



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 06:53 am GMT

PDB ID : 4GMT
Title : Crystal structure of heterosubtypic Fab S139/1
Authors : Lee, P.S.; Ekiert, D.C.; Wilson, I.A.
Deposited on : 2012-08-16
Resolution : 2.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

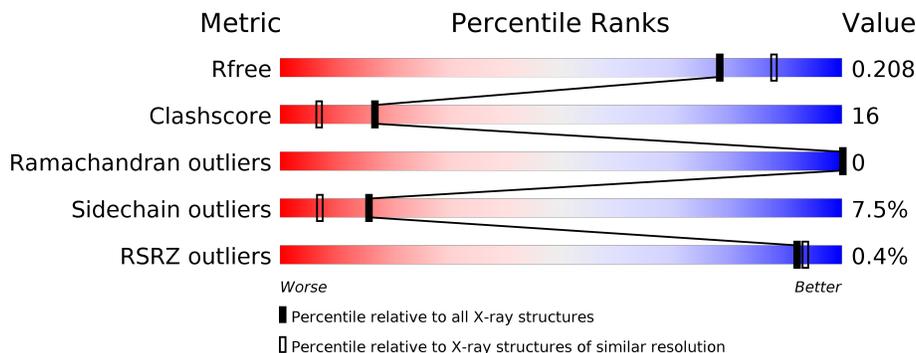
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	100719	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (2.04-2.04)

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	L	214	
1	M	214	
2	H	225	
2	I	225	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6690 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 S139/1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	213	1662	1031	278	346	7	0	0	0
1	M	213	1662	1031	278	346	7	0	0	0

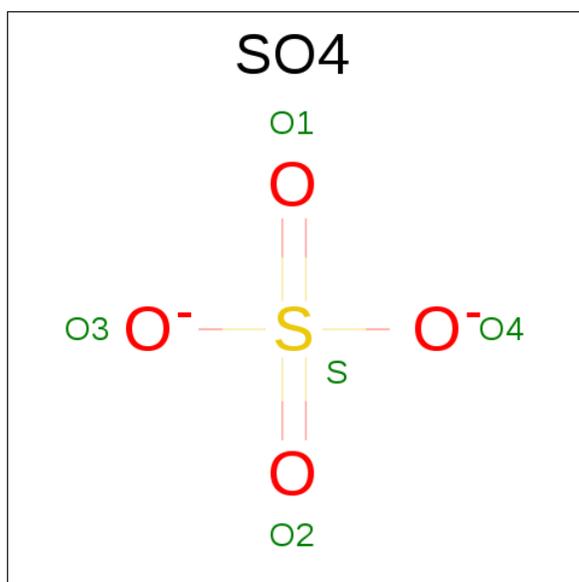
- Molecule 2 is a protein called Fab S139/1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	213	1635	1046	262	320	7	0	0	0
2	I	213	1635	1046	262	320	7	0	0	0

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

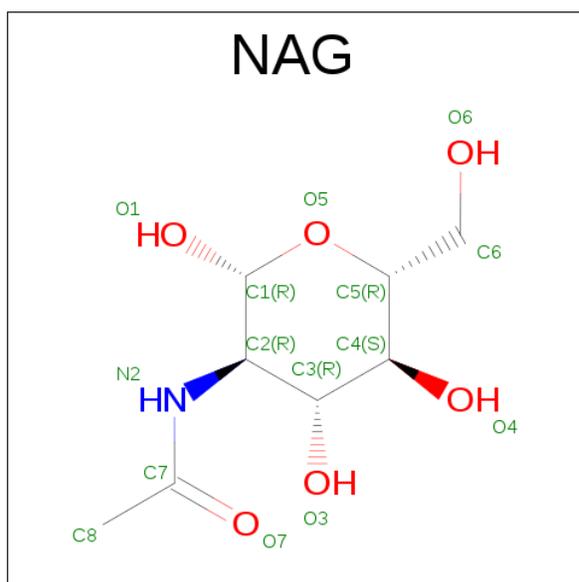
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	H	2	28	16	2	10	0	0

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



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

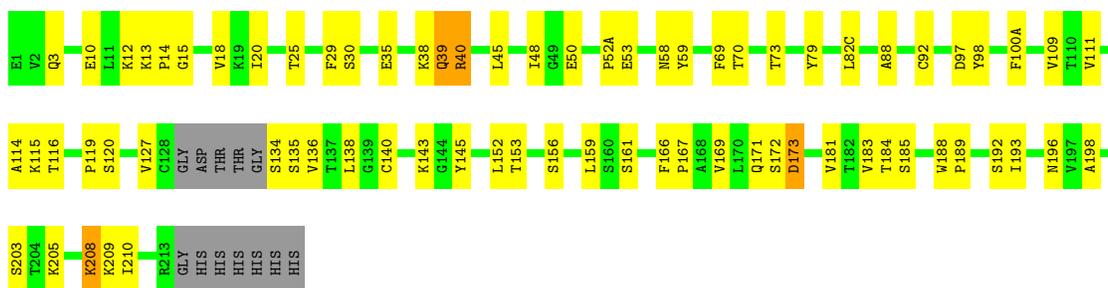
- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	11	Total 11	O 11	0	0
6	H	8	Total 8	O 8	0	0
6	M	15	Total 15	O 15	0	0
6	I	10	Total 10	O 10	0	0



4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	106.84Å 106.84Å 185.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.29 – 2.05 46.29 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.29-2.05) 93.5 (46.29-2.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.05Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.158 , 0.209 0.158 , 0.208	Depositor DCC
R_{free} test set	3998 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	37.9	Xtrriage
Anisotropy	0.109	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.487 for -h,-k,l	Xtrriage
Reported twinning fraction	0.497 for -h,-k,l	Depositor
Outliers	0 of 75882 reflections	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6690	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: PCA, NAG, 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	L	0.42	0/1698	0.58	0/2306
1	M	0.46	0/1698	0.59	0/2306
2	H	0.41	0/1674	0.59	0/2291
2	I	0.42	0/1674	0.59	0/2291
All	All	0.43	0/6744	0.58	0/9194

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	L	1662	0	1575	62	0
1	M	1662	0	1575	42	0
2	H	1635	0	1587	47	2
2	I	1635	0	1587	58	2
3	H	28	0	25	2	0
4	H	5	0	0	0	0
4	I	5	0	0	0	0
5	I	14	0	13	0	0
6	H	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	10	0	0	1	0
6	L	11	0	0	0	0
6	M	15	0	0	0	0
All	All	6690	0	6362	204	2

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 16.

The worst 5 of 204 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:L:83:LEU:HD11	1:L:106:ILE:HD11	1.60	0.81
1:M:151:ASP:HA	1:M:191:SER:HB3	1.70	0.72
2:H:196:ASN:ND2	2:H:207:ASP:OD1	2.26	0.68
2:H:11:LEU:HD21	2:H:146:PHE:CE2	2.30	0.67
1:L:83:LEU:HD11	1:L:106:ILE:CD1	2.26	0.66

All (2) 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)
2:H:98:TYR:OH	2:I:53:GLU:OE1[5_555]	2.13	0.07
2:H:53:GLU:OE1	2:I:98:TYR:OH[5_555]	2.15	0.05

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	L	211/214 (99%)	201 (95%)	10 (5%)	0	100 100
1	M	211/214 (99%)	205 (97%)	6 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	209/225 (93%)	203 (97%)	6 (3%)	0	100	100
2	I	209/225 (93%)	204 (98%)	5 (2%)	0	100	100
All	All	840/878 (96%)	813 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	L	191/192 (100%)	177 (93%)	14 (7%)	16	8
1	M	191/192 (100%)	177 (93%)	14 (7%)	16	8
2	H	184/193 (95%)	169 (92%)	15 (8%)	13	6
2	I	184/193 (95%)	171 (93%)	13 (7%)	17	9
All	All	750/770 (97%)	694 (92%)	56 (8%)	16	7

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	195	CYS
1	M	105	GLU
2	I	140	CYS
2	H	206	VAL
2	H	211	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	137	ASN
2	I	171	GLN
1	M	190	ASN
2	H	164	HIS
2	I	81	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
2	PCA	H	1	2	8,8,9	2.27	3 (37%)	9,10,12	1.95	4 (44%)
2	PCA	I	1	2	8,8,9	1.86	2 (25%)	9,10,12	2.03	5 (55%)

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
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1
2	PCA	I	1	2	-	0/0/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	PCA	CA-C	2.16	1.53	1.50
2	I	1	PCA	CA-N	2.58	1.49	1.46
2	H	1	PCA	CA-N	3.98	1.51	1.46
2	I	1	PCA	CD-N	4.09	1.46	1.34
2	H	1	PCA	CD-N	4.44	1.47	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1	PCA	CA-N-CD	-2.93	103.55	113.58
2	H	1	PCA	OE-CD-CG	-2.85	121.62	126.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	PCA	CA-N-CD	-2.75	104.15	113.58
2	I	1	PCA	OE-CD-CG	-2.70	121.88	126.86
2	I	1	PCA	CB-CA-C	-2.68	109.01	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

2 carbohydrates 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
3	NAG	H	301	3,2	14,14,15	0.59	0	15,19,21	0.85	0
3	NAG	H	302	3	14,14,15	0.66	0	15,19,21	0.90	1 (6%)

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
3	NAG	H	301	3,2	-	0/6/23/26	0/1/1/1
3	NAG	H	302	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	302	NAG	C2-N2-C7	-2.48	119.33	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	301	NAG	2	0
3	H	302	NAG	2	0

5.6 Ligand geometry [i](#)

3 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	H	303	-	4,4,4	0.18	0	6,6,6	0.23	0
5	NAG	I	301	2	14,14,15	0.53	0	15,19,21	0.80	1 (6%)
4	SO4	I	302	-	4,4,4	0.19	0	6,6,6	0.15	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	SO4	H	303	-	-	0/0/0/0	0/0/0/0
5	NAG	I	301	2	-	0/6/23/26	0/1/1/1
4	SO4	I	302	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	I	301	NAG	C1-O5-C5	2.36	115.42	112.17

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	L	213/214 (99%)	-0.20	2 (0%) 84 86	34, 55, 96, 130	0
1	M	213/214 (99%)	-0.34	1 (0%) 90 92	31, 46, 84, 107	0
2	H	212/225 (94%)	-0.35	0 100 100	31, 52, 75, 104	0
2	I	212/225 (94%)	-0.37	0 100 100	32, 48, 71, 95	0
All	All	850/878 (96%)	-0.31	3 (0%) 92 93	31, 51, 84, 130	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	205	ILE	3.5
1	L	202	THR	2.4
1	M	1	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	PCA	I	1	8/9	0.98	0.11	-	55,65,70,78	0
2	PCA	H	1	8/9	0.96	0.12	-	68,72,74,77	0

6.3 Carbohydrates [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(Å ²)	Q<0.9
3	NAG	H	302	14/15	0.89	0.19	-	93,106,114,119	0
3	NAG	H	301	14/15	0.93	0.11	-	66,76,87,99	0

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(Å ²)	Q<0.9
4	SO4	H	303	5/5	0.97	0.10	0.96	77,85,87,91	0
4	SO4	I	302	5/5	0.99	0.09	-1.08	72,73,77,80	0
5	NAG	I	301	14/15	0.88	0.19	-	106,126,131,135	0

6.5 Other polymers [i](#)

There are no such residues in this entry.