Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:34 PM GMT

PDB ID	:	4UV7
Title	:	The complex structure of extracellular domain of EGFR and GC1118A
Authors	:	Yoo, J.H.; Cho, H.S.
Deposited on	:	2014-08-05
Resolution	:	2.10 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:

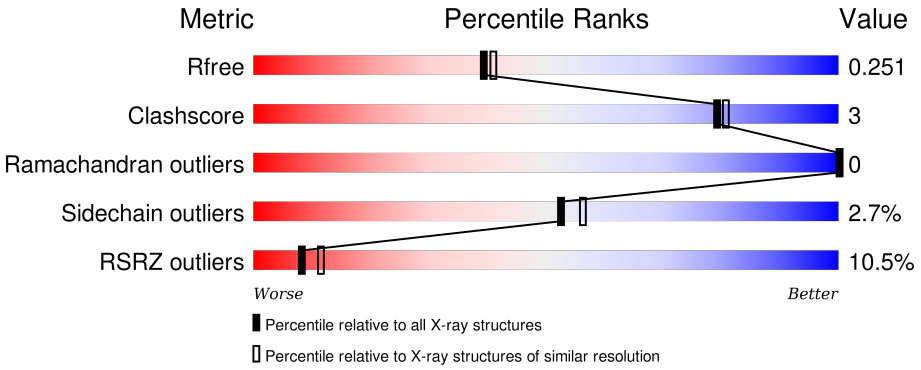
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 <=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	621	13% 87% 8%
2	H	225	8% 84% 11%
3	L	219	5% 88% 9%

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
6	NAG	A	4201	-	-	-	X
6	NAG	A	5441	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8385 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 EPIDERMAL GROWTH FACTOR RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	0	0
			4583	2829	818	879	57			

- Molecule 2 is a protein called GC1118A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1640	1034	279	321	6			

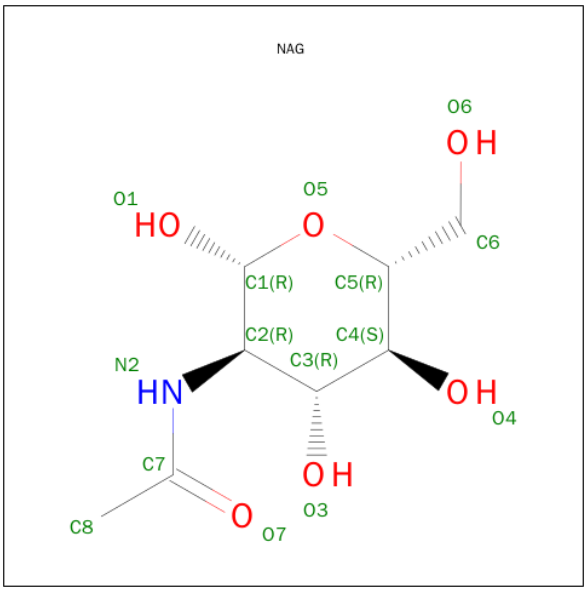
- Molecule 3 is a protein called GC1118A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	216	Total	C	N	O	S	0	0	0
			1683	1056	288	333	6			

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		

- 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	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is water.

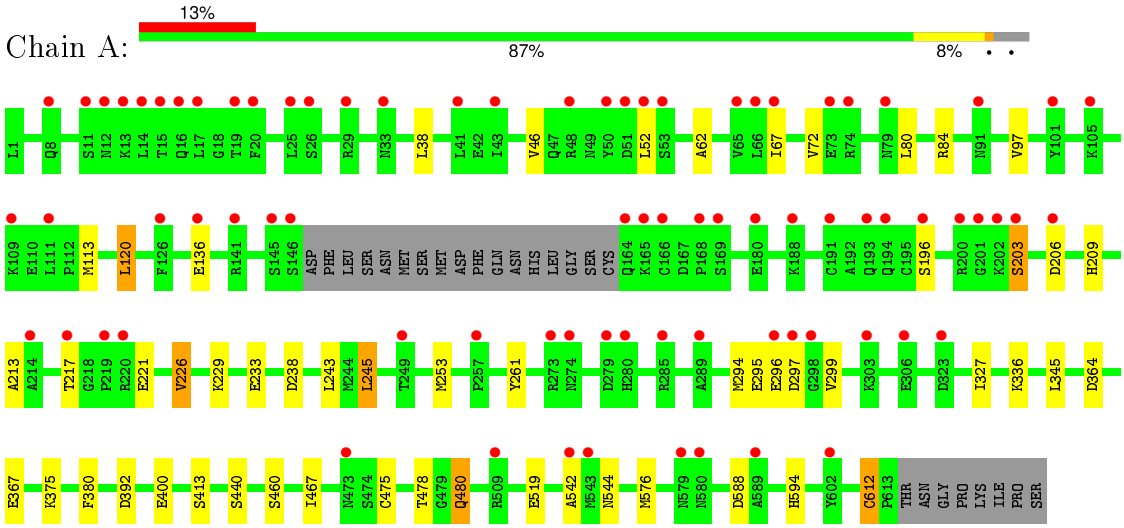
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	158	Total	O	0	0
			158	158		
7	H	73	Total	O	0	0
			73	73		
7	L	139	Total	O	0	0
			139	139		

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 errors 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.

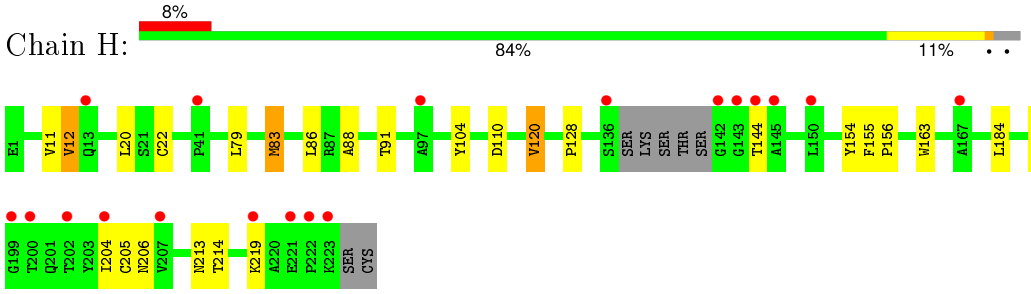
- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR

Chain A:



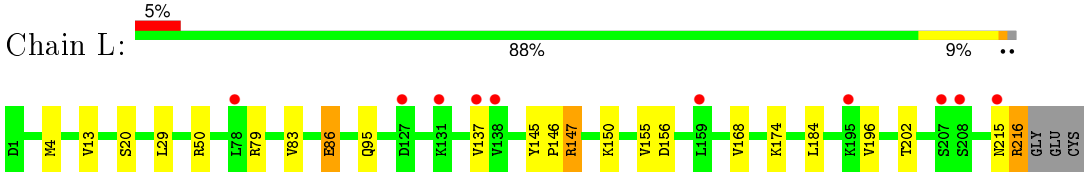
- Molecule 2: GC1118A

Chain H:



- Molecule 3: GC1118A

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.39Å 84.17Å 97.79Å 90.00° 97.11° 90.00°	Depositor
Resolution (Å)	19.75 – 2.10 19.75 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.75-2.10) 99.8 (19.75-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.01 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.202 , 0.248 0.208 , 0.251	Depositor DCC
R_{free} test set	3710 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 73613 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8385	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: BMA, 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	A	0.69	0/4671	0.73	2/6319 (0.0%)
2	H	0.85	0/1681	0.79	2/2287 (0.1%)
3	L	0.91	1/1724 (0.1%)	0.80	3/2346 (0.1%)
All	All	0.78	1/8076 (0.0%)	0.76	7/10952 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	20	SER	CB-OG	-5.71	1.34	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	110	ASP	CB-CG-OD1	5.96	123.66	118.30
3	L	50	ARG	NE-CZ-NH1	5.76	123.18	120.30
3	L	147	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	612	CYS	CA-CB-SG	-5.52	104.07	114.00
2	H	83	MET	CG-SD-CE	-5.21	91.87	100.20
1	A	392	ASP	CB-CG-OD1	5.16	122.94	118.30
3	L	147	ARG	NE-CZ-NH1	5.06	122.83	120.30

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	4583	0	4428	26	0
2	H	1640	0	1592	13	0
3	L	1683	0	1630	13	0
4	A	39	0	34	1	0
5	A	14	0	13	1	0
6	A	56	0	50	2	0
7	A	158	0	0	0	0
7	H	73	0	0	0	0
7	L	139	0	0	2	0
All	All	8385	0	7747	55	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 (55) 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:91:THR:HG22	2:H:120:VAL:H	1.38	0.88
1:A:213:ALA:HB3	1:A:226:VAL:HG23	1.71	0.73
1:A:542:ALA:O	1:A:544:ASN:ND2	2.21	0.73
1:A:475:CYS:O	1:A:478:THR:HG22	1.90	0.72
3:L:13:VAL:HG11	3:L:83:VAL:HG21	1.76	0.68
1:A:327:ILE:HD11	1:A:345:LEU:HD22	1.79	0.64
6:A:5441:NAG:O3	6:A:5442:NAG:O5	2.16	0.63
3:L:150:LYS:HB3	3:L:202:THR:HB	1.80	0.63
1:A:375:LYS:NZ	1:A:400:GLU:OE2	2.27	0.58
2:H:204:ILE:HG12	2:H:219:LYS:HG2	1.86	0.57
3:L:137:VAL:HG13	3:L:184:LEU:HB3	1.86	0.56
3:L:215:ASN:O	3:L:216:ARG:HB2	2.06	0.56
1:A:364:ASP:HB3	1:A:367:GLU:HG3	1.88	0.55
1:A:336:LYS:HG2	5:A:3371:NAG:H82	1.87	0.55
1:A:380:PHE:CD1	1:A:413:SER:HA	2.42	0.54
2:H:194:PRO:HB2	2:H:197:SER:HB2	1.90	0.53
3:L:13:VAL:HG11	3:L:83:VAL:CG2	2.41	0.51
1:A:229:LYS:NZ	1:A:238:ASP:O	2.40	0.51
1:A:67:ILE:O	1:A:97:VAL:HA	2.12	0.49
2:H:11:VAL:HG21	2:H:156:PRO:HG3	1.94	0.49
1:A:243:LEU:HD21	1:A:261:TYR:CE2	2.48	0.48
6:A:5441:NAG:H62	6:A:5442:NAG:H82	1.96	0.48
3:L:196:VAL:HG22	3:L:215:ASN:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:VAL:O	2:H:120:VAL:HA	2.14	0.47
1:A:209:HIS:CD2	1:A:221:GLU:HG3	2.50	0.47
3:L:29:LEU:HD22	3:L:95:GLN:HG2	1.97	0.46
1:A:38:LEU:O	1:A:62:ALA:HB3	2.16	0.46
2:H:163:TRP:CH2	2:H:205:CYS:HB3	2.51	0.46
1:A:233:GLU:OE1	1:A:233:GLU:HA	2.16	0.45
3:L:155:VAL:O	3:L:156:ASP:C	2.54	0.44
2:H:83:MET:HB3	2:H:86:LEU:HD21	2.00	0.44
1:A:440:SER:HA	1:A:467:ILE:O	2.18	0.44
1:A:588:ASP:OD2	1:A:594:HIS:NE2	2.40	0.44
1:A:46:VAL:HG11	1:A:52:LEU:HD11	1.99	0.44
2:H:128:PRO:HD2	2:H:214:THR:HG21	2.00	0.44
3:L:147:ARG:NH2	3:L:168:VAL:HG11	2.32	0.44
1:A:80:LEU:HD23	1:A:113:MET:CE	2.48	0.44
1:A:478:THR:HG23	1:A:480:GLN:NE2	2.33	0.43
2:H:128:PRO:HB3	2:H:154:TYR:HB3	2.00	0.43
3:L:4:MET:HE2	3:L:95:GLN:HB2	2.00	0.43
3:L:79:ARG:NE	7:L:2034:HOH:O	2.41	0.43
1:A:203:SER:HB3	1:A:206:ASP:OD1	2.19	0.43
2:H:155:PHE:HA	2:H:156:PRO:HA	1.86	0.43
1:A:296:GLU:HA	1:A:297:ASP:HA	1.75	0.42
1:A:84:ARG:HA	1:A:120:LEU:HB2	2.02	0.42
3:L:86:GLU:HB3	7:L:2090:HOH:O	2.19	0.42
1:A:245:LEU:O	1:A:253:MET:HA	2.20	0.41
2:H:22:CYS:HB3	2:H:79:LEU:HB3	2.02	0.41
1:A:67:ILE:HB	1:A:97:VAL:HB	2.02	0.41
2:H:88:ALA:O	2:H:91:THR:HG23	2.21	0.41
4:A:3282:NAG:H61	4:A:3283:BMA:C1	2.51	0.41
1:A:295:GLU:HA	1:A:299:VAL:O	2.21	0.41
2:H:20:LEU:HD11	2:H:83:MET:HE1	2.02	0.41
3:L:145:TYR:CG	3:L:146:PRO:HA	2.56	0.41
1:A:46:VAL:HG12	1:A:72:VAL:HB	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	A	592/621 (95%)	570 (96%)	22 (4%)	0	100	100
2	H	214/225 (95%)	208 (97%)	6 (3%)	0	100	100
3	L	214/219 (98%)	210 (98%)	4 (2%)	0	100	100
All	All	1020/1065 (96%)	988 (97%)	32 (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	A	519/542 (96%)	506 (98%)	13 (2%)	55	59
2	H	180/187 (96%)	172 (96%)	8 (4%)	35	33
3	L	192/194 (99%)	189 (98%)	3 (2%)	70	76
All	All	891/923 (96%)	867 (97%)	24 (3%)	52	56

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

Mol	Chain	Res	Type
1	A	120	LEU
1	A	136	GLU
1	A	196	SER
1	A	203	SER
1	A	217	THR
1	A	226	VAL
1	A	245	LEU
1	A	294	MET
1	A	460	SER
1	A	480	GLN
1	A	519	GLU

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Mol	Chain	Res	Type
1	A	576	MET
1	A	612	CYS
2	H	12	VAL
2	H	104	TYR
2	H	120	VAL
2	H	144	THR
2	H	184	LEU
2	H	193	VAL
2	H	206	ASN
2	H	213	ASN
3	L	86	GLU
3	L	174	LYS
3	L	216	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	544	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)

7 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	A	3281	1,4	14,14,15	1.04	1 (7%)	15,19,21	0.84	0
4	NAG	A	3282	4	14,14,15	0.62	0	15,19,21	0.93	0
4	BMA	A	3283	4	11,11,12	0.60	0	15,15,17	1.15	2 (13%)
6	NAG	A	4201	1,6	14,14,15	0.60	0	15,19,21	0.92	0
6	NAG	A	4202	6	14,14,15	0.52	0	15,19,21	0.60	0
6	NAG	A	5441	1,6	14,14,15	1.04	2 (14%)	15,19,21	1.44	2 (13%)
6	NAG	A	5442	6	14,14,15	1.18	1 (7%)	15,19,21	1.56	4 (26%)

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	3281	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	3282	4	-	0/6/23/26	0/1/1/1
4	BMA	A	3283	4	-	0/2/19/22	0/1/1/1
6	NAG	A	4201	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	4202	6	-	0/6/23/26	0/1/1/1
6	NAG	A	5441	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	5442	6	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3281	NAG	O5-C1	-3.31	1.38	1.43
6	A	5441	NAG	O5-C5	-2.36	1.38	1.43
6	A	5441	NAG	O5-C1	-2.35	1.39	1.43
6	A	5442	NAG	O5-C1	4.04	1.50	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	5441	NAG	O5-C5-C4	-3.09	105.01	110.13
6	A	5442	NAG	O7-C7-C8	-2.79	116.93	122.07
6	A	5441	NAG	O6-C6-C5	-2.27	103.72	111.30
6	A	5442	NAG	C1-O5-C5	-2.03	109.15	112.14
6	A	5442	NAG	O7-C7-N2	2.01	125.94	121.84
4	A	3283	BMA	O3-C3-C2	2.06	113.79	110.01
4	A	3283	BMA	C1-C2-C3	2.31	112.35	109.55
6	A	5442	NAG	C2-N2-C7	2.70	126.61	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3282	NAG	1	0
4	A	3283	BMA	1	0
6	A	5441	NAG	2	0
6	A	5442	NAG	2	0

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
5	NAG	A	3371	1	14,14,15	0.58	0	15,19,21	1.31	2 (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
5	NAG	A	3371	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	3371	NAG	O5-C5-C6	2.59	112.88	107.34
5	A	3371	NAG	C1-O5-C5	2.72	116.14	112.14

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
5	A	3371	NAG	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, 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	596/621 (95%)	0.66	79 (13%) 4 6	21, 50, 82, 108	0
2	H	218/225 (96%)	0.54	19 (8%) 13 17	21, 42, 75, 88	0
3	L	216/219 (98%)	0.29	10 (4%) 36 45	19, 33, 59, 75	0
All	All	1030/1065 (96%)	0.56	108 (10%) 8 11	19, 44, 78, 108	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	ASN	6.7
1	A	194	GLN	6.1
1	A	220	ARG	5.0
2	H	200	THR	4.9
1	A	43	ILE	4.7
2	H	223	LYS	4.5
1	A	509	ARG	4.4
1	A	12	ASN	4.3
3	L	127	ASP	4.3
2	H	41	PRO	4.2
2	H	143	GLY	4.2
2	H	219	LYS	4.2
1	A	17	LEU	4.2
1	A	67	ILE	4.1
1	A	191	CYS	4.1
1	A	15	THR	4.0
1	A	164	GLN	3.8
1	A	193	GLN	3.8
1	A	101	TYR	3.7
1	A	146	SER	3.6
1	A	542	ALA	3.5
1	A	166	CYS	3.5
1	A	33	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	202	LYS	3.5
1	A	543	MET	3.5
1	A	16	GLN	3.5
1	A	13	LYS	3.5
3	L	215	ASN	3.4
2	H	199	GLY	3.3
1	A	219	PRO	3.3
1	A	579	ASN	3.3
3	L	159	LEU	3.3
2	H	202	THR	3.3
1	A	165	LYS	3.3
1	A	249	THR	3.3
1	A	280	HIS	3.2
1	A	273	ARG	3.2
1	A	602	TYR	3.2
1	A	180	GLU	3.2
1	A	8	GLN	3.2
2	H	144	THR	3.1
1	A	289	ALA	3.1
1	A	11	SER	3.1
1	A	48	ARG	3.0
1	A	196	SER	3.0
1	A	25	LEU	3.0
1	A	50	TYR	2.9
1	A	297	ASP	2.9
1	A	66	LEU	2.9
2	H	142	GLY	2.9
2	H	136	SER	2.9
1	A	141	ARG	2.8
3	L	208	SER	2.8
1	A	20	PHE	2.8
1	A	296	GLU	2.8
1	A	298	GLY	2.8
1	A	168	PRO	2.7
1	A	41	LEU	2.7
1	A	145	SER	2.7
1	A	214	ALA	2.7
1	A	109	LYS	2.7
1	A	26	SER	2.7
1	A	206	ASP	2.6
1	A	14	LEU	2.6
1	A	51	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	473	ASN	2.5
1	A	53	SER	2.5
3	L	138	VAL	2.5
3	L	131	LYS	2.5
1	A	169	SER	2.5
2	H	97	ALA	2.4
1	A	65	VAL	2.4
1	A	303	LYS	2.4
3	L	207	SER	2.4
1	A	279	ASP	2.4
2	H	222	PRO	2.4
2	H	204	ILE	2.3
1	A	111	LEU	2.3
1	A	589	ALA	2.3
1	A	19	THR	2.2
1	A	52	LEU	2.2
2	H	167	ALA	2.2
2	H	150	LEU	2.2
1	A	74	ARG	2.2
1	A	79	ASN	2.2
1	A	91	ASN	2.2
3	L	78	LEU	2.2
3	L	137	VAL	2.2
1	A	188	LYS	2.2
1	A	203	SER	2.2
1	A	73	GLU	2.1
1	A	323	ASP	2.1
1	A	257	PRO	2.1
1	A	580	ASN	2.1
1	A	201	GLY	2.1
1	A	217	THR	2.1
3	L	195	LYS	2.1
1	A	285	ARG	2.0
1	A	306	GLU	2.0
1	A	126	PHE	2.0
1	A	105	LYS	2.0
1	A	136	GLU	2.0
2	H	221	GLU	2.0
2	H	145	ALA	2.0
1	A	29	ARG	2.0
1	A	200	ARG	2.0
2	H	13	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	207	VAL	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)

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, 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	LLDF	B-factors(Å^2)	Q<0.9
6	NAG	A	5441	14/15	0.82	0.28	2.57	57,66,76,78	0
6	NAG	A	4201	14/15	0.88	0.20	2.56	48,53,60,73	0
6	NAG	A	5442	14/15	0.74	0.36	1.00	58,64,68,69	0
4	NAG	A	3281	14/15	0.88	0.14	0.03	34,40,46,50	0
4	NAG	A	3282	14/15	0.88	0.23	-	43,54,68,81	0
6	NAG	A	4202	14/15	0.74	0.45	-	82,96,105,107	0
4	BMA	A	3283	11/12	0.59	0.39	-	80,92,108,111	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, 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	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	A	3371	14/15	0.85	0.34	-	58,66,84,91	0

6.5 Other polymers (i)

There are no such residues in this entry.