



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:20 AM GMT

PDB ID : 2WR1
Title : STRUCTURE OF INFLUENZA H2 HEMAGGLUTININ WITH HUMAN RECEPTOR
Authors : Liu, J.; Stevens, D.J.; Haire, L.F.; Walker, P.A.; Coombs, P.J.; Russell, R.J.; Gamblin, S.J.; Skehel, J.J.
Deposited on : 2009-08-29
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 (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

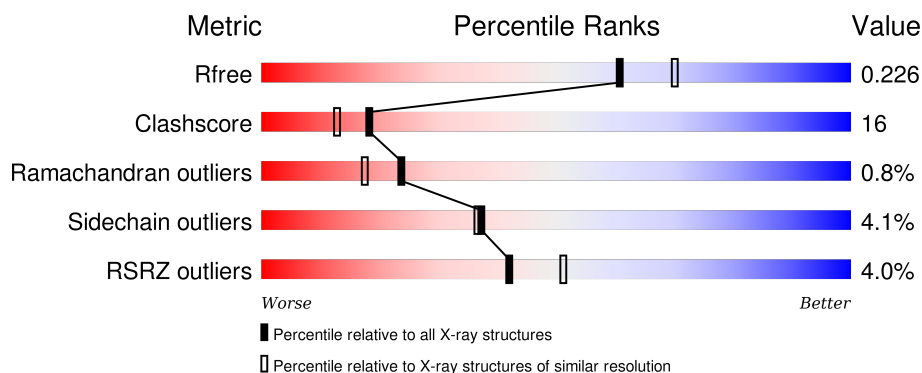
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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 $\leq 5\%$. 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	509	<div> <div>4%</div> <div>75% 17% • •</div> </div>
1	B	509	<div> <div>5%</div> <div>72% 21% • • •</div> </div>
1	C	509	<div> <div>3%</div> <div>73% 19% • 5%</div> </div>

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
2	NAG	C	1500	-	-	-	X
3	SIA	B	1499	-	-	-	X
4	NAG	B	1502	-	-	-	X
5	NAG	B	1504	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13094 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 HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	4	0	0
			3882	2436	671	753	22			
1	B	490	Total	C	N	O	S	0	0	0
			3879	2434	670	753	22			
1	C	485	Total	C	N	O	S	0	0	0
			3844	2413	664	745	22			

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	3	Total	C	N	O	0	0
			46	25	2	19		
3	C	3	Total	C	N	O	0	0
			46	25	2	19		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	4	Total	C	N	O	0	0
			40	23	2	15		

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	4	Total	C	N	O	0	0
			50	28	2	20		

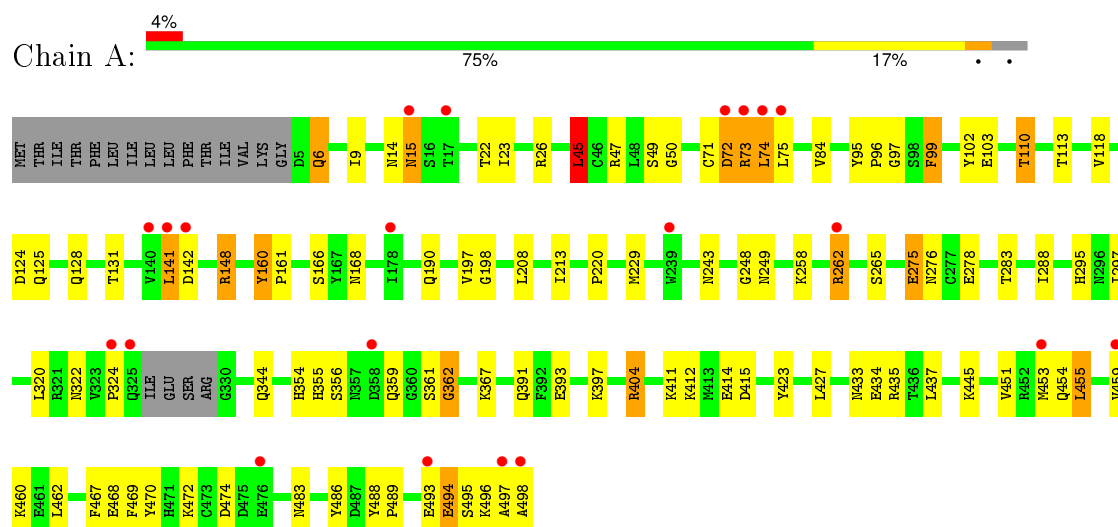
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	433	Total	O	0	0
			433	433		
7	B	406	Total	O	0	0
			406	406		
7	C	398	Total	O	0	0
			398	398		

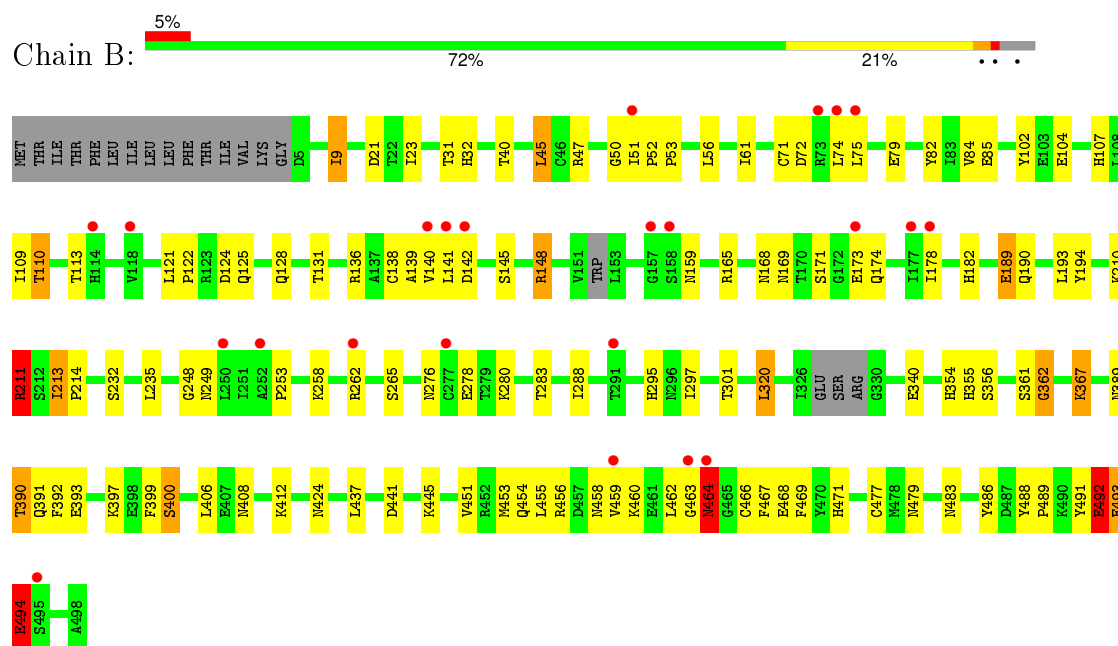
3 Residue-property plots

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.

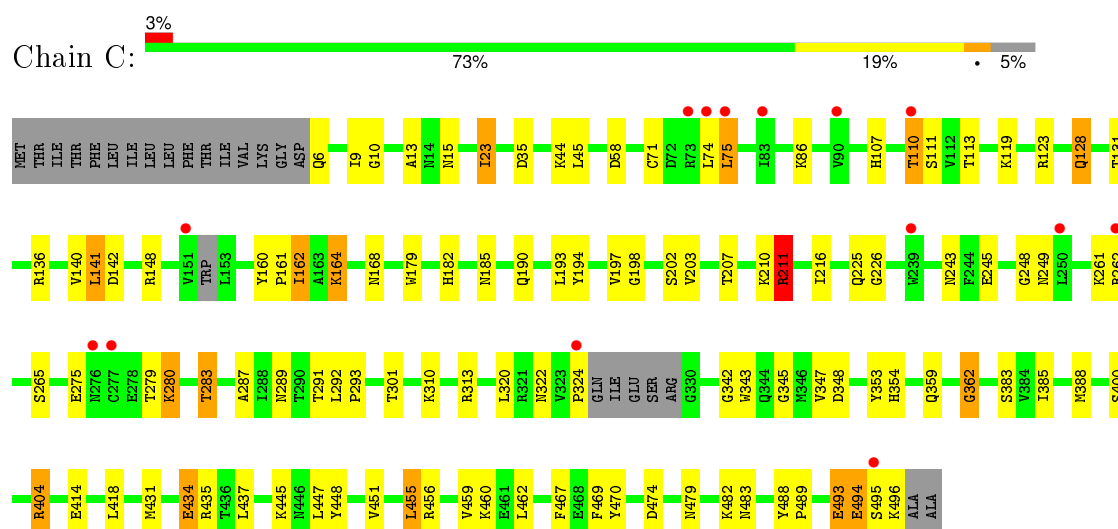
• Molecule 1: HEMAGGLUTININ



• Molecule 1: HEMAGGLUTININ



• Molecule 1: HEMAGGLUTININ



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.56Å 141.46Å 199.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.10) 99.8 (30.00-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.10Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.196 , 0.230 0.192 , 0.226	Depositor DCC
R_{free} test set	5776 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 115319 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13094	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, SIA, BMA, NAG, 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	1.02	2/3968 (0.1%)	0.79	2/5372 (0.0%)
1	B	1.04	5/3962 (0.1%)	0.82	6/5361 (0.1%)
1	C	0.94	2/3927 (0.1%)	0.77	3/5313 (0.1%)
All	All	1.00	9/11857 (0.1%)	0.79	11/16046 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	400	SER	CB-OG	6.17	1.50	1.42
1	B	464	ASN	CG-ND2	6.06	1.48	1.32
1	C	434	GLU	CD-OE1	5.84	1.32	1.25
1	B	102	TYR	CE2-CZ	5.42	1.45	1.38
1	A	160	TYR	CE2-CZ	5.32	1.45	1.38
1	B	173	GLU	CD-OE2	5.25	1.31	1.25
1	C	400	SER	CB-OG	5.23	1.49	1.42
1	B	104	GLU	CG-CD	5.06	1.59	1.51
1	A	103	GLU	CD-OE1	5.00	1.31	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	211	ARG	NE-CZ-NH1	-9.17	115.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	404	ARG	NE-CZ-NH1	-7.38	116.61	120.30
1	B	211	ARG	NE-CZ-NH1	-7.28	116.66	120.30
1	B	462	LEU	CB-CG-CD2	-7.04	99.03	111.00
1	C	23	ILE	CG1-CB-CG2	-6.26	97.62	111.40
1	B	464	ASN	CB-CA-C	-5.81	98.78	110.40
1	B	493	GLU	N-CA-C	-5.80	95.33	111.00
1	B	441	ASP	CB-CG-OD1	5.74	123.47	118.30
1	C	211	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	A	45	LEU	CA-CB-CG	5.33	127.56	115.30
1	B	189	GLU	OE1-CD-OE2	-5.04	117.25	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	492	GLU	Peptide

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	3882	0	3742	104	0
1	B	3879	0	3749	130	0
1	C	3844	0	3718	126	0
2	A	28	0	26	6	0
2	C	14	0	13	3	0
3	B	46	0	40	5	0
3	C	46	0	40	6	0
4	B	28	0	25	7	0
5	B	40	0	33	7	0
6	C	50	0	43	6	0
7	A	433	0	0	21	0
7	B	406	0	0	27	0
7	C	398	0	0	29	0
All	All	13094	0	11429	362	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 16.

All (362) 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:C:483:ASN:HD21	6:C:1501:NAG:C1	1.51	1.21
1:B:168:ASN:HD21	4:B:1502:NAG:C1	1.56	1.19
1:C:168:ASN:HD21	2:C:1500:NAG:C1	1.58	1.17
1:B:477:CYS:SG	7:B:2394:HOH:O	2.04	1.13
1:A:148:ARG:HG2	1:A:148:ARG:HH11	1.03	1.09
1:A:445:LYS:HG2	7:A:2392:HOH:O	1.52	1.09
7:B:2347:HOH:O	1:C:431:MET:SD	2.10	1.07
1:B:459:VAL:HG22	1:B:469:PHE:HA	1.39	1.05
1:B:464:ASN:ND2	1:B:466:CYS:SG	2.30	1.03
1:C:202:SER:OG	1:C:211:ARG:NH1	1.93	1.01
1:C:483:ASN:ND2	6:C:1501:NAG:C1	2.25	0.99
1:B:459:VAL:HG11	1:B:467:PHE:HB3	1.46	0.97
1:B:463:GLY:C	1:B:464:ASN:OD1	2.02	0.96
1:B:148:ARG:HD2	7:B:2075:HOH:O	1.66	0.94
1:C:190:GLN:HE22	1:C:249:ASN:HD21	1.12	0.94
1:A:459:VAL:HG11	1:A:467:PHE:HB3	1.47	0.93
1:A:110:THR:CG2	1:A:265:SER:H	1.83	0.92
1:A:148:ARG:HG2	1:A:148:ARG:NH1	1.83	0.91
1:C:148:ARG:CD	7:C:2134:HOH:O	2.19	0.91
1:C:211:ARG:HH11	1:C:211:ARG:HB2	1.36	0.91
1:B:453:MET:SD	7:B:2364:HOH:O	2.28	0.90
1:B:168:ASN:ND2	4:B:1502:NAG:C1	2.35	0.89
1:A:14:ASN:HA	1:A:344:GLN:HE21	1.34	0.89
1:A:434:GLU:HG2	7:C:2340:HOH:O	1.73	0.88
1:B:459:VAL:HG13	1:B:468:GLU:O	1.75	0.86
1:C:148:ARG:HD3	7:C:2134:HOH:O	1.74	0.86
1:A:496:LYS:HG2	7:A:2426:HOH:O	1.74	0.85
1:B:113:THR:HG23	1:B:262:ARG:HB2	1.59	0.85
1:C:211:ARG:HH11	1:C:211:ARG:CB	1.89	0.85
1:B:464:ASN:HD21	1:B:466:CYS:CB	1.89	0.85
1:B:110:THR:CG2	1:B:265:SER:H	1.90	0.85
1:C:148:ARG:NE	7:C:2134:HOH:O	2.11	0.84
1:A:470:TYR:HB3	1:A:496:LYS:H	1.42	0.84
1:C:168:ASN:ND2	2:C:1500:NAG:C1	2.41	0.83
1:C:211:ARG:HH11	1:C:211:ARG:CG	1.89	0.83
1:B:390:THR:C	7:B:2310:HOH:O	2.16	0.82
5:B:1504:NAG:H83	5:B:1504:NAG:H3	1.60	0.82
1:A:470:TYR:HB3	1:A:496:LYS:N	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:THR:CG2	1:C:265:SER:H	1.93	0.81
1:C:202:SER:HG	1:C:211:ARG:HH12	1.26	0.81
1:A:72:ASP:HA	7:A:2067:HOH:O	1.79	0.81
1:C:141:LEU:N	1:C:142:ASP:HA	1.96	0.81
1:B:211:ARG:NH1	1:C:216:ILE:O	2.13	0.81
1:A:148:ARG:CG	1:A:148:ARG:HH11	1.89	0.80
1:B:124:ASP:OD2	7:B:2126:HOH:O	1.99	0.79
1:C:262:ARG:HG2	1:C:262:ARG:O	1.82	0.79
1:A:278:GLU:HB2	7:A:2283:HOH:O	1.81	0.79
1:C:35:ASP:OD1	7:C:2031:HOH:O	2.01	0.78
1:B:168:ASN:HD21	4:B:1502:NAG:C2	1.94	0.78
1:C:493:GLU:C	1:C:494:GLU:HG3	2.02	0.78
1:B:464:ASN:HD21	1:B:466:CYS:HB2	1.48	0.78
1:C:140:VAL:C	1:C:142:ASP:HA	2.05	0.77
1:B:389:ASN:OD1	7:B:2310:HOH:O	2.02	0.77
1:A:190:GLN:HE22	1:A:249:ASN:HD21	1.29	0.77
1:A:15:ASN:ND2	7:A:2008:HOH:O	2.18	0.77
3:C:1499:NAG:O6	7:C:2386:HOH:O	2.03	0.76
1:A:168:ASN:HD21	2:A:1500:NAG:C5	1.98	0.76
1:A:168:ASN:ND2	2:A:1500:NAG:O5	2.15	0.75
1:A:445:LYS:CG	7:A:2392:HOH:O	2.16	0.74
1:B:190:GLN:HE22	1:B:249:ASN:HD21	1.33	0.74
1:C:483:ASN:ND2	6:C:1501:NAG:H83	2.03	0.73
1:A:453:MET:SD	7:A:2398:HOH:O	2.47	0.72
1:A:110:THR:HG21	1:A:265:SER:H	1.53	0.72
1:C:6:GLN:N	7:C:2002:HOH:O	2.21	0.72
1:C:459:VAL:HG21	1:C:467:PHE:HB3	1.71	0.72
1:B:340:GLU:OE1	7:B:2284:HOH:O	2.08	0.71
1:C:141:LEU:O	7:C:2125:HOH:O	2.08	0.71
1:A:141:LEU:N	1:A:142:ASP:HA	2.06	0.71
1:A:278:GLU:HG3	7:A:2285:HOH:O	1.92	0.70
1:B:483:ASN:ND2	5:B:1504:NAG:O5	2.23	0.69
1:A:354:HIS:HA	1:A:362:GLY:O	1.92	0.69
1:B:397:LYS:NZ	7:B:2316:HOH:O	2.25	0.69
1:C:23:ILE:HD11	1:C:431:MET:HG3	1.73	0.68
1:B:488:TYR:HB3	1:B:489:PRO:HD3	1.75	0.68
1:A:483:ASN:HD21	2:A:1499:NAG:C1	2.07	0.68
1:C:459:VAL:HG23	1:C:469:PHE:HA	1.76	0.68
1:A:455:LEU:HG	1:A:459:VAL:HG21	1.74	0.68
1:B:189:GLU:OE2	3:B:1499:SIA:C9	2.42	0.68
1:B:40:THR:O	7:B:2047:HOH:O	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ASP:OD2	7:B:2023:HOH:O	2.12	0.67
1:A:208:LEU:HD12	7:A:2211:HOH:O	1.94	0.67
1:B:459:VAL:HG12	1:B:460:LYS:N	2.09	0.67
1:B:459:VAL:HG13	1:B:468:GLU:C	2.15	0.67
2:A:1500:NAG:O3	7:A:2433:HOH:O	2.13	0.67
3:B:1499:SIA:H6	3:B:1499:SIA:O1B	1.95	0.66
6:C:1504:MAN:O2	7:C:2394:HOH:O	2.11	0.66
1:C:148:ARG:HH11	1:C:148:ARG:HG2	1.59	0.66
1:A:355:HIS:CE1	1:A:362:GLY:HA2	2.30	0.66
1:C:128:GLN:HB3	7:C:2114:HOH:O	1.94	0.66
1:B:141:LEU:N	1:B:142:ASP:HA	2.11	0.66
1:C:324:PRO:O	7:C:2257:HOH:O	2.12	0.66
1:A:9:ILE:HD11	1:A:451:VAL:HG21	1.76	0.66
1:B:491:TYR:C	1:B:492:GLU:OE1	2.35	0.66
1:B:72:ASP:OD1	7:B:2075:HOH:O	2.13	0.65
1:A:262:ARG:O	1:A:262:ARG:HG2	1.95	0.65
1:B:493:GLU:O	1:B:494:GLU:HB2	1.96	0.65
1:C:110:THR:HG21	1:C:265:SER:H	1.59	0.65
1:B:355:HIS:O	1:B:361:SER:HB2	1.96	0.65
1:A:47:ARG:NH1	7:A:2042:HOH:O	2.28	0.65
1:C:404:ARG:NH1	7:C:2317:HOH:O	2.29	0.65
1:C:207:THR:OG1	7:C:2171:HOH:O	2.10	0.63
1:C:211:ARG:NH1	1:C:211:ARG:CG	2.61	0.63
1:C:107:HIS:HE1	7:C:2094:HOH:O	1.81	0.62
1:B:400:SER:HB3	7:B:2321:HOH:O	1.99	0.62
1:A:414:GLU:HG3	7:A:2150:HOH:O	1.99	0.62
1:A:110:THR:HG23	1:A:265:SER:H	1.65	0.62
1:C:482:LYS:HE3	7:C:2370:HOH:O	1.99	0.62
1:B:262:ARG:HH11	1:B:262:ARG:HB3	1.65	0.62
1:C:211:ARG:NH1	1:C:211:ARG:HB2	2.11	0.61
1:B:74:LEU:O	1:B:74:LEU:HD23	2.00	0.61
1:C:162:ILE:HD13	1:C:164:LYS:HE3	1.81	0.61
1:B:463:GLY:O	1:B:464:ASN:OD1	2.18	0.61
1:B:110:THR:HG23	1:B:265:SER:HB3	1.81	0.61
1:C:168:ASN:HD21	2:C:1500:NAG:C2	2.11	0.61
1:B:464:ASN:OD1	1:B:464:ASN:N	2.32	0.61
1:B:174:GLN:OE1	1:B:235:LEU:HD13	2.01	0.61
1:C:494:GLU:O	1:C:496:LYS:N	2.34	0.61
1:C:128:GLN:HG3	1:C:161:PRO:HG2	1.83	0.60
1:C:455:LEU:HD23	1:C:459:VAL:HG11	1.82	0.60
5:B:1504:NAG:C8	5:B:1504:NAG:H3	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:ASN:ND2	1:B:466:CYS:HB2	2.16	0.60
1:B:464:ASN:ND2	1:B:466:CYS:CB	2.64	0.60
1:C:140:VAL:HG12	1:C:141:LEU:HB2	1.83	0.60
1:A:99:PHE:HB3	1:A:102:TYR:HB2	1.84	0.60
1:B:459:VAL:CG1	1:B:460:LYS:N	2.64	0.59
1:B:391:GLN:N	7:B:2310:HOH:O	2.32	0.59
1:B:492:GLU:OE1	1:B:492:GLU:N	2.34	0.59
1:C:160:TYR:CZ	1:C:248:GLY:HA2	2.38	0.59
1:A:110:THR:CG2	1:A:265:SER:N	2.61	0.59
1:A:71:CYS:O	1:A:74:LEU:HB2	2.03	0.59
1:B:47:ARG:HH12	1:B:276:ASN:HA	1.66	0.59
1:B:110:THR:HG21	1:B:265:SER:H	1.68	0.59
1:C:479:ASN:ND2	7:C:2370:HOH:O	2.36	0.59
1:B:141:LEU:HD22	7:B:2138:HOH:O	2.02	0.58
1:A:74:LEU:O	1:A:74:LEU:HD23	2.03	0.58
1:B:171:SER:HB2	1:B:258:LYS:HD2	1.84	0.58
3:C:1497:SIA:O7	3:C:1497:SIA:H113	2.04	0.57
1:A:496:LYS:O	1:A:497:ALA:HB3	2.04	0.57
1:C:488:TYR:HB3	1:C:489:PRO:HD3	1.86	0.57
1:B:85:GLU:OE2	7:B:2081:HOH:O	2.18	0.57
1:A:110:THR:HG23	1:A:265:SER:N	2.20	0.57
1:A:14:ASN:CA	1:A:344:GLN:HE21	2.12	0.57
1:C:128:GLN:NE2	7:C:2114:HOH:O	2.29	0.57
1:C:182:HIS:CD2	1:C:194:TYR:OH	2.59	0.56
1:C:74:LEU:O	1:C:75:LEU:HB2	2.03	0.56
1:C:494:GLU:C	1:C:496:LYS:H	2.08	0.56
1:B:107:HIS:HE1	7:B:2230:HOH:O	1.88	0.56
1:A:404:ARG:NH1	7:A:2370:HOH:O	2.25	0.56
1:A:295:HIS:HD2	1:A:297:ILE:H	1.52	0.55
1:B:424:ASN:ND2	7:B:2344:HOH:O	1.92	0.55
1:C:225:GLN:HE22	3:C:1498:GAL:H62	1.71	0.55
1:C:493:GLU:C	1:C:493:GLU:OE2	2.45	0.55
1:B:492:GLU:HA	1:B:494:GLU:HB2	1.88	0.55
1:A:488:TYR:HB3	1:A:489:PRO:HD3	1.89	0.55
1:A:397:LYS:NZ	1:B:408:ASN:HD21	2.05	0.55
1:C:185:ASN:HD21	1:C:226:GLY:C	2.11	0.55
1:C:211:ARG:HH11	1:C:211:ARG:HG3	1.71	0.55
1:B:47:ARG:NH1	1:B:276:ASN:HA	2.22	0.55
1:B:320:LEU:HD23	1:B:320:LEU:H	1.72	0.55
1:C:123:ARG:HD3	7:C:2107:HOH:O	2.07	0.55
1:B:295:HIS:HD2	1:B:297:ILE:H	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:ARG:NH2	1:C:460:LYS:HG2	2.21	0.54
1:A:393:GLU:HB3	1:B:412:LYS:HE2	1.90	0.54
1:A:6:GLN:HB3	1:A:468:GLU:HA	1.89	0.54
1:C:313:ARG:NH2	7:C:2250:HOH:O	2.40	0.54
1:A:168:ASN:HD21	2:A:1500:NAG:C1	2.19	0.54
1:A:355:HIS:O	1:A:361:SER:HB2	2.08	0.54
1:B:400:SER:CB	7:B:2321:HOH:O	2.54	0.54
1:C:320:LEU:H	1:C:320:LEU:HD23	1.73	0.54
1:C:58:ASP:HB3	1:C:86:LYS:HD2	1.90	0.54
1:B:79:GLU:HG3	1:B:113:THR:HA	1.88	0.54
1:A:468:GLU:OE2	7:A:2413:HOH:O	2.17	0.54
1:C:353:TYR:OH	1:C:447:LEU:HD11	2.09	0.53
1:A:14:ASN:HA	1:A:344:GLN:NE2	2.16	0.53
1:B:399:PHE:CE1	1:B:406:LEU:HG	2.43	0.53
1:B:140:VAL:HG13	1:B:141:LEU:HD23	1.89	0.53
1:A:470:TYR:CD1	1:A:496:LYS:HA	2.44	0.53
1:B:463:GLY:O	1:B:464:ASN:CG	2.46	0.53
1:B:262:ARG:NH1	1:B:262:ARG:HB3	2.23	0.53
1:B:479:ASN:HB3	5:B:1504:NAG:H61	1.91	0.53
1:C:9:ILE:HG13	1:C:448:TYR:HA	1.91	0.53
1:A:472:LYS:NZ	7:A:2414:HOH:O	2.41	0.53
3:C:1497:SIA:H112	3:C:1499:NAG:H83	1.90	0.53
1:A:397:LYS:HZ1	1:B:408:ASN:HD21	1.56	0.53
1:A:95:TYR:CD2	1:A:96:PRO:HD2	2.45	0.52
1:C:456:ARG:NH1	7:C:2356:HOH:O	2.36	0.52
1:B:458:ASN:OD1	1:B:494:GLU:HG2	2.09	0.52
1:A:213:ILE:O	1:A:213:ILE:HG13	2.08	0.52
1:C:293:PRO:HG3	1:C:385:ILE:HA	1.91	0.52
1:B:56:LEU:HD23	1:B:74:LEU:HD21	1.91	0.52
1:B:460:LYS:NZ	7:B:2373:HOH:O	2.11	0.52
1:C:148:ARG:CG	1:C:148:ARG:HH11	2.22	0.52
1:C:197:VAL:HG12	1:C:198:GLY:N	2.25	0.52
1:C:110:THR:CG2	1:C:265:SER:N	2.69	0.52
1:A:45:LEU:HD21	1:A:84:VAL:HG21	1.91	0.52
1:B:71:CYS:O	1:B:74:LEU:HB2	2.10	0.51
1:B:493:GLU:O	1:B:494:GLU:CB	2.52	0.51
1:A:460:LYS:HE3	1:C:456:ARG:HH22	1.76	0.51
1:C:359:GLN:OE1	1:C:474:ASP:HB2	2.10	0.51
1:A:462:LEU:HD22	1:A:462:LEU:H	1.75	0.51
1:B:445:LYS:HE3	7:B:2280:HOH:O	2.11	0.51
1:B:463:GLY:C	1:B:464:ASN:CG	2.70	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:THR:CG2	1:B:262:ARG:HB2	2.37	0.51
1:A:454:GLN:NE2	1:A:486:TYR:H	2.08	0.51
1:C:483:ASN:HD22	6:C:1501:NAG:H83	1.74	0.50
1:C:10:GLY:HA3	1:C:343:TRP:CZ3	2.46	0.50
1:B:492:GLU:N	7:B:2395:HOH:O	2.44	0.50
1:B:110:THR:CG2	1:B:265:SER:N	2.69	0.50
1:B:45:LEU:HD12	1:B:82:TYR:OH	2.12	0.50
1:C:451:VAL:HG12	1:C:455:LEU:HD22	1.94	0.50
1:B:283:THR:HG22	1:B:301:THR:HG22	1.93	0.50
1:A:26:ARG:NH2	1:C:383:SER:OG	2.39	0.50
1:C:111:SER:HB2	1:C:265:SER:HB2	1.93	0.49
1:C:494:GLU:C	1:C:496:LYS:N	2.65	0.49
1:C:434:GLU:CD	7:C:2336:HOH:O	2.50	0.49
3:B:1500:GAL:O5	3:B:1501:NAG:O3	2.26	0.49
1:C:110:THR:HG23	1:C:265:SER:HB3	1.93	0.49
1:B:392:PHE:O	1:B:393:GLU:HG3	2.12	0.49
1:A:128:GLN:HB3	1:A:161:PRO:HG2	1.94	0.49
1:B:463:GLY:O	1:B:464:ASN:CB	2.61	0.49
1:C:262:ARG:NH2	7:C:2216:HOH:O	2.45	0.49
1:A:276:ASN:HA	7:A:2042:HOH:O	2.13	0.49
1:B:136:ARG:HG2	1:B:136:ARG:HH11	1.78	0.49
1:A:248:GLY:C	1:A:249:ASN:HD22	2.16	0.49
1:C:462:LEU:N	1:C:462:LEU:HD22	2.28	0.49
1:B:75:LEU:HD23	1:B:75:LEU:O	2.13	0.49
1:A:455:LEU:CG	1:A:459:VAL:HG21	2.42	0.49
1:C:310:LYS:HG3	1:C:418:LEU:HD21	1.95	0.48
1:B:483:ASN:HD21	5:B:1504:NAG:C1	2.25	0.48
1:B:138:CYS:O	1:B:145:SER:HB3	2.12	0.48
1:B:354:HIS:HA	1:B:362:GLY:O	2.13	0.48
1:B:211:ARG:CG	1:B:211:ARG:HH11	2.25	0.48
1:C:74:LEU:O	1:C:75:LEU:CB	2.61	0.48
1:C:345:GLY:O	7:C:2273:HOH:O	2.20	0.48
1:C:211:ARG:HG3	1:C:211:ARG:NH1	2.27	0.48
1:A:493:GLU:O	1:A:494:GLU:HB2	2.13	0.48
1:A:166:SER:HB3	1:A:243:ASN:OD1	2.13	0.48
1:C:289:ASN:ND2	7:C:2231:HOH:O	2.39	0.48
1:B:494:GLU:HA	1:B:494:GLU:OE1	2.13	0.48
1:C:280:LYS:HD2	1:C:280:LYS:N	2.29	0.48
1:C:459:VAL:CG2	1:C:467:PHE:HB3	2.41	0.47
1:B:213:ILE:HG13	1:B:213:ILE:O	2.13	0.47
1:A:72:ASP:C	1:A:74:LEU:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:VAL:CG1	1:B:141:LEU:HD23	2.44	0.47
1:B:9:ILE:HD11	1:B:451:VAL:HG21	1.97	0.47
1:C:354:HIS:HA	1:C:362:GLY:O	2.14	0.47
1:C:136:ARG:HD3	7:C:2122:HOH:O	2.14	0.47
1:C:279:THR:OG1	1:C:287:ALA:HB1	2.15	0.47
1:C:248:GLY:C	1:C:249:ASN:HD22	2.18	0.47
1:C:110:THR:HG23	1:C:265:SER:N	2.30	0.47
1:C:493:GLU:C	1:C:494:GLU:CG	2.80	0.47
1:A:124:ASP:OD1	1:A:125:GLN:HG3	2.15	0.47
1:A:220:PRO:HD3	1:C:243:ASN:HD22	1.80	0.47
1:A:278:GLU:CG	7:A:2285:HOH:O	2.57	0.47
1:B:182:HIS:CD2	1:B:194:TYR:OH	2.68	0.47
1:C:470:TYR:HB3	1:C:494:GLU:O	2.15	0.46
1:B:45:LEU:HD21	1:B:84:VAL:HG21	1.97	0.46
5:B:1504:NAG:H83	5:B:1505:NAG:H83	1.97	0.46
1:A:113:THR:CG2	1:A:262:ARG:HB3	2.46	0.46
1:A:496:LYS:O	1:A:497:ALA:CB	2.64	0.46
1:B:210:LYS:NZ	1:B:232:SER:OG	2.48	0.46
1:C:140:VAL:O	1:C:142:ASP:HA	2.14	0.46
1:C:44:LYS:HG2	1:C:275:GLU:OE1	2.15	0.46
1:C:113:THR:CG2	1:C:262:ARG:HB2	2.46	0.46
1:A:6:GLN:NE2	1:A:356:SER:HB3	2.31	0.46
1:B:178:ILE:O	1:B:253:PRO:HB3	2.16	0.46
1:A:455:LEU:HG	1:A:459:VAL:CG2	2.44	0.46
1:A:22:THR:HG22	1:A:433:ASN:HB3	1.98	0.46
1:A:355:HIS:O	1:A:361:SER:CB	2.63	0.46
1:A:275:GLU:O	1:A:275:GLU:OE2	2.34	0.46
1:C:193:LEU:HD22	3:C:1497:SIA:H111	1.97	0.46
1:A:411:LYS:NZ	1:A:415:ASP:OD2	2.50	0.45
1:B:168:ASN:ND2	4:B:1502:NAG:C2	2.74	0.45
1:B:320:LEU:N	1:B:320:LEU:HD23	2.31	0.45
1:A:462:LEU:HD22	1:A:462:LEU:N	2.31	0.45
7:A:2075:HOH:O	1:B:213:ILE:HD11	2.16	0.45
1:C:445:LYS:NZ	7:C:2344:HOH:O	2.36	0.45
1:B:121:LEU:O	1:B:122:PRO:C	2.54	0.45
1:A:322:ASN:O	1:A:324:PRO:HD3	2.17	0.45
1:B:159:ASN:ND2	7:B:2152:HOH:O	2.48	0.45
1:C:9:ILE:HD12	1:C:447:LEU:HG	1.99	0.45
1:B:53:PRO:HG3	1:B:82:TYR:CZ	2.51	0.45
1:A:494:GLU:N	7:A:2423:HOH:O	2.42	0.45
1:A:459:VAL:CG1	1:A:467:PHE:HB3	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ILE:HD12	1:B:23:ILE:HG23	1.62	0.45
1:C:283:THR:HG22	1:C:301:THR:HG22	1.99	0.45
1:A:148:ARG:CG	1:A:148:ARG:NH1	2.57	0.45
1:B:454:GLN:NE2	1:B:486:TYR:H	2.15	0.45
1:C:179:TRP:CE2	1:C:203:VAL:HG21	2.52	0.45
1:A:50:GLY:HA2	1:A:278:GLU:OE1	2.16	0.44
1:C:182:HIS:HD2	1:C:194:TYR:OH	1.99	0.44
1:A:359:GLN:OE1	1:A:474:ASP:HB2	2.17	0.44
1:A:495:SER:O	1:A:498:ALA:O	2.35	0.44
1:A:262:ARG:O	1:A:262:ARG:CG	2.65	0.44
1:C:162:ILE:HD11	1:C:245:GLU:CG	2.47	0.44
3:C:1497:SIA:O1B	3:C:1497:SIA:H6	2.17	0.44
1:C:185:ASN:HD21	1:C:226:GLY:CA	2.31	0.44
1:C:470:TYR:CZ	1:C:496:LYS:HG2	2.53	0.43
1:B:295:HIS:CD2	1:B:297:ILE:H	2.36	0.43
1:B:125:GLN:NE2	1:B:165:ARG:NH2	2.66	0.43
1:C:13:ALA:HB2	1:C:342:GLY:HA3	2.00	0.43
1:B:459:VAL:CG2	1:B:469:PHE:CD1	3.01	0.43
1:A:459:VAL:HG12	1:A:460:LYS:N	2.34	0.43
1:A:295:HIS:CD2	1:A:297:ILE:H	2.34	0.43
1:A:73:ARG:O	1:A:75:LEU:N	2.52	0.43
1:C:261:LYS:HB3	1:C:261:LYS:HE3	1.77	0.43
1:A:110:THR:HG23	1:A:265:SER:HB3	2.00	0.43
1:C:119:LYS:NZ	7:C:2104:HOH:O	2.50	0.43
1:C:322:ASN:C	1:C:324:PRO:HD3	2.38	0.43
1:C:10:GLY:HA3	1:C:343:TRP:CH2	2.54	0.43
1:B:483:ASN:ND2	5:B:1504:NAG:C1	2.82	0.43
1:C:15:ASN:ND2	7:C:2011:HOH:O	2.51	0.43
1:A:435:ARG:HH11	1:C:435:ARG:NH1	2.16	0.43
1:A:435:ARG:NE	7:A:2386:HOH:O	2.42	0.42
1:C:141:LEU:N	1:C:142:ASP:CA	2.77	0.42
1:C:71:CYS:O	1:C:74:LEU:HB2	2.19	0.42
1:C:483:ASN:ND2	6:C:1501:NAG:C2	2.81	0.42
1:B:56:LEU:CD2	1:B:74:LEU:HD21	2.50	0.42
1:C:185:ASN:HD21	1:C:226:GLY:HA3	1.84	0.42
1:B:367:LYS:HA	1:B:367:LYS:HD2	1.59	0.42
1:B:460:LYS:CE	7:B:2373:HOH:O	2.64	0.42
1:B:136:ARG:HA	1:B:139:ALA:HB2	2.01	0.42
1:A:197:VAL:HG12	1:A:198:GLY:N	2.34	0.42
1:A:160:TYR:CZ	1:A:248:GLY:HA2	2.54	0.42
1:B:280:LYS:HA	1:B:280:LYS:HD3	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:LEU:HA	1:C:293:PRO:HD3	1.87	0.41
1:C:462:LEU:H	1:C:462:LEU:HD22	1.84	0.41
1:B:51:ILE:HA	1:B:52:PRO:HD3	1.77	0.41
1:A:118:VAL:HG21	1:A:258:LYS:HD2	2.02	0.41
1:B:397:LYS:HD3	7:B:2316:HOH:O	2.20	0.41
1:B:210:LYS:HE2	7:B:2199:HOH:O	2.20	0.41
1:A:97:GLY:HA3	1:A:229:MET:O	2.20	0.41
4:B:1503:NAG:H81	7:B:2405:HOH:O	2.19	0.41
1:B:168:ASN:HD21	4:B:1502:NAG:H2	1.80	0.41
1:B:193:LEU:HD21	3:B:1499:SIA:H113	2.02	0.41
1:A:498:ALA:HB2	7:A:2190:HOH:O	2.19	0.41
1:B:50:GLY:N	1:B:278:GLU:OE2	2.35	0.41
1:A:168:ASN:ND2	2:A:1500:NAG:C5	2.77	0.41
1:B:248:GLY:C	1:B:249:ASN:HD22	2.22	0.41
1:C:164:LYS:HB2	1:C:164:LYS:HE3	1.62	0.41
1:B:213:ILE:HA	1:B:214:PRO:HD3	1.91	0.41
1:B:491:TYR:O	1:B:494:GLU:OE2	2.38	0.41
1:B:211:ARG:NH1	1:B:211:ARG:CG	2.83	0.41
1:C:35:ASP:CG	7:C:2031:HOH:O	2.55	0.41
1:B:471:HIS:HD2	1:B:494:GLU:OE2	2.04	0.41
1:C:459:VAL:HG23	1:C:469:PHE:CA	2.48	0.41
1:C:310:LYS:HB3	1:C:310:LYS:HE2	1.94	0.41
1:A:412:LYS:HE3	1:C:414:GLU:OE2	2.21	0.41
1:A:423:TYR:CE1	1:C:388:MET:HE1	2.56	0.41
1:A:470:TYR:O	1:A:495:SER:HA	2.20	0.41
1:B:56:LEU:HA	1:B:74:LEU:HD11	2.03	0.41
1:B:168:ASN:ND2	4:B:1502:NAG:O5	2.48	0.40
1:A:459:VAL:HG22	1:A:469:PHE:HA	2.02	0.40
1:B:356:SER:HA	1:B:361:SER:HB3	2.02	0.40
1:C:353:TYR:CD2	1:C:482:LYS:HG2	2.55	0.40
1:A:23:ILE:HD12	1:A:23:ILE:HG23	1.65	0.40
1:A:288:ILE:HG12	1:A:297:ILE:HD13	2.04	0.40
1:B:61:ILE:HG21	1:B:109:ILE:HD11	2.04	0.40
3:B:1499:SIA:C6	3:B:1499:SIA:O1B	2.65	0.40
1:B:31:THR:OG1	1:B:32:HIS:HD2	2.04	0.40
1:C:148:ARG:CG	1:C:148:ARG:NH1	2.85	0.40
1:B:288:ILE:HG12	1:B:297:ILE:HD13	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	A	486/509 (96%)	465 (96%)	17 (4%)	4 (1%)	24	17
1	B	484/509 (95%)	462 (96%)	18 (4%)	4 (1%)	24	17
1	C	479/509 (94%)	452 (94%)	24 (5%)	3 (1%)	30	24
All	All	1449/1527 (95%)	1379 (95%)	59 (4%)	11 (1%)	24	17

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	ASP
1	A	494	GLU
1	B	464	ASN
1	B	494	GLU
1	C	495	SER
1	A	74	LEU
1	C	75	LEU
1	A	362	GLY
1	B	362	GLY
1	C	362	GLY
1	B	169	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	A	427/447 (96%)	408 (96%)	19 (4%)	35	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	428/447 (96%)	413 (96%)	15 (4%)	43	44
1	C	425/447 (95%)	406 (96%)	19 (4%)	34	32
All	All	1280/1341 (96%)	1227 (96%)	53 (4%)	37	36

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	15	ASN
1	A	45	LEU
1	A	49	SER
1	A	73	ARG
1	A	99	PHE
1	A	110	THR
1	A	131	THR
1	A	141	LEU
1	A	148	ARG
1	A	262	ARG
1	A	275	GLU
1	A	283	THR
1	A	320	LEU
1	A	367	LYS
1	A	391	GLN
1	A	427	LEU
1	A	437	LEU
1	A	455	LEU
1	B	9	ILE
1	B	45	LEU
1	B	110	THR
1	B	128	GLN
1	B	131	THR
1	B	148	ARG
1	B	211	ARG
1	B	213	ILE
1	B	320	LEU
1	B	367	LYS
1	B	390	THR
1	B	437	LEU
1	B	455	LEU
1	B	492	GLU
1	B	494	GLU

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Mol	Chain	Res	Type
1	C	45	LEU
1	C	110	THR
1	C	128	GLN
1	C	131	THR
1	C	141	LEU
1	C	162	ILE
1	C	164	LYS
1	C	210	LYS
1	C	211	ARG
1	C	280	LYS
1	C	283	THR
1	C	291	THR
1	C	347	VAL
1	C	348	ASP
1	C	404	ARG
1	C	437	LEU
1	C	455	LEU
1	C	493	GLU
1	C	494	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	32	HIS
1	A	91	ASN
1	A	182	HIS
1	A	249	ASN
1	A	295	HIS
1	A	344	GLN
1	A	382	ASN
1	A	389	ASN
1	A	408	ASN
1	A	454	GLN
1	B	32	HIS
1	B	88	ASN
1	B	114	HIS
1	B	125	GLN
1	B	159	ASN
1	B	168	ASN
1	B	182	HIS
1	B	249	ASN

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Mol	Chain	Res	Type
1	B	295	HIS
1	B	382	ASN
1	B	408	ASN
1	B	454	GLN
1	B	479	ASN
1	C	32	HIS
1	C	100	ASN
1	C	128	GLN
1	C	143	ASN
1	C	168	ASN
1	C	182	HIS
1	C	185	ASN
1	C	243	ASN
1	C	249	ASN
1	C	382	ASN
1	C	408	ASN
1	C	454	GLN
1	C	479	ASN
1	C	483	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 ⓘ

Of 16 carbohydrates modelled in this entry, 1 is modelled with single atom - leaving 15 for Mogul analysis.

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	SIA	B	1499	1,3	16,20,21	0.70	0	18,28,31	1.72	3 (16%)
3	GAL	B	1500	3	11,11,12	0.52	0	14,15,17	1.77	4 (28%)
3	NAG	B	1501	3	15,15,15	1.10	1 (6%)	17,21,21	1.88	4 (23%)
4	NAG	B	1502	4	14,14,15	0.66	0	15,19,21	1.40	2 (13%)
4	NAG	B	1503	4	14,14,15	0.73	0	15,19,21	1.40	3 (20%)
5	NAG	B	1504	5	14,14,15	0.67	0	15,19,21	2.04	5 (33%)
5	NAG	B	1505	5	14,14,15	0.50	0	15,19,21	0.94	1 (6%)
5	BMA	B	1506	5	11,11,12	0.73	0	14,15,17	0.64	0
3	SIA	C	1497	3	16,20,21	0.94	1 (6%)	18,28,31	1.69	4 (22%)
3	GAL	C	1498	3	11,11,12	0.72	0	14,15,17	3.25	8 (57%)
3	NAG	C	1499	3	15,15,15	1.53	3 (20%)	17,21,21	3.31	11 (64%)
6	NAG	C	1501	6	14,14,15	0.53	0	15,19,21	1.64	2 (13%)
6	NAG	C	1502	6	14,14,15	0.61	0	15,19,21	1.02	0
6	BMA	C	1503	6	11,11,12	0.76	0	14,15,17	0.99	1 (7%)
6	MAN	C	1504	6	11,11,12	0.77	0	14,15,17	1.93	4 (28%)

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	SIA	B	1499	1,3	-	0/14/34/38	0/1/1/1
3	GAL	B	1500	3	-	0/2/19/22	0/1/1/1
3	NAG	B	1501	3	-	0/6/26/26	0/1/1/1
4	NAG	B	1502	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1503	4	-	0/6/23/26	0/1/1/1
5	NAG	B	1504	5	-	0/6/23/26	0/1/1/1
5	NAG	B	1505	5	-	0/6/23/26	0/1/1/1
5	BMA	B	1506	5	-	0/2/19/22	0/1/1/1
3	SIA	C	1497	3	-	0/14/34/38	0/1/1/1
3	GAL	C	1498	3	-	0/2/19/22	0/1/1/1
3	NAG	C	1499	3	-	0/6/26/26	0/1/1/1
6	NAG	C	1501	6	-	0/6/23/26	0/1/1/1
6	NAG	C	1502	6	-	0/6/23/26	0/1/1/1
6	BMA	C	1503	6	-	0/2/19/22	0/1/1/1
6	MAN	C	1504	6	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1497	SIA	O6-C6	-2.61	1.39	1.43
3	B	1501	NAG	C8-C7	2.17	1.54	1.50
3	C	1499	NAG	C1-C2	2.17	1.55	1.53
3	C	1499	NAG	C8-C7	2.68	1.55	1.50
3	C	1499	NAG	C2-N2	4.08	1.52	1.45

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1499	NAG	C6-C5-C4	-8.76	91.40	113.02
3	C	1498	GAL	C1-O5-C5	-7.63	102.57	112.25
3	C	1497	SIA	C3-C4-C5	-4.95	105.96	111.47
6	C	1501	NAG	C1-O5-C5	-4.83	106.12	112.25
3	B	1499	SIA	C7-C6-C5	-4.78	107.09	114.32
3	C	1498	GAL	C2-C3-C4	-4.73	103.00	111.04
3	C	1498	GAL	O6-C6-C5	-4.42	96.72	111.33
6	C	1504	MAN	O3-C3-C2	-4.36	102.11	110.00
3	C	1498	GAL	O2-C2-C1	-3.81	101.57	109.21
3	B	1501	NAG	C6-C5-C4	-3.72	103.85	113.02
3	C	1499	NAG	C4-C3-C2	-3.70	105.30	110.43
3	C	1499	NAG	C3-C2-N2	-3.46	103.51	110.66
4	B	1503	NAG	C2-N2-C7	-3.24	118.88	123.04
3	C	1499	NAG	O3-C3-C4	-3.13	103.28	110.34
5	B	1504	NAG	O7-C7-C8	-3.08	116.42	122.06
3	B	1499	SIA	C3-C4-C5	-3.04	108.08	111.47
3	B	1501	NAG	O3-C3-C2	-3.04	103.46	109.66
3	B	1499	SIA	O9-C9-C8	-2.99	104.60	111.10
3	C	1499	NAG	O3-C3-C2	-2.96	103.63	109.66
3	C	1498	GAL	C6-C5-C4	-2.96	105.72	113.02
3	C	1497	SIA	C7-C6-C5	-2.79	110.10	114.32
3	B	1500	GAL	C1-O5-C5	-2.73	108.78	112.25
3	B	1500	GAL	O3-C3-C4	-2.68	104.31	110.34
3	C	1498	GAL	O2-C2-C3	-2.65	104.79	110.12
3	B	1500	GAL	O3-C3-C2	-2.63	105.24	110.00
3	C	1498	GAL	O5-C5-C6	-2.58	101.76	107.35
4	B	1503	NAG	C4-C3-C2	-2.33	107.60	111.23
6	C	1501	NAG	O4-C4-C3	-2.29	105.17	110.34
3	C	1497	SIA	C4-C5-N5	-2.28	105.46	110.41
6	C	1503	BMA	C1-C2-C3	-2.26	106.86	109.54
5	B	1505	NAG	C2-N2-C7	-2.17	120.25	123.04
3	B	1500	GAL	O2-C2-C1	-2.16	104.87	109.21
3	C	1499	NAG	O5-C5-C4	-2.15	105.64	109.68
3	C	1498	GAL	C3-C4-C5	-2.14	106.47	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1499	NAG	O7-C7-C8	-2.12	118.17	122.06
3	B	1501	NAG	C4-C3-C2	-2.03	107.62	110.43
3	C	1497	SIA	O7-C7-C8	-2.00	103.70	108.75
4	B	1502	NAG	C1-O5-C5	-2.00	109.70	112.25
3	C	1499	NAG	O7-C7-N2	2.26	126.47	121.86
6	C	1504	MAN	C2-C3-C4	2.28	114.91	111.04
6	C	1504	MAN	C3-C4-C5	2.77	115.03	110.20
5	B	1504	NAG	C2-N2-C7	2.89	126.75	123.04
4	B	1503	NAG	C1-O5-C5	2.97	116.01	112.25
3	C	1499	NAG	O4-C4-C3	3.11	117.35	110.34
5	B	1504	NAG	C8-C7-N2	3.15	122.14	116.11
5	B	1504	NAG	C4-C3-C2	3.57	116.78	111.23
4	B	1502	NAG	C3-C4-C5	3.61	116.48	110.20
5	B	1504	NAG	C3-C4-C5	3.71	116.66	110.20
6	C	1504	MAN	C1-C2-C3	3.71	113.93	109.54
3	C	1499	NAG	C3-C4-C5	4.20	117.52	110.20
3	C	1499	NAG	O5-C5-C6	4.75	118.37	106.36
3	B	1501	NAG	O5-C5-C6	5.13	119.33	106.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1499	SIA	4	0
3	B	1500	GAL	1	0
3	B	1501	NAG	1	0
4	B	1502	NAG	6	0
4	B	1503	NAG	1	0
5	B	1504	NAG	7	0
5	B	1505	NAG	1	0
3	C	1497	SIA	4	0
3	C	1498	GAL	1	0
3	C	1499	NAG	2	0
6	C	1501	NAG	5	0
6	C	1504	MAN	1	0

5.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	1499	-	14,14,15	0.52	0	15,19,21	0.83	1 (6%)
2	NAG	A	1500	-	14,14,15	0.67	0	15,19,21	0.72	0
2	NAG	C	1500	-	14,14,15	0.63	0	15,19,21	1.01	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	1499	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1500	-	-	0/6/23/26	0/1/1/1
2	NAG	C	1500	-	-	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(°)	Ideal(°)
2	C	1500	NAG	C6-C5-C4	-2.24	107.49	113.02
2	A	1499	NAG	C1-O5-C5	2.32	115.19	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1499	NAG	1	0
2	A	1500	NAG	5	0
2	C	1500	NAG	3	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	490/509 (96%)	-0.01	21 (4%)	39 48	22, 36, 65, 153	1 (0%)
1	B	490/509 (96%)	0.06	23 (4%)	35 44	24, 38, 66, 139	0
1	C	485/509 (95%)	-0.01	14 (2%)	55 63	25, 39, 64, 145	0
All	All	1465/1527 (95%)	0.01	58 (3%)	42 51	22, 38, 66, 153	1 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	LEU	7.9
1	A	493	GLU	5.4
1	A	453	MET	5.3
1	B	74	LEU	5.0
1	A	73	ARG	4.8
1	B	141	LEU	4.5
1	B	262	ARG	4.4
1	B	73	ARG	4.3
1	A	72	ASP	4.2
1	B	140	VAL	4.1
1	A	262	ARG	4.1
1	C	73	ARG	4.1
1	A	74	LEU	3.9
1	C	75	LEU	3.7
1	C	83	ILE	3.7
1	A	142	ASP	3.7
1	A	324	PRO	3.6
1	B	463	GLY	3.5
1	B	75	LEU	3.4
1	A	178	ILE	3.4
1	A	498	ALA	3.3
1	C	151	VAL	3.2
1	C	262	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	75	LEU	3.2
1	A	325	GLN	3.1
1	B	178	ILE	3.1
1	A	459	VAL	3.0
1	C	74	LEU	3.0
1	C	276	ASN	3.0
1	A	15	ASN	2.9
1	C	495	SER	2.8
1	B	51	ILE	2.8
1	A	17	THR	2.8
1	B	158	SER	2.7
1	B	142	ASP	2.6
1	B	277	CYS	2.5
1	C	90	VAL	2.5
1	B	252	ALA	2.5
1	B	177	ILE	2.5
1	B	173	GLU	2.4
1	C	277	CYS	2.4
1	B	250	LEU	2.4
1	A	497	ALA	2.4
1	B	495	SER	2.4
1	C	250	LEU	2.3
1	B	464	ASN	2.3
1	B	459	VAL	2.3
1	C	324	PRO	2.3
1	A	358	ASP	2.2
1	C	239	TRP	2.2
1	C	110	THR	2.2
1	B	157	GLY	2.2
1	A	476	GLU	2.1
1	A	140	VAL	2.1
1	B	114	HIS	2.1
1	A	239	TRP	2.0
1	B	291	THR	2.0
1	B	118	VAL	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	B	1502	14/15	0.71	0.25	4.47	74,75,75,76	0
3	SIA	B	1499	20/21	0.88	0.19	2.51	60,65,72,73	0
6	NAG	C	1501	14/15	0.83	0.18	1.67	56,57,57,58	0
3	SIA	C	1497	20/21	0.95	0.11	-0.26	35,40,46,48	0
6	NAG	C	1502	14/15	0.90	0.18	-	55,56,56,56	0
3	NAG	B	1501	15/15	0.74	0.31	-	87,90,92,95	0
6	MAN	C	1504	11/12	0.75	0.20	-	56,56,56,57	0
4	NAG	B	1503	14/15	0.81	0.46	-	75,76,76,76	0
3	GAL	C	1498	11/12	0.79	0.20	-	47,55,58,58	0
6	BMA	C	1503	11/12	0.88	0.23	-	55,56,57,57	0
3	NAG	C	1499	15/15	0.69	0.40	-	62,65,66,69	0
5	BMA	B	1506	11/12	0.72	0.42	-	88,88,89,89	0
3	GAL	B	1500	11/12	0.88	0.32	-	73,80,83,83	0
5	BMA	B	1507	1/12	0.88	0.50	-	89,89,89,89	0
5	NAG	B	1504	14/15	0.65	0.37	-	86,88,88,88	0
5	NAG	B	1505	14/15	0.64	0.29	-	87,87,88,88	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	C	1500	14/15	0.84	0.23	2.60	61,63,63,63	0
2	NAG	A	1500	14/15	0.78	0.21	-	59,61,62,62	0
2	NAG	A	1499	14/15	0.74	0.26	-	92,94,95,95	0

6.5 Other polymers

There are no such residues in this entry.