



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 10, 2014 – 12:23 PM EDT

PDB ID : 4LIQ
Title : Structure of the extracellular domain of human CSF-1 receptor in complex with the Fab fragment of RG7155
Authors : Benz, J.; Gorr, I.H.; Hertenberger, H.; Ries, C.H.
Deposited on : 2013-07-03
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

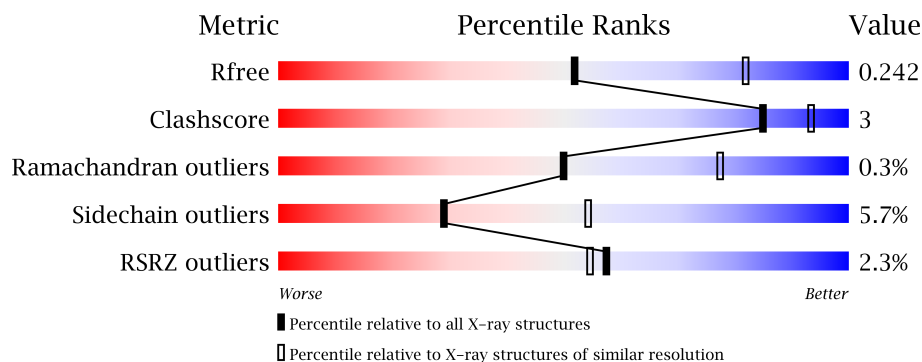
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23161
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	E	553	
2	H	223	
3	L	213	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	NAG	E	807	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7268 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Macrophage colony-stimulating factor 1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	469	Total	C	N	O	S	0	0	0
			3671	2336	632	688	15			

- Molecule 2 is a protein called Fab fragment RG7155 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	212	Total	C	N	O	S	0	1	0
			1594	1003	266	318	7			

- Molecule 3 is a protein called Fab fragment RG7155 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1643	1027	274	336	6			

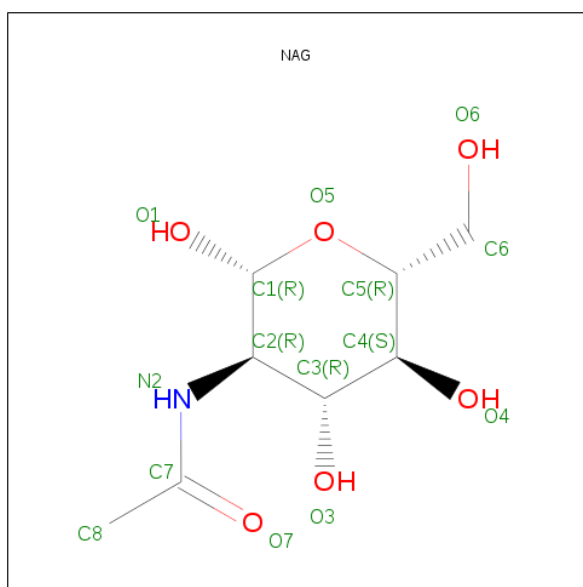
- Molecule 4 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

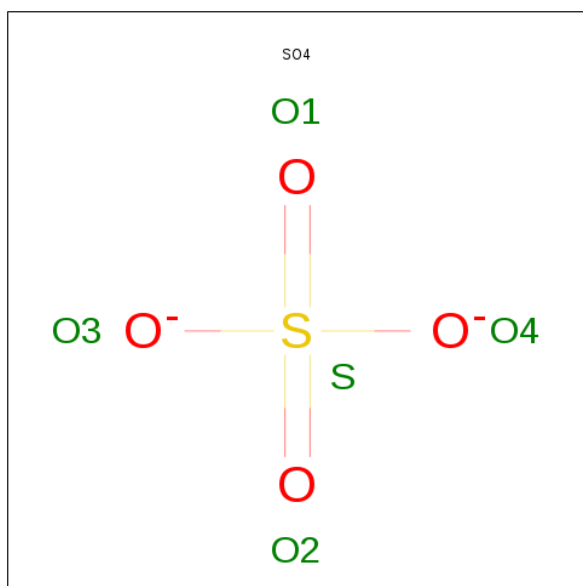
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 7 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	139	Total 139	O 139	0	0
8	H	72	Total 72	O 72	0	0
8	L	57	Total 57	O 57	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.17Å 113.58Å 146.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.07 – 2.60 49.29 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.07-2.60) 100.0 (49.29-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.186 , 0.237 0.191 , 0.242	Depositor DCC
R_{free} test set	2144 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 42980 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7268	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	E	0.47	0/3769	0.72	0/5148
2	H	0.46	0/1633	0.71	0/2228
3	L	0.46	0/1679	0.72	0/2280
All	All	0.47	0/7081	0.72	0/9656

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3671	0	3563	30	0
2	H	1594	0	1560	4	0
3	L	1643	0	1586	4	0
4	E	49	0	43	2	0
5	E	24	0	22	0	0
6	E	14	0	13	0	0
7	L	5	0	0	0	0
8	E	139	0	0	0	0
8	H	72	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	57	0	0	0	0
All	All	7268	0	6787	38	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (38) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:347:PRO:HA	1:E:350:LYS:HD3	1.50	0.94
1:E:323:VAL:HG21	1:E:381:PHE:CD1	2.39	0.58
1:E:75:THR:HG22	1:E:77:GLN:H	1.68	0.58
3:L:18:ARG:HG3	3:L:76:SER:HA	1.84	0.58
1:E:54:PRO:HB2	1:E:57:HIS:CD2	2.39	0.57
1:E:399:ARG:HB3	1:E:491:VAL:HG21	1.87	0.56
1:E:324:MET:HG3	1:E:363:THR:HG22	1.87	0.56
1:E:269:ASP:H	1:E:272:HIS:HD2	1.54	0.55
2:H:202:ASN:HD21	2:H:209:LYS:HE2	1.72	0.54
1:E:336:TRP:CD1	1:E:351:LEU:HD13	2.43	0.54
1:E:138:VAL:HG13	1:E:162:PHE:CZ	2.45	0.51
1:E:332:GLN:HG2	1:E:385:ASN:HA	1.92	0.51
3:L:8:PRO:HG3	3:L:11:LEU:HD13	1.92	0.51
3:L:36:TYR:HE2	3:L:89:GLN:HE21	1.60	0.50
1:E:48:VAL:HG12	1:E:86:GLU:HG2	1.92	0.50
1:E:109:ASN:HB3	1:E:128:LEU:HB2	1.93	0.50
1:E:138:VAL:HG13	1:E:162:PHE:HZ	1.77	0.49
1:E:118:PHE:HB3	1:E:198:VAL:HG22	1.95	0.48
1:E:436:GLY:O	1:E:482:THR:HG22	2.13	0.48
1:E:55:SER:HA	1:E:57:HIS:H	1.78	0.48
2:H:122:PRO:HB3	2:H:148:TYR:HB3	1.96	0.47
1:E:477:LEU:HD12	1:E:500:PRO:HG3	1.96	0.47
3:L:2:ILE:HG12	3:L:27:GLU:HG2	1.97	0.47
1:E:269:ASP:N	1:E:272:HIS:HD2	2.13	0.46
1:E:346:GLN:HG2	4:E:801:NAG:H81	1.99	0.45
1:E:408:TRP:HZ3	1:E:474:VAL:HG13	1.80	0.45
1:E:313:VAL:HG13	1:E:317:GLU:HB2	2.00	0.43
1:E:431:TRP:HB2	1:E:450:TRP:HB2	2.02	0.42
2:H:36:TRP:CE2	2:H:80:MET:HB2	2.55	0.42
1:E:406:VAL:HG23	1:E:496:TRP:HB3	2.02	0.41
1:E:303:LEU:HD13	1:E:390:ARG:HB2	2.00	0.41
1:E:346:GLN:HG2	4:E:801:NAG:C8	2.50	0.41
1:E:111:LEU:HB2	1:E:126:PRO:HB2	2.03	0.41
1:E:169:PHE:CD1	1:E:197:LYS:HG3	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:191:SER:HA	2:H:194:THR:HG23	2.02	0.41
1:E:419:CYS:HB2	1:E:431:TRP:CH2	2.56	0.41
1:E:338:TYR:CZ	1:E:340:GLY:HA3	2.55	0.40
1:E:142:ARG:HD3	1:E:149:MET:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	E	459/553 (83%)	439 (96%)	18 (4%)	2 (0%)	43	72
2	H	209/223 (94%)	203 (97%)	6 (3%)	0	100	100
3	L	211/213 (99%)	199 (94%)	11 (5%)	1 (0%)	38	67
All	All	879/989 (89%)	841 (96%)	35 (4%)	3 (0%)	50	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	340	GLY
1	E	56	PRO
3	L	137	ASN

5.3.2 Protein sidechains ⓘ

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	E	410/474 (86%)	385 (94%)	25 (6%)	26	50
2	H	180/190 (95%)	174 (97%)	6 (3%)	50	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	188/188 (100%)	175 (93%)	13 (7%)	22	42
All	All	778/852 (91%)	734 (94%)	44 (6%)	29	54

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	41	ARG
1	E	55	SER
1	E	86	GLU
1	E	133	VAL
1	E	138	VAL
1	E	148	LEU
1	E	149	MET
1	E	205	LEU
1	E	216	ARG
1	E	224	CYS
1	E	256	ARG
1	E	287	HIS
1	E	297	GLU
1	E	324	MET
1	E	326	GLU
1	E	332	GLN
1	E	346	GLN
1	E	351	LEU
1	E	437	HIS
1	E	440	ARG
1	E	461	GLU
1	E	474	VAL
1	E	475	GLU
1	E	478	GLU
1	E	499	ILE
2	H	25	SER
2	H	35	SER
2	H	43	GLN
2	H	172	VAL
2	H	194	THR
2	H	202	ASN
3	L	1	ASP
3	L	10	SER
3	L	19	VAL
3	L	34	SER
3	L	53	ASN

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Mol	Chain	Res	Type
3	L	67	SER
3	L	89	GLN
3	L	104	GLU
3	L	105	ILE
3	L	113	SER
3	L	144	LYS
3	L	166	ASP
3	L	189	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	57	HIS
1	E	253	HIS
1	E	272	HIS
1	E	320	ASN
1	E	469	GLN
2	H	202	ASN
3	L	89	GLN
3	L	209	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

6 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
4	NAG	E	801	1,4	12,14,15	0.42	0	15,19,21	0.54	0
4	FUC	E	802	4	9,10,11	0.43	0	10,14,16	0.52	0
4	NAG	E	803	4	12,14,15	0.42	0	15,19,21	0.52	0
4	BMA	E	804	4	10,11,12	0.42	0	11,15,17	0.44	0
5	NAG	E	805	1,5	12,14,15	0.37	0	15,19,21	0.64	0
5	FUC	E	806	5	9,10,11	0.41	0	10,14,16	0.38	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	NAG	E	801	1,4	-	0/6/23/26	0/1/1/1
4	FUC	E	802	4	-	0/0/17/20	0/1/1/1
4	NAG	E	803	4	-	0/6/23/26	0/1/1/1
4	BMA	E	804	4	-	0/2/19/22	0/1/1/1
5	NAG	E	805	1,5	-	0/6/23/26	0/1/1/1
5	FUC	E	806	5	-	0/0/17/20	0/1/1/1

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.

5.6 Ligand geometry ⓘ

2 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
6	NAG	E	807	1	12,14,15	0.41	0	15,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	L	301	-	4,4,4	0.15	0	6,6,6	0.13	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
6	NAG	E	807	1	-	0/6/23/26	0/1/1/1
7	SO4	L	301	-	-	0/0/0/0	0/0/0/0

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.

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, 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	E	469/553 (84%)	0.08	20 (4%) 34 30	34, 57, 98, 135	0
2	H	212/223 (95%)	-0.18	1 (0%) 88 90	32, 50, 80, 119	0
3	L	213/213 (100%)	-0.19	0 100 100	31, 50, 71, 113	0
All	All	894/989 (90%)	-0.05	21 (2%) 57 54	31, 52, 91, 135	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	56	PRO	5.6
1	E	54	PRO	4.8
1	E	61	TYR	4.6
1	E	20	ILE	3.9
1	E	479	HIS	3.8
1	E	53	PRO	3.3
1	E	68	ILE	3.2
1	E	52	GLY	3.2
1	E	500	PRO	3.1
1	E	26	SER	2.8
1	E	478	GLU	2.7
2	H	131	SER	2.6
1	E	170	ILE	2.6
1	E	444	ALA	2.6
1	E	169	PHE	2.5
1	E	58	TRP	2.5
1	E	408	TRP	2.4
1	E	151	HIS	2.3
1	E	43	VAL	2.2
1	E	86	GLU	2.1
1	E	41	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	E	805	14/15	0.15	0.36	58,64,69,73	0
5	FUC	E	806	10/11	0.13	-0.53	61,64,68,69	0
4	FUC	E	802	10/11	0.12	-0.75	66,67,68,70	0
4	NAG	E	801	14/15	0.12	-1.10	57,62,66,69	0
4	NAG	E	803	14/15	0.14	-4.60	72,77,82,88	0
4	BMA	E	804	11/12	0.17	-	92,99,102,103	0

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	NAG	E	807	14/15	0.28	5.64	100,102,113,113	0
7	SO4	L	301	5/5	0.17	0.02	105,107,107,109	0

6.5 Other polymers ⓘ

There are no such residues in this entry.