WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2020 – 12:26 PM BST

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)

The following versions of software and data (see references (i)) 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	:	2.13.1
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)	:	2.13.1

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 2.60 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.
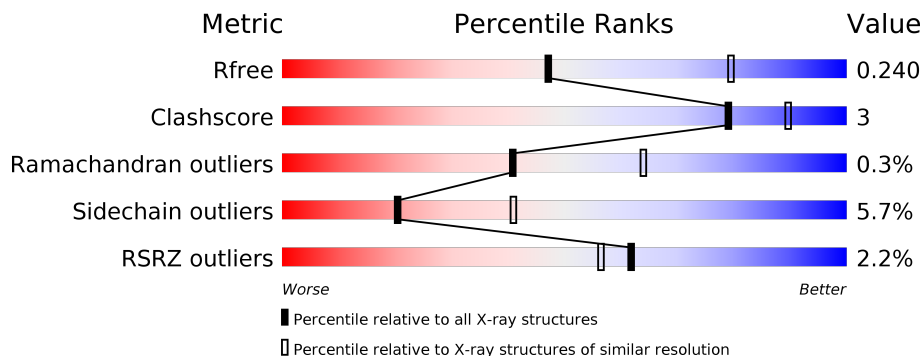
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	E	553	3% / 73% / 10% · 15%
2	H	223	90% · · 5%
3	L	213	90% 9%
4	A	4	25% 75%
5	B	2	100%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7268 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 Macrophage colony-stimulating factor 1 receptor.

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

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	MET	-	expression tag	UNP P07333
E	0	GLY	-	expression tag	UNP P07333
E	1	SER	-	expression tag	UNP P07333
E	513	ALA	-	expression tag	UNP P07333
E	514	ALA	-	expression tag	UNP P07333
E	515	ALA	-	expression tag	UNP P07333
E	516	LEU	-	expression tag	UNP P07333
E	517	GLU	-	expression tag	UNP P07333
E	518	VAL	-	expression tag	UNP P07333
E	519	LEU	-	expression tag	UNP P07333
E	520	PHE	-	expression tag	UNP P07333
E	521	GLN	-	expression tag	UNP P07333
E	522	GLY	-	expression tag	UNP P07333
E	523	PRO	-	expression tag	UNP P07333
E	524	GLY	-	expression tag	UNP P07333
E	525	THR	-	expression tag	UNP P07333
E	526	HIS	-	expression tag	UNP P07333
E	527	HIS	-	expression tag	UNP P07333
E	528	HIS	-	expression tag	UNP P07333
E	529	HIS	-	expression tag	UNP P07333
E	530	HIS	-	expression tag	UNP P07333
E	531	HIS	-	expression tag	UNP P07333
E	532	HIS	-	expression tag	UNP P07333
E	533	HIS	-	expression tag	UNP P07333
E	534	HIS	-	expression tag	UNP P07333
E	535	HIS	-	expression tag	UNP P07333
E	536	ILE	-	expression tag	UNP P07333

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Chain	Residue	Modelled	Actual	Comment	Reference
E	537	GLY	-	expression tag	UNP P07333
E	538	LEU	-	expression tag	UNP P07333
E	539	ASN	-	expression tag	UNP P07333
E	540	ASP	-	expression tag	UNP P07333
E	541	ILE	-	expression tag	UNP P07333
E	542	PHE	-	expression tag	UNP P07333
E	543	GLU	-	expression tag	UNP P07333
E	544	ALA	-	expression tag	UNP P07333
E	545	GLN	-	expression tag	UNP P07333
E	546	LYS	-	expression tag	UNP P07333
E	547	ILE	-	expression tag	UNP P07333
E	548	GLU	-	expression tag	UNP P07333
E	549	TRP	-	expression tag	UNP P07333
E	550	HIS	-	expression tag	UNP P07333
E	551	GLU	-	expression tag	UNP P07333

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

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

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

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

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.
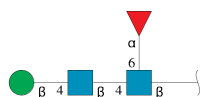
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	A	4	49	28	2	19	0	0	0

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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: O_4S).

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

- 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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Macrophage colony-stimulating factor 1 receptor
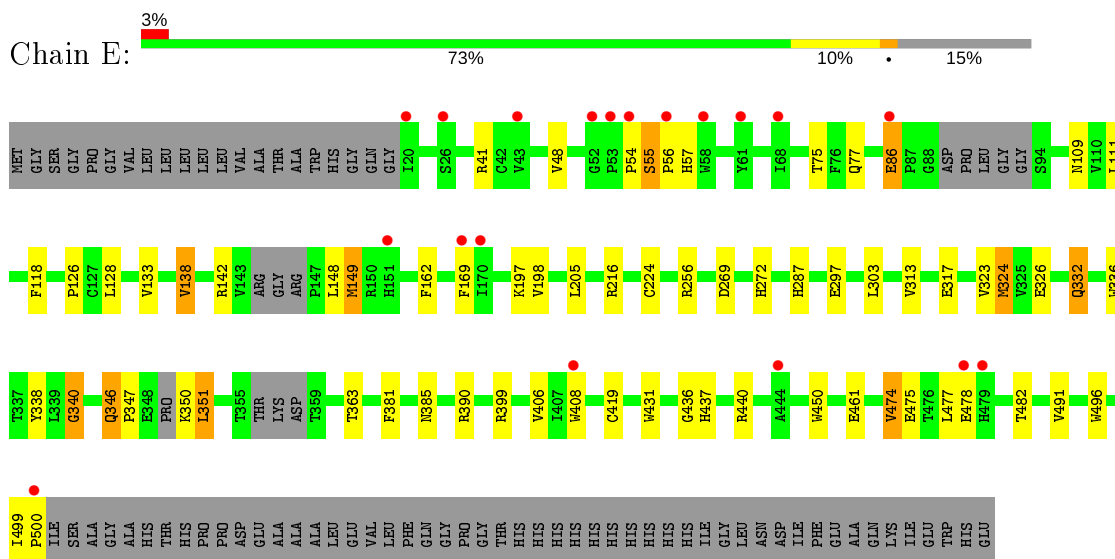
Chain E:

• Molecule 2: Fab fragment RG7155 heavy chain
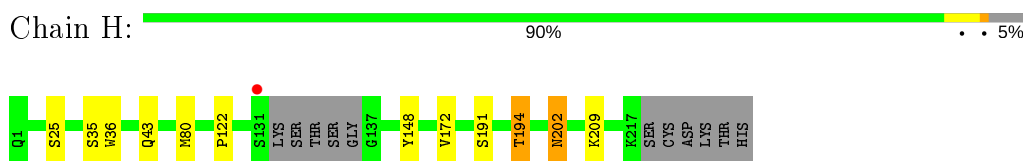
Chain H:

• Molecule 3: Fab fragment RG7155 light chain

Chain L:
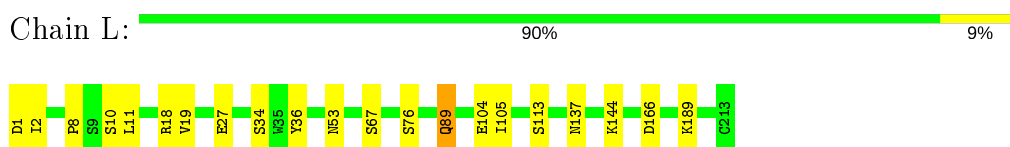
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:

NAG1 NAG2 BMA3 FUC4

- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

100%

NAG1 FUC2

4 Data and refinement statistics (i)

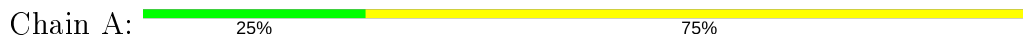| Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.17Å 113.58Å 146.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.07 – 2.60	Depositor
	49.29 – 2.60	EDS
% Data completeness	100.0 (38.07-2.60)	Depositor
(in resolution range)	100.0 (49.29-2.60)	EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.95 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.186 , 0.237	Depositor
	0.190 , 0.240	DCC
R_{free} test set	2144 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	55.1	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.6	EDS
L-test for twinning[2]	$<|L|>=0.48$, $<L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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[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 (i)

5.1 Standard geometry (i)

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 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	E	3671	0	3563	30	0
2	H	1594	0	1560	4	0
3	L	1643	0	1586	4	0
4	A	49	0	43	2	0
5	B	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
8	L	57	0	0	0	0
All	All	7268	0	6787	38	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 3.

All (38) 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: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:A:1: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:A:1: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:ARG:HD3	1:E:149:MET:HA	2.03	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	E	459/553 (83%)	439 (96%)	18 (4%)	2 (0%)	34	57
2	H	209/223 (94%)	203 (97%)	6 (3%)	0	100	100
3	L	211/213 (99%)	199 (94%)	11 (5%)	1 (0%)	29	52
All	All	879/989 (89%)	841 (96%)	35 (4%)	3 (0%)	41	64

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 (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	E	410/474 (86%)	385 (94%)	25 (6%)	18	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	180/190 (95%)	174 (97%)	6 (3%)	38	64
3	L	188/188 (100%)	175 (93%)	13 (7%)	15	31
All	All	778/852 (91%)	734 (94%)	44 (6%)	20	41

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

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Mol	Chain	Res	Type
3	L	34	SER
3	L	53	ASN
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 (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)

6 monosaccharides 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	A	1	1,4	14,14,15	0.37	0	17,19,21	0.66	0
4	NAG	A	2	4	14,14,15	0.31	0	17,19,21	1.03	2 (11%)
4	BMA	A	3	4	11,11,12	0.41	0	15,15,17	0.82	1 (6%)
4	FUC	A	4	4	10,10,11	0.52	0	14,14,16	0.79	0
5	NAG	B	1	1,5	14,14,15	0.32	0	17,19,21	0.83	1 (5%)
5	FUC	B	2	5	10,10,11	0.45	0	14,14,16	0.98	1 (7%)

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	A	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1
4	BMA	A	3	4	-	0/2/19/22	0/1/1/1
4	FUC	A	4	4	-	-	0/1/1/1
5	NAG	B	1	1,5	-	0/6/23/26	0/1/1/1
5	FUC	B	2	5	-	-	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	2	FUC	C1-O5-C5	3.12	119.85	112.78
4	A	3	BMA	C1-O5-C5	2.59	115.70	112.19
4	A	2	NAG	O5-C1-C2	2.52	115.26	111.29
5	B	1	NAG	C1-O5-C5	2.47	115.54	112.19
4	A	2	NAG	C1-C2-N2	-2.26	106.63	110.49

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2	NAG	O5-C5-C6-O6
4	A	2	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	NAG	2	0

5.6 Ligand geometry (i)

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	14,14,15	0.37	0	17,19,21	0.41	0
7	SO4	L	301	-	4,4,4	0.20	0	6,6,6	0.07	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

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 (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(Å²)	Q<0.9
1	E	469/553 (84%)	0.06	19 (4%)	37	30	34, 57, 98, 135	0
2	H	212/223 (95%)	-0.19	1 (0%)	91	89	32, 50, 80, 119	0
3	L	213/213 (100%)	-0.23	0	100	100	31, 50, 71, 113	0
All	All	894/989 (90%)	-0.07	20 (2%)	62	56	31, 52, 91, 135	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	56	PRO	6.2
1	E	20	ILE	5.2
1	E	54	PRO	4.9
1	E	61	TYR	4.1
1	E	479	HIS	3.6
1	E	478	GLU	3.0
2	H	131	SER	2.9
1	E	53	PRO	2.8
1	E	26	SER	2.8
1	E	151	HIS	2.7
1	E	52	GLY	2.6
1	E	444	ALA	2.5
1	E	58	TRP	2.4
1	E	170	ILE	2.3
1	E	169	PHE	2.2
1	E	500	PRO	2.2
1	E	43	VAL	2.2
1	E	68	ILE	2.2
1	E	408	TRP	2.1
1	E	86	GLU	2.1

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)

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	BMA	A	3	11/12	0.76	0.18	92,99,102,103	0
5	NAG	B	1	14/15	0.95	0.16	58,64,69,73	0
4	NAG	A	2	14/15	0.96	0.14	72,77,82,88	0
4	NAG	A	1	14/15	0.96	0.14	57,62,66,69	0
4	FUC	A	4	10/11	0.96	0.12	66,67,68,70	0
5	FUC	B	2	10/11	0.97	0.14	61,64,68,69	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. 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
6	NAG	E	807	14/15	0.81	0.28	100,102,113,113	0
7	SO4	L	301	5/5	0.96	0.18	105,107,107,109	0

6.5 Other polymers (i)

There are no such residues in this entry.