



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:54 AM GMT

PDB ID : 3CIG
Title : Crystal structure of mouse TLR3 ectodomain
Authors : Liu, L.; Botos, I.; Wang, Y.; Leonard, J.N.; Shiloach, J.; Segal, D.M.; Davies, D.R.
Deposited on : 2008-03-11
Resolution : 2.66 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

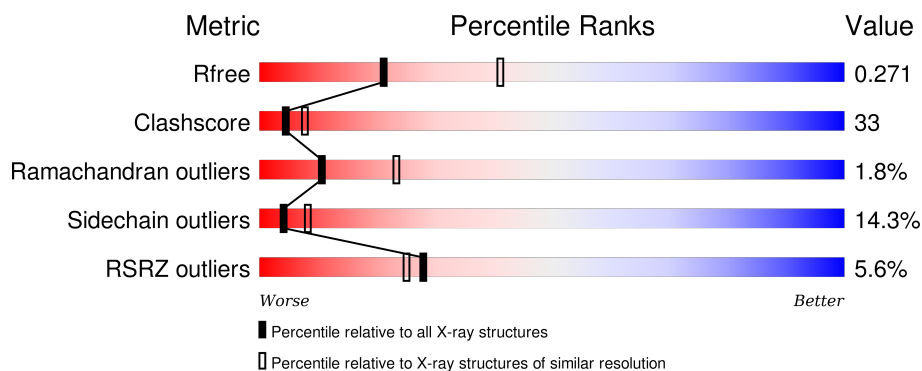
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	697	

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	NAG	A	2521	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 5736 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 Toll-like receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	663	Total	C	N	O	S	0	0	0
			5330	3404	908	1004	14			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	704	ASN	-	EXPRESSION TAG	UNP Q99MB1
A	705	LEU	-	EXPRESSION TAG	UNP Q99MB1
A	706	TYR	-	EXPRESSION TAG	UNP Q99MB1
A	707	PHE	-	EXPRESSION TAG	UNP Q99MB1
A	708	GLN	-	EXPRESSION TAG	UNP Q99MB1
A	709	GLY	-	EXPRESSION TAG	UNP Q99MB1
A	710	HIS	-	EXPRESSION TAG	UNP Q99MB1
A	711	HIS	-	EXPRESSION TAG	UNP Q99MB1
A	712	HIS	-	EXPRESSION TAG	UNP Q99MB1
A	713	HIS	-	EXPRESSION TAG	UNP Q99MB1
A	714	HIS	-	EXPRESSION TAG	UNP Q99MB1
A	715	HIS	-	EXPRESSION TAG	UNP Q99MB1
A	716	TRP	-	EXPRESSION TAG	UNP Q99MB1
A	717	SER	-	EXPRESSION TAG	UNP Q99MB1
A	718	HIS	-	EXPRESSION TAG	UNP Q99MB1
A	719	PRO	-	EXPRESSION TAG	UNP Q99MB1
A	720	GLN	-	EXPRESSION TAG	UNP Q99MB1
A	721	PHE	-	EXPRESSION TAG	UNP Q99MB1
A	722	GLU	-	EXPRESSION TAG	UNP Q99MB1
A	723	LYS	-	EXPRESSION TAG	UNP Q99MB1

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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

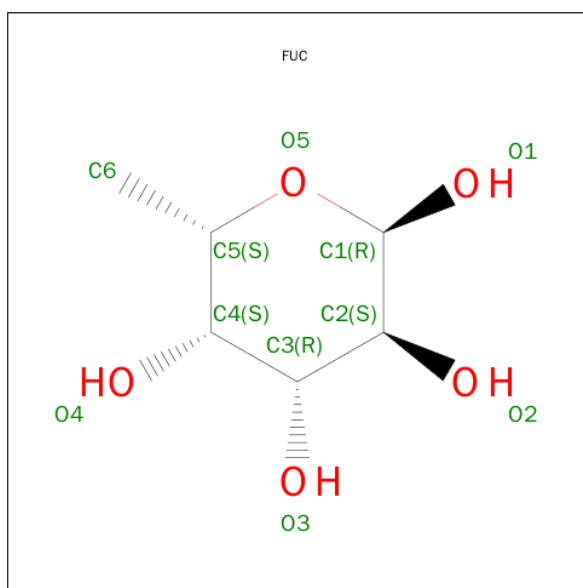
- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			38	22	2	14		

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

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

- Molecule 6 is SUGAR (ALPHA-L-FUCOSE) (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	5	Total	C	N	O	0	0
			61	34	2	25		

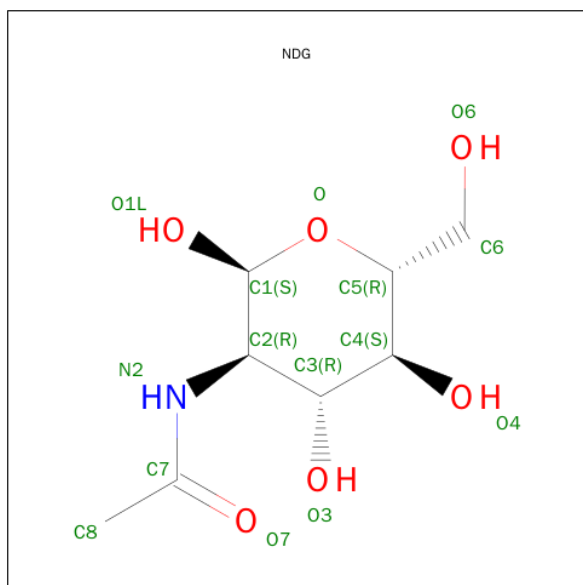
- Molecule 8 is a polymer of unknown type called SUGAR (4-MER).

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

- Molecule 9 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 10 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



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

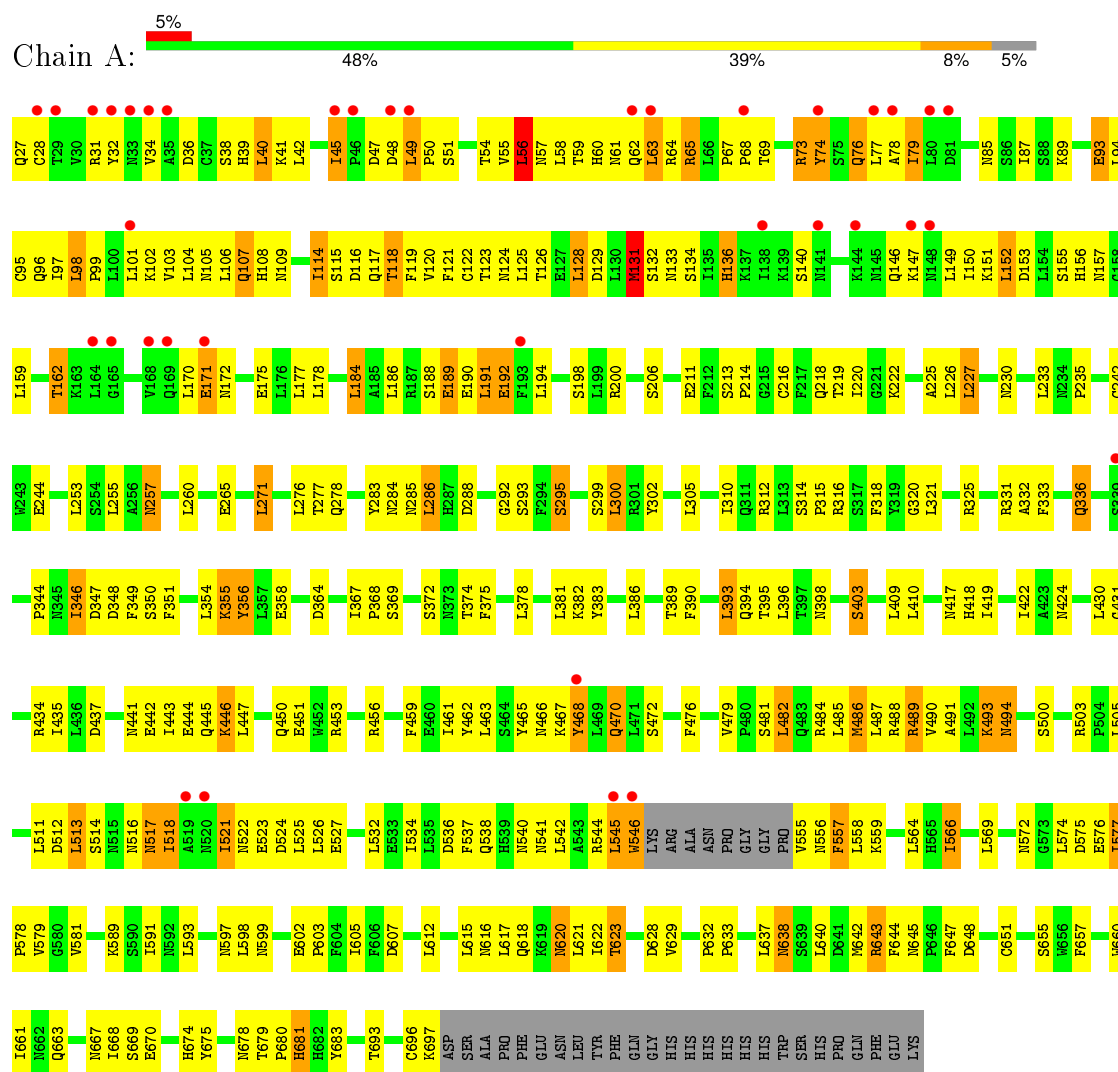
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	79	Total	O	0	0
			79	79		

3 Residue-property plots

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: Toll-like receptor 3



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.68Å 158.02Å 185.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.66 49.48 – 2.66	Depositor EDS
% Data completeness (in resolution range)	95.2 (50.00-2.66) 95.2 (49.48-2.66)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.244 , 0.272 0.246 , 0.271	Depositor DCC
R_{free} test set	1693 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 33494 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5736	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: BMA, NAG, NDG, FUC, FUL, MAN

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	0.43	0/5440	0.83	4/7386 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	286	LEU	CB-CG-CD1	-5.85	101.06	111.00
1	A	227	LEU	CB-CG-CD1	-5.36	101.89	111.00
1	A	489	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	393	LEU	CB-CG-CD2	-5.22	102.13	111.00

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	5330	0	5334	347	0
2	A	42	0	39	3	0
3	A	56	0	50	9	0
4	A	38	0	34	0	0
5	A	28	0	25	1	0
6	A	11	0	12	1	0
7	A	61	0	52	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	49	0	43	5	0
9	A	28	0	25	3	0
10	A	14	0	13	1	0
11	A	79	0	0	5	1
All	All	5736	0	5627	367	1

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 33.

All (367) 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:A:556:ASN:HB2	11:A:6725:HOH:O	1.51	1.11
1:A:393:LEU:HD21	1:A:396:LEU:HD23	1.34	1.08
1:A:107:GLN:NE2	1:A:107:GLN:H	1.52	1.06
1:A:107:GLN:N	1:A:107:GLN:HE21	1.60	0.97
1:A:77:LEU:HB2	1:A:98:LEU:HD21	1.43	0.97
1:A:422:ILE:H	1:A:445:GLN:HE22	0.99	0.93
1:A:393:LEU:HD21	1:A:396:LEU:CD2	1.97	0.93
1:A:42:LEU:H	1:A:61:ASN:HD22	1.18	0.91
1:A:107:GLN:HE21	1:A:107:GLN:H	0.91	0.89
1:A:76:GLN:HA	1:A:76:GLN:HE21	1.40	0.86
1:A:451:GLU:CD	1:A:451:GLU:H	1.79	0.86
1:A:105:ASN:O	1:A:106:LEU:HD12	1.76	0.85
1:A:93:GLU:HA	1:A:96:GLN:HE21	1.42	0.84
1:A:150:ILE:HG22	1:A:151:LYS:HG3	1.60	0.83
1:A:122:CYS:HB3	1:A:125:LEU:HD22	1.61	0.83
1:A:422:ILE:H	1:A:445:GLN:NE2	1.76	0.82
1:A:534:ILE:HG12	1:A:566:ILE:HG23	1.62	0.82
1:A:147:LYS:HE2	1:A:147:LYS:HA	1.62	0.81
1:A:450:GLN:HG3	8:A:4241:NDG:H6C2	1.62	0.80
1:A:640:LEU:HD11	1:A:642:MET:CE	2.13	0.79
1:A:555:VAL:HG12	1:A:556:ASN:H	1.47	0.78
1:A:555:VAL:HG12	1:A:556:ASN:N	1.98	0.77
1:A:443:ILE:H	1:A:466:ASN:HD22	1.32	0.76
1:A:42:LEU:HG	1:A:61:ASN:ND2	2.01	0.76
1:A:643:ARG:HB2	1:A:674:HIS:O	1.85	0.76
7:A:4132:NDG:O6	7:A:4133:MAN:O4	2.02	0.76
1:A:133:ASN:H	1:A:157:ASN:HD21	1.33	0.76
1:A:603:PRO:HA	1:A:629:VAL:HG22	1.69	0.74
8:A:4242:NDG:H4	8:A:4243:BMA:O2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASN:C	1:A:106:LEU:HD12	2.07	0.74
1:A:147:LYS:NZ	1:A:171:GLU:HG2	2.02	0.74
3:A:2521:NAG:C6	3:A:2521:NAG:H2	2.18	0.73
1:A:521:ILE:CD1	1:A:525:LEU:HD22	2.18	0.73
1:A:393:LEU:HD23	1:A:394:GLN:N	2.04	0.73
1:A:461:ILE:HG22	1:A:463:LEU:CD2	2.20	0.72
1:A:598:LEU:H	1:A:620:ASN:ND2	1.86	0.72
1:A:468:TYR:C	1:A:468:TYR:CD1	2.63	0.72
1:A:348:ASP:O	1:A:349:PHE:HB2	1.88	0.72
1:A:76:GLN:HA	1:A:76:GLN:NE2	2.05	0.71
1:A:638:ASN:N	1:A:638:ASN:HD22	1.89	0.71
1:A:622:ILE:H	1:A:645:ASN:ND2	1.89	0.71
1:A:85:ASN:HB2	1:A:87:ILE:HD13	1.73	0.71
1:A:117:GLN:HA	1:A:120:VAL:HG21	1.73	0.70
1:A:575:ASP:O	1:A:576:GLU:HG3	1.92	0.70
1:A:242:CYS:HB3	1:A:271:LEU:HD13	1.74	0.69
1:A:541:ASN:HD21	1:A:544:ARG:HD2	1.56	0.69
1:A:444:GLU:HG3	1:A:468:TYR:CE2	2.27	0.68
1:A:525:LEU:O	1:A:526:LEU:HB2	1.93	0.68
1:A:105:ASN:HB3	1:A:107:GLN:HE22	1.57	0.68
3:A:2521:NAG:H4	3:A:2522:NDG:H5	1.76	0.68
1:A:151:LYS:HG2	1:A:175:GLU:HB3	1.76	0.67
1:A:536:ASP:HB3	1:A:538:GLN:HE22	1.59	0.67
1:A:220:ILE:N	1:A:220:ILE:HD12	2.09	0.67
10:A:6621:NDG:H6C1	11:A:6746:HOH:O	1.94	0.67
1:A:622:ILE:H	1:A:645:ASN:HD22	1.40	0.67
1:A:314:SER:HB2	1:A:315:PRO:HD2	1.75	0.67
1:A:40:LEU:O	1:A:41:LYS:HB2	1.94	0.67
1:A:76:GLN:CA	1:A:76:GLN:HE21	2.07	0.67
1:A:93:GLU:O	1:A:96:GLN:HG2	1.94	0.67
1:A:55:VAL:HG12	1:A:56:LEU:N	2.11	0.66
1:A:577:ILE:HG12	1:A:577:ILE:O	1.95	0.66
1:A:56:LEU:CD2	1:A:58:LEU:HG	2.26	0.66
1:A:147:LYS:HZ3	1:A:171:GLU:HG2	1.59	0.66
1:A:521:ILE:HG23	1:A:545:LEU:HG	1.78	0.66
1:A:198:SER:OG	1:A:222:LYS:HD3	1.96	0.66
1:A:278:GLN:HG3	1:A:302:TYR:HB2	1.77	0.65
1:A:461:ILE:CG2	1:A:463:LEU:CD2	2.75	0.65
1:A:95:CYS:HB2	1:A:121:PHE:HB2	1.78	0.65
1:A:134:SER:N	1:A:157:ASN:HD22	1.94	0.65
1:A:446:LYS:N	1:A:446:LYS:HD3	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:H	1:A:61:ASN:ND2	1.94	0.64
1:A:64:ARG:HD3	1:A:65:ARG:HH21	1.62	0.64
1:A:51:SER:HB3	1:A:73:ARG:HE	1.63	0.64
1:A:214:PRO:HA	1:A:244:GLU:OE1	1.98	0.64
7:A:4132:NDG:H4	7:A:4133:MAN:O4	1.98	0.63
1:A:540:ASN:O	1:A:541:ASN:C	2.37	0.63
1:A:87:ILE:HD12	1:A:87:ILE:H	1.63	0.63
1:A:115:SER:O	1:A:118:THR:HG22	1.98	0.63
1:A:93:GLU:HA	1:A:96:GLN:NE2	2.12	0.63
1:A:28:CYS:HB2	1:A:49:LEU:HD11	1.79	0.63
1:A:575:ASP:HB3	1:A:597:ASN:HB2	1.80	0.63
1:A:36:ASP:C	1:A:36:ASP:OD1	2.37	0.62
9:A:5071:NDG:O3	9:A:5072:NAG:H61	1.98	0.62
1:A:444:GLU:HG3	1:A:468:TYR:CD2	2.34	0.62
1:A:598:LEU:N	1:A:620:ASN:HD22	1.98	0.62
1:A:667:ASN:HB2	2:A:6671:NAG:HN2	1.64	0.62
1:A:598:LEU:H	1:A:620:ASN:HD22	1.46	0.62
1:A:265:GLU:HG3	1:A:292:GLY:O	2.00	0.62
1:A:393:LEU:O	1:A:394:GLN:HB2	1.98	0.62
1:A:522:ASN:OD1	1:A:524:ASP:HB2	2.00	0.62
1:A:441:ASN:HB2	1:A:466:ASN:HD21	1.65	0.61
1:A:375:PHE:H	1:A:403:SER:HB2	1.65	0.61
1:A:87:ILE:H	1:A:87:ILE:CD1	2.14	0.61
1:A:257:ASN:HA	1:A:283:TYR:O	2.01	0.60
3:A:2521:NAG:H4	3:A:2522:NDG:H3	1.83	0.60
1:A:512:ASP:HA	1:A:536:ASP:HB2	1.82	0.60
1:A:56:LEU:HB2	1:A:77:LEU:HD21	1.83	0.60
1:A:64:ARG:HH11	1:A:64:ARG:HG3	1.67	0.60
9:A:5071:NDG:H6C2	9:A:5072:NAG:H83	1.82	0.59
1:A:615:LEU:O	1:A:640:LEU:HD12	2.02	0.59
1:A:42:LEU:N	1:A:61:ASN:HD22	1.94	0.59
1:A:638:ASN:N	1:A:638:ASN:ND2	2.50	0.59
1:A:516:ASN:O	1:A:517:ASN:O	2.21	0.59
1:A:640:LEU:HD11	1:A:642:MET:HE3	1.85	0.59
1:A:191:LEU:HD12	1:A:194:LEU:HD12	1.83	0.59
1:A:175:GLU:HG2	1:A:177:LEU:CD1	2.33	0.58
1:A:87:ILE:HD12	1:A:87:ILE:N	2.17	0.58
1:A:152:LEU:HD23	1:A:153:ASP:N	2.19	0.58
1:A:93:GLU:CA	1:A:96:GLN:HE21	2.15	0.57
1:A:616:ASN:OD1	1:A:618:GLN:HG2	2.04	0.57
1:A:344:PRO:HG2	1:A:367:ILE:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:ILE:HD11	1:A:525:LEU:HD22	1.85	0.57
1:A:129:ASP:OD2	1:A:131:MET:HB2	2.05	0.57
1:A:578:PRO:HG2	1:A:581:VAL:HG13	1.86	0.57
3:A:2521:NAG:C6	3:A:2521:NAG:C2	2.83	0.57
1:A:117:GLN:HA	1:A:120:VAL:CG2	2.34	0.56
1:A:451:GLU:CD	1:A:451:GLU:N	2.53	0.56
1:A:312:ARG:HG2	1:A:312:ARG:HH11	1.71	0.56
1:A:54:THR:HG22	1:A:76:GLN:O	2.05	0.56
1:A:133:ASN:H	1:A:157:ASN:ND2	2.01	0.56
1:A:74:TYR:C	1:A:76:GLN:H	2.08	0.56
1:A:109:ASN:HB2	1:A:133:ASN:HD21	1.69	0.56
1:A:461:ILE:CG2	1:A:463:LEU:HD21	2.36	0.56
1:A:49:LEU:HD22	1:A:49:LEU:H	1.70	0.56
1:A:640:LEU:HD11	1:A:642:MET:HE2	1.87	0.55
1:A:40:LEU:N	1:A:40:LEU:HD12	2.22	0.55
1:A:465:TYR:HD1	1:A:489:ARG:HD3	1.71	0.55
1:A:40:LEU:N	1:A:40:LEU:CD1	2.68	0.55
1:A:55:VAL:HG12	1:A:56:LEU:H	1.72	0.55
1:A:643:ARG:HB3	1:A:675:TYR:CE1	2.42	0.55
1:A:450:GLN:CG	8:A:4241:NDG:H6C2	2.33	0.54
1:A:620:ASN:CB	1:A:645:ASN:HD21	2.21	0.54
1:A:65:ARG:HD2	1:A:65:ARG:C	2.28	0.54
1:A:105:ASN:CB	1:A:107:GLN:HE22	2.21	0.54
1:A:513:LEU:HD23	1:A:513:LEU:H	1.72	0.54
1:A:623:THR:HG23	1:A:648:ASP:HB2	1.90	0.54
1:A:484:ARG:HB3	1:A:486:MET:CE	2.38	0.53
1:A:437:ASP:OD2	1:A:462:TYR:CD2	2.61	0.53
1:A:657:PHE:CE1	1:A:661:ILE:HD11	2.44	0.53
1:A:63:LEU:N	1:A:63:LEU:HD12	2.24	0.53
5:A:2911:NAG:O6	6:A:2916:FUC:H5	2.09	0.53
1:A:277:THR:C	1:A:300:LEU:HD23	2.29	0.53
3:A:2521:NAG:C4	3:A:2522:NDG:H5	2.37	0.53
1:A:678:ASN:HD22	1:A:679:THR:HG23	1.74	0.53
1:A:38:SER:O	1:A:59:THR:O	2.27	0.53
1:A:446:LYS:H	1:A:446:LYS:HD3	1.74	0.53
1:A:696:CYS:C	1:A:697:LYS:HG2	2.29	0.53
1:A:63:LEU:N	1:A:63:LEU:CD1	2.72	0.52
1:A:461:ILE:HG22	1:A:463:LEU:HD23	1.90	0.52
1:A:670:GLU:OE1	1:A:674:HIS:HD2	1.93	0.52
1:A:63:LEU:CD1	1:A:63:LEU:H	2.21	0.52
1:A:56:LEU:HD22	1:A:58:LEU:HG	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:TYR:CD1	1:A:468:TYR:O	2.63	0.52
1:A:632:PRO:HB2	1:A:633:PRO:HD3	1.92	0.52
1:A:393:LEU:HD23	1:A:393:LEU:C	2.30	0.52
1:A:422:ILE:N	1:A:445:GLN:HE22	1.84	0.52
1:A:244:GLU:HA	1:A:244:GLU:OE2	2.09	0.52
1:A:545:LEU:O	1:A:546:TRP:CD1	2.63	0.52
1:A:312:ARG:HG2	1:A:312:ARG:NH1	2.24	0.52
1:A:108:HIS:HA	1:A:132:SER:HB2	1.92	0.52
1:A:123:THR:C	1:A:125:LEU:H	2.13	0.52
1:A:39:HIS:C	1:A:40:LEU:HD12	2.30	0.52
1:A:511:LEU:HG	1:A:513:LEU:HD22	1.92	0.51
1:A:77:LEU:HD12	1:A:98:LEU:HD21	1.92	0.51
1:A:465:TYR:CD1	1:A:489:ARG:HD3	2.46	0.51
1:A:186:LEU:O	1:A:216:CYS:HB3	2.10	0.51
1:A:351:PHE:HB3	1:A:378:LEU:HD21	1.93	0.51
1:A:541:ASN:ND2	1:A:544:ARG:HD2	2.25	0.51
1:A:114:ILE:CD1	1:A:118:THR:HG21	2.40	0.51
1:A:462:TYR:HD1	1:A:486:MET:HG3	1.76	0.51
1:A:253:LEU:HG	1:A:255:LEU:CD1	2.41	0.51
1:A:537:PHE:HB3	1:A:569:LEU:HD23	1.93	0.51
1:A:386:LEU:HD13	1:A:390:PHE:CE2	2.46	0.51
1:A:59:THR:CG2	1:A:60:HIS:HD2	2.24	0.51
1:A:55:VAL:CG1	1:A:56:LEU:N	2.74	0.50
1:A:220:ILE:N	1:A:220:ILE:CD1	2.74	0.50
1:A:484:ARG:HB3	1:A:486:MET:HE1	1.93	0.50
1:A:189:GLU:O	1:A:192:GLU:HG3	2.11	0.50
1:A:93:GLU:O	1:A:97:ILE:HG12	2.11	0.50
1:A:85:ASN:CB	1:A:87:ILE:HD13	2.42	0.50
1:A:525:LEU:O	1:A:526:LEU:CB	2.57	0.50
1:A:514:SER:HA	1:A:540:ASN:HD21	1.77	0.50
1:A:542:LEU:H	1:A:572:ASN:HB3	1.76	0.50
1:A:314:SER:CB	1:A:315:PRO:HD2	2.42	0.50
1:A:325:ARG:NH1	1:A:356:TYR:CD1	2.80	0.50
1:A:632:PRO:HB2	1:A:633:PRO:CD	2.42	0.49
1:A:56:LEU:HB2	1:A:77:LEU:CD2	2.42	0.49
1:A:640:LEU:HD21	1:A:642:MET:HE3	1.94	0.49
1:A:620:ASN:C	1:A:645:ASN:ND2	2.66	0.49
1:A:64:ARG:HB3	1:A:65:ARG:HE	1.76	0.49
1:A:73:ARG:HH11	1:A:73:ARG:HG3	1.77	0.49
1:A:660:TRP:CZ3	1:A:661:ILE:HD13	2.47	0.49
1:A:393:LEU:CD2	1:A:394:GLN:N	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:ASP:OD2	1:A:462:TYR:HD2	1.96	0.49
1:A:32:TYR:O	1:A:34:VAL:HG13	2.12	0.49
1:A:382:LYS:HE3	1:A:383:TYR:CE1	2.48	0.49
1:A:603:PRO:HA	1:A:629:VAL:CG2	2.39	0.49
1:A:386:LEU:HD13	1:A:390:PHE:HE2	1.77	0.49
1:A:333:PHE:HB3	1:A:344:PRO:HG3	1.93	0.49
1:A:134:SER:HB2	1:A:136:HIS:HE1	1.77	0.49
1:A:465:TYR:OH	1:A:488:ARG:NH1	2.45	0.49
1:A:68:PRO:HB3	1:A:94:LEU:HG	1.94	0.49
1:A:521:ILE:O	1:A:521:ILE:HG13	2.13	0.48
1:A:540:ASN:H	1:A:572:ASN:ND2	2.11	0.48
1:A:660:TRP:CE3	1:A:661:ILE:HD13	2.48	0.48
1:A:79:ILE:O	1:A:79:ILE:CG1	2.61	0.48
1:A:593:LEU:HB2	1:A:617:LEU:HD23	1.95	0.48
1:A:597:ASN:HA	1:A:621:LEU:HD13	1.96	0.48
1:A:346:ILE:HD11	1:A:374:THR:HG23	1.95	0.48
1:A:284:ASN:O	1:A:285:ASN:HB2	2.13	0.48
1:A:147:LYS:HZ1	1:A:171:GLU:H	1.61	0.48
1:A:681:HIS:HB3	11:A:6741:HOH:O	2.13	0.48
1:A:555:VAL:CG1	1:A:556:ASN:N	2.70	0.48
1:A:42:LEU:HG	1:A:61:ASN:HD21	1.74	0.48
1:A:470:GLN:HG2	1:A:493:LYS:HB2	1.95	0.48
1:A:394:GLN:HG3	1:A:418:HIS:O	2.13	0.48
1:A:536:ASP:HB3	1:A:538:GLN:NE2	2.26	0.48
1:A:65:ARG:H	1:A:65:ARG:HD2	1.79	0.48
1:A:522:ASN:OD1	1:A:524:ASP:CB	2.62	0.48
1:A:253:LEU:HG	1:A:255:LEU:HD11	1.96	0.48
1:A:355:LYS:HD2	1:A:355:LYS:C	2.34	0.48
1:A:133:ASN:O	1:A:134:SER:C	2.52	0.48
3:A:2521:NAG:H2	3:A:2521:NAG:H62	1.93	0.48
3:A:2521:NAG:H4	3:A:2522:NDG:C5	2.42	0.47
1:A:310:ILE:HB	1:A:333:PHE:CD1	2.49	0.47
1:A:470:GLN:HA	1:A:493:LYS:HB2	1.95	0.47
1:A:157:ASN:HB2	1:A:159:LEU:HD22	1.95	0.47
1:A:450:GLN:HE22	1:A:453:ARG:HD3	1.80	0.47
1:A:431:GLY:HA3	1:A:456:ARG:HH21	1.79	0.47
1:A:74:TYR:CD1	1:A:74:TYR:N	2.83	0.47
1:A:534:ILE:HG12	1:A:566:ILE:CG2	2.41	0.47
1:A:443:ILE:HG13	1:A:466:ASN:ND2	2.30	0.47
1:A:79:ILE:HB	1:A:103:VAL:HB	1.96	0.47
1:A:393:LEU:HD21	1:A:396:LEU:HD21	1.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:4132:NDG:HB	7:A:4133:MAN:C1	2.28	0.47
1:A:109:ASN:CB	1:A:133:ASN:HD21	2.28	0.47
1:A:468:TYR:HA	1:A:490:VAL:O	2.15	0.47
1:A:316:ARG:HD2	1:A:316:ARG:HA	1.75	0.47
1:A:602:GLU:O	1:A:605:ILE:HG12	2.15	0.46
1:A:55:VAL:CG1	1:A:56:LEU:H	2.28	0.46
8:A:4242:NDG:C4	8:A:4243:BMA:O2	2.62	0.46
1:A:85:ASN:HB2	1:A:109:ASN:HD21	1.80	0.46
1:A:87:ILE:CD1	1:A:87:ILE:N	2.78	0.46
1:A:598:LEU:N	1:A:620:ASN:ND2	2.58	0.46
1:A:188:SER:HA	1:A:216:CYS:HA	1.96	0.46
1:A:162:THR:HG22	1:A:178:LEU:HD13	1.96	0.46
1:A:443:ILE:H	1:A:466:ASN:ND2	2.06	0.46
1:A:615:LEU:HB3	1:A:637:LEU:HD21	1.98	0.46
1:A:63:LEU:HD13	1:A:85:ASN:OD1	2.16	0.46
1:A:637:LEU:C	1:A:638:ASN:HD22	2.20	0.46
1:A:119:PHE:CE1	1:A:128:LEU:HD21	2.51	0.46
1:A:67:PRO:C	1:A:69:THR:H	2.20	0.46
1:A:147:LYS:HZ1	1:A:171:GLU:HG2	1.76	0.45
1:A:643:ARG:HG3	1:A:644:PHE:CD2	2.51	0.45
1:A:450:GLN:NE2	1:A:453:ARG:HD3	2.31	0.45
1:A:184:LEU:HD12	1:A:184:LEU:H	1.81	0.45
1:A:65:ARG:N	1:A:65:ARG:HD2	2.30	0.45
1:A:481:SER:HB3	9:A:5071:NDG:H8C2	1.97	0.45
1:A:295:SER:HA	1:A:320:GLY:HA3	1.99	0.45
1:A:348:ASP:O	1:A:349:PHE:CB	2.56	0.45
1:A:206:SER:HA	1:A:230:ASN:O	2.17	0.45
1:A:591:ILE:HG13	1:A:612:LEU:HD11	1.99	0.45
1:A:513:LEU:N	1:A:513:LEU:HD23	2.31	0.45
1:A:27:GLN:OE1	1:A:48:ASP:OD1	2.35	0.45
1:A:118:THR:HG23	1:A:119:PHE:H	1.82	0.45
1:A:434:ARG:C	1:A:435:ILE:HD12	2.37	0.45
1:A:485:LEU:HD11	1:A:487:LEU:HD21	1.98	0.45
1:A:147:LYS:CE	1:A:147:LYS:HA	2.42	0.44
1:A:191:LEU:HG	1:A:220:ILE:HD11	1.99	0.44
1:A:79:ILE:HG12	1:A:79:ILE:O	2.16	0.44
1:A:235:PRO:HA	1:A:260:LEU:CD1	2.47	0.44
1:A:637:LEU:HD12	1:A:637:LEU:HA	1.81	0.44
1:A:645:ASN:O	1:A:647:PHE:N	2.48	0.44
1:A:479:VAL:O	1:A:482:LEU:HB2	2.17	0.44
1:A:628:ASP:OD1	1:A:628:ASP:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:C	1:A:227:LEU:HD23	2.37	0.44
1:A:155:SER:O	1:A:156:HIS:C	2.56	0.44
1:A:56:LEU:HD21	1:A:58:LEU:HG	1.98	0.44
1:A:516:ASN:HB2	1:A:518:ILE:HD13	1.99	0.44
1:A:73:ARG:HD3	1:A:73:ARG:C	2.38	0.44
1:A:375:PHE:H	1:A:403:SER:CB	2.31	0.44
1:A:59:THR:CG2	1:A:60:HIS:CD2	3.00	0.44
1:A:54:THR:O	1:A:55:VAL:HG23	2.18	0.44
1:A:200:ARG:O	1:A:225:ALA:HB3	2.18	0.44
1:A:93:GLU:CD	1:A:93:GLU:H	2.19	0.43
1:A:394:GLN:HA	1:A:419:ILE:HA	2.00	0.43
1:A:104:LEU:HG	1:A:106:LEU:HD13	2.00	0.43
1:A:122:CYS:O	1:A:146:GLN:NE2	2.51	0.43
1:A:285:ASN:HA	1:A:285:ASN:HD22	1.64	0.43
1:A:45:ILE:HG22	2:A:724:NAG:O7	2.19	0.43
1:A:490:VAL:O	1:A:491:ALA:HB3	2.18	0.43
1:A:462:TYR:CD1	1:A:486:MET:HG3	2.52	0.43
1:A:97:ILE:O	1:A:99:PRO:HD3	2.19	0.43
1:A:409:LEU:HA	1:A:409:LEU:HD23	1.91	0.43
1:A:74:TYR:C	1:A:76:GLN:N	2.72	0.43
1:A:620:ASN:HB2	1:A:645:ASN:HD21	1.84	0.43
1:A:27:GLN:OE1	1:A:48:ASP:CG	2.57	0.43
1:A:500:SER:HB3	1:A:503:ARG:NH1	2.34	0.43
1:A:355:LYS:HE3	1:A:356:TYR:CD2	2.53	0.43
1:A:77:LEU:HD12	1:A:98:LEU:CD2	2.48	0.43
1:A:444:GLU:CG	1:A:468:TYR:CE2	3.01	0.43
1:A:93:GLU:CB	1:A:96:GLN:HE21	2.32	0.42
1:A:667:ASN:HB2	2:A:6671:NAG:N2	2.33	0.42
1:A:42:LEU:O	1:A:62:GLN:HB2	2.19	0.42
1:A:93:GLU:HB3	1:A:96:GLN:HE21	1.84	0.42
3:A:2521:NAG:H4	3:A:2522:NDG:C3	2.48	0.42
1:A:521:ILE:HG23	1:A:545:LEU:HB3	2.00	0.42
1:A:310:ILE:HG12	1:A:332:ALA:O	2.19	0.42
1:A:419:ILE:HG13	1:A:441:ASN:OD1	2.18	0.42
1:A:77:LEU:CB	1:A:98:LEU:HD21	2.30	0.42
1:A:64:ARG:NH2	11:A:6687:HOH:O	2.29	0.42
1:A:57:ASN:OD1	1:A:59:THR:HB	2.19	0.42
1:A:73:ARG:HD3	1:A:73:ARG:O	2.20	0.42
1:A:693:THR:O	1:A:696:CYS:HB2	2.20	0.42
1:A:578:PRO:HG2	1:A:581:VAL:CG1	2.49	0.42
1:A:286:LEU:HD12	1:A:286:LEU:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2521:NAG:H61	3:A:2521:NAG:H2	1.98	0.42
1:A:446:LYS:HB3	1:A:470:GLN:HB3	2.01	0.42
1:A:393:LEU:O	1:A:395:THR:N	2.51	0.42
1:A:527:GLU:OE2	1:A:559:LYS:NZ	2.50	0.42
1:A:54:THR:O	1:A:78:ALA:HB3	2.19	0.42
1:A:450:GLN:HG3	8:A:4241:NDG:C6	2.42	0.42
7:A:4133:MAN:H4	7:A:4134:BMA:C2	2.49	0.42
1:A:65:ARG:O	1:A:65:ARG:HD2	2.19	0.42
1:A:513:LEU:CD2	1:A:513:LEU:N	2.83	0.42
1:A:680:PRO:HD2	1:A:683:TYR:HD2	1.85	0.42
1:A:599:ASN:ND2	11:A:6681:HOH:O	2.52	0.42
1:A:102:LYS:HG2	1:A:124:ASN:O	2.20	0.42
1:A:162:THR:OG1	1:A:190:GLU:HG3	2.20	0.41
1:A:42:LEU:HD23	1:A:42:LEU:N	2.36	0.41
1:A:521:ILE:HD13	1:A:525:LEU:HD22	1.99	0.41
1:A:470:GLN:HG2	1:A:493:LYS:CB	2.50	0.41
1:A:355:LYS:HE3	1:A:356:TYR:HD2	1.85	0.41
1:A:417:ASN:O	1:A:418:HIS:HB2	2.20	0.41
1:A:95:CYS:HB3	1:A:122:CYS:N	2.35	0.41
1:A:482:LEU:CD1	1:A:485:LEU:HB2	2.50	0.41
1:A:97:ILE:C	1:A:99:PRO:HD3	2.41	0.41
1:A:150:ILE:CG2	1:A:150:ILE:O	2.68	0.41
1:A:622:ILE:N	1:A:645:ASN:HD22	2.13	0.41
1:A:64:ARG:CB	1:A:65:ARG:HE	2.33	0.41
1:A:494:ASN:HA	1:A:494:ASN:HD22	1.67	0.41
1:A:126:THR:C	1:A:149:LEU:HD12	2.40	0.41
1:A:521:ILE:HG23	1:A:545:LEU:CG	2.49	0.41
1:A:516:ASN:O	1:A:517:ASN:C	2.59	0.41
1:A:393:LEU:CD2	1:A:396:LEU:CD2	2.85	0.41
1:A:446:LYS:CD	1:A:446:LYS:H	2.34	0.41
1:A:351:PHE:HB3	1:A:354:LEU:HD12	2.02	0.41
1:A:331:ARG:HD2	1:A:364:ASP:O	2.21	0.41
1:A:107:GLN:N	1:A:107:GLN:NE2	2.34	0.41
1:A:620:ASN:C	1:A:621:LEU:HD12	2.41	0.41
1:A:386:LEU:HD22	1:A:389:THR:HG21	2.02	0.41
1:A:383:TYR:N	1:A:383:TYR:CD1	2.89	0.41
1:A:479:VAL:O	1:A:479:VAL:HG23	2.20	0.41
1:A:476:PHE:HB3	1:A:505:LEU:HD21	2.03	0.41
1:A:558:LEU:HD12	1:A:581:VAL:O	2.21	0.41
1:A:336:GLN:HB2	1:A:336:GLN:HE21	1.77	0.41
1:A:314:SER:HA	1:A:347:ASP:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:HB3	1:A:32:TYR:H	1.74	0.40
1:A:368:PRO:O	1:A:369:SER:HB3	2.20	0.40
1:A:542:LEU:H	1:A:572:ASN:HD22	1.70	0.40
1:A:318:PHE:HB3	1:A:321:LEU:HD12	2.02	0.40
1:A:396:LEU:HD11	1:A:419:ILE:HD13	2.03	0.40
7:A:4133:MAN:H62	7:A:4135:MAN:H2	1.96	0.40
1:A:620:ASN:HB3	1:A:621:LEU:H	1.64	0.40
1:A:468:TYR:C	1:A:468:TYR:HD1	2.22	0.40
1:A:114:ILE:HD12	1:A:118:THR:HG21	2.03	0.40
1:A:678:ASN:ND2	1:A:679:THR:HG23	2.36	0.40

All (1) 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)
11:A:6718:HOH:O	11:A:6718:HOH:O[2_655]	1.90	0.30

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	659/697 (94%)	546 (83%)	101 (15%)	12 (2%)	11 23

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	517	ASN
1	A	131	MET
1	A	372	SER
1	A	398	ASN
1	A	56	LEU
1	A	170	LEU

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Mol	Chain	Res	Type
1	A	171	GLU
1	A	350	SER
1	A	557	PHE
1	A	140	SER
1	A	424	ASN
1	A	50	PRO

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	A	622/651 (96%)	533 (86%)	89 (14%)	4 8

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	45	ILE
1	A	47	ASP
1	A	49	LEU
1	A	56	LEU
1	A	63	LEU
1	A	65	ARG
1	A	73	ARG
1	A	74	TYR
1	A	76	GLN
1	A	79	ILE
1	A	89	LYS
1	A	93	GLU
1	A	98	LEU
1	A	101	LEU
1	A	107	GLN
1	A	114	ILE
1	A	116	ASP
1	A	118	THR
1	A	128	LEU

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Mol	Chain	Res	Type
1	A	131	MET
1	A	136	HIS
1	A	152	LEU
1	A	162	THR
1	A	172	ASN
1	A	184	LEU
1	A	189	GLU
1	A	191	LEU
1	A	192	GLU
1	A	211	GLU
1	A	213	SER
1	A	218	GLN
1	A	219	THR
1	A	233	LEU
1	A	257	ASN
1	A	271	LEU
1	A	276	LEU
1	A	288	ASP
1	A	293	SER
1	A	295	SER
1	A	299	SER
1	A	300	LEU
1	A	305	LEU
1	A	336	GLN
1	A	346	ILE
1	A	355	LYS
1	A	356	TYR
1	A	358	GLU
1	A	381	LEU
1	A	403	SER
1	A	410	LEU
1	A	430	LEU
1	A	442	GLU
1	A	446	LYS
1	A	447	LEU
1	A	459	PHE
1	A	467	LYS
1	A	468	TYR
1	A	470	GLN
1	A	472	SER
1	A	482	LEU
1	A	486	MET

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Mol	Chain	Res	Type
1	A	493	LYS
1	A	494	ASN
1	A	513	LEU
1	A	518	ILE
1	A	521	ILE
1	A	523	GLU
1	A	532	LEU
1	A	545	LEU
1	A	546	TRP
1	A	557	PHE
1	A	564	LEU
1	A	566	ILE
1	A	574	LEU
1	A	577	ILE
1	A	579	VAL
1	A	589	LYS
1	A	607	ASP
1	A	620	ASN
1	A	623	THR
1	A	638	ASN
1	A	643	ARG
1	A	651	CYS
1	A	655	SER
1	A	663	GLN
1	A	668	ILE
1	A	669	SER
1	A	681	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	61	ASN
1	A	76	GLN
1	A	96	GLN
1	A	105	ASN
1	A	107	GLN
1	A	109	ASN
1	A	113	GLN
1	A	133	ASN
1	A	157	ASN
1	A	169	GLN

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Mol	Chain	Res	Type
1	A	218	GLN
1	A	230	ASN
1	A	278	GLN
1	A	285	ASN
1	A	309	ASN
1	A	445	GLN
1	A	450	GLN
1	A	466	ASN
1	A	483	GLN
1	A	494	ASN
1	A	538	GLN
1	A	541	ASN
1	A	565	HIS
1	A	572	ASN
1	A	609	GLN
1	A	620	ASN
1	A	638	ASN
1	A	645	ASN
1	A	678	ASN

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 ⓘ

20 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	A	2521	1,3	14,14,15	0.43	0	15,19,21	1.40	2 (13%)
3	NDG	A	2522	3	14,14,15	0.52	0	15,19,21	1.79	3 (20%)
4	NAG	A	2751	1,4	14,14,15	0.50	0	15,19,21	1.40	1 (6%)
4	NAG	A	2752	4	14,14,15	0.53	0	15,19,21	1.63	2 (13%)
4	FUL	A	2756	4	10,10,11	0.54	0	14,14,16	0.92	1 (7%)
5	NAG	A	2911	1,5	14,14,15	0.62	0	15,19,21	1.62	2 (13%)
5	NAG	A	2912	5	14,14,15	0.50	0	15,19,21	1.04	0
3	NAG	A	3981	1,3	14,14,15	0.46	0	15,19,21	1.20	2 (13%)
3	NDG	A	3982	3	14,14,15	0.48	0	15,19,21	0.99	1 (6%)
7	NDG	A	4131	1,7	14,14,15	0.67	0	15,19,21	1.69	3 (20%)
7	NDG	A	4132	7	14,14,15	0.53	0	15,19,21	1.05	2 (13%)
7	MAN	A	4133	7	11,11,12	0.56	0	14,15,17	2.03	4 (28%)
7	BMA	A	4134	7	11,11,12	0.56	0	14,15,17	1.07	1 (7%)
7	MAN	A	4135	7	11,11,12	0.54	0	14,15,17	1.26	1 (7%)
8	NDG	A	4241	1,8	14,14,15	0.45	0	15,19,21	1.04	1 (6%)
8	NDG	A	4242	8	14,14,15	0.51	0	15,19,21	0.80	1 (6%)
8	BMA	A	4243	8	11,11,12	0.60	0	14,15,17	1.28	2 (14%)
8	FUL	A	4246	8	10,10,11	0.60	0	14,14,16	1.36	1 (7%)
9	NDG	A	5071	9,1	14,14,15	0.50	0	15,19,21	1.73	3 (20%)
9	NAG	A	5072	9	14,14,15	0.44	0	15,19,21	1.59	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
3	NAG	A	2521	1,3	-	0/6/23/26	0/1/1/1
3	NDG	A	2522	3	-	0/6/23/26	0/1/1/1
4	NAG	A	2751	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2752	4	-	0/6/23/26	0/1/1/1
4	FUL	A	2756	4	-	0/0/17/20	0/1/1/1
5	NAG	A	2911	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2912	5	-	0/6/23/26	0/1/1/1
3	NAG	A	3981	1,3	-	2/6/23/26	0/1/1/1
3	NDG	A	3982	3	-	1/6/23/26	0/1/1/1
7	NDG	A	4131	1,7	-	0/6/23/26	0/1/1/1
7	NDG	A	4132	7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	A	4133	7	-	0/2/19/22	0/1/1/1
7	BMA	A	4134	7	-	0/2/19/22	0/1/1/1
7	MAN	A	4135	7	-	0/2/19/22	0/1/1/1
8	NDG	A	4241	1,8	-	0/6/23/26	0/1/1/1
8	NDG	A	4242	8	-	1/6/23/26	0/1/1/1
8	BMA	A	4243	8	-	0/2/19/22	0/1/1/1
8	FUL	A	4246	8	-	0/0/17/20	0/1/1/1
9	NDG	A	5071	9,1	-	0/6/23/26	0/1/1/1
9	NAG	A	5072	9	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2911	NAG	C3-C4-C5	-4.57	102.23	110.20
4	A	2752	NAG	C2-N2-C7	-3.70	118.29	123.04
7	A	4131	NDG	C3-C2-N2	-3.53	102.11	110.56
9	A	5071	NDG	C3-C4-C5	-3.17	104.66	110.20
4	A	2752	NAG	C4-C3-C2	-3.01	106.55	111.23
3	A	2522	NDG	O7-C7-C8	-2.86	116.82	122.06
9	A	5071	NDG	C4-C3-C2	-2.85	106.80	111.23
7	A	4132	NDG	C3-C2-N2	-2.22	105.25	110.56
9	A	5072	NAG	O7-C7-C8	-2.20	118.02	122.06
5	A	2911	NAG	C3-C2-N2	-2.17	105.36	110.56
7	A	4133	MAN	O2-C2-C1	-2.13	104.93	109.21
7	A	4131	NDG	C3-C4-C5	-2.12	106.50	110.20
8	A	4242	NDG	C3-C4-C5	-2.07	106.58	110.20
3	A	3981	NAG	C2-N2-C7	-2.06	120.39	123.04
8	A	4246	FUL	C1-C2-C3	2.01	111.92	109.54
9	A	5072	NAG	O5-C5-C6	2.12	111.95	107.35
7	A	4133	MAN	O5-C1-C2	2.13	114.31	110.86
7	A	4132	NDG	O-C5-C6	2.13	111.97	107.35
9	A	5072	NAG	C2-N2-C7	2.27	125.96	123.04
3	A	2521	NAG	O5-C5-C6	2.31	112.35	107.35
8	A	4241	NDG	O-C5-C6	2.44	112.64	107.35
8	A	4243	BMA	C1-C2-C3	2.50	112.50	109.54
3	A	3982	NDG	C1-O-C5	2.51	115.44	112.25
3	A	2522	NDG	C1-O-C5	2.55	115.48	112.25
4	A	2756	FUL	O5-C5-C6	2.63	110.48	106.13
7	A	4134	BMA	C1-O5-C5	2.66	115.62	112.25
3	A	3981	NAG	C1-O5-C5	2.77	115.77	112.25
8	A	4243	BMA	C1-O5-C5	3.28	116.41	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	4131	NDG	C1-O-C5	3.48	116.66	112.25
7	A	4133	MAN	C1-C2-C3	3.56	113.75	109.54
7	A	4135	MAN	C1-O5-C5	4.00	117.33	112.25
9	A	5072	NAG	C1-O5-C5	4.15	117.52	112.25
3	A	2521	NAG	C1-O5-C5	4.33	117.74	112.25
9	A	5071	NDG	C1-O-C5	4.44	117.88	112.25
3	A	2522	NDG	C2-N2-C7	4.58	128.92	123.04
4	A	2751	NAG	C1-O5-C5	4.90	118.46	112.25
7	A	4133	MAN	C1-O5-C5	4.96	118.54	112.25

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	4242	NDG	O7-C7-N2-C2
3	A	3982	NDG	O7-C7-N2-C2
3	A	3981	NAG	C8-C7-N2-C2
3	A	3981	NAG	O7-C7-N2-C2

There are no ring outliers.

12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2521	NAG	9	0
3	A	2522	NDG	5	0
5	A	2911	NAG	1	0
7	A	4132	NDG	3	0
7	A	4133	MAN	5	0
7	A	4134	BMA	1	0
7	A	4135	MAN	1	0
8	A	4241	NDG	3	0
8	A	4242	NDG	2	0
8	A	4243	BMA	2	0
9	A	5071	NDG	3	0
9	A	5072	NAG	2	0

5.6 Ligand geometry

5 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	$\# Z > 2$
2	NAG	A	1961	1	14,14,15	0.46	0	15,19,21	1.38	2 (13%)
6	FUC	A	2916	-	11,11,11	0.59	0	16,16,16	1.22	3 (18%)
10	NDG	A	6621	1	14,14,15	0.49	0	15,19,21	0.66	0
2	NAG	A	6671	1	14,14,15	0.48	0	15,19,21	1.41	1 (6%)
2	NAG	A	724	1	14,14,15	0.49	0	15,19,21	1.00	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
2	NAG	A	1961	1	-	0/6/23/26	0/1/1/1
6	FUC	A	2916	-	-	0/0/20/20	0/1/1/1
10	NDG	A	6621	1	-	1/6/23/26	0/1/1/1
2	NAG	A	6671	1	-	0/6/23/26	0/1/1/1
2	NAG	A	724	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1961	NAG	C2-N2-C7	-2.37	119.99	123.04
6	A	2916	FUC	C1-C2-C3	2.00	113.41	110.43
6	A	2916	FUC	C3-C4-C5	2.14	113.33	109.72
6	A	2916	FUC	O5-C5-C4	2.74	114.28	109.53
2	A	724	NAG	C1-O5-C5	3.14	116.23	112.25
2	A	1961	NAG	C1-O5-C5	4.12	117.48	112.25
2	A	6671	NAG	C1-O5-C5	4.23	117.62	112.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	6621	NDG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2916	FUC	1	0
10	A	6621	NDG	1	0
2	A	6671	NAG	2	0
2	A	724	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, 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	663/697 (95%)	0.45	37 (5%) 28 25	38, 59, 95, 115	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	46	PRO	5.5
1	A	33	ASN	5.3
1	A	78	ALA	5.1
1	A	164	LEU	5.0
1	A	49	LEU	4.5
1	A	28	CYS	4.3
1	A	74	TYR	4.1
1	A	77	LEU	3.9
1	A	34	VAL	3.9
1	A	31	ARG	3.6
1	A	45	ILE	3.5
1	A	141	ASN	3.3
1	A	165	GLY	3.2
1	A	63	LEU	3.2
1	A	519	ALA	3.1
1	A	168	VAL	3.1
1	A	80	LEU	3.0
1	A	32	TYR	2.9
1	A	29	THR	2.9
1	A	62	GLN	2.8
1	A	48	ASP	2.7
1	A	35	ALA	2.7
1	A	147	LYS	2.6
1	A	169	GLN	2.6
1	A	171	GLU	2.6
1	A	81	ASP	2.6
1	A	101	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	148	ASN	2.5
1	A	520	ASN	2.5
1	A	468	TYR	2.5
1	A	144	LYS	2.5
1	A	545	LEU	2.4
1	A	339	SER	2.4
1	A	546	TRP	2.3
1	A	138	ILE	2.2
1	A	68	PRO	2.1
1	A	193	PHE	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, 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	NAG	A	2751	14/15	0.88	0.16	-0.04	60,64,73,83	0
7	NDG	A	4131	14/15	0.95	0.14	-1.64	34,54,64,78	0
5	NAG	A	2911	14/15	0.92	0.14	-3.61	70,75,81,83	0
9	NAG	A	5072	14/15	0.88	0.17	-	82,87,91,92	0
7	BMA	A	4134	11/12	0.42	0.50	-	113,120,121,123	0
3	NAG	A	2521	14/15	0.87	0.13	-	74,82,88,96	0
8	NDG	A	4242	14/15	0.71	0.30	-	90,91,93,95	0
7	MAN	A	4133	11/12	0.62	0.38	-	108,115,120,124	0
7	MAN	A	4135	11/12	0.47	0.36	-	112,126,127,127	0
8	NDG	A	4241	14/15	0.90	0.16	-	72,76,87,91	0
4	FUL	A	2756	10/11	0.88	0.22	-	86,91,93,95	0
3	NDG	A	3982	14/15	0.58	0.50	-	106,109,111,114	0
3	NDG	A	2522	14/15	0.49	0.28	-	96,104,109,109	0
8	BMA	A	4243	11/12	0.75	0.18	-	79,83,88,90	0
4	NAG	A	2752	14/15	0.90	0.16	-	51,62,65,66	0
8	FUL	A	4246	10/11	0.70	0.63	-	97,99,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	A	2912	14/15	0.82	0.17	-	85,91,94,95	0
3	NAG	A	3981	14/15	0.83	0.31	-	90,99,104,105	0
9	NDG	A	5071	14/15	0.94	0.15	-	55,67,74,80	0
7	NDG	A	4132	14/15	0.89	0.28	-	73,84,93,105	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(\AA^2)	Q<0.9
2	NAG	A	724	14/15	0.79	0.30	0.27	86,89,91,91	0
10	NDG	A	6621	14/15	0.57	0.41	-	67,79,81,82	0
2	NAG	A	1961	14/15	0.64	0.39	-	74,83,87,88	0
6	FUC	A	2916	11/11	0.57	0.41	-	105,113,116,116	0
2	NAG	A	6671	14/15	0.71	0.32	-	79,81,84,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.