Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:38 am BST

PDB ID	:	4CNI
Title	:	Crystal structure of the Fab portion of Olokizumab in complex with IL- 6
Authors	:	Shaw, S.; Bourne, T.; Meier, C.; Carrington, B.; Gelinas, R.; Henry, A.; Popplewell, A.; Adams, R.; Baker, T.; Rapecki, S.; Marshall, D.; Neale, H.; Lawson, A.
Deposited on	:	2014-01-22
Resolution	:	2.20 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:

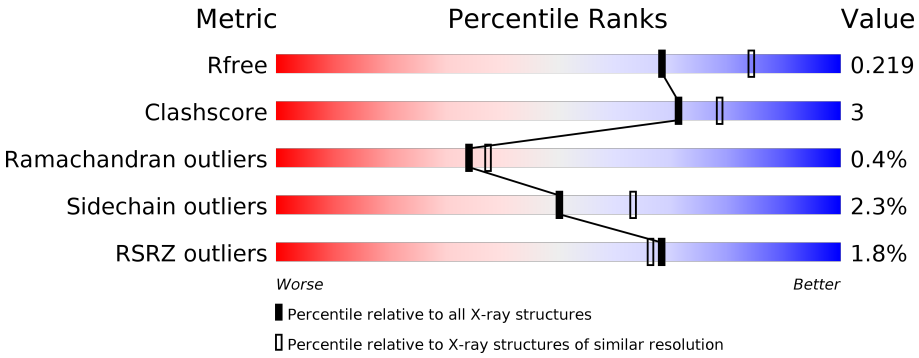
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	220	92% 8%
1	H	220	91% 7%
2	B	214	% 95% 5%
2	L	214	90% 10%
3	C	171	8% 94% 6%
3	D	171	4% 89% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TAM	A	1221	-	-	X	-
4	TAM	H	1220	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10999 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 OLOKIZUMAB HEAVY CHAIN, FAB PORTION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	2	0
			1685	1061	279	336	9			
1	H	219	Total	C	N	O	S	0	1	0
			1678	1057	278	334	9			

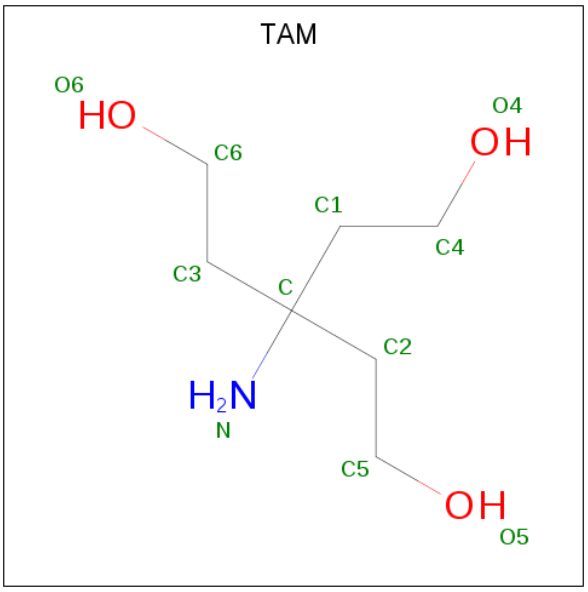
- Molecule 2 is a protein called OLOKIZUMAB LIGHT CHAIN, FAB PORTION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	2	0
			1639	1022	274	336	7			
2	L	214	Total	C	N	O	S	0	2	0
			1643	1025	273	339	6			

- Molecule 3 is a protein called INTERLEUKIN-6.

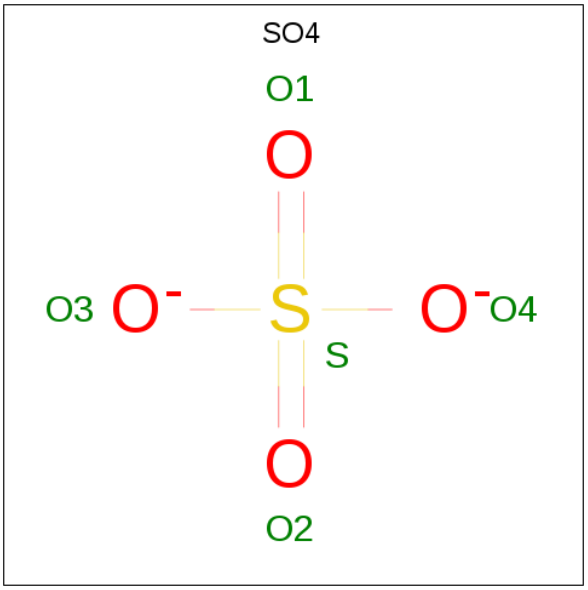
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	171	Total	C	N	O	S	0	1	0
			1355	849	234	263	9			
3	D	171	Total	C	N	O	S	0	1	0
			1365	855	234	266	10			

- Molecule 4 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 11 7 1 3	0	0
4	H	1	Total C N O 11 7 1 3	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

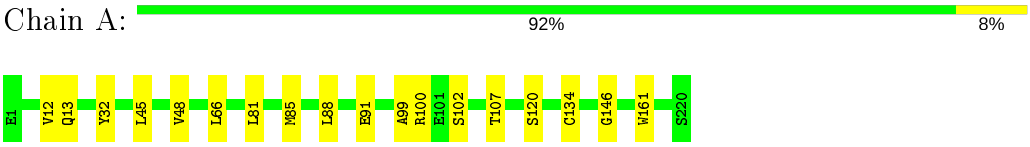
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	353	Total O 353 353	0	0
6	B	257	Total O 257 257	0	0
6	C	205	Total O 205 205	0	0
6	D	193	Total O 193 193	0	0
6	H	314	Total O 314 314	0	0
6	L	265	Total O 265 265	0	0

3 Residue-property plots (i)

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

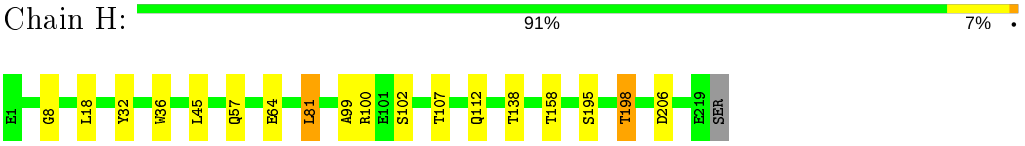
• Molecule 1: OLOKIZUMAB HEAVY CHAIN, FAB PORTION

Chain A:



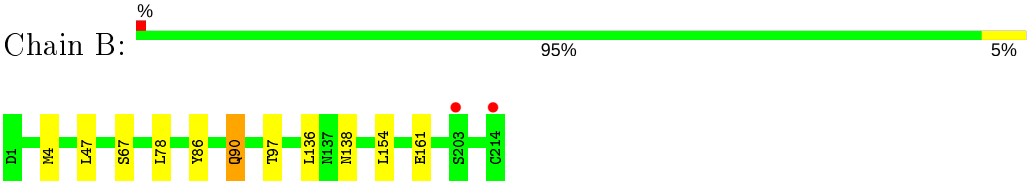
• Molecule 1: OLOKIZUMAB HEAVY CHAIN, FAB PORTION

Chain H:



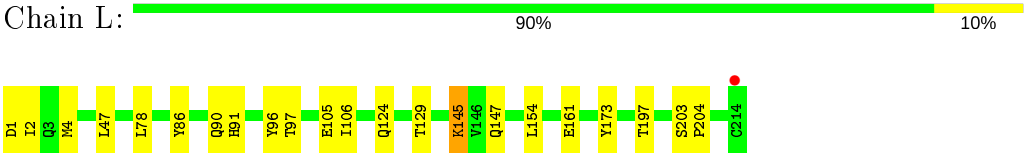
• Molecule 2: OLOKIZUMAB LIGHT CHAIN, FAB PORTION

Chain B:



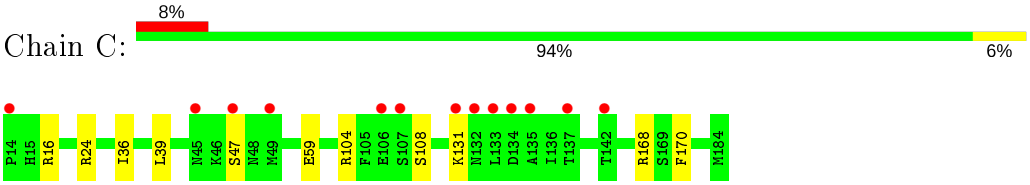
• Molecule 2: OLOKIZUMAB LIGHT CHAIN, FAB PORTION

Chain L:



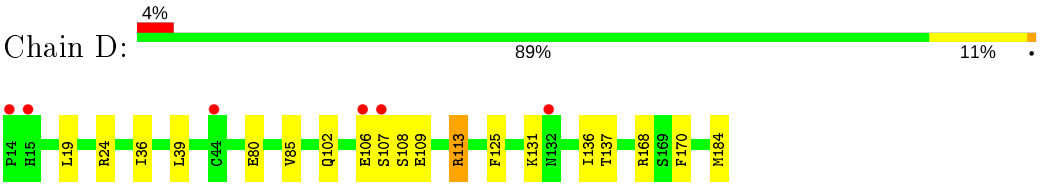
• Molecule 3: INTERLEUKIN-6

Chain C:



• Molecule 3: INTERLEUKIN-6

Chain D:


4%
89%
11%
P14
H15
L19
R24
I36
L39
C44
E80
V85
Q102
E106
S107
S108
E109
R113
F125
K131
N132
I136
T137
R168
S169
F170
M184

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α, β, γ	241.99Å 241.99Å 76.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.5 (30.00-2.20) 97.5 (29.95-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.59 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.176 , 0.215 0.178 , 0.219	Depositor DCC
R_{free} test set	6411 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	19.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10999	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: TAM, 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	0.41	0/1732	0.55	0/2358
1	H	0.42	0/1722	0.58	0/2343
2	B	0.42	0/1679	0.56	0/2281
2	L	0.42	0/1683	0.57	0/2285
3	C	0.40	0/1375	0.51	0/1852
3	D	0.41	0/1386	0.52	0/1866
All	All	0.42	0/9577	0.55	0/12985

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

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	1685	0	1611	13	0
1	H	1678	0	1606	15	0
2	B	1639	0	1575	4	0
2	L	1643	0	1587	17	0
3	C	1355	0	1354	6	0
3	D	1365	0	1364	7	0
4	A	11	0	17	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	11	0	17	8	0
5	C	10	0	0	0	0
5	D	10	0	0	0	0
5	H	5	0	0	0	0
6	A	353	0	0	4	1
6	B	257	0	0	2	0
6	C	205	0	0	3	1
6	D	193	0	0	1	0
6	H	314	0	0	2	0
6	L	265	0	0	2	0
All	All	10999	0	9131	64	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 3.

All (64) 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:H:100:ARG:HH21	4:H:1220:TAM:H21	1.02	1.17
1:H:100:ARG:NH2	4:H:1220:TAM:H21	1.83	0.92
1:H:102:SER:HA	4:H:1220:TAM:H51	1.51	0.92
1:A:100:ARG:HH21	4:A:1221:TAM:H52	1.45	0.79
3:D:106:GLU:O	3:D:107:SER:HB3	1.81	0.78
1:H:100:ARG:HH21	4:H:1220:TAM:C2	1.93	0.76
3:D:168:ARG:NH1	6:D:2072:HOH:O	2.20	0.74
2:L:161:GLU:HG3	6:L:2219:HOH:O	1.87	0.74
2:L:2:ILE:O	2:L:97:THR:HG21	1.93	0.68
2:L:90:GLN:HE21	2:L:97:THR:HG22	1.64	0.62
6:H:2139:HOH:O	2:L:1:ASP:HB3	1.99	0.62
3:D:24:ARG:HD3	3:D:125:PHE:CZ	2.35	0.61
3:C:24:ARG:HD2	6:C:2030:HOH:O	1.99	0.60
1:H:32:TYR:HE2	4:H:1220:TAM:H52	1.66	0.60
2:L:105[B]:GLU:HG3	2:L:173:TYR:OH	2.02	0.60
1:H:102:SER:HA	4:H:1220:TAM:C5	2.30	0.59
1:A:100:ARG:NH2	4:A:1221:TAM:H52	2.16	0.59
1:A:85:MET:HB3	1:A:88:LEU:HD21	1.86	0.57
1:H:36:TRP:NE1	1:H:81:LEU:HD13	2.24	0.53
3:D:36:ILE:HD11	3:D:170:PHE:CD2	2.43	0.53
2:L:197:THR:HG22	2:L:204:PRO:HG3	1.90	0.53
3:D:102:GLN:HG3	3:D:113:ARG:HH21	1.74	0.52
1:A:99:ALA:HB1	1:A:107:THR:CG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:VAL:HG13	1:A:66:LEU:HD11	1.92	0.51
4:A:1221:TAM:H32	6:A:2069:HOH:O	2.10	0.50
1:H:158:THR:OG1	1:H:206:ASP:HB3	2.12	0.50
2:L:105[B]:GLU:HG2	2:L:106:ILE:N	2.27	0.49
2:L:197:THR:HG23	6:L:2179:HOH:O	2.11	0.49
1:H:32:TYR:CE2	4:H:1220:TAM:H52	2.47	0.49
2:B:161:GLU:HG3	6:B:2213:HOH:O	2.11	0.49
1:A:134:CYS:HB3	6:A:2231:HOH:O	2.13	0.48
1:H:195:SER:O	1:H:198:THR:HB	2.14	0.48
1:H:99:ALA:HB1	1:H:107:THR:CG2	2.45	0.47
1:A:99:ALA:HB1	1:A:107:THR:HG23	1.95	0.47
2:L:145:LYS:CB	2:L:197:THR:OG1	2.64	0.46
4:A:1221:TAM:H62	6:A:2353:HOH:O	2.15	0.46
3:C:36:ILE:HD11	3:C:170:PHE:CD2	2.50	0.46
3:D:80:GLU:HG3	3:D:184:MET:HG2	1.98	0.45
1:H:99:ALA:HB1	1:H:107:THR:HG23	1.97	0.45
1:A:91:GLU:HG3	6:A:2078:HOH:O	2.16	0.45
2:B:138:ASN:ND2	6:B:2170:HOH:O	2.49	0.45
1:H:64:GLU:HB3	6:H:2139:HOH:O	2.17	0.45
3:C:104:ARG:CZ	3:C:104:ARG:HA	2.47	0.45
1:A:146:GLY:HA2	1:A:161:TRP:CH2	2.52	0.44
2:L:197:THR:HG22	2:L:204:PRO:HB3	1.99	0.44
2:L:47:LEU:HD11	2:L:86:TYR:HE2	1.83	0.44
1:A:13[A]:GLN:OE1	1:A:120:SER:HA	2.18	0.44
1:H:102:SER:CA	4:H:1220:TAM:H51	2.36	0.44
2:L:145:LYS:HB2	2:L:197:THR:OG1	2.18	0.44
2:B:47:LEU:HD11	2:B:86:TYR:HE2	1.83	0.44
1:A:12:VAL:HG11	1:A:88:LEU:HD13	2.00	0.43
3:C:16:ARG:NH2	6:C:2009:HOH:O	2.51	0.43
2:L:124:GLN:HG2	2:L:129:THR:O	2.19	0.43
2:L:47:LEU:HD11	2:L:86:TYR:CE2	2.54	0.43
3:C:168:ARG:NH1	6:C:2191:HOH:O	2.51	0.42
2:B:4:MET:SD	2:B:90:GLN:HB2	2.60	0.42
2:L:91:HIS:HA	2:L:96:TYR:CD1	2.54	0.42
2:L:147:GLN:CG	2:L:154:LEU:HD22	2.50	0.41
1:A:102:SER:CB	4:A:1221:TAM:H22	2.50	0.41
1:H:8:GLY:O	1:H:18:LEU:HD21	2.20	0.41
3:C:104:ARG:NE	3:C:104:ARG:HA	2.35	0.41
1:A:32:TYR:HE2	4:A:1221:TAM:H51	1.85	0.41
2:L:4:MET:HG2	2:L:97:THR:HG23	2.03	0.41
3:D:85:VAL:HG13	3:D:136:ILE:HD13	2.04	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)
6:A:2032:HOH:O	6:C:2036:HOH:O[5_556]	2.19	0.01

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	220/220 (100%)	219 (100%)	1 (0%)	0	100	100
1	H	218/220 (99%)	217 (100%)	1 (0%)	0	100	100
2	B	214/214 (100%)	206 (96%)	8 (4%)	0	100	100
2	L	214/214 (100%)	207 (97%)	7 (3%)	0	100	100
3	C	170/171 (99%)	164 (96%)	3 (2%)	3 (2%)	8	5
3	D	170/171 (99%)	165 (97%)	3 (2%)	2 (1%)	13	10
All	All	1206/1210 (100%)	1178 (98%)	23 (2%)	5 (0%)	34	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	131	LYS
3	D	131	LYS
3	C	47	SER
3	D	108	SER
3	C	108	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	188/188 (100%)	186 (99%)	2 (1%)	73 85
1	H	187/188 (100%)	181 (97%)	6 (3%)	39 50
2	B	186/187 (100%)	180 (97%)	6 (3%)	39 50
2	L	188/187 (100%)	185 (98%)	3 (2%)	62 76
3	C	150/156 (96%)	148 (99%)	2 (1%)	69 81
3	D	153/156 (98%)	148 (97%)	5 (3%)	38 49
All	All	1052/1062 (99%)	1028 (98%)	24 (2%)	50 63

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	81	LEU
2	B	67	SER
2	B	78	LEU
2	B	90	GLN
2	B	97	THR
2	B	136	LEU
2	B	154	LEU
3	C	39	LEU
3	C	59	GLU
3	D	19	LEU
3	D	39	LEU
3	D	109	GLU
3	D	113	ARG
3	D	137	THR
1	H	45	LEU
1	H	57	GLN
1	H	81	LEU
1	H	112	GLN
1	H	138	THR
1	H	198	THR
2	L	78	LEU
2	L	145	LYS
2	L	203	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	103	ASN
1	H	13	GLN
2	L	147	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 carbohydrates in this entry.

5.6 Ligand geometry

7 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	TAM	A	1221	-	7,10,10	0.52	0	9,12,12	0.71	0
5	SO4	C	1185	-	4,4,4	0.16	0	6,6,6	0.15	0
5	SO4	D	1185	-	4,4,4	0.12	0	6,6,6	0.17	0
5	SO4	C	1186	-	4,4,4	0.13	0	6,6,6	0.09	0
5	SO4	D	1186	-	4,4,4	0.14	0	6,6,6	0.06	0
4	TAM	H	1220	-	7,10,10	0.46	0	9,12,12	1.32	1 (11%)
5	SO4	H	1221	-	4,4,4	0.15	0	6,6,6	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TAM	H	1220	-	-	7/12/12/12	-
4	TAM	A	1221	-	-	1/12/12/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1220	TAM	C3-C-C1	2.89	115.60	110.50

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1221	TAM	C-C3-C6-O6
4	H	1220	TAM	C3-C-C1-C4
4	H	1220	TAM	C1-C-C3-C6
4	H	1220	TAM	C2-C-C3-C6
4	H	1220	TAM	N-C-C3-C6
4	H	1220	TAM	C-C1-C4-O4
4	H	1220	TAM	C2-C-C1-C4
4	H	1220	TAM	N-C-C1-C4

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1221	TAM	6	0
4	H	1220	TAM	8	0

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	220/220 (100%)	-0.58	0 100 100	9, 18, 32, 39	2 (0%)
1	H	219/220 (99%)	-0.67	0 100 100	7, 18, 33, 44	3 (1%)
2	B	214/214 (100%)	-0.63	2 (0%) 84 83	9, 20, 32, 37	0
2	L	214/214 (100%)	-0.73	1 (0%) 91 90	7, 17, 31, 45	0
3	C	171/171 (100%)	-0.16	13 (7%) 13 12	10, 22, 55, 60	3 (1%)
3	D	171/171 (100%)	-0.27	6 (3%) 44 42	7, 19, 51, 57	3 (1%)
All	All	1209/1210 (99%)	-0.53	22 (1%) 68 66	7, 19, 42, 60	11 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	47	SER	5.8
3	C	14	PRO	4.6
3	C	132	ASN	4.2
3	C	107	SER	3.8
3	D	132	ASN	3.8
3	D	106	GLU	3.6
3	D	107	SER	3.5
3	D	14	PRO	3.3
3	C	49	MET	3.1
3	C	133	LEU	3.0
2	B	214	CYS	2.9
2	L	214	CYS	2.9
3	C	135	ALA	2.9
3	D	15	HIS	2.9
3	C	142	THR	2.6
3	C	131	LYS	2.4
3	C	137	THR	2.4
3	C	106	GLU	2.3
3	C	134	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	44	CYS	2.2
3	C	45	ASN	2.0
2	B	203	SER	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, 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	TAM	A	1221	11/11	0.70	0.34	52,57,59,61	0
4	TAM	H	1220	11/11	0.84	0.25	41,49,52,54	0
5	SO4	C	1186	5/5	0.90	0.20	92,92,92,92	0
5	SO4	C	1185	5/5	0.94	0.14	58,58,60,61	0
5	SO4	D	1186	5/5	0.96	0.19	90,91,91,91	0
5	SO4	D	1185	5/5	0.98	0.07	41,42,44,45	0
5	SO4	H	1221	5/5	0.99	0.11	48,49,50,51	0

6.5 Other polymers (i)

There are no such residues in this entry.