



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:29 PM GMT

PDB ID : 5D6C
Title : Structure of 4497 Fab bound to synthetic wall teichoic acid fragment
Authors : Lupardus, P.J.; Fong, R.
Deposited on : 2015-08-12
Resolution : 1.72 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
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

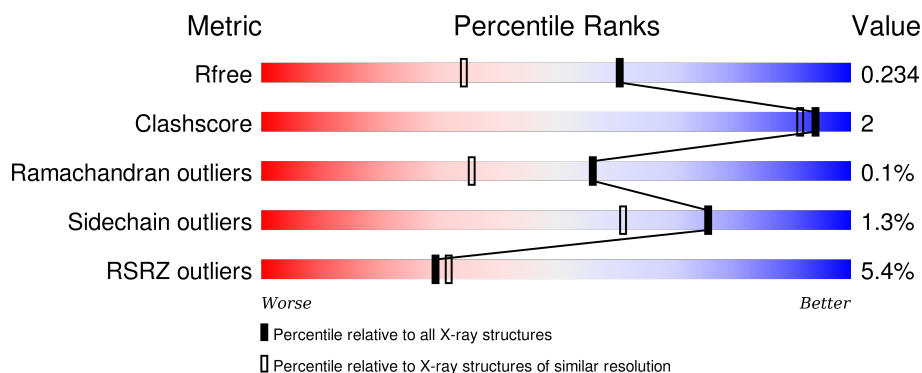
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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}	91344	3998 (1.74-1.70)
Clashscore	102246	4425 (1.74-1.70)
Ramachandran outliers	100387	4360 (1.74-1.70)
Sidechain outliers	100360	4360 (1.74-1.70)
RSRZ outliers	91569	4010 (1.74-1.70)

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. 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	220	<div> <div>7%</div> <div>94%</div> <div>5%</div> </div>
1	L	220	<div> <div>3%</div> <div>93%</div> <div>6%</div> </div>
2	B	224	<div> <div>7%</div> <div>92%</div> <div>6%</div> </div>
2	H	224	<div> <div>4%</div> <div>92%</div> <div>6%</div> </div>

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
3	CA	L	301	-	-	-	X
5	ACT	H	302	-	-	-	X
5	ACT	L	302	-	-	-	X
6	GOL	H	303	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7481 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 4497 antibody IgK (VL and CL).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	3	0
			1736	1090	302	340	4			
1	L	219	Total	C	N	O	S	0	5	0
			1742	1095	299	344	4			

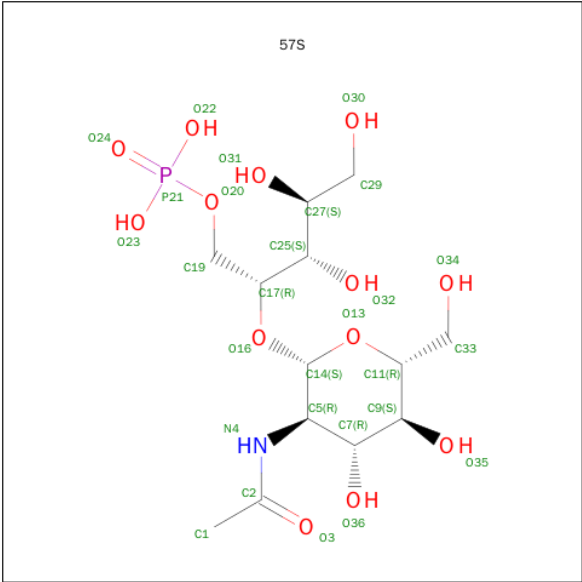
- Molecule 2 is a protein called 4497 antibody IgG1 (VH and CH1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	2	0
			1575	995	266	308	6			
2	H	219	Total	C	N	O	S	0	5	0
			1652	1040	279	326	7			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

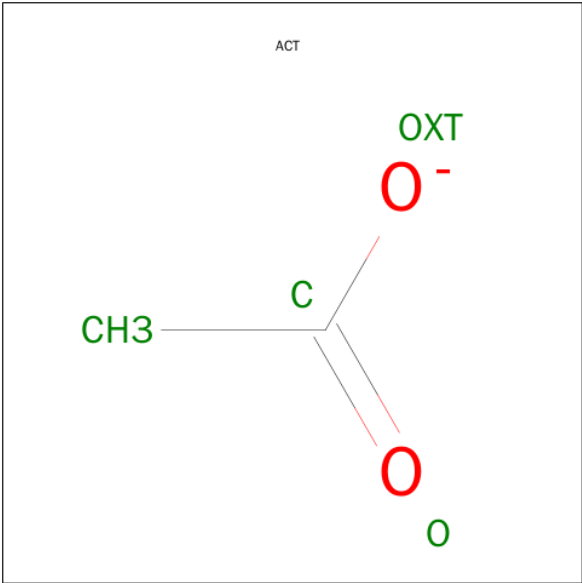
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	Ca	0	0
			1	1		
3	A	2	Total	Ca	0	0
			2	2		
3	L	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 4-O-[2-(acetylamino)-2-deoxy-beta-D-glucopyranosyl]-5-O-phosphono-D-ribitol (three-letter code: 57S) (formula: C₁₃H₂₆NO₁₃P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			28	13	1	13	1		
4	L	1	Total	C	N	O	P	0	0
			28	13	1	13	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			4	2	2		
5	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

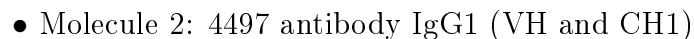
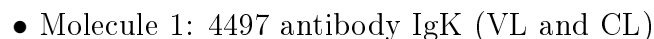


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	138	Total	O	0	0
			138	138		
7	B	171	Total	O	0	0
			171	171		
7	H	196	Total	O	0	0
			196	196		
7	L	197	Total	O	0	0
			197	197		

- Molecule 1: 4497 antibody IgK (VL and CL)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.71Å 111.47Å 158.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.64 – 1.72 33.64 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.64-1.72) 99.9 (33.64-1.72)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.72Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.203 , 0.238 0.203 , 0.234	Depositor DCC
R_{free} test set	6101 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 120150 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7481	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 57S, GOL, CA, ACT

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	0.46	0/1784	0.66	0/2420
1	L	0.52	0/1796	0.68	0/2438
2	B	0.51	0/1618	0.69	0/2205
2	H	0.61	1/1705 (0.1%)	0.69	0/2321
All	All	0.53	1/6903 (0.0%)	0.68	0/9384

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	130	THR	C-N	-5.39	1.21	1.34

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	1736	0	1703	8	0
1	L	1742	0	1713	6	0
2	B	1575	0	1531	2	0
2	H	1652	0	1621	8	0
3	A	2	0	0	0	0
3	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1	0	0	0	0
4	B	28	0	24	0	0
4	L	28	0	24	0	0
5	H	4	0	3	0	0
5	L	4	0	3	0	0
6	H	6	0	8	1	0
7	A	138	0	0	0	0
7	B	171	0	0	0	0
7	H	196	0	0	1	0
7	L	197	0	0	1	0
All	All	7481	0	6630	24	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 2.

All (24) 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:208[A]:LYS:HE3	6:H:303:GOL:O2	1.71	0.89
1:A:142[B]:ARG:HD3	1:A:163:VAL:HG11	1.68	0.74
2:B:83:ARG:HG3	2:B:85:GLU:HG2	1.73	0.69
7:H:496:HOH:O	1:L:129:GLU:HG3	2.04	0.57
1:A:78:LEU:HD11	1:A:104:LEU:HD21	1.89	0.55
1:A:145:LYS:HB3	1:A:197:THR:HB	1.90	0.53
2:H:47:TRP:HZ2	2:H:50:PHE:HB3	1.73	0.53
2:H:100[B]:ASP:HB3	2:H:101:ASP:OD2	2.11	0.49
2:B:51:THR:OG1	2:B:54:GLY:HA2	2.13	0.48
1:L:8:PRO:HG2	1:L:11:LEU:HG	1.95	0.47
1:L:155:LYS:HG3	7:L:512:HOH:O	2.14	0.46
2:H:34:MET:HB3	2:H:78:LEU:HD22	1.97	0.46
1:L:11:LEU:HD13	1:L:110:LEU:HD13	1.98	0.46
1:A:108[B]:ARG:HD3	1:A:109:THR:O	2.16	0.45
1:A:120:PRO:HG3	1:A:130:ALA:HB1	1.99	0.45
2:H:22:CYS:HB3	2:H:78:LEU:HB3	1.99	0.44
2:H:120:VAL:O	2:H:208[B]:LYS:HE3	2.18	0.43
1:A:108[A]:ARG:HD3	1:A:109:THR:O	2.18	0.43
2:H:51:THR:OG1	2:H:54:GLY:HA2	2.20	0.42
1:L:148[A]:ARG:CZ	1:L:169[A]:VAL:HG21	2.50	0.41
1:A:108[B]:ARG:HG2	1:A:171:SER:HB2	2.02	0.41
2:H:120:VAL:HG12	2:H:208[B]:LYS:HD2	2.03	0.41
1:L:151:LYS:HB3	1:L:203:THR:HB	2.01	0.41

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	220/220 (100%)	213 (97%)	7 (3%)	0	100	100
1	L	222/220 (101%)	216 (97%)	5 (2%)	1 (0%)	34	15
2	B	208/224 (93%)	203 (98%)	5 (2%)	0	100	100
2	H	222/224 (99%)	217 (98%)	5 (2%)	0	100	100
All	All	872/888 (98%)	849 (97%)	22 (2%)	1 (0%)	56	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	57	ALA

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	197/196 (100%)	196 (100%)	1 (0%)	92	87
1	L	200/196 (102%)	194 (97%)	6 (3%)	48	25
2	B	175/188 (93%)	174 (99%)	1 (1%)	90	84
2	H	187/188 (100%)	185 (99%)	2 (1%)	80	68
All	All	759/768 (99%)	749 (99%)	10 (1%)	76	61

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	TYR
2	B	100	ASP
2	H	4	LEU
2	H	131	SER
1	L	11	LEU
1	L	27(F)	SER
1	L	45	ARG
1	L	69	SER
1	L	97	TYR
1	L	187	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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	57S	B	301	-	28,28,28	1.02	1 (3%)	36,40,40	0.94	1 (2%)
5	ACT	H	302	-	0,3,3	0.00	-	0,3,3	0.00	-
6	GOL	H	303	-	5,5,5	0.25	0	5,5,5	0.81	0
5	ACT	L	302	-	0,3,3	0.00	-	0,3,3	0.00	-
4	57S	L	303	-	28,28,28	1.07	2 (7%)	36,40,40	1.31	5 (13%)

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	57S	B	301	-	-	0/26/46/46	0/1/1/1
5	ACT	H	302	-	-	0/0/0/0	0/0/0/0
6	GOL	H	303	-	-	0/4/4/4	0/0/0/0
5	ACT	L	302	-	-	0/0/0/0	0/0/0/0
4	57S	L	303	-	-	0/26/46/46	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	303	57S	P21-O23	2.05	1.61	1.54
4	L	303	57S	P21-O24	3.28	1.61	1.50
4	B	301	57S	P21-O24	3.49	1.61	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	57S	C14-C5-N4	-3.03	105.31	111.01
4	L	303	57S	C14-C5-N4	-2.57	106.18	111.01
4	L	303	57S	O3-C2-C1	-2.21	118.01	122.07
4	L	303	57S	C29-C27-C25	2.03	117.45	112.43
4	L	303	57S	C27-C25-C17	2.75	118.79	113.10
4	L	303	57S	O16-C17-C25	3.43	114.12	107.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	303	GOL	1	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, 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	219/220 (99%)	0.35	15 (6%)	20 22	25, 39, 61, 92	0
1	L	219/220 (99%)	0.09	7 (3%)	51 56	19, 31, 52, 66	0
2	B	210/224 (93%)	0.36	16 (7%)	17 19	19, 34, 64, 78	0
2	H	219/224 (97%)	0.13	9 (4%)	41 45	18, 31, 56, 89	0
All	All	867/888 (97%)	0.23	47 (5%)	29 32	18, 34, 59, 92	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	132	GLY	6.5
1	L	73	PHE	5.3
2	H	131	SER	5.1
2	B	186	SER	4.9
1	L	27(E)	THR	4.5
2	B	190	THR	4.4
2	H	130	THR	4.4
1	L	27(C)	PHE	4.4
2	B	187	SER	4.0
2	B	209	LYS	3.7
1	A	212	GLY	3.6
1	A	67	PHE	3.5
1	A	184	ALA	3.5
2	B	193	TYR	3.5
1	A	56	SER	3.5
2	B	126	SER	3.3
2	H	127	SER	3.3
2	B	157	ALA	3.2
2	B	192	THR	3.2
1	A	188	LYS	3.1
2	B	194	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
2	H	129	SER	3.0
2	B	74	ALA	3.0
1	A	191	VAL	3.0
2	B	188	LEU	2.8
2	H	83	ARG	2.7
2	B	3	GLN	2.7
2	B	156	GLY	2.7
1	A	203	SER	2.6
1	A	126	LYS	2.6
1	A	210	ASN	2.6
2	H	99	LEU	2.5
1	L	98	PHE	2.4
1	A	29	ASN	2.3
2	B	55	THR	2.2
2	H	133	GLY	2.2
1	A	154	LEU	2.2
2	B	1	GLU	2.2
2	B	211	GLU	2.2
1	A	152	ASN	2.1
1	L	3	GLN	2.1
1	A	192	TYR	2.0
1	A	135	LEU	2.0
1	A	157	GLY	2.0
1	L	218	GLY	2.0
2	H	82(B)	ASN	2.0
1	L	1	ASP	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
5	ACT	L	302	4/4	0.91	0.22	10.92	44,49,49,52	0
3	CA	L	301	1/1	0.98	0.16	7.28	44,44,44,44	0
6	GOL	H	303	6/6	0.82	0.26	6.50	41,45,53,55	0
5	ACT	H	302	4/4	0.83	0.17	5.24	63,65,66,69	0
4	57S	B	301	28/28	0.89	0.14	1.88	36,51,68,70	0
4	57S	L	303	28/28	0.84	0.14	0.87	38,57,73,74	0
3	CA	H	301	1/1	0.97	0.07	-2.06	41,41,41,41	0
3	CA	A	301	1/1	0.99	0.04	-3.25	35,35,35,35	0
3	CA	A	302	1/1	0.99	0.04	-3.50	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.