Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 09:36 PM BST

PDB ID	:	6F7T
Title	:	Crystal Structure of an Fab fragment in complex with a peptide from Bacillus subtilis RNase Y
Authors	:	Golinelli-Pimpaneau, B.; Hardouin, P.
Deposited on	:	2017-12-11
Resolution	:	2.60 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 ⓘ) were used in the production of this report:

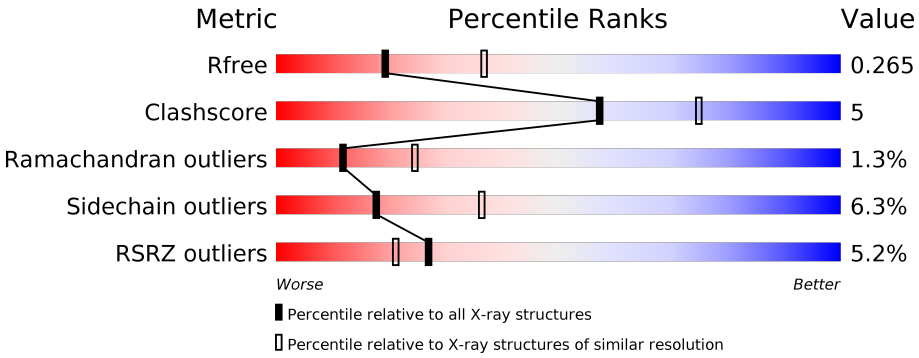
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	218	4% 87% 11% ·
1	L	218	4% 85% 14% ·
2	B	211	9% 79% 17% ·
2	H	211	4% 77% 19% ·
3	C	12	92% 8%
3	D	12	92% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7016 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 RY79-90, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	1	0
			1658	1039	277	336	6			
1	L	218	Total	C	N	O	S	0	1	0
			1663	1041	276	340	6			

- Molecule 2 is a protein called FAB RY79-90, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1604	1022	259	316	7			
2	H	211	Total	C	N	O	S	0	1	0
			1610	1027	260	316	7			

- Molecule 3 is a protein called Ribonuclease Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	0	0	0
			111	63	26	22			
3	D	12	Total	C	N	O	0	0	0
			111	63	26	22			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	58	Total	O	0	0
			58	58		

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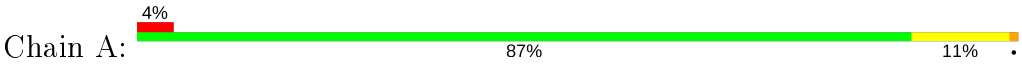
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	45	Total O 45 45	0	0
5	C	14	Total O 14 14	0	0
5	D	2	Total O 2 2	0	0
5	H	53	Total O 53 53	0	0
5	L	86	Total O 86 86	0	0

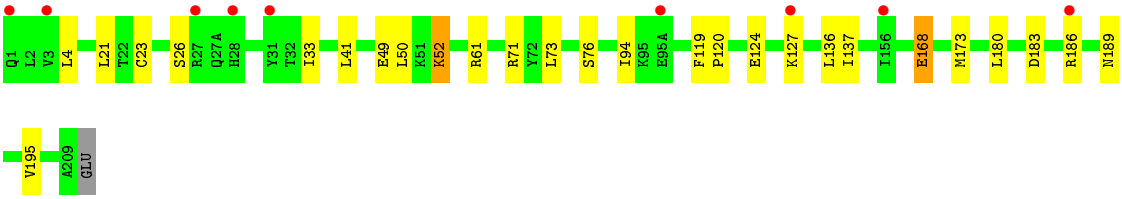
3 Residue-property plots (i)

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: FAB RY79-90, LIGHT CHAIN

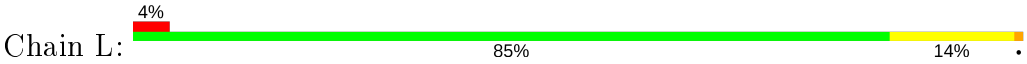
Chain A:

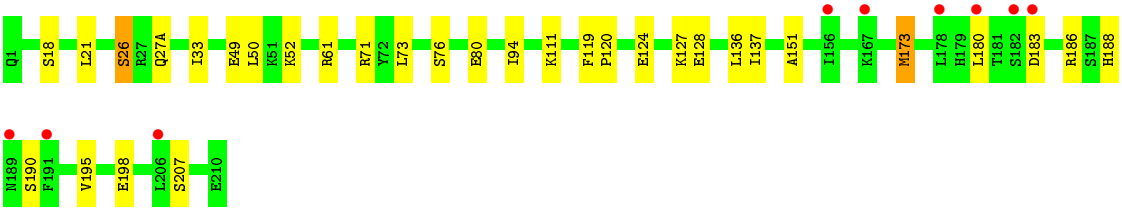




- Molecule 1: FAB RY79-90, LIGHT CHAIN

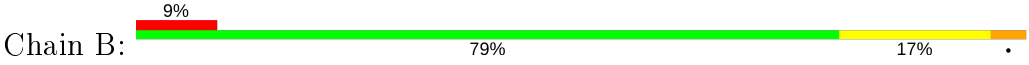
Chain L:

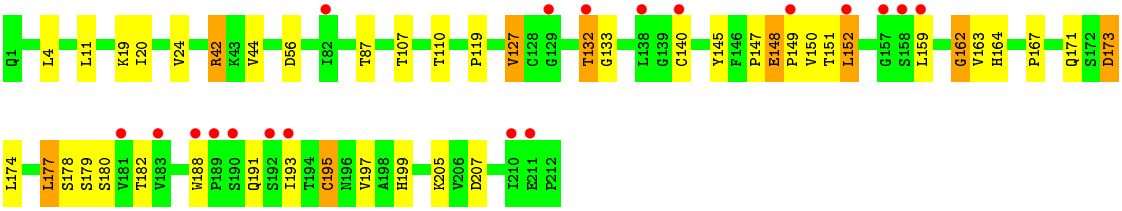




- Molecule 2: FAB RY79-90, HEAVY CHAIN

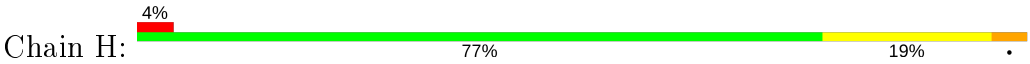
Chain B:

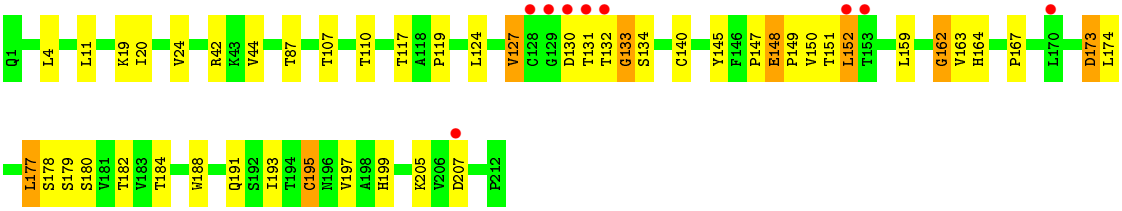




- Molecule 2: FAB RY79-90, HEAVY CHAIN

Chain H:





- Molecule 3: Ribonuclease Y

Chain C:

- Molecule 3: Ribonuclease Y

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	98.68Å 130.45Å 72.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.15 – 2.60 43.42 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.15-2.60) 100.0 (43.42-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.202 , 0.253 0.212 , 0.265	Depositor DCC
R_{free} test set	1464 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	71.0	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 72.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7016	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 6.91% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.49	0/1699	0.74	0/2308
1	L	0.53	0/1703	0.75	0/2313
2	B	0.50	0/1648	0.76	1/2255 (0.0%)
2	H	0.51	0/1657	0.76	0/2266
3	C	0.54	0/110	0.66	0/143
3	D	0.54	0/110	0.67	0/143
All	All	0.51	0/6927	0.75	1/9428 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	42	ARG	C-N-CA	5.13	134.54	121.70

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	1613	12	0
1	L	1663	0	1617	16	0
2	B	1604	0	1567	21	0
2	H	1610	0	1580	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	111	0	111	0	0
3	D	111	0	111	0	0
4	L	1	0	0	0	0
5	A	58	0	0	2	0
5	B	45	0	0	0	0
5	C	14	0	0	0	0
5	D	2	0	0	0	0
5	H	53	0	0	0	0
5	L	86	0	0	1	0
All	All	7016	0	6599	66	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 (66) 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:H:119:PRO:HB3	2:H:145:TYR:HB3	1.81	0.63
2:H:4:LEU:HD22	2:H:24:VAL:HG22	1.81	0.62
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.80	0.62
1:L:151:ALA:HB1	1:L:188:HIS:HD2	1.64	0.60
2:H:127:VAL:HG13	1:L:120:PRO:HG3	1.83	0.60
2:B:4:LEU:HD22	2:B:24:VAL:HG22	1.84	0.59
1:L:33:ILE:HG12	1:L:71:ARG:HG3	1.84	0.58
1:A:33:ILE:HG12	1:A:71:ARG:HG3	1.88	0.56
2:H:163:VAL:HA	2:H:180:SER:O	2.08	0.54
1:A:168:GLU:HB2	1:A:173:MET:HG2	1.90	0.54
2:B:163:VAL:HA	2:B:180:SER:O	2.07	0.53
1:A:120:PRO:HG3	2:B:127:VAL:HG13	1.90	0.53
2:H:87:THR:HG23	2:H:110:THR:HA	1.90	0.53
1:A:137:ILE:HG12	1:A:195:VAL:HG21	1.89	0.53
2:H:117:THR:HG21	2:H:174:LEU:HD22	1.91	0.52
1:L:111:LYS:HE2	1:L:198:GLU:HG3	1.92	0.52
1:A:183:ASP:HA	1:A:186:ARG:HB2	1.92	0.52
2:B:11:LEU:HD12	2:B:110:THR:HB	1.92	0.52
2:B:152:LEU:HD13	2:B:179:SER:HB3	1.93	0.51
2:H:152:LEU:HD13	2:H:179:SER:HB3	1.92	0.51
1:L:137:ILE:HG12	1:L:195:VAL:HG21	1.93	0.51
2:H:173:ASP:HB3	2:H:174:LEU:HG	1.93	0.50
1:L:183:ASP:HA	1:L:186:ARG:HB2	1.92	0.50
2:B:87:THR:HG23	2:B:110:THR:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:11:LEU:HD12	2:H:110:THR:HB	1.95	0.49
2:B:42:ARG:HG3	2:B:44:VAL:HG22	1.93	0.49
5:A:320:HOH:O	2:B:164:HIS:HA	2.13	0.48
2:B:24:VAL:O	2:H:134:SER:HB2	2.13	0.48
1:L:124:GLU:HA	1:L:127:LYS:HE3	1.95	0.48
1:A:52:LYS:H	1:A:52:LYS:HD3	1.78	0.48
1:L:151:ALA:HB1	1:L:188:HIS:CD2	2.46	0.48
1:L:21:LEU:HD12	1:L:73:LEU:HD23	1.96	0.48
1:L:61:ARG:HB2	1:L:76:SER:O	2.14	0.47
2:B:173:ASP:HB3	2:B:174:LEU:HG	1.95	0.47
1:A:124:GLU:HA	1:A:127:LYS:HE3	1.95	0.47
2:B:147:PRO:C	2:B:149:PRO:HD3	2.35	0.47
2:H:167:PRO:HD3	1:L:173:MET:HE3	1.97	0.47
1:A:61:ARG:HB2	1:A:76:SER:O	2.16	0.46
1:A:21:LEU:HD12	1:A:73:LEU:HD23	1.97	0.46
2:B:177:LEU:HG	2:B:178:SER:N	2.31	0.46
2:H:177:LEU:HG	2:H:178:SER:N	2.30	0.46
2:H:195:CYS:O	2:H:207:ASP:HA	2.16	0.46
2:B:162:GLY:HA3	2:B:182:THR:H	1.81	0.46
2:H:164:HIS:HA	5:L:439:HOH:O	2.16	0.46
2:H:149:PRO:HD2	2:H:199:HIS:CD2	2.50	0.46
2:H:162:GLY:HA3	2:H:182:THR:H	1.81	0.45
2:B:149:PRO:HD2	2:B:199:HIS:CD2	2.52	0.45
2:H:127:VAL:HG11	1:L:207:SER:H	1.83	0.44
2:B:195:CYS:O	2:B:207:ASP:HA	2.17	0.44
2:H:197:VAL:O	2:H:205:LYS:HA	2.18	0.44
1:L:119:PHE:HE2	1:L:136:LEU:HD12	1.82	0.44
2:H:147:PRO:C	2:H:149:PRO:HD3	2.38	0.44
2:H:188:TRP:CD1	2:H:193:ILE:HD12	2.53	0.43
1:L:50:LEU:HD23	1:L:71:ARG:HB3	2.00	0.43
2:B:188:TRP:CD1	2:B:193:ILE:HD12	2.54	0.43
2:H:20:ILE:HG12	2:H:107:THR:HG21	2.01	0.43
2:B:197:VAL:O	2:B:205:LYS:HA	2.19	0.42
2:H:131:THR:C	2:H:133:GLY:H	2.22	0.42
1:L:26:SER:O	1:L:27(A):GLN:O	2.38	0.42
1:A:4:LEU:HD22	1:A:23:CYS:SG	2.59	0.42
2:B:20:ILE:HG12	2:B:107:THR:HG21	2.01	0.42
1:A:119:PHE:HE2	1:A:136:LEU:HD12	1.85	0.41
1:A:50:LEU:HD23	1:A:71:ARG:HB3	2.02	0.41
5:A:331:HOH:O	2:B:167:PRO:HD2	2.21	0.41
2:H:124:LEU:HB3	1:L:119:PHE:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:VAL:O	2:H:134:SER:CB	2.69	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	216/218 (99%)	206 (95%)	9 (4%)	1 (0%)	29 52
1	L	217/218 (100%)	206 (95%)	9 (4%)	2 (1%)	17 35
2	B	209/211 (99%)	186 (89%)	19 (9%)	4 (2%)	8 15
2	H	210/211 (100%)	187 (89%)	19 (9%)	4 (2%)	8 15
3	C	10/12 (83%)	8 (80%)	2 (20%)	0	100 100
3	D	10/12 (83%)	8 (80%)	2 (20%)	0	100 100
All	All	872/882 (99%)	801 (92%)	60 (7%)	11 (1%)	12 24

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	132	THR
2	B	132	THR
2	B	162	GLY
2	H	133	GLY
2	H	162	GLY
1	L	190	SER
2	B	148	GLU
2	H	148	GLU
2	B	133	GLY
1	A	94	ILE
1	L	94	ILE

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	191/191 (100%)	184 (96%)	7 (4%)	34	60
1	L	192/191 (100%)	184 (96%)	8 (4%)	30	55
2	B	181/181 (100%)	166 (92%)	15 (8%)	11	22
2	H	182/181 (101%)	166 (91%)	16 (9%)	10	19
3	C	12/12 (100%)	11 (92%)	1 (8%)	11	22
3	D	12/12 (100%)	11 (92%)	1 (8%)	11	22
All	All	770/768 (100%)	722 (94%)	48 (6%)	18	37

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	41	LEU
1	A	49	GLU
1	A	52	LYS
1	A	168	GLU
1	A	180	LEU
1	A	189	ASN
2	B	19	LYS
2	B	56	ASP
2	B	127	VAL
2	B	132	THR
2	B	140	CYS
2	B	148	GLU
2	B	150	VAL
2	B	151	THR
2	B	152	LEU
2	B	159	LEU
2	B	171	GLN
2	B	173	ASP
2	B	177	LEU
2	B	191	GLN
2	B	195	CYS

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Mol	Chain	Res	Type
3	C	3	ARG
3	D	3	ARG
2	H	19	LYS
2	H	42	ARG
2	H	44	VAL
2	H	127	VAL
2	H	130	ASP
2	H	140	CYS
2	H	148	GLU
2	H	150	VAL
2	H	151	THR
2	H	152	LEU
2	H	159	LEU
2	H	173	ASP
2	H	177	LEU
2	H	184	THR
2	H	191	GLN
2	H	195	CYS
1	L	18	SER
1	L	26	SER
1	L	49	GLU
1	L	52	LYS
1	L	80	GLU
1	L	128	GLU
1	L	173	MET
1	L	180	LEU

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

Mol	Chain	Res	Type
2	H	31	ASN
1	L	188	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	217/218 (99%)	0.05	9 (4%) 37 30	48, 79, 122, 163	0
1	L	218/218 (100%)	0.23	9 (4%) 37 30	47, 74, 133, 155	0
2	B	211/211 (100%)	0.46	19 (9%) 9 6	54, 84, 138, 153	1 (0%)
2	H	211/211 (100%)	0.24	9 (4%) 35 28	51, 82, 130, 152	0
3	C	12/12 (100%)	0.17	0 100 100	62, 73, 104, 110	0
3	D	12/12 (100%)	0.07	0 100 100	61, 83, 109, 130	0
All	All	881/882 (99%)	0.24	46 (5%) 27 21	47, 81, 132, 163	1 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	189	ASN	6.1
2	B	129	GLY	5.8
1	A	1	GLN	5.5
2	B	138	LEU	5.5
1	L	156	ILE	5.3
2	B	132	THR	4.7
2	B	192	SER	4.4
2	B	210	ILE	4.3
2	B	158	SER	4.0
2	B	159	LEU	3.7
2	B	193	ILE	3.6
2	B	183	VAL	3.6
2	B	189	PRO	3.5
1	A	127	LYS	3.5
2	B	152	LEU	3.3
1	A	28	HIS	3.1
2	H	129	GLY	3.1
2	H	152	LEU	3.1
2	H	128	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	190	SER	2.9
1	L	180	LEU	2.9
2	H	170	LEU	2.9
2	B	82	ILE	2.8
2	H	130	ASP	2.7
1	L	183	ASP	2.7
1	L	206	LEU	2.7
2	H	153	THR	2.7
1	A	31	TYR	2.5
2	H	207	ASP	2.5
2	B	157	GLY	2.5
1	A	156	ILE	2.5
1	L	182	SER	2.4
2	H	131	THR	2.4
2	H	132	THR	2.4
2	B	188	TRP	2.4
2	B	149	PRO	2.4
1	L	167	LYS	2.4
1	A	186	ARG	2.3
1	L	191	PHE	2.3
2	B	211	GLU	2.3
2	B	140	CYS	2.2
1	A	27	ARG	2.2
1	L	178	LEU	2.1
2	B	181	VAL	2.1
1	A	95(A)	GLU	2.0
1	A	3	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	L	301	1/1	0.87	0.58	89,89,89,89	1

6.5 Other polymers (i)

There are no such residues in this entry.