TYR:HB3	2:D:94:TYR:OH	2.06	0.56
1:E:1:GLU:HG2	1:E:3:GLN:HG3	1.87	0.56
1:E:67:ARG:NH2	1:E:90:ASP:OD2	2.34	0.56
2:L:89:GLN:HE21	2:L:96:VAL:HB	1.72	0.55
2:B:185:ASP:HA	2:B:188:LYS:HE2	1.89	0.54
1:A:142:SER:HA	1:A:196:SER:OG	2.07	0.54
2:D:10:THR:OG1	3:D:301:HOH:O	2.17	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ARG:NH2	1:A:90:ASP:OD2	2.26	0.54
1:E:1:GLU:O	1:E:26:GLY:HA3	2.09	0.53
1:H:60:TYR:HB2	1:H:65:LYS:HD2	1.89	0.53
1:E:73:ASP:OD2	1:E:76:LYS:HE3	2.08	0.53
2:L:30:SER:OG	2:L:31:SER:N	2.40	0.53
2:F:185:ASP:HA	2:F:188:LYS:HD2	1.91	0.53
2:L:145:LYS:NZ	3:L:307:HOH:O	2.40	0.52
2:B:61:ARG:HB2	2:B:76:SER:O	2.10	0.52
2:D:189:HIS:O	2:D:211:ARG:NH1	2.33	0.51
1:A:203:THR:CG2	1:A:220:LYS:HD2	2.41	0.50
1:C:55:GLY:O	1:C:58:LYS:NZ	2.42	0.50
2:F:37:GLN:HB2	2:F:47:LEU:HD11	1.94	0.50
1:H:203:THR:HG21	1:H:220:LYS:HD2	1.93	0.49
2:F:89:GLN:HE21	2:F:96:VAL:HB	1.76	0.49
1:E:100:TYR:HD2	1:E:111:ASP:HB3	1.78	0.48
1:A:105:TRP:CD2	1:A:106:LEU:HD12	2.48	0.48
2:L:37:GLN:HG2	3:L:325:HOH:O	2.13	0.48
1:E:147:ALA:HB2	1:E:193:THR:HG22	1.95	0.48
1:C:100:TYR:CD2	1:C:111:ASP:HB3	2.48	0.48
1:E:129:PRO:HB3	1:E:155:TYR:HB3	1.95	0.48
2:D:20:THR:HG23	2:D:72:THR:HG23	1.96	0.48
2:F:39:LYS:HB2	2:F:42:LYS:HE3	1.96	0.48
1:C:205:ILE:HG12	1:C:220:LYS:HG2	1.95	0.47
2:L:196:VAL:HB	2:L:205:VAL:HG13	1.96	0.47
1:A:100:TYR:CD1	1:A:111:ASP:HB3	2.50	0.47
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.96	0.47
1:H:1:GLU:O	1:H:1:GLU:HG2	2.15	0.47
1:A:11:VAL:HG22	1:A:120:THR:HB	1.97	0.47
1:A:205:ILE:HG12	1:A:220:LYS:HD3	1.97	0.47
2:D:186:TYR:CE2	2:D:211:ARG:HD3	2.49	0.47
1:E:1:GLU:HG2	1:E:3:GLN:CG	2.44	0.47
2:L:169:LYS:HB2	2:L:169:LYS:HE2	1.77	0.47
2:B:145:LYS:HB3	2:B:197:THR:OG1	2.15	0.47
1:C:166:SER:HB3	2:F:9:SER:HB2	1.97	0.47
1:A:104:ARG:HD3	1:A:104:ARG:HA	1.65	0.46
2:F:197:THR:HG22	2:F:204:PRO:HG3	1.96	0.46
1:H:176:PHE:HB3	2:L:162:SER:OG	2.15	0.46
1:C:198:SER:HB2	1:C:202:GLN:HB2	1.97	0.46
2:D:196:VAL:HB	2:D:205:VAL:HG13	1.97	0.46
2:F:105:ASP:HB2	2:F:166:GLN:OE1	2.15	0.46
1:H:19:ARG:HD2	3:D:364:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:SER:N	1:A:145:THR:O	2.48	0.46
2:B:20:THR:HG23	2:B:72:THR:HG23	1.98	0.45
2:B:183:LYS:O	2:B:187:GLU:HG3	2.17	0.45
1:E:68:PHE:CZ	1:E:83:MET:HE2	2.51	0.45
2:L:168:SER:OG	2:L:169:LYS:HD3	2.16	0.45
1:E:2:VAL:HG13	1:E:27:PHE:CD1	2.52	0.45
1:H:129:PRO:HB3	1:H:155:TYR:HB3	1.97	0.45
1:E:104:ARG:HB2	3:E:302:HOH:O	2.16	0.45
1:H:216:LYS:HB2	1:H:216:LYS:HE2	1.74	0.44
1:C:211:LYS:HE2	1:C:211:LYS:HB2	1.80	0.44
2:L:28:SER:HB2	2:L:68:GLY:CA	2.45	0.44
2:F:154:LEU:HD12	2:F:154:LEU:HA	1.66	0.44
2:F:201:LEU:HB2	3:F:373:HOH:O	2.18	0.44
2:L:147:GLN:CG	2:L:154:LEU:HD11	2.49	0.43
1:C:211:LYS:HG2	2:F:3:GLN:HG3	1.99	0.43
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.99	0.43
1:C:100:TYR:HB3	1:C:103:LYS:HG3	2.01	0.43
2:F:140:TYR:CD2	2:F:141:PRO:HA	2.53	0.43
1:E:11:VAL:HG22	1:E:120:THR:HB	2.00	0.43
2:F:183:LYS:NZ	3:F:312:HOH:O	2.48	0.43
2:D:123:GLU:HA	2:D:126:LYS:HD2	2.01	0.43
1:E:76:LYS:NZ	1:E:80:TYR:OH	2.50	0.43
2:L:140:TYR:CG	2:L:141:PRO:HA	2.54	0.43
1:E:2:VAL:HG22	1:E:27:PHE:HB3	2.01	0.43
1:H:220:LYS:HB3	1:H:220:LYS:HE3	1.85	0.43
1:E:194:VAL:O	1:E:196:SER:N	2.48	0.43
2:F:140:TYR:CG	2:F:141:PRO:HA	2.54	0.42
2:L:20:THR:HG23	2:L:72:THR:HG23	2.01	0.42
2:L:18:ARG:HG3	2:L:76:SER:HA	2.01	0.42
1:C:70:ILE:HD11	1:C:79:LEU:HD11	2.02	0.42
2:L:186:TYR:CZ	2:L:211:ARG:HG3	2.55	0.42
1:E:83:MET:HE2	1:E:86:LEU:HD21	2.02	0.42
2:L:85:SER:HA	2:L:102:THR:O	2.20	0.42
1:C:129:PRO:C	3:C:301:HOH:O	2.58	0.42
1:A:153:LYS:NZ	1:A:181:GLN:OE1	2.53	0.41
2:L:39:LYS:HG3	3:L:325:HOH:O	2.20	0.41
1:A:129:PRO:HB3	1:A:155:TYR:HB3	2.02	0.41
2:B:140:TYR:CG	2:B:141:PRO:HA	2.56	0.41
1:C:144:GLY:O	1:C:195:PRO:HA	2.21	0.41
2:F:45:LYS:NZ	3:F:309:HOH:O	2.42	0.41
1:H:165:ASN:OD1	1:H:205:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ALA:HB3	1:C:43:LYS:HD3	2.03	0.41
2:L:10:THR:HG23	2:L:103:LYS:HB3	2.03	0.41
2:L:29:ILE:HB	2:L:92:ASN:HB2	2.03	0.41
2:D:89:GLN:HB2	2:D:98:PHE:CD2	2.56	0.41
2:F:105:ASP:OD2	2:F:173:TYR:OH	2.30	0.41
2:D:201:LEU:HD13	2:D:205:VAL:HG12	2.03	0.41
2:L:35:TRP:CE2	2:L:73:LEU:HB2	2.56	0.40
2:B:6:GLN:OE1	2:B:87:CYS:HA	2.21	0.40
2:B:149:LYS:HG2	2:B:154:LEU:HD23	2.04	0.40
2:F:103:LYS:NZ	3:F:311:HOH:O	2.46	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:308:HOH:O	3:F:392:HOH:O[2_445]	2.15	0.05

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	217/229 (95%)	210 (97%)	5 (2%)	2 (1%)	17 7
1	C	216/229 (94%)	211 (98%)	4 (2%)	1 (0%)	29 17
1	E	209/229 (91%)	205 (98%)	3 (1%)	1 (0%)	29 17
1	H	214/229 (93%)	209 (98%)	4 (2%)	1 (0%)	29 17
2	B	211/214 (99%)	205 (97%)	6 (3%)	0	100 100
2	D	210/214 (98%)	202 (96%)	8 (4%)	0	100 100
2	F	211/214 (99%)	202 (96%)	9 (4%)	0	100 100
2	L	212/214 (99%)	204 (96%)	8 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1700/1772 (96%)	1648 (97%)	47 (3%)	5 (0%)	41 30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	LEU
1	A	108	PRO
1	E	108	PRO
1	H	108	PRO
1	C	108	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	A	187/195 (96%)	187 (100%)	0	100 100
1	C	186/195 (95%)	185 (100%)	1 (0%)	88 88
1	E	183/195 (94%)	179 (98%)	4 (2%)	52 43
1	H	185/195 (95%)	182 (98%)	3 (2%)	62 56
2	B	188/189 (100%)	185 (98%)	3 (2%)	62 56
2	D	187/189 (99%)	185 (99%)	2 (1%)	73 70
2	F	188/189 (100%)	186 (99%)	2 (1%)	73 70
2	L	189/189 (100%)	183 (97%)	6 (3%)	39 27
All	All	1493/1536 (97%)	1472 (99%)	21 (1%)	67 62

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	99	SER
1	H	189	SER
1	H	207	ASN
2	L	14	SER
2	L	33	LEU

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Mol	Chain	Res	Type
2	L	78	LEU
2	L	100	GLN
2	L	107	LYS
2	L	156	SER
2	B	33	LEU
2	B	94	TYR
2	B	199	GLN
1	C	211	LYS
2	D	94	TYR
2	D	156	SER
1	E	3	GLN
1	E	99	SER
1	E	189	SER
1	E	207	ASN
2	F	94	TYR
2	F	156	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	3	GLN
1	E	202	GLN

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 (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	221/229 (96%)	-0.09	10 (4%)	33	34	18, 32, 57, 97	0
1	C	220/229 (96%)	-0.03	7 (3%)	47	49	18, 38, 62, 97	0
1	E	215/229 (93%)	0.25	18 (8%)	11	12	20, 37, 82, 107	0
1	H	218/229 (95%)	-0.03	10 (4%)	32	34	21, 35, 67, 81	0
2	B	213/214 (99%)	-0.13	1 (0%)	91	91	22, 34, 57, 90	0
2	D	212/214 (99%)	-0.07	7 (3%)	46	47	19, 32, 68, 100	0
2	F	213/214 (99%)	0.06	5 (2%)	60	62	18, 38, 64, 96	0
2	L	214/214 (100%)	0.13	6 (2%)	53	54	24, 43, 65, 110	0
All	All	1726/1772 (97%)	0.01	64 (3%)	41	43	18, 36, 67, 110	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	214	CYS	6.2
1	E	144	GLY	5.7
1	C	143	GLY	5.6
1	E	195	PRO	5.4
1	A	141	THR	5.4
1	E	1	GLU	4.5
1	E	137	SER	4.5
2	F	169	LYS	4.4
1	A	140	SER	4.3
1	E	138	SER	4.1
1	H	137	SER	3.9
1	C	200	GLY	3.9
1	E	197	SER	3.8
1	A	143	GLY	3.8
1	C	144	GLY	3.7
2	F	212	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	212	GLY	3.6
1	C	139	LYS	3.6
2	B	94	TYR	3.5
1	C	201	THR	3.5
2	L	213	GLU	3.4
1	E	3	GLN	3.3
2	F	205	VAL	3.3
1	E	166	SER	3.3
2	L	28	SER	3.2
1	A	1	GLU	3.2
1	H	1	GLU	3.1
1	E	194	VAL	3.1
1	H	105	TRP	3.0
2	F	94	TYR	3.0
1	A	142	SER	3.0
1	A	105	TRP	3.0
1	C	138	SER	3.0
1	H	200	GLY	2.9
1	E	216	LYS	2.9
1	E	170	THR	2.8
1	C	199	LEU	2.7
2	D	94	TYR	2.6
1	H	104	ARG	2.5
1	A	137	SER	2.5
2	D	126	LYS	2.5
1	H	222	GLU	2.5
1	H	168	ALA	2.4
1	E	169	LEU	2.4
1	E	104	ARG	2.4
2	L	94	TYR	2.4
2	D	127	SER	2.3
2	D	181	LEU	2.3
1	E	106	LEU	2.2
1	H	56	ARG	2.2
2	D	184	ALA	2.2
1	E	148	LEU	2.2
1	H	224	LYS	2.2
1	E	145	THR	2.2
1	E	203	THR	2.2
1	A	214	ASN	2.2
2	F	126	LYS	2.1
1	A	216	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	198	SER	2.1
1	A	104	ARG	2.1
2	D	122	ASP	2.1
1	H	106	LEU	2.1
2	L	24	ARG	2.0
2	L	123	GLU	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.