Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2022 – 12:46 PM EDT

PDB ID	:	7T98
Title	:	Crystal structure of engineered CYS-CYS fab dimer VL-108 (LC33)
Authors	:	Harris, S.F.; Boenig, G.D.L.
Deposited on	:	2021-12-18
Resolution	:	2.97 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:

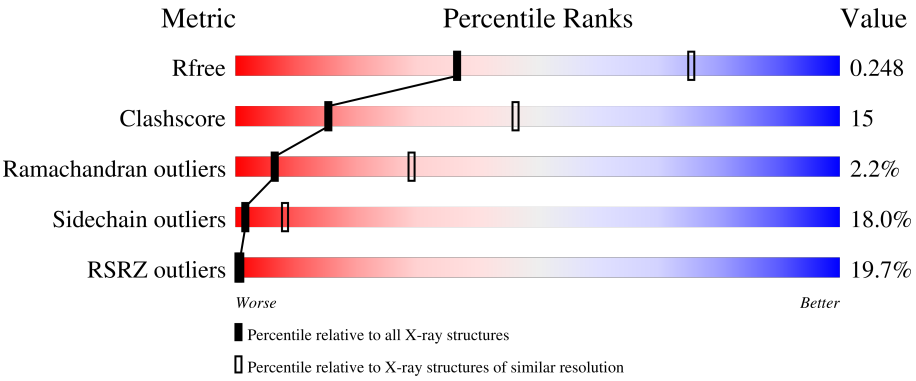
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.97 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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	228	17% 48% 44%
1	H	228	17% 53% 39% 5%
2	B	214	23% 60% 35%
2	L	214	21% 53% 39% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6634 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 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	1	0
			1658	1048	280	324	6			
1	H	221	Total	C	N	O	S	0	1	0
			1658	1048	280	324	6			

- Molecule 2 is a protein called FAB Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	1	0
			1637	1026	275	329	7			
2	L	212	Total	C	N	O	S	0	1	0
			1637	1026	275	329	7			

- Molecule 3 is water.

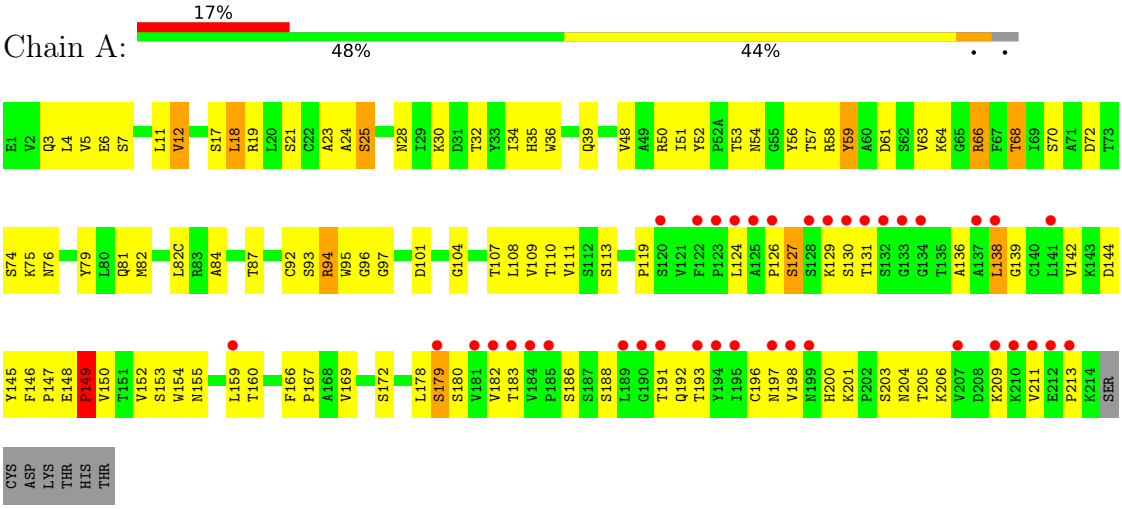
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	15	Total	O	0	0
			15	15		
3	H	6	Total	O	0	0
			6	6		
3	L	13	Total	O	0	0
			13	13		

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.

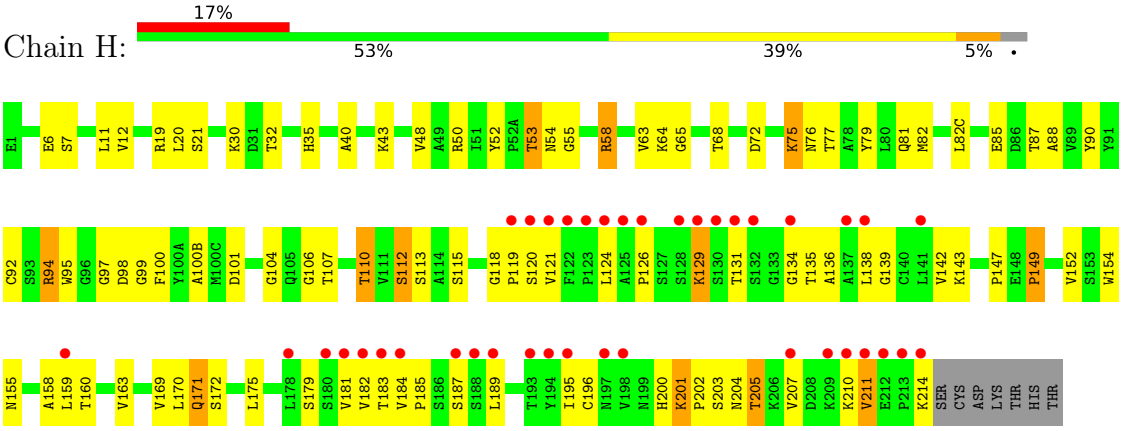
• Molecule 1: FAB Heavy Chain

Chain A:



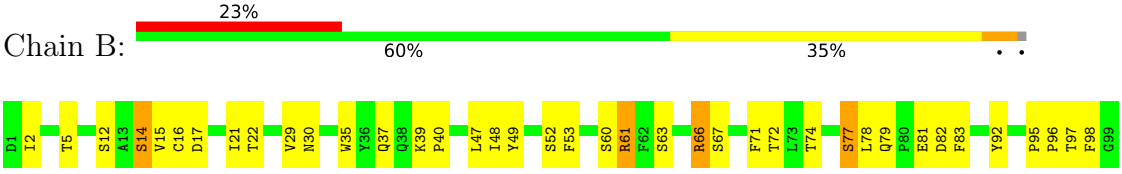
• Molecule 1: FAB Heavy Chain

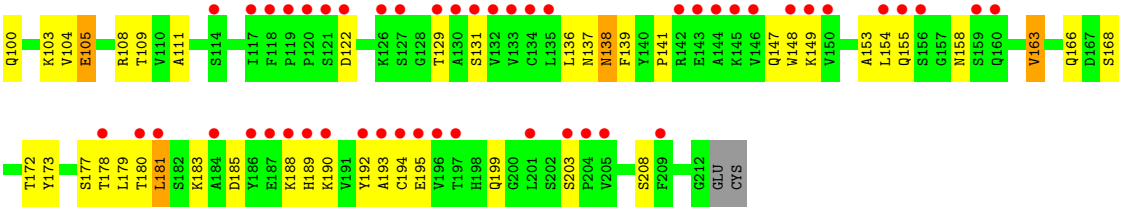
Chain H:



• Molecule 2: FAB Light Chain

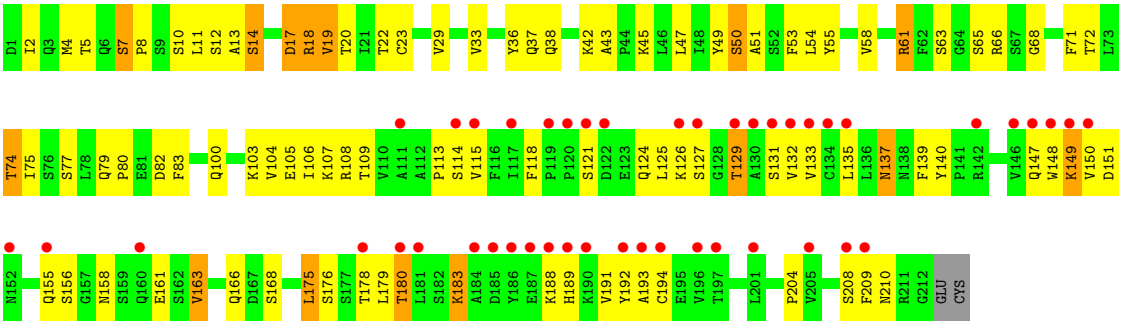
Chain B:





• Molecule 2: FAB Light Chain

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	99.63Å 99.63Å 212.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	70.89 – 2.97 70.89 – 2.97	Depositor EDS
% Data completeness (in resolution range)	69.5 (70.89-2.97) 71.5 (70.89-2.97)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.192 , 0.274 0.184 , 0.248	Depositor DCC
R_{free} test set	924 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	65.2	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 84.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.289 for -h,-k,l	Xtriage
Reported twinning fraction	0.578 for H, K, L 0.422 for -h,-k,l	Depositor
Outliers	2 of 18593 reflections (0.011%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6634	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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	0.87	0/1700	1.06	3/2317 (0.1%)
1	H	0.85	0/1700	1.09	3/2317 (0.1%)
2	B	0.82	0/1677	1.06	1/2280 (0.0%)
2	L	0.82	0/1677	1.05	0/2280
All	All	0.84	0/6754	1.07	7/9194 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	149	PRO	N-CA-CB	-5.90	96.11	102.60
1	A	58	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	149	PRO	N-CA-CB	-5.74	96.29	102.60
1	H	58	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	66	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	H	94	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	B	98	PHE	CB-CA-C	-5.07	100.25	110.40

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	1658	0	1619	51	1
1	H	1658	0	1619	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1637	0	1595	45	1
2	L	1637	0	1595	52	0
3	A	10	0	0	3	0
3	B	15	0	0	2	0
3	H	6	0	0	0	0
3	L	13	0	0	1	0
All	All	6634	0	6428	194	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 15.

All (194) 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:87:THR:HG23	1:A:110:THR:HA	1.62	0.79
1:H:75:LYS:O	1:H:77:THR:OG1	2.03	0.77
1:A:138:LEU:HB2	1:A:211:VAL:HG21	1.68	0.74
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.67	0.74
2:B:61:ARG:NH2	2:B:82:ASP:OD1	2.20	0.73
2:L:161:GLU:HA	2:L:176:SER:O	1.89	0.71
2:B:147:GLN:O	2:B:195:GLU:N	2.23	0.71
2:L:151:ASP:OD1	2:L:189:HIS:ND1	2.23	0.71
2:L:115:VAL:HA	2:L:135:LEU:O	1.92	0.69
2:L:61:ARG:O	2:L:75:ILE:HA	1.93	0.68
1:H:6:GLU:OE1	1:H:106:GLY:N	2.24	0.67
2:B:30:ASN:N	3:B:301:HOH:O	2.28	0.65
1:A:54:ASN:OD1	1:A:56:TYR:N	2.28	0.65
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.78	0.64
1:H:121:VAL:HG21	1:H:207:VAL:HB	1.79	0.64
1:A:82:MET:HB3	1:A:82(C):LEU:HD21	1.80	0.63
1:A:188:SER:HA	1:A:191:THR:HG23	1.80	0.63
1:A:159:LEU:HD21	1:A:182:VAL:HG21	1.79	0.62
1:H:82:MET:HB3	1:H:82(C):LEU:HD21	1.80	0.62
2:B:141:PRO:HD2	2:B:199:GLN:HB3	1.82	0.62
2:B:14:SER:O	2:B:17:ASP:HB2	2.01	0.60
2:B:35:TRP:HB2	2:B:48:ILE:HB	1.84	0.60
1:H:159:LEU:HD21	1:H:182:VAL:HG21	1.84	0.60
1:H:131:THR:HA	1:H:136:ALA:HB2	1.83	0.59
1:A:3:GLN:HB2	1:A:25:SER:OG	2.03	0.59
2:L:14:SER:HB3	2:L:107:LYS:O	2.03	0.59
2:B:149:LYS:HA	2:B:153:ALA:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:49:TYR:CZ	2:L:53:PHE:HB3	2.38	0.59
1:H:120:SER:O	1:H:142:VAL:HA	2.04	0.58
2:B:49:TYR:CZ	2:B:53:PHE:HB3	2.40	0.57
1:H:119:PRO:HB2	1:H:142:VAL:HG13	1.87	0.57
2:B:79:GLN:O	2:B:82:ASP:HB2	2.05	0.56
2:B:166:GLN:HG3	2:B:173:TYR:CE1	2.41	0.56
1:A:32:THR:HG22	1:A:97:GLY:HA2	1.86	0.56
1:H:19:ARG:HB2	1:H:81:GLN:OE1	2.06	0.56
1:A:196:CYS:SG	1:A:196:CYS:O	2.64	0.56
1:A:119:PRO:HA	1:A:144:ASP:O	2.07	0.55
1:H:98:ASP:O	1:H:100:PHE:N	2.34	0.55
2:L:148:TRP:CD2	2:L:179:LEU:HD13	2.43	0.54
1:A:188:SER:HA	1:A:191:THR:CG2	2.37	0.54
1:H:30:LYS:HE2	1:H:53:THR:HA	1.88	0.54
1:H:159:LEU:CD2	1:H:182:VAL:HG21	2.37	0.54
1:A:6:GLU:HA	3:A:301:HOH:O	2.08	0.53
2:L:131:SER:HA	2:L:179:LEU:O	2.09	0.52
1:A:124:LEU:O	1:A:211:VAL:HG23	2.09	0.52
1:H:75:LYS:O	1:H:76:ASN:C	2.47	0.52
1:H:118:GLY:HA2	1:H:203:SER:OG	2.10	0.52
1:A:24:ALA:HB3	1:A:76:ASN:O	2.10	0.52
2:L:55:TYR:O	2:L:58:VAL:HG23	2.10	0.52
2:B:141:PRO:HG3	2:B:199:GLN:OE1	2.10	0.52
1:H:6:GLU:HB3	1:H:107:THR:HB	1.92	0.51
1:H:203:SER:O	1:H:205:THR:N	2.44	0.51
2:L:53:PHE:N	2:L:53:PHE:CD1	2.76	0.51
2:L:158:ASN:HB3	2:L:180:THR:O	2.10	0.51
2:B:189:HIS:HB2	2:B:192:TYR:OH	2.11	0.51
2:L:113:PRO:HA	2:L:137:ASN:O	2.11	0.51
1:A:11:LEU:HB2	1:A:147:PRO:HG3	1.92	0.50
2:L:106:ILE:O	2:L:166:GLN:NE2	2.43	0.50
2:L:194:CYS:SG	2:L:194:CYS:O	2.69	0.50
1:A:32:THR:HB	1:A:95:TRP:O	2.11	0.50
1:A:35:HIS:O	1:A:92:CYS:HA	2.11	0.50
2:L:38:GLN:HG3	2:L:42:LYS:O	2.12	0.50
1:H:32:THR:HG22	1:H:97:GLY:HA2	1.92	0.50
2:B:96:PRO:HG3	3:B:306:HOH:O	2.11	0.50
1:A:21:SER:HG	1:A:79:TYR:HD1	1.59	0.49
1:A:59:TYR:HE2	1:A:68:THR:HA	1.77	0.49
1:H:87:THR:HG23	1:H:110:THR:HA	1.93	0.49
1:H:126:PRO:HG3	1:H:138:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:13:ALA:O	2:L:106:ILE:HA	2.12	0.49
2:L:150:VAL:HG13	2:L:192:TYR:CD2	2.48	0.49
1:H:6:GLU:OE2	1:H:104:GLY:HA3	2.12	0.49
1:H:88:ALA:HB3	1:H:90:TYR:CE1	2.48	0.49
2:L:149:LYS:O	2:L:193:ALA:HB3	2.12	0.49
1:H:196:CYS:SG	1:H:196:CYS:O	2.71	0.49
1:A:6:GLU:CA	3:A:301:HOH:O	2.59	0.49
1:A:139:GLY:HA2	1:A:154:TRP:CZ2	2.48	0.49
1:H:138:LEU:HB2	1:H:211:VAL:HG21	1.94	0.49
2:L:53:PHE:N	2:L:53:PHE:HD1	2.09	0.49
2:B:83:PHE:HD1	2:B:104:VAL:O	1.96	0.48
1:A:126:PRO:O	1:A:127:SER:O	2.30	0.48
2:L:132:VAL:HB	2:L:179:LEU:HB3	1.95	0.48
1:A:51:ILE:O	1:A:51:ILE:HG23	2.13	0.48
2:B:39:LYS:NZ	2:B:81:GLU:O	2.32	0.48
2:B:199:GLN:HG2	2:B:199:GLN:O	2.13	0.48
2:L:19:VAL:CG2	2:L:75:ILE:HB	2.42	0.48
2:B:53:PHE:CD1	2:B:53:PHE:N	2.82	0.47
1:H:124:LEU:HD22	2:L:118:PHE:HB3	1.96	0.47
2:L:20:THR:HG23	2:L:74:THR:HG23	1.96	0.47
1:A:4:LEU:HA	1:A:23:ALA:O	2.14	0.47
1:A:18:LEU:HD12	1:A:109:VAL:HG13	1.96	0.47
1:H:139:GLY:HA2	1:H:154:TRP:CZ2	2.49	0.47
2:B:148:TRP:HA	2:B:194:CYS:HA	1.97	0.47
2:B:193:ALA:HB2	2:B:208:SER:HB3	1.97	0.47
1:H:155:ASN:O	1:H:158:ALA:HB3	2.15	0.47
1:A:6:GLU:HB3	1:A:107:THR:HB	1.97	0.47
2:B:136:LEU:HD12	2:B:136:LEU:N	2.30	0.47
1:A:203:SER:O	1:A:205:THR:N	2.48	0.47
1:A:36:TRP:O	1:A:48:VAL:HB	2.15	0.46
2:B:12:SER:HA	2:B:105:GLU:O	2.16	0.46
2:L:107:LYS:HA	2:L:140:TYR:OH	2.16	0.46
1:A:72:ASP:OD2	1:A:74:SER:HB2	2.15	0.46
2:B:61:ARG:HD2	2:B:77:SER:O	2.14	0.46
2:B:148:TRP:CG	2:B:179:LEU:HD13	2.51	0.46
1:H:54:ASN:OD1	1:H:55:GLY:N	2.48	0.46
2:B:53:PHE:N	2:B:53:PHE:HD1	2.13	0.46
2:B:158:ASN:HB3	2:B:180:THR:N	2.31	0.46
1:H:195:ILE:HG12	1:H:210:LYS:HA	1.97	0.46
2:B:66:ARG:HB2	2:B:71:PHE:CE2	2.51	0.46
1:A:63:VAL:O	1:A:66:ARG:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:SER:O	1:A:205:THR:OG1	2.32	0.46
2:B:137:ASN:ND2	2:B:138:ASN:OD1	2.49	0.46
2:B:139:PHE:CD2	2:B:139:PHE:O	2.69	0.46
2:B:149:LYS:HE2	2:B:154:LEU:HD11	1.98	0.46
2:L:36:TYR:HA	2:L:45:LYS:O	2.16	0.46
1:H:12:VAL:HG11	1:H:82(C):LEU:HD12	1.97	0.45
1:A:108:LEU:HD12	1:A:109:VAL:N	2.30	0.45
1:A:6:GLU:N	3:A:301:HOH:O	2.49	0.45
1:A:145:TYR:OH	1:A:178:LEU:HD23	2.17	0.45
1:A:155:ASN:ND2	1:A:193:THR:O	2.49	0.45
1:H:20:LEU:O	1:H:79:TYR:HA	2.16	0.45
2:L:49:TYR:O	2:L:50:SER:C	2.54	0.45
2:L:79:GLN:O	2:L:82:ASP:HB2	2.16	0.45
1:A:131:THR:HA	1:A:136:ALA:HB2	1.99	0.45
2:B:147:GLN:HE21	2:B:154:LEU:HD23	1.82	0.45
2:B:181:LEU:HD22	2:B:185:ASP:CB	2.46	0.45
1:H:201:LYS:N	1:H:202:PRO:CD	2.80	0.45
1:A:94:ARG:HG2	1:A:95:TRP:N	2.32	0.45
1:A:84:ALA:HA	1:A:111:VAL:HB	1.97	0.45
1:A:150:VAL:O	1:A:150:VAL:HG12	2.17	0.44
1:A:19:ARG:HD3	1:A:81:GLN:OE1	2.18	0.44
2:B:15:VAL:HA	2:B:78:LEU:O	2.17	0.44
1:A:146:PHE:O	1:A:200:HIS:HE1	2.00	0.44
2:B:147:GLN:N	2:B:195:GLU:O	2.48	0.44
2:L:12:SER:HA	2:L:105:GLU:O	2.18	0.44
1:A:12:VAL:HG21	1:A:82(C):LEU:HD12	1.99	0.44
2:B:15:VAL:C	2:B:17:ASP:H	2.22	0.43
1:H:30:LYS:O	1:H:53:THR:OG1	2.35	0.43
1:H:35:HIS:O	1:H:92:CYS:HA	2.17	0.43
2:L:125:LEU:HD22	2:L:183:LYS:CE	2.48	0.43
1:A:34:ILE:O	1:A:50:ARG:HA	2.18	0.43
2:L:80:PRO:HB2	2:L:168:SER:O	2.18	0.43
1:H:104:GLY:O	2:L:43:ALA:HB2	2.17	0.43
1:H:72:ASP:OD2	1:H:75:LYS:HB2	2.18	0.43
2:L:4:MET:HB3	2:L:23:CYS:SG	2.58	0.43
2:L:150:VAL:HA	2:L:192:TYR:HA	2.00	0.43
1:H:163:VAL:HA	1:H:181:VAL:O	2.19	0.43
1:A:142:VAL:HG22	1:A:198:VAL:HG21	2.01	0.43
1:H:171:GLN:HB2	1:H:175:LEU:O	2.19	0.43
2:B:181:LEU:HD22	2:B:185:ASP:CG	2.39	0.43
2:L:10:SER:HA	2:L:103:LYS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:48:VAL:HG13	1:H:63:VAL:HG21	2.00	0.42
2:L:18:ARG:HG3	3:L:304:HOH:O	2.19	0.42
2:B:21:ILE:O	2:B:72:THR:HA	2.19	0.42
2:L:124:GLN:HG2	2:L:129:THR:O	2.19	0.42
2:L:118:PHE:HB2	2:L:133:VAL:HB	2.02	0.42
2:L:158:ASN:HB2	2:L:179:LEU:HA	2.00	0.42
2:L:191:VAL:HA	2:L:210:ASN:OD1	2.19	0.42
2:L:83:PHE:O	2:L:83:PHE:CD2	2.71	0.42
2:L:163:VAL:HG13	2:L:175:LEU:CD1	2.49	0.42
1:H:40:ALA:HB3	1:H:43:LYS:HB2	2.00	0.42
2:L:13:ALA:HB1	2:L:17:ASP:OD2	2.20	0.42
2:L:137:ASN:HD22	2:L:137:ASN:HA	1.64	0.42
2:B:77:SER:HB3	2:B:79:GLN:HE21	1.84	0.42
2:L:11:LEU:HD22	2:L:104:VAL:HG13	2.02	0.42
2:L:148:TRP:CE3	2:L:194:CYS:HB3	2.55	0.42
1:H:90:TYR:CD1	1:H:90:TYR:N	2.88	0.42
1:A:166:PHE:HD1	1:A:179:SER:O	2.03	0.42
1:H:11:LEU:HB2	1:H:147:PRO:HG3	2.01	0.42
2:L:113:PRO:HB3	2:L:139:PHE:HB3	2.01	0.42
1:A:153:SER:O	1:A:197:ASN:N	2.48	0.42
2:B:148:TRP:CE3	2:B:194:CYS:HB3	2.55	0.42
2:L:33:VAL:HG21	2:L:71:PHE:CE2	2.56	0.41
2:B:158:ASN:OD1	2:B:158:ASN:N	2.52	0.41
1:H:129:LYS:HG2	2:L:208:SER:O	2.20	0.41
1:A:28:ASN:OD1	1:A:30:LYS:HB2	2.21	0.41
2:B:111:ALA:O	2:B:139:PHE:HA	2.20	0.41
1:H:32:THR:HB	1:H:95:TRP:O	2.20	0.41
2:L:37:GLN:CB	2:L:47:LEU:HD11	2.45	0.41
1:A:17:SER:HA	1:A:82:MET:O	2.20	0.41
2:B:95:PRO:HG2	2:B:97:THR:CG2	2.50	0.41
1:H:189:LEU:HD23	1:H:189:LEU:HA	1.97	0.41
2:B:181:LEU:HD13	2:B:185:ASP:HB3	2.03	0.41
1:H:100:PHE:CE1	1:H:100(B):ALA:HB3	2.56	0.41
1:H:124:LEU:HD23	1:H:124:LEU:HA	1.97	0.41
1:H:135:THR:HA	1:H:185:PRO:HA	2.03	0.41
2:L:33:VAL:HG21	2:L:71:PHE:CD2	2.55	0.41
2:B:138:ASN:HA	2:B:172:THR:HB	2.04	0.40
1:H:32:THR:HG22	1:H:97:GLY:CA	2.51	0.40
1:H:120:SER:HB2	1:H:143:LYS:HB3	2.03	0.40
1:H:200:HIS:CD2	1:H:202:PRO:HD2	2.56	0.40
1:A:131:THR:HA	1:A:136:ALA:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:PRO:HG2	2:B:163:VAL:O	2.21	0.40
2:L:7:SER:HA	2:L:8:PRO:HA	1.90	0.40
1:A:6:GLU:OE2	1:A:104:GLY:HA3	2.21	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)
1:A:57:THR:O	2:B:92:TYR:OH[4_645]	2.11	0.09

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	219/228 (96%)	188 (86%)	26 (12%)	5 (2%)	6	28
1	H	219/228 (96%)	195 (89%)	18 (8%)	6 (3%)	5	24
2	B	211/214 (99%)	187 (89%)	20 (10%)	4 (2%)	8	33
2	L	211/214 (99%)	191 (90%)	16 (8%)	4 (2%)	8	33
All	All	860/884 (97%)	761 (88%)	80 (9%)	19 (2%)	6	29

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	SER
1	A	204	ASN
2	B	203	SER
1	H	204	ASN
1	A	96	GLY
1	H	99	GLY
2	L	68	GLY

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Mol	Chain	Res	Type
2	B	138	ASN
1	H	112	SER
2	L	50	SER
2	L	51	ALA
2	L	204	PRO
1	A	213	PRO
2	B	16	CYS
2	B	40	PRO
1	H	134	GLY
1	H	65	GLY
1	A	149	PRO
1	H	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	A	182/189 (96%)	147 (81%)	35 (19%)	1 7
1	H	182/189 (96%)	151 (83%)	31 (17%)	2 9
2	B	189/190 (100%)	159 (84%)	30 (16%)	2 11
2	L	189/190 (100%)	151 (80%)	38 (20%)	1 6
All	All	742/758 (98%)	608 (82%)	134 (18%)	1 8

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	7	SER
1	A	12	VAL
1	A	18	LEU
1	A	25	SER
1	A	39	GLN
1	A	52	TYR
1	A	53	THR
1	A	59	TYR

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Mol	Chain	Res	Type
1	A	61	ASP
1	A	64	LYS
1	A	68	THR
1	A	70	SER
1	A	75	LYS
1	A	93	SER
1	A	94	ARG
1	A	101	ASP
1	A	113	SER
1	A	129	LYS
1	A	130	SER
1	A	138	LEU
1	A	148	GLU
1	A	149	PRO
1	A	152	VAL
1	A	160	THR
1	A	169	VAL
1	A	172	SER
1	A	179	SER
1	A	180	SER
1	A	183	THR
1	A	186	SER
1	A	192	GLN
1	A	201	LYS
1	A	206	LYS
1	A	209	LYS
2	B	2	ILE
2	B	5	THR
2	B	14	SER
2	B	22	THR
2	B	29	VAL
2	B	52	SER
2	B	60	SER
2	B	61	ARG
2	B	63	SER
2	B	66	ARG
2	B	67	SER
2	B	74	THR
2	B	77	SER
2	B	100	GLN
2	B	103	LYS
2	B	105	GLU

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Mol	Chain	Res	Type
2	B	108	ARG
2	B	109	THR
2	B	122	ASP
2	B	129	THR
2	B	131	SER
2	B	155	GLN
2	B	163	VAL
2	B	168	SER
2	B	177	SER
2	B	178	THR
2	B	181	LEU
2	B	183	LYS
2	B	188	LYS
2	B	190	LYS
1	H	7	SER
1	H	21	SER
1	H	50	ARG
1	H	52	TYR
1	H	53	THR
1	H	58	ARG
1	H	64	LYS
1	H	68	THR
1	H	75	LYS
1	H	85[A]	GLU
1	H	94	ARG
1	H	101	ASP
1	H	110	THR
1	H	112	SER
1	H	113	SER
1	H	115	SER
1	H	129	LYS
1	H	152	VAL
1	H	160	THR
1	H	169	VAL
1	H	170	LEU
1	H	171	GLN
1	H	172	SER
1	H	179	SER
1	H	183	THR
1	H	184	VAL
1	H	187	SER
1	H	201	LYS

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Mol	Chain	Res	Type
1	H	205	THR
1	H	211	VAL
1	H	214	LYS
2	L	2	ILE
2	L	5	THR
2	L	7	SER
2	L	14	SER
2	L	17	ASP
2	L	18	ARG
2	L	19	VAL
2	L	22	THR
2	L	29	VAL
2	L	54	LEU
2	L	61	ARG
2	L	63	SER
2	L	65	SER
2	L	66	ARG
2	L	72	THR
2	L	74	THR
2	L	77	SER
2	L	100	GLN
2	L	108	ARG
2	L	109	THR
2	L	114	SER
2	L	121	SER
2	L	126	LYS
2	L	127	SER
2	L	129	THR
2	L	137	ASN
2	L	147	GLN
2	L	149	LYS
2	L	155	GLN
2	L	156[A]	SER
2	L	156[B]	SER
2	L	163	VAL
2	L	175	LEU
2	L	178	THR
2	L	180	THR
2	L	183	LYS
2	L	188	LYS
2	L	209	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	HIS
1	A	199	ASN
2	B	30	ASN
2	B	79	GLN
2	B	137	ASN
2	B	147	GLN
1	H	164	HIS
2	L	27	GLN
2	L	137	ASN
2	L	155	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

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	221/228 (96%)	0.93	38 (17%)	1	1	26, 69, 172, 199	0
1	H	221/228 (96%)	0.95	39 (17%)	1	1	27, 66, 158, 185	0
2	B	212/214 (99%)	1.02	49 (23%)	0	0	29, 68, 165, 181	0
2	L	212/214 (99%)	1.04	45 (21%)	0	0	28, 67, 165, 180	0
All	All	866/884 (97%)	0.99	171 (19%)	1	0	26, 68, 166, 199	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	130	SER	13.2
1	H	193	THR	9.4
2	B	119	PRO	8.7
1	A	130	SER	8.4
2	L	120	PRO	8.2
1	H	211	VAL	8.0
1	H	183	THR	7.5
1	A	194	TYR	7.5
1	A	138	LEU	7.5
1	H	138	LEU	7.4
2	B	134	CYS	7.3
2	L	119	PRO	7.2
2	B	196	VAL	7.1
2	B	135	LEU	6.5
2	L	121	SER	6.4
1	A	137	ALA	6.3
1	H	123	PRO	6.3
2	L	186	TYR	6.2
2	L	122	ASP	6.2
2	L	190	LYS	6.2
1	H	194	TYR	6.0

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Mol	Chain	Res	Type	RSRZ
1	H	124	LEU	6.0
1	A	126	PRO	5.9
2	B	155	GLN	5.7
1	H	187	SER	5.7
1	A	123	PRO	5.7
2	B	146	VAL	5.6
2	L	196	VAL	5.6
2	L	127	SER	5.6
2	L	117	ILE	5.5
2	B	127	SER	5.5
1	A	122	PHE	5.5
2	L	209	PHE	5.5
2	L	132	VAL	5.4
1	H	184	VAL	5.4
1	H	125	ALA	5.2
1	A	212	GLU	5.1
2	L	188	LYS	5.1
1	A	128	SER	5.0
1	A	210	LYS	5.0
2	B	193	ALA	4.9
1	A	195	ILE	4.9
2	L	197	THR	4.9
2	B	209	PHE	4.9
1	A	141	LEU	4.9
2	B	132	VAL	4.8
1	A	134	GLY	4.8
2	L	193	ALA	4.8
1	A	211	VAL	4.7
1	A	183	THR	4.6
2	L	134	CYS	4.6
2	L	131	SER	4.6
1	A	179	SER	4.6
2	L	180	THR	4.5
1	A	159	LEU	4.5
1	H	137	ALA	4.5
1	H	128	SER	4.4
2	B	192	TYR	4.4
2	B	131	SER	4.2
2	L	126	LYS	4.2
1	H	210	LYS	4.1
2	L	192	TYR	4.1
2	L	181	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	184	ALA	4.1
1	H	189	LEU	4.0
2	L	148	TRP	4.0
2	L	130	ALA	4.0
1	A	132	SER	4.0
1	H	141	LEU	4.0
2	L	133	VAL	4.0
1	A	131	THR	3.9
2	B	120	PRO	3.8
2	B	201	LEU	3.8
1	A	209	LYS	3.8
2	B	186	TYR	3.7
1	H	209	LYS	3.7
1	A	133	GLY	3.7
1	H	180	SER	3.7
1	H	122	PHE	3.7
1	H	132	SER	3.6
1	H	212	GLU	3.6
2	L	184	ALA	3.5
1	H	121	VAL	3.5
2	L	187	GLU	3.4
2	L	129	THR	3.4
2	B	122	ASP	3.4
1	H	120	SER	3.4
1	H	188	SER	3.3
2	L	155	GLN	3.3
2	L	146	VAL	3.3
2	L	178	THR	3.3
1	A	124	LEU	3.3
1	A	197	ASN	3.2
1	H	134	GLY	3.2
1	A	125	ALA	3.2
1	A	189	LEU	3.2
2	B	126	LYS	3.2
2	L	150	VAL	3.2
2	B	144	ALA	3.2
2	B	180	THR	3.1
2	L	135	LEU	3.1
1	H	213	PRO	3.1
1	H	181	VAL	3.1
2	L	185	ASP	3.0
2	B	118	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	181	LEU	3.0
2	B	145	LYS	3.0
2	B	160	GLN	3.0
1	H	182	VAL	3.0
2	B	121	SER	2.9
2	B	178	THR	2.9
1	A	213	PRO	2.9
1	A	207	VAL	2.8
1	H	119	PRO	2.8
2	B	188	LYS	2.7
2	B	148	TRP	2.7
1	H	159	LEU	2.7
2	L	194	CYS	2.7
2	B	117	ILE	2.7
1	A	129	LYS	2.7
1	A	198	VAL	2.7
2	L	189	HIS	2.6
1	A	185	PRO	2.6
2	L	149	LYS	2.6
2	B	195	GLU	2.6
2	B	204	PRO	2.6
1	A	193	THR	2.6
1	H	195	ILE	2.6
2	L	201	LEU	2.6
1	A	190	GLY	2.6
1	A	191	THR	2.6
2	B	189	HIS	2.6
1	H	126	PRO	2.5
2	B	114	SER	2.5
2	B	154	LEU	2.5
2	B	129	THR	2.5
2	L	160	GLN	2.5
1	A	182	VAL	2.5
2	B	194	CYS	2.5
1	H	178	LEU	2.5
1	H	131	THR	2.4
2	L	114	SER	2.4
2	B	150	VAL	2.4
2	B	142	ARG	2.4
2	B	130	ALA	2.4
1	A	184	VAL	2.4
2	B	156[A]	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	L	147	GLN	2.4
1	H	207	VAL	2.4
1	A	199	ASN	2.4
2	B	197	THR	2.3
1	A	120	SER	2.3
2	B	133	VAL	2.3
2	L	142	ARG	2.3
1	H	198	VAL	2.2
1	H	129	LYS	2.2
2	L	111	ALA	2.2
2	B	205	VAL	2.2
1	A	181	VAL	2.2
2	B	190	LYS	2.2
2	B	159	SER	2.2
2	L	205	VAL	2.2
1	H	214	LYS	2.2
2	B	187	GLU	2.2
2	B	143	GLU	2.2
1	H	197	ASN	2.1
2	B	203	SER	2.1
2	L	208	SER	2.1
2	B	149	LYS	2.1
2	L	152	ASN	2.1
2	L	115	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides 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.