



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:06 pm BST

PDB ID : 6PE8
Title : Crystal structure of CD40/ABBV-323 FAB complex
Authors : Argiriadi, M.A.
Deposited on : 2019-06-20
Resolution : 2.84 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

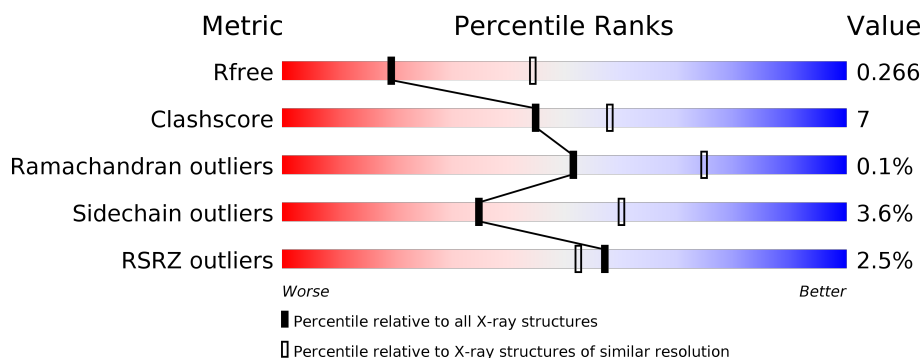
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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 $\leq 5\%$. 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	223	<div> <div>0%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>•</div> </div> </div>
1	H	223	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>5%</div> </div> </div>
2	B	220	<div> <div></div> <div> <div></div> <div>87%</div> <div>13%</div> </div> </div>
2	L	220	<div> <div></div> <div> <div></div> <div>80%</div> <div>18%</div> <div>•</div> </div> </div>
3	T	173	<div> <div>8%</div> <div> <div></div> <div>68%</div> <div>23%</div> <div>•</div> <div>8%</div> </div> </div>
3	U	173	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9151 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	213	Total	C	N	O	S	0	0	0
			1598	1012	269	310	7			
1	H	212	Total	C	N	O	S	0	0	0
			1588	1006	267	309	6			

- Molecule 2 is a protein called FAB Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	220	Total	C	N	O	S	0	1	0
			1713	1071	288	348	6			
2	L	219	Total	C	N	O	S	0	1	0
			1707	1068	287	347	5			

- Molecule 3 is a protein called Tumor necrosis factor receptor superfamily member 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	159	Total	C	N	O	S	0	0	0
			1170	707	202	241	20			
3	U	160	Total	C	N	O	S	0	0	0
			1204	733	205	246	20			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	T	1	Total	O	S	0	0
			5	4	1		
4	T	1	Total	O	S	0	0
			5	4	1		
4	U	1	Total	O	S	0	0
			5	4	1		
4	U	1	Total	O	S	0	0
			5	4	1		

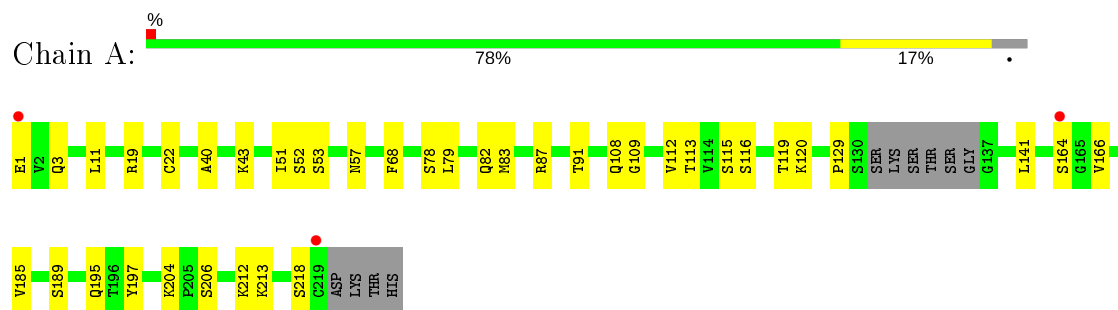
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total	O	0	0
			23	23		
5	B	39	Total	O	0	0
			39	39		
5	H	23	Total	O	0	0
			23	23		
5	L	41	Total	O	0	0
			41	41		
5	T	16	Total	O	0	0
			16	16		
5	U	9	Total	O	0	0
			9	9		

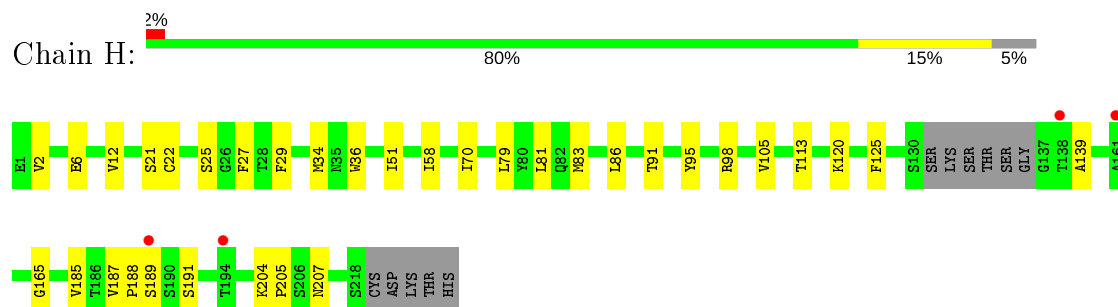
3 Residue-property plots [i](#)

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.

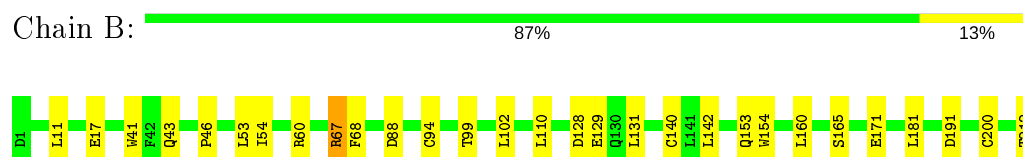
- Molecule 1: FAB Heavy chain



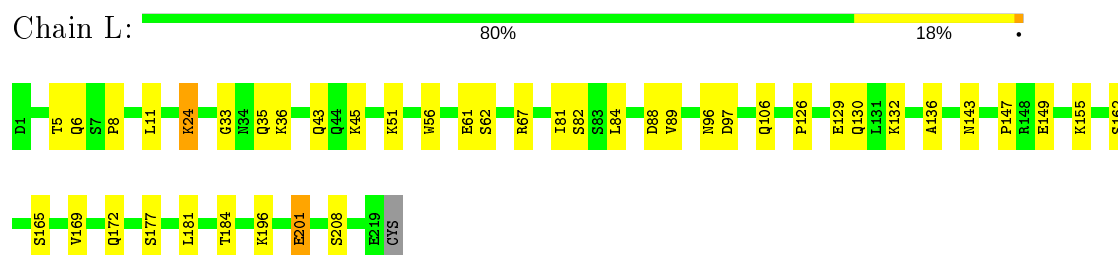
- Molecule 1: FAB Heavy chain



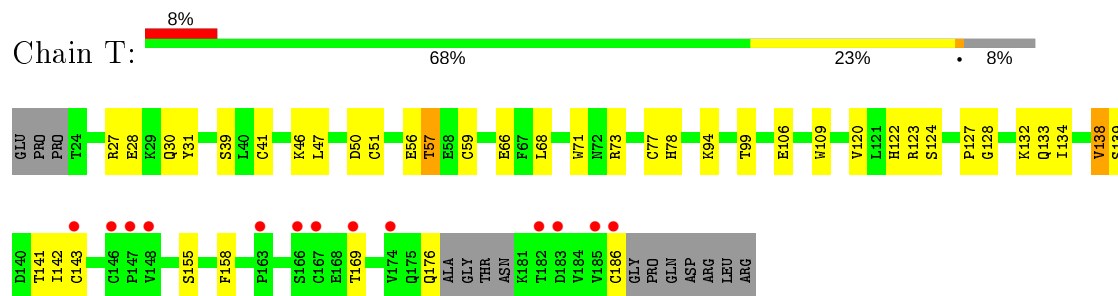
- Molecule 2: FAB Light chain



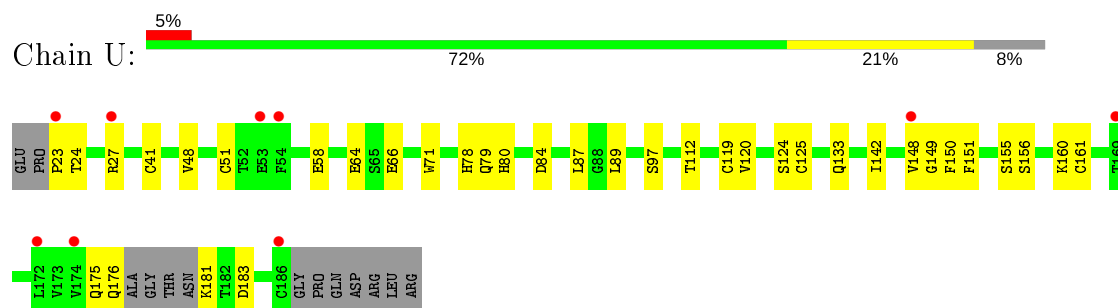
- Molecule 2: FAB Light chain



- Molecule 3: Tumor necrosis factor receptor superfamily member 5



- Molecule 3: Tumor necrosis factor receptor superfamily member 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	173.31Å 75.96Å 126.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.98 – 2.84 37.98 – 2.84	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.98-2.84) 100.0 (37.98-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.85Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.205 , 0.265 0.206 , 0.266	Depositor DCC
R_{free} test set	1925 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9151	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.45	0/1637	0.62	0/2228
1	H	0.46	0/1627	0.64	0/2216
2	B	0.48	0/1749	0.59	0/2375
2	L	0.49	0/1743	0.62	0/2367
3	T	0.49	0/1192	0.62	0/1621
3	U	0.46	0/1230	0.60	0/1671
All	All	0.47	0/9178	0.61	0/12478

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1598	0	1560	21	0
1	H	1588	0	1545	21	0
2	B	1713	0	1661	15	0
2	L	1707	0	1657	27	0
3	T	1170	0	1027	20	0
3	U	1204	0	1069	18	0
4	T	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	U	10	0	0	0	0
5	A	23	0	0	0	0
5	B	39	0	0	0	0
5	H	23	0	0	0	0
5	L	41	0	0	0	0
5	T	16	0	0	0	0
5	U	9	0	0	0	0
All	All	9151	0	8519	114	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (114) 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)
3:U:176:GLN:HA	3:U:181:LYS:N	1.81	0.95
3:T:127:PRO:HD3	3:T:155:SER:HB3	1.73	0.71
1:A:91:THR:HG23	1:A:113:THR:HA	1.72	0.71
2:B:46:PRO:HB3	2:B:171:GLU:HG3	1.71	0.71
1:A:83:MET:HE1	1:A:112:VAL:HG21	1.73	0.70
1:H:98:ARG:HG2	1:H:105:VAL:HB	1.77	0.67
3:U:176:GLN:CA	3:U:181:LYS:N	2.58	0.67
2:L:155:LYS:NZ	2:L:201:GLU:HB3	2.11	0.65
2:B:129:GLU:HG3	1:H:120:LYS:HA	1.80	0.64
2:L:5:THR:HB	2:L:24:LYS:HG3	1.81	0.62
1:H:139:ALA:HB2	1:H:189:SER:HB3	1.80	0.62
2:L:36:LYS:HE3	2:L:56:TRP:CE2	2.35	0.61
3:T:39:SER:O	3:T:57:THR:HG21	2.00	0.61
1:A:53:SER:OG	3:U:64:GLU:HB3	2.03	0.59
2:L:35:GLN:HG3	2:L:35:GLN:O	2.03	0.58
1:A:120:LYS:HB2	2:L:132:LYS:HD3	1.85	0.57
3:T:120:VAL:HG21	3:T:122:HIS:CE1	2.41	0.56
2:L:149:GLU:OE2	2:L:149:GLU:N	2.29	0.55
3:T:106:GLU:HG3	3:T:109:TRP:CD1	2.42	0.54
3:U:133:GLN:HB2	3:U:142:ILE:HB	1.90	0.54
1:H:34:MET:HB3	1:H:79:LEU:HD22	1.89	0.54
1:H:83:MET:HB3	1:H:86:LEU:HD21	1.90	0.54
1:H:139:ALA:HB3	1:H:187:VAL:O	2.08	0.53
1:H:51:ILE:HD12	1:H:58:ILE:HD11	1.90	0.53
2:B:142:LEU:HB2	2:B:181:LEU:HB3	1.91	0.52
1:A:129:PRO:HG3	1:A:141:LEU:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:ASP:HA	2:B:131:LEU:HD12	1.92	0.51
1:H:12:VAL:HG11	1:H:86:LEU:HD13	1.93	0.51
1:A:52:SER:HB3	1:A:57:ASN:HB2	1.93	0.51
1:A:119:THR:HG22	1:A:206:SER:HB3	1.93	0.50
3:U:124:SER:HB2	3:U:156:SER:C	2.32	0.50
2:B:41:TRP:CZ3	2:B:94:CYS:HB3	2.47	0.50
1:H:91:THR:HG23	1:H:113:THR:HA	1.93	0.50
1:A:108:GLN:HG3	1:A:109:GLY:O	2.12	0.49
2:L:67:ARG:HB2	2:L:82[B]:SER:O	2.12	0.49
1:H:2:VAL:HG13	1:H:27:PHE:CD1	2.47	0.49
2:B:43:GLN:HB2	2:B:53:LEU:HD11	1.93	0.49
2:L:67:ARG:HB2	2:L:82[A]:SER:O	2.13	0.49
3:T:123:ARG:HG2	3:T:141:THR:HB	1.93	0.49
2:L:43:GLN:OE1	2:L:45:LYS:HE2	2.13	0.48
2:B:99:THR:O	2:B:102:LEU:HD23	2.13	0.48
1:H:70:ILE:HD11	1:H:79:LEU:HD11	1.96	0.48
1:A:120:LYS:HA	2:L:129:GLU:HG3	1.95	0.48
3:U:125:CYS:O	3:U:155:SER:HA	2.14	0.48
3:T:27:ARG:HG3	3:T:28:GLU:H	1.78	0.48
3:U:84:ASP:HB3	3:U:87:LEU:HG	1.94	0.48
3:T:134:ILE:HD11	3:T:158:PHE:CD1	2.49	0.47
3:U:23:PRO:O	3:U:24:THR:HG23	2.14	0.47
3:T:133:GLN:HB2	3:T:142:ILE:HB	1.97	0.47
2:L:61:GLU:HG3	2:L:62:SER:O	2.15	0.47
2:L:81:ILE:O	2:L:84:LEU:HD12	2.15	0.47
3:T:56:GLU:OE1	3:T:57:THR:HG22	2.13	0.47
1:A:11:LEU:HD11	1:A:115:SER:HB3	1.96	0.47
2:L:165:SER:HA	2:L:184:THR:O	2.15	0.47
1:A:108:GLN:CG	1:A:109:GLY:N	2.78	0.47
2:B:53:LEU:C	2:B:54:ILE:HG13	2.35	0.46
3:T:169:THR:O	3:T:186:CYS:HA	2.16	0.46
2:L:67:ARG:NH1	2:L:88:ASP:OD1	2.49	0.46
3:U:175:GLN:C	3:U:181:LYS:N	2.69	0.45
3:U:175:GLN:O	3:U:181:LYS:N	2.48	0.45
3:T:31:TYR:CD2	3:T:73:ARG:HD2	2.51	0.45
3:U:148:VAL:HA	3:U:149:GLY:HA2	1.60	0.45
1:H:22:CYS:HB3	1:H:79:LEU:HB3	1.98	0.45
2:B:140:CYS:HB2	2:B:154:TRP:CH2	2.51	0.45
2:B:60:ARG:HD3	2:B:68:PHE:O	2.15	0.45
1:A:40:ALA:HB3	1:A:43:LYS:HB2	1.98	0.44
2:L:89:VAL:HG21	2:L:172:GLN:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:27:PHE:CE2	1:H:29:PHE:HA	2.53	0.44
2:B:67:ARG:NH2	2:B:88:ASP:OD1	2.50	0.44
3:U:66:GLU:HA	3:U:78:HIS:O	2.18	0.44
2:B:11:LEU:HD23	2:B:110:LEU:HD13	1.98	0.44
3:T:41:CYS:O	3:T:71:TRP:HA	2.18	0.43
2:B:140:CYS:HB2	2:B:154:TRP:CZ2	2.53	0.43
1:A:166:VAL:HG22	1:A:185:VAL:HB	2.00	0.43
2:B:200:CYS:O	2:B:212:THR:HA	2.18	0.43
1:A:68:PHE:CE1	1:A:83:MET:HB3	2.54	0.43
1:A:195:GLN:HG3	1:A:197:TYR:CZ	2.54	0.43
1:H:188:PRO:O	1:H:191:SER:OG	2.27	0.43
3:T:30:GLN:HG2	3:T:39:SER:HA	2.01	0.43
1:A:1:GLU:CD	1:A:3:GLN:HE21	2.22	0.43
2:L:147:PRO:HB2	2:L:149:GLU:OE2	2.19	0.42
2:L:24:LYS:H	2:L:24:LYS:HG2	1.72	0.42
2:L:97:ASP:OD1	3:T:94:LYS:NZ	2.50	0.42
3:T:46:LYS:O	3:T:59:CYS:HA	2.18	0.42
1:H:125:PHE:CE2	2:L:130:GLN:HG3	2.55	0.42
2:L:126:PRO:HG3	2:L:136:ALA:HB1	2.02	0.42
2:L:169:VAL:HG22	2:L:181:LEU:HD12	2.01	0.42
1:A:22:CYS:HB3	1:A:79:LEU:HB3	2.01	0.42
3:U:41:CYS:O	3:U:71:TRP:HA	2.20	0.42
3:U:48:VAL:HB	3:U:58:GLU:HG3	2.02	0.42
2:L:33:GLY:HA3	3:T:99:THR:HG21	2.02	0.41
2:B:153:GLN:HG2	2:B:160:LEU:HD11	2.01	0.41
1:H:204:LYS:N	1:H:205:PRO:HD2	2.35	0.41
3:U:150:PHE:HB3	3:U:161:CYS:HB3	2.01	0.41
1:A:51:ILE:HA	1:A:57:ASN:O	2.20	0.41
3:T:128:GLY:HA2	3:T:176:GLN:C	2.40	0.41
3:T:66:GLU:HA	3:T:78:HIS:O	2.20	0.41
1:A:68:PHE:HA	1:A:82:GLN:O	2.20	0.41
3:U:151:PHE:CZ	3:U:183:ASP:HB2	2.55	0.41
2:L:155:LYS:HZ3	2:L:201:GLU:HB3	1.83	0.41
3:U:89:LEU:HD23	3:U:119:CYS:SG	2.61	0.41
1:H:6:GLU:HA	1:H:21:SER:O	2.21	0.41
1:H:6:GLU:OE1	1:H:95:TYR:HA	2.21	0.41
2:L:81:ILE:O	2:L:84:LEU:CD1	2.69	0.41
3:T:68:LEU:HG	3:T:77:CYS:SG	2.60	0.41
2:L:6:GLN:HB2	2:L:106:GLN:NE2	2.36	0.41
1:A:213:LYS:HB3	1:H:207:ASN:HB3	2.02	0.41
2:L:8:PRO:HG3	2:L:11:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ARG:HG3	1:A:19:ARG:HH11	1.86	0.40
1:H:36:TRP:NE1	1:H:81:LEU:HB2	2.36	0.40
2:L:155:LYS:HZ1	2:L:201:GLU:HB3	1.85	0.40
3:T:132:LYS:HB3	3:T:142:ILE:HG22	2.03	0.40
3:U:112:THR:HG22	3:U:120:VAL:HG13	2.03	0.40
1:H:165:GLY:O	1:H:185:VAL:HA	2.21	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	209/223 (94%)	198 (95%)	11 (5%)	0	100	100
1	H	208/223 (93%)	202 (97%)	6 (3%)	0	100	100
2	B	219/220 (100%)	210 (96%)	9 (4%)	0	100	100
2	L	218/220 (99%)	210 (96%)	8 (4%)	0	100	100
3	T	155/173 (90%)	146 (94%)	8 (5%)	1 (1%)	25	46
3	U	156/173 (90%)	144 (92%)	12 (8%)	0	100	100
All	All	1165/1232 (95%)	1110 (95%)	54 (5%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	T	138	VAL

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	176/185 (95%)	168 (96%)	8 (4%)	27	51
1	H	174/185 (94%)	173 (99%)	1 (1%)	86	93
2	B	196/195 (100%)	192 (98%)	4 (2%)	55	76
2	L	195/195 (100%)	186 (95%)	9 (5%)	27	51
3	T	133/157 (85%)	125 (94%)	8 (6%)	19	37
3	U	139/157 (88%)	133 (96%)	6 (4%)	29	54
All	All	1013/1074 (94%)	977 (96%)	36 (4%)	35	60

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	SER
1	A	87	ARG
1	A	116	SER
1	A	164	SER
1	A	189	SER
1	A	204	LYS
1	A	212	LYS
1	A	218	SER
2	B	17	GLU
2	B	67	ARG
2	B	165	SER
2	B	191	ASP
1	H	25	SER
2	L	24	LYS
2	L	51	LYS
2	L	96	ASN
2	L	143	ASN
2	L	162	SER
2	L	177	SER
2	L	196	LYS
2	L	201	GLU
2	L	208	SER
3	T	47	LEU
3	T	50	ASP
3	T	51	CYS
3	T	57	THR

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Mol	Chain	Res	Type
3	T	124	SER
3	T	138	VAL
3	T	139	SER
3	T	143	CYS
3	U	27	ARG
3	U	51	CYS
3	U	79	GLN
3	U	80	HIS
3	U	97	SER
3	U	160	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	108	GLN
2	L	48	GLN
3	T	42	GLN
3	T	122	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	T	202	-	4,4,4	0.14	0	6,6,6	0.17	0
4	SO4	T	201	-	4,4,4	0.27	0	6,6,6	0.50	0
4	SO4	U	202	-	4,4,4	0.12	0	6,6,6	0.41	0
4	SO4	U	201	-	4,4,4	0.20	0	6,6,6	0.60	0

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 [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, 95th 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	213/223 (95%)	-0.03	3 (1%) 75 71	34, 52, 81, 127	0
1	H	212/223 (95%)	-0.21	4 (1%) 66 62	27, 43, 87, 131	0
2	B	220/220 (100%)	-0.26	1 (0%) 91 89	29, 46, 70, 123	0
2	L	219/220 (99%)	-0.15	0 100 100	29, 45, 70, 84	0
3	T	159/173 (91%)	0.32	13 (8%) 11 6	32, 58, 118, 133	0
3	U	160/173 (92%)	0.22	9 (5%) 24 17	30, 58, 109, 119	0
All	All	1183/1232 (96%)	-0.05	30 (2%) 57 52	27, 50, 90, 133	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	T	166	SER	4.7
3	U	186	CYS	4.4
1	H	194	THR	3.8
3	U	172	LEU	3.6
3	T	183	ASP	3.5
3	U	174	VAL	3.3
3	T	174	VAL	3.2
3	U	53	GLU	3.1
3	U	148	VAL	3.1
3	T	185	VAL	3.1
1	H	189	SER	3.0
1	A	164	SER	2.9
3	T	148	VAL	2.8
3	T	182	THR	2.8
3	T	169	THR	2.7
3	U	27	ARG	2.6
3	T	167	CYS	2.5
1	H	138	THR	2.4
2	B	220	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1	GLU	2.4
3	U	23	PRO	2.3
3	U	169	THR	2.3
3	T	147	PRO	2.2
1	A	219	CYS	2.2
1	H	161	ALA	2.2
3	T	186	CYS	2.1
3	T	163	PRO	2.1
3	U	54	PHE	2.1
3	T	146	CYS	2.0
3	T	143	CYS	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 [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, 95th 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	SO4	T	202	5/5	0.92	0.17	92,93,93,98	0
4	SO4	U	202	5/5	0.98	0.15	48,50,54,57	0
4	SO4	T	201	5/5	0.99	0.13	33,37,39,41	0
4	SO4	U	201	5/5	0.99	0.15	41,45,51,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.