



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:45 AM UTC

PDB ID : 4KPS / pdb_00004kps
Title : Structure and receptor binding specificity of the hemagglutinin H13 from avian influenza A virus H13N6
Authors : Lu, X.; Qi, J.; Shi, Y.; Gao, G.
Deposited on : 2013-05-14
Resolution : 2.59 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

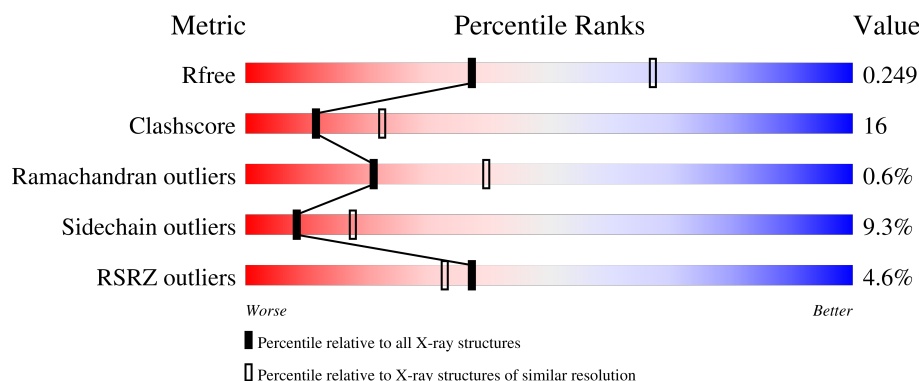
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	324	4% 70% 26% • •
1	C	324	5% 72% 25% •
1	E	324	4% 69% 27% •
2	B	165	4% 64% 32% •
2	D	165	6% 72% 24% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	165	7% 72% 24%
3	G	2	50% 50%
4	H	3	33% 33% 33%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11796 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	324	Total	C	N	O	S	0	0	0
			2555	1610	448	485	12			
1	C	324	Total	C	N	O	S	0	0	0
			2555	1610	448	485	12			
1	E	324	Total	C	N	O	S	0	0	0
			2555	1610	448	485	12			

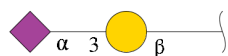
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	ILE	-	expression tag	UNP P13103
A	5	GLN	-	expression tag	UNP P13103
C	4	ILE	-	expression tag	UNP P13103
C	5	GLN	-	expression tag	UNP P13103
E	4	ILE	-	expression tag	UNP P13103
E	5	GLN	-	expression tag	UNP P13103

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	165	Total	C	N	O	S	0	0	0
			1312	811	229	265	7			
2	D	165	Total	C	N	O	S	0	0	0
			1312	811	229	265	7			
2	F	165	Total	C	N	O	S	0	0	0
			1312	811	229	265	7			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose.



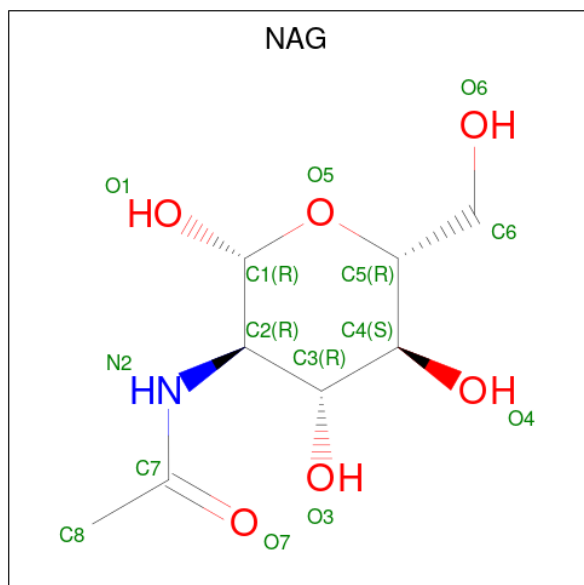
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			32	17	1	14			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

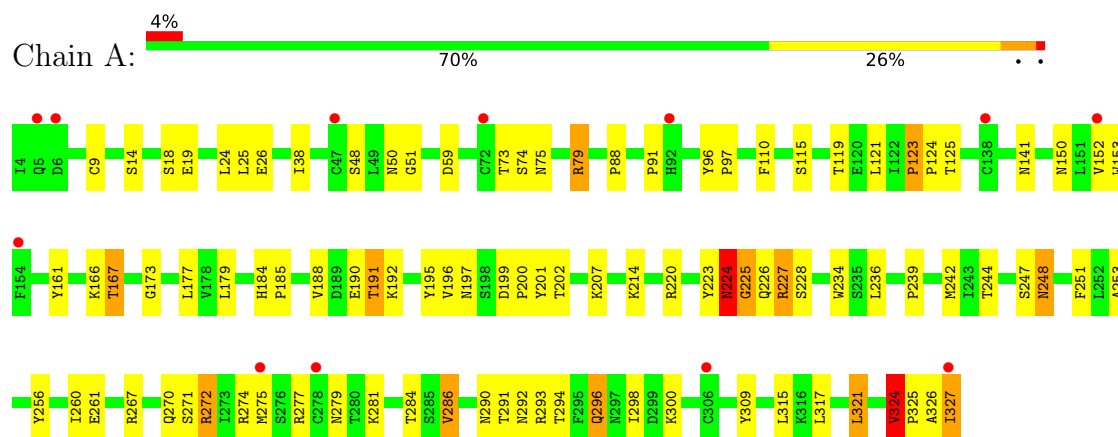
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	15	Total 15	O 15	0	0
6	B	19	Total 19	O 19	0	0
6	C	20	Total 20	O 20	0	0
6	D	13	Total 13	O 13	0	0
6	E	25	Total 25	O 25	0	0
6	F	11	Total 11	O 11	0	0

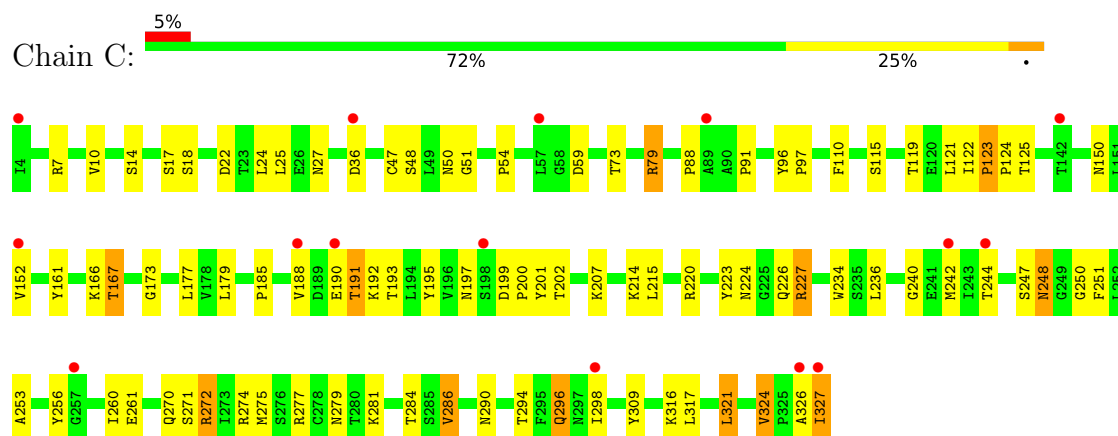
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

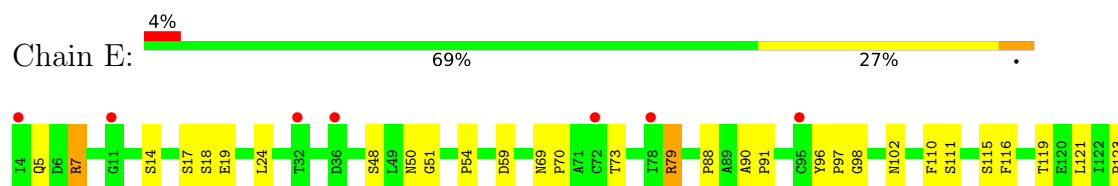
• Molecule 1: Hemagglutinin

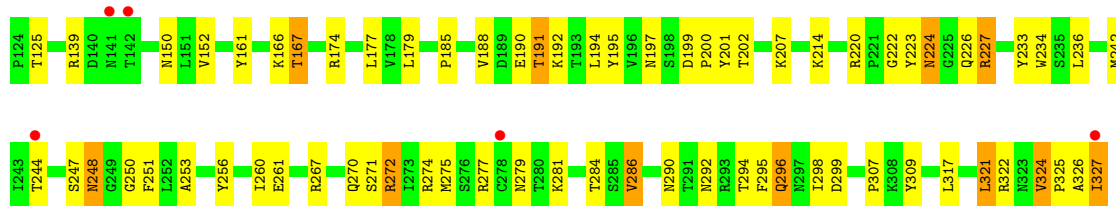


• Molecule 1: Hemagglutinin

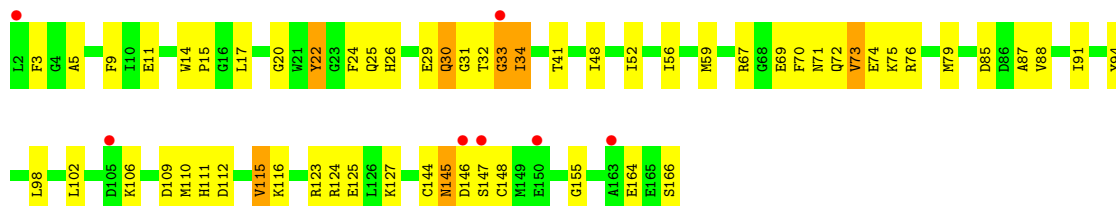


• Molecule 1: Hemagglutinin

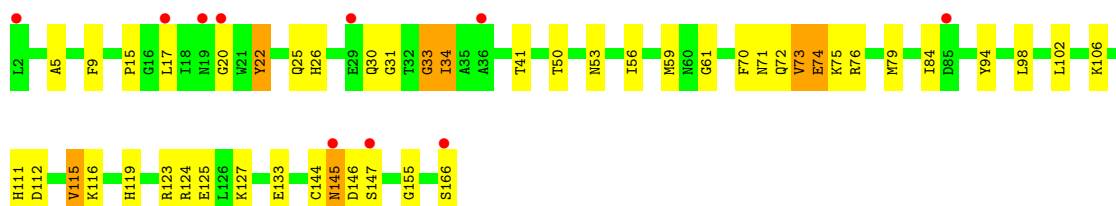




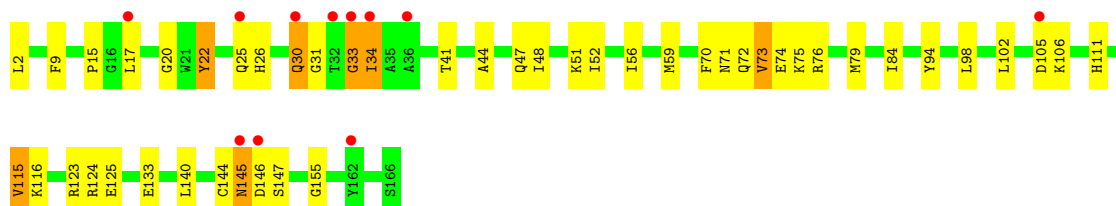
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



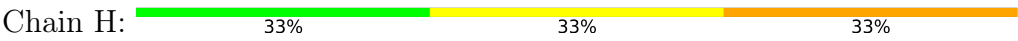
• Molecule 2: Hemagglutinin



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose



• Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.64Å 76.80Å 76.38Å 85.60° 82.67° 87.52°	Depositor
Resolution (Å)	42.45 – 2.59 42.45 – 2.59	Depositor EDS
% Data completeness (in resolution range)	90.3 (42.45-2.59) 95.2 (42.45-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.216 , 0.255 0.216 , 0.249	Depositor DCC
R_{free} test set	2576 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11796	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: SIA, GAL, 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	0.42	0/2619	0.73	4/3560 (0.1%)
1	C	0.31	0/2619	0.72	4/3560 (0.1%)
1	E	0.42	0/2619	0.74	2/3560 (0.1%)
2	B	0.43	1/1333 (0.1%)	0.71	2/1798 (0.1%)
2	D	0.31	0/1333	0.70	2/1798 (0.1%)
2	F	0.30	0/1333	0.70	1/1798 (0.1%)
All	All	0.38	1/11856 (0.0%)	0.72	15/16074 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	14	TRP	C-O	-5.06	1.20	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	31	GLY	N-CA-C	6.14	119.57	111.52
2	F	31	GLY	N-CA-C	6.10	119.51	111.52
2	D	31	GLY	N-CA-C	6.04	119.43	111.52
1	C	123	PRO	CA-C-N	5.77	125.45	119.56
1	C	123	PRO	C-N-CA	5.77	125.45	119.56
1	A	123	PRO	CA-C-N	5.71	125.38	119.56
1	A	123	PRO	C-N-CA	5.71	125.38	119.56
1	E	123	PRO	CA-C-N	5.69	125.36	119.56
1	E	123	PRO	C-N-CA	5.69	125.36	119.56
2	D	127	LYS	CB-CA-C	-5.56	110.18	116.63
2	B	127	LYS	CB-CA-C	-5.38	110.39	116.63
1	C	324	VAL	CA-C-N	5.12	125.11	119.89
1	C	324	VAL	C-N-CA	5.12	125.11	119.89
1	A	324	VAL	CA-C-N	5.01	125.00	119.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	VAL	C-N-CA	5.01	125.00	119.89

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	2555	0	2476	86	0
1	C	2555	0	2476	79	0
1	E	2555	0	2474	85	0
2	B	1312	0	1240	69	0
2	D	1312	0	1240	38	0
2	F	1312	0	1240	41	0
3	G	32	0	27	1	0
4	H	46	0	39	2	0
5	E	14	0	13	0	0
6	A	15	0	0	24	0
6	B	19	0	0	38	0
6	C	20	0	0	22	0
6	D	13	0	0	3	0
6	E	25	0	0	22	0
6	F	11	0	0	11	0
All	All	11796	0	11225	367	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 (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:C:47:CYS:HB2	6:C:409:HOH:O	1.14	1.32
2:B:106:LYS:HB2	6:B:218:HOH:O	1.15	1.29
2:B:30:GLN:HG2	6:B:207:HOH:O	1.30	1.25
6:A:903:HOH:O	2:D:50:THR:HG21	1.38	1.24

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:SER:HB3	6:B:215:HOH:O	1.42	1.19
1:A:25:LEU:C	6:A:903:HOH:O	1.85	1.18
1:C:316:LYS:HG2	6:C:412:HOH:O	1.46	1.13
2:B:148:CYS:N	6:B:215:HOH:O	1.82	1.11
2:B:109:ASP:CA	6:B:206:HOH:O	1.98	1.11
1:C:274:ARG:NH1	6:C:408:HOH:O	1.86	1.09
2:B:30:GLN:N	6:B:207:HOH:O	1.83	1.09
1:E:277:ARG:N	6:E:716:HOH:O	1.86	1.08
6:A:903:HOH:O	2:D:50:THR:CG2	1.93	1.08
1:E:277:ARG:CB	6:E:716:HOH:O	2.06	1.04
1:A:296:GLN:NE2	6:A:908:HOH:O	1.91	1.04
2:B:147:SER:CB	6:B:215:HOH:O	2.02	1.03
2:B:147:SER:CA	6:B:215:HOH:O	2.06	1.02
2:B:109:ASP:N	6:B:206:HOH:O	1.91	1.02
1:A:150:ASN:HD22	1:A:256:TYR:HB2	1.26	1.01
1:A:293:ARG:CD	6:A:907:HOH:O	2.08	1.00
1:E:277:ARG:CA	6:E:716:HOH:O	2.09	1.00
2:B:30:GLN:CG	6:B:207:HOH:O	1.94	0.99
1:E:150:ASN:HD22	1:E:256:TYR:HB2	1.25	0.98
1:C:150:ASN:HD22	1:C:256:TYR:HB2	1.25	0.98
1:A:293:ARG:HD3	6:A:907:HOH:O	1.61	0.97
2:B:147:SER:C	6:B:215:HOH:O	2.05	0.97
1:A:224:ASN:N	1:A:224:ASN:HD22	1.58	0.96
1:A:38:ILE:C	6:A:907:HOH:O	2.07	0.96
1:C:294:THR:OG1	6:C:410:HOH:O	1.83	0.95
2:B:110:MET:N	6:B:206:HOH:O	1.98	0.95
2:B:109:ASP:HB2	6:B:206:HOH:O	1.64	0.94
1:C:48:SER:O	6:C:409:HOH:O	1.86	0.93
2:B:164:GLU:O	6:B:208:HOH:O	1.85	0.93
2:F:47:GLN:NE2	6:F:201:HOH:O	2.03	0.92
1:E:277:ARG:HB2	6:E:716:HOH:O	1.68	0.92
2:D:61:GLY:O	6:D:205:HOH:O	1.86	0.92
1:A:239:PRO:O	6:A:912:HOH:O	1.88	0.91
1:A:296:GLN:CD	6:A:908:HOH:O	2.13	0.91
1:C:240:GLY:O	6:C:411:HOH:O	1.89	0.90
1:A:296:GLN:OE1	6:A:908:HOH:O	1.90	0.89
1:E:167:THR:HB	1:E:244:THR:HG22	1.56	0.89
1:C:27:ASN:OD1	6:C:418:HOH:O	1.91	0.88
6:A:903:HOH:O	2:D:50:THR:CB	2.17	0.88
1:E:307:PRO:O	6:E:703:HOH:O	1.90	0.88
1:A:167:THR:HB	1:A:244:THR:HG22	1.55	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:GLY:O	6:E:707:HOH:O	1.92	0.87
1:C:167:THR:HB	1:C:244:THR:HG22	1.57	0.87
2:B:88:VAL:O	6:B:211:HOH:O	1.94	0.86
2:B:69:GLU:OE2	6:B:214:HOH:O	1.92	0.85
1:C:122:ILE:O	6:C:403:HOH:O	1.93	0.85
1:E:102:ASN:OD1	6:E:705:HOH:O	1.93	0.84
1:A:25:LEU:O	6:A:903:HOH:O	1.85	0.84
2:B:88:VAL:C	6:B:211:HOH:O	2.21	0.82
1:C:240:GLY:C	6:C:411:HOH:O	2.24	0.80
2:B:109:ASP:CB	6:B:206:HOH:O	2.13	0.80
1:C:22:ASP:HB3	6:C:418:HOH:O	1.81	0.79
2:B:87:ALA:O	6:B:211:HOH:O	2.00	0.78
1:E:59:ASP:OD1	6:E:723:HOH:O	2.01	0.78
1:A:224:ASN:HD22	1:A:224:ASN:H	1.30	0.78
1:C:200:PRO:O	6:C:413:HOH:O	2.02	0.78
1:E:19:GLU:OE1	6:E:712:HOH:O	2.02	0.78
1:E:59:ASP:CG	6:E:723:HOH:O	2.28	0.77
2:D:166:SER:N	6:D:203:HOH:O	2.18	0.77
2:B:30:GLN:CB	6:B:207:HOH:O	2.25	0.76
2:F:74:GLU:OE2	6:F:205:HOH:O	2.05	0.75
1:C:51:GLY:H	1:C:279:ASN:HD21	1.35	0.75
1:A:79:ARG:HB3	1:A:79:ARG:NH1	2.03	0.74
1:C:79:ARG:HB3	1:C:79:ARG:NH1	2.02	0.74
1:E:207:LYS:HE3	1:E:242:MET:HE3	1.70	0.74
1:E:59:ASP:OD2	6:E:723:HOH:O	2.05	0.74
2:B:106:LYS:N	6:B:218:HOH:O	1.82	0.73
1:E:51:GLY:H	1:E:279:ASN:HD21	1.35	0.73
1:C:201:TYR:H	1:C:248:ASN:HD21	1.37	0.73
1:A:173:GLY:HA2	6:A:915:HOH:O	1.88	0.73
1:A:201:TYR:H	1:A:248:ASN:HD21	1.37	0.73
1:A:207:LYS:HE3	1:A:242:MET:HE3	1.71	0.72
1:A:51:GLY:H	1:A:279:ASN:HD21	1.36	0.72
1:A:96:TYR:CE1	1:A:226:GLN:HG3	2.24	0.72
2:B:106:LYS:O	6:B:206:HOH:O	2.06	0.72
1:E:277:ARG:CD	6:E:716:HOH:O	2.37	0.72
1:A:293:ARG:HD2	6:A:907:HOH:O	1.80	0.72
1:C:47:CYS:CB	6:C:409:HOH:O	1.91	0.72
1:C:207:LYS:HE3	1:C:242:MET:HE3	1.71	0.72
1:E:227:ARG:HG2	1:E:227:ARG:HH11	1.55	0.72
1:E:322:ARG:O	6:E:713:HOH:O	2.07	0.71
1:C:96:TYR:CE1	1:C:226:GLN:HG3	2.25	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ALA:HB2	2:B:15:PRO:HD3	1.73	0.71
1:E:272:ARG:H	1:E:272:ARG:HD2	1.56	0.71
1:A:274:ARG:HG3	1:A:275:MET:N	2.06	0.70
1:A:79:ARG:HB3	1:A:79:ARG:HH11	1.55	0.70
6:A:903:HOH:O	2:D:50:THR:HB	1.86	0.70
1:E:96:TYR:CE1	1:E:226:GLN:HG3	2.26	0.70
1:C:79:ARG:HB3	1:C:79:ARG:HH11	1.56	0.70
2:B:91:ILE:HB	6:B:211:HOH:O	1.90	0.70
1:C:272:ARG:H	1:C:272:ARG:HD2	1.55	0.70
1:E:201:TYR:H	1:E:248:ASN:HD21	1.38	0.70
2:B:69:GLU:CD	6:B:214:HOH:O	2.35	0.69
1:E:233:TYR:OH	6:E:718:HOH:O	2.06	0.69
1:A:97:PRO:HA	1:A:223:TYR:CZ	2.27	0.69
1:C:215:LEU:HG	6:C:413:HOH:O	1.93	0.68
1:C:240:GLY:HA3	6:C:411:HOH:O	1.93	0.68
1:A:38:ILE:O	6:A:907:HOH:O	2.04	0.68
1:A:236:LEU:HD21	1:A:260:ILE:HD11	1.76	0.68
1:C:236:LEU:HD21	1:C:260:ILE:HD11	1.76	0.67
1:A:272:ARG:H	1:A:272:ARG:HD2	1.59	0.67
2:F:2:LEU:N	6:F:202:HOH:O	2.26	0.67
1:C:47:CYS:C	6:C:409:HOH:O	2.39	0.66
1:A:224:ASN:N	1:A:224:ASN:ND2	2.30	0.65
1:E:236:LEU:HD21	1:E:260:ILE:HD11	1.78	0.65
1:A:150:ASN:ND2	1:A:256:TYR:HB2	2.07	0.64
1:C:17:SER:N	6:C:420:HOH:O	2.17	0.64
1:E:224:ASN:N	1:E:224:ASN:HD22	1.93	0.64
1:E:227:ARG:HG2	1:E:227:ARG:NH1	2.09	0.63
1:C:274:ARG:HG3	1:C:275:MET:N	2.11	0.63
1:A:173:GLY:N	6:A:915:HOH:O	2.31	0.63
1:E:97:PRO:HA	1:E:223:TYR:CZ	2.34	0.63
1:E:194:LEU:HD21	4:H:3:SIA:O10	1.99	0.62
2:B:166:SER:C	6:B:208:HOH:O	2.41	0.62
1:A:24:LEU:HD22	2:B:102:LEU:HD23	1.81	0.62
1:E:150:ASN:ND2	1:E:256:TYR:HB2	2.08	0.62
2:B:91:ILE:N	6:B:211:HOH:O	1.91	0.62
2:B:106:LYS:CB	6:B:218:HOH:O	1.85	0.62
1:C:272:ARG:HD2	1:C:272:ARG:N	2.16	0.61
1:E:326:ALA:HB2	2:F:15:PRO:HD3	1.82	0.61
1:C:201:TYR:H	1:C:248:ASN:ND2	1.97	0.61
1:A:201:TYR:H	1:A:248:ASN:ND2	1.97	0.60
1:E:201:TYR:H	1:E:248:ASN:ND2	1.99	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:THR:N	6:E:715:HOH:O	2.18	0.60
1:E:327:ILE:HD12	1:E:327:ILE:H	1.66	0.60
2:F:70:PHE:HB3	2:F:74:GLU:HG3	1.84	0.60
1:C:327:ILE:HD12	1:C:327:ILE:H	1.67	0.60
1:A:327:ILE:HD12	1:A:327:ILE:H	1.67	0.60
2:B:106:LYS:CA	6:B:218:HOH:O	2.15	0.60
1:C:48:SER:HB2	1:C:279:ASN:HD22	1.67	0.59
1:E:272:ARG:HD2	1:E:272:ARG:N	2.16	0.59
1:A:272:ARG:HD2	1:A:272:ARG:N	2.18	0.59
1:A:48:SER:HB2	1:A:279:ASN:HD22	1.66	0.59
1:A:74:SER:HA	6:A:914:HOH:O	2.02	0.59
1:C:36:ASP:OD1	6:C:412:HOH:O	2.16	0.59
1:C:150:ASN:ND2	1:C:256:TYR:HB2	2.08	0.58
4:H:3:SIA:O1B	4:H:3:SIA:H6	2.02	0.58
1:E:174:ARG:HD3	6:E:706:HOH:O	2.03	0.58
1:A:173:GLY:CA	6:A:915:HOH:O	2.47	0.58
1:A:195:TYR:O	1:A:196:VAL:HB	2.04	0.58
2:B:70:PHE:HB3	2:B:74:GLU:HG3	1.85	0.58
2:B:29:GLU:C	6:B:207:HOH:O	2.36	0.58
2:B:145:ASN:CB	6:B:215:HOH:O	2.52	0.57
2:B:147:SER:N	6:B:215:HOH:O	2.30	0.57
1:C:97:PRO:HA	1:C:223:TYR:CZ	2.40	0.57
2:D:76:ARG:NH2	6:F:205:HOH:O	2.32	0.57
1:E:48:SER:HB2	1:E:279:ASN:HD22	1.68	0.57
2:B:59:MET:HG3	2:F:94:TYR:CE1	2.40	0.56
2:B:91:ILE:CB	6:B:211:HOH:O	2.47	0.56
1:C:173:GLY:N	6:C:406:HOH:O	2.11	0.56
1:C:240:GLY:CA	6:C:411:HOH:O	2.45	0.56
2:D:70:PHE:HB3	2:D:74:GLU:HG3	1.86	0.56
2:F:2:LEU:C	6:F:202:HOH:O	2.48	0.56
1:E:7:ARG:NH2	2:F:133:GLU:OE2	2.38	0.56
1:A:223:TYR:C	1:A:224:ASN:O	2.47	0.56
1:A:97:PRO:HA	1:A:223:TYR:CE1	2.41	0.55
1:E:24:LEU:HD22	2:F:102:LEU:HD23	1.88	0.55
1:A:248:ASN:HD22	1:A:248:ASN:H	1.54	0.54
1:C:326:ALA:HB2	2:D:15:PRO:HD3	1.89	0.54
2:B:85:ASP:OD2	6:B:205:HOH:O	2.19	0.54
1:E:185:PRO:HG2	1:E:191:THR:HB	1.90	0.54
1:E:248:ASN:H	1:E:248:ASN:HD22	1.55	0.54
1:C:115:SER:HB2	1:C:261:GLU:HB3	1.91	0.53
2:F:74:GLU:CD	6:F:205:HOH:O	2.49	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:SER:HB2	1:A:261:GLU:HB3	1.90	0.53
1:E:277:ARG:HD2	6:E:716:HOH:O	2.06	0.53
1:A:199:ASP:N	1:A:200:PRO:HD3	2.24	0.53
1:E:115:SER:HB2	1:E:261:GLU:HB3	1.90	0.53
1:E:161:TYR:OH	6:E:720:HOH:O	2.18	0.53
1:C:248:ASN:HD22	1:C:248:ASN:H	1.56	0.53
2:B:145:ASN:HB3	6:B:215:HOH:O	2.09	0.52
2:D:94:TYR:CE1	2:F:59:MET:HG3	2.44	0.52
1:C:24:LEU:HD22	2:D:102:LEU:HD23	1.91	0.52
1:C:327:ILE:H	1:C:327:ILE:CD1	2.23	0.52
1:C:188:VAL:HA	1:C:191:THR:HG23	1.92	0.52
1:A:220:ARG:O	1:A:227:ARG:HG3	2.09	0.52
1:C:220:ARG:O	1:C:227:ARG:HG3	2.10	0.52
1:A:326:ALA:HB2	2:B:15:PRO:CD	2.38	0.52
2:F:105:ASP:CG	6:F:204:HOH:O	2.52	0.52
1:A:79:ARG:N	6:A:910:HOH:O	1.98	0.52
1:E:188:VAL:HA	1:E:191:THR:HG23	1.92	0.51
2:F:2:LEU:O	6:F:202:HOH:O	2.19	0.51
1:A:9:CYS:O	2:B:24:PHE:HA	2.11	0.51
2:B:145:ASN:HB2	6:B:215:HOH:O	2.09	0.51
1:C:185:PRO:HG2	1:C:191:THR:HB	1.91	0.51
1:A:185:PRO:HG2	1:A:191:THR:HB	1.92	0.51
1:A:195:TYR:O	1:A:197:ASN:N	2.43	0.51
2:B:94:TYR:CE1	2:D:59:MET:HG3	2.45	0.51
1:C:25:LEU:HD21	2:F:51:LYS:HE3	1.92	0.51
1:E:199:ASP:N	1:E:200:PRO:HD3	2.25	0.51
1:A:188:VAL:HA	1:A:191:THR:HG23	1.92	0.50
1:C:199:ASP:N	1:C:200:PRO:HD3	2.25	0.50
1:C:7:ARG:NH2	2:D:133:GLU:OE2	2.45	0.50
1:A:50:ASN:HD21	1:A:281:LYS:HB3	1.77	0.50
1:A:223:TYR:O	1:A:224:ASN:O	2.30	0.50
1:E:59:ASP:O	1:E:91:PRO:HD2	2.12	0.50
1:E:202:THR:HG23	1:E:247:SER:HB2	1.93	0.50
1:E:299:ASP:HA	6:E:704:HOH:O	2.12	0.50
1:A:26:GLU:N	6:A:903:HOH:O	2.27	0.49
2:B:34:ILE:HD12	2:B:34:ILE:O	2.12	0.49
2:B:3:PHE:CE2	6:F:202:HOH:O	2.64	0.49
2:F:105:ASP:HB3	6:F:204:HOH:O	2.11	0.49
2:B:164:GLU:C	6:B:208:HOH:O	2.44	0.49
1:C:202:THR:HG23	1:C:247:SER:HB2	1.94	0.49
2:D:75:LYS:HB3	2:D:79:MET:HE2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:O	1:A:91:PRO:HD2	2.12	0.49
1:C:50:ASN:HD21	1:C:281:LYS:HB3	1.78	0.49
2:D:102:LEU:HD22	2:F:106:LYS:NZ	2.28	0.49
1:A:75:ASN:N	6:A:914:HOH:O	2.06	0.49
2:B:102:LEU:HD22	2:D:106:LYS:NZ	2.27	0.48
2:B:75:LYS:HB3	2:B:79:MET:HE2	1.94	0.48
1:E:50:ASN:HD21	1:E:281:LYS:HB3	1.77	0.48
2:B:111:HIS:O	2:B:115:VAL:HG13	2.13	0.48
1:C:59:ASP:O	1:C:91:PRO:HD2	2.12	0.48
2:D:34:ILE:O	2:D:34:ILE:HD12	2.12	0.48
1:E:5:GLN:OE1	2:F:140:LEU:O	2.31	0.48
1:A:202:THR:HG23	1:A:247:SER:HB2	1.95	0.48
2:D:111:HIS:O	2:D:115:VAL:HG13	2.14	0.48
2:F:34:ILE:O	2:F:34:ILE:HD12	2.13	0.48
2:F:75:LYS:HB3	2:F:79:MET:HE2	1.94	0.48
2:F:26:HIS:C	2:F:26:HIS:CD2	2.92	0.48
1:A:197:ASN:H	1:A:197:ASN:ND2	2.11	0.48
1:C:294:THR:HG23	2:D:56:ILE:HG23	1.95	0.48
2:F:111:HIS:O	2:F:115:VAL:HG13	2.14	0.47
1:E:294:THR:HG23	2:F:56:ILE:HG23	1.96	0.47
1:A:321:LEU:HD23	1:A:321:LEU:H	1.78	0.47
2:B:76:ARG:HA	2:B:79:MET:HE3	1.96	0.47
2:D:26:HIS:C	2:D:26:HIS:CD2	2.92	0.47
1:A:24:LEU:HD22	2:B:102:LEU:CD2	2.43	0.47
2:B:26:HIS:C	2:B:26:HIS:CD2	2.93	0.47
1:C:223:TYR:O	1:C:224:ASN:HB2	2.14	0.47
2:D:20:GLY:HA2	2:D:41:THR:HG21	1.97	0.47
2:D:84:ILE:HD13	2:F:84:ILE:HD13	1.97	0.47
2:F:76:ARG:HA	2:F:79:MET:HE3	1.96	0.47
1:C:197:ASN:ND2	1:C:197:ASN:H	2.12	0.46
1:C:123:PRO:HA	1:C:124:PRO:HD3	1.80	0.46
2:B:9:PHE:HB3	2:D:124:ARG:CZ	2.45	0.46
1:C:296:GLN:HG2	1:C:298:ILE:H	1.80	0.46
1:E:220:ARG:O	1:E:227:ARG:HG2	2.15	0.46
1:A:224:ASN:O	1:A:225:GLY:C	2.56	0.46
2:D:53:ASN:ND2	6:D:210:HOH:O	2.09	0.46
2:D:102:LEU:HD22	2:F:106:LYS:HZ1	1.80	0.46
1:E:296:GLN:HG2	1:E:298:ILE:H	1.81	0.46
2:F:20:GLY:HA2	2:F:41:THR:HG21	1.98	0.46
1:A:248:ASN:HD22	1:A:248:ASN:N	2.13	0.46
1:A:327:ILE:H	1:A:327:ILE:CD1	2.23	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:ASN:HB3	2:B:147:SER:H	1.81	0.46
1:E:197:ASN:ND2	1:E:197:ASN:H	2.13	0.46
1:C:197:ASN:H	1:C:197:ASN:HD22	1.63	0.46
1:A:272:ARG:H	1:A:272:ARG:CD	2.23	0.46
1:A:48:SER:CB	1:A:279:ASN:HD22	2.29	0.45
1:A:291:THR:N	6:A:906:HOH:O	2.37	0.45
1:A:294:THR:HG23	2:B:56:ILE:HG23	1.98	0.45
1:E:261:GLU:OE1	6:E:706:HOH:O	2.21	0.45
1:E:110:PHE:CE2	1:E:177:LEU:HD22	2.51	0.45
2:F:145:ASN:HB3	2:F:147:SER:H	1.82	0.45
1:A:296:GLN:HG2	1:A:298:ILE:H	1.81	0.45
1:A:284:THR:C	1:A:286:VAL:H	2.25	0.45
1:C:88:PRO:HG3	1:C:270:GLN:HB3	1.99	0.45
1:C:48:SER:CB	1:C:279:ASN:HD22	2.30	0.45
1:C:272:ARG:H	1:C:272:ARG:CD	2.21	0.45
2:D:145:ASN:HB3	2:D:147:SER:H	1.81	0.45
1:C:110:PHE:CE2	1:C:177:LEU:HD22	2.52	0.45
1:C:195:TYR:CZ	1:C:250:GLY:HA2	2.51	0.45
1:A:110:PHE:CE2	1:A:177:LEU:HD22	2.51	0.45
1:A:321:LEU:HD23	1:A:321:LEU:N	2.32	0.45
2:F:71:ASN:OD1	2:F:73:VAL:HG23	2.17	0.45
2:B:20:GLY:HA2	2:B:41:THR:HG21	1.98	0.45
2:D:76:ARG:HA	2:D:79:MET:HE3	1.98	0.45
1:E:201:TYR:N	1:E:248:ASN:HD21	2.12	0.44
1:E:324:VAL:HG12	6:E:713:HOH:O	2.17	0.44
1:A:153:TRP:CE3	3:G:2:SIA:H112	2.52	0.44
1:A:197:ASN:H	1:A:197:ASN:HD22	1.64	0.44
1:A:277:ARG:H	1:A:277:ARG:HD2	1.82	0.44
1:E:326:ALA:HB2	2:F:15:PRO:CD	2.46	0.44
2:B:71:ASN:OD1	2:B:73:VAL:HG23	2.17	0.44
2:B:124:ARG:CZ	2:F:9:PHE:HB3	2.48	0.44
1:C:277:ARG:H	1:C:277:ARG:HD2	1.82	0.44
2:D:71:ASN:OD1	2:D:73:VAL:HG23	2.17	0.44
1:E:277:ARG:HD2	1:E:277:ARG:H	1.82	0.44
1:C:122:ILE:HB	6:C:403:HOH:O	2.18	0.44
1:E:284:THR:C	1:E:286:VAL:H	2.25	0.44
1:E:195:TYR:CZ	1:E:250:GLY:HA2	2.53	0.44
1:E:197:ASN:H	1:E:197:ASN:HD22	1.64	0.44
1:C:54:PRO:HG2	1:C:275:MET:HE3	2.00	0.44
1:E:224:ASN:N	1:E:224:ASN:ND2	2.64	0.44
2:B:106:LYS:NZ	2:F:102:LEU:HD22	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:321:LEU:HD23	1:E:321:LEU:H	1.82	0.43
1:A:88:PRO:HG3	1:A:270:GLN:HB3	1.99	0.43
2:D:125:GLU:OE2	2:D:155:GLY:HA2	2.17	0.43
1:E:327:ILE:H	1:E:327:ILE:CD1	2.22	0.43
1:A:315:LEU:HA	6:A:905:HOH:O	2.18	0.43
2:B:25:GLN:HA	2:B:33:GLY:O	2.19	0.43
2:B:125:GLU:OE2	2:B:155:GLY:HA2	2.18	0.43
1:C:188:VAL:HA	1:C:191:THR:CG2	2.49	0.43
1:C:201:TYR:N	1:C:248:ASN:HD21	2.11	0.43
1:E:48:SER:CB	1:E:279:ASN:HD22	2.30	0.43
2:D:22:TYR:CD1	2:D:115:VAL:HG12	2.54	0.43
1:C:193:THR:OG1	6:C:405:HOH:O	1.91	0.43
1:E:161:TYR:HB3	1:E:197:ASN:ND2	2.33	0.43
1:C:24:LEU:HD22	2:D:102:LEU:CD2	2.49	0.43
1:E:88:PRO:HG3	1:E:270:GLN:HB3	2.00	0.43
2:F:125:GLU:OE2	2:F:155:GLY:HA2	2.18	0.43
1:E:295:PHE:N	6:E:715:HOH:O	2.51	0.42
1:C:321:LEU:HD23	1:C:321:LEU:H	1.83	0.42
1:E:90:ALA:HA	1:E:91:PRO:HD3	1.93	0.42
1:E:321:LEU:HD23	1:E:321:LEU:N	2.34	0.42
1:C:161:TYR:HB3	1:C:197:ASN:ND2	2.34	0.42
1:C:152:VAL:CG2	1:C:253:ALA:HB3	2.49	0.42
1:C:321:LEU:HD23	1:C:321:LEU:N	2.35	0.42
1:A:161:TYR:HB3	1:A:197:ASN:ND2	2.34	0.42
1:C:10:VAL:HG21	2:D:119:HIS:HA	2.02	0.42
2:F:25:GLN:HA	2:F:33:GLY:O	2.19	0.42
2:D:25:GLN:HA	2:D:33:GLY:O	2.19	0.42
1:E:251:PHE:CZ	1:E:253:ALA:HA	2.55	0.42
1:A:251:PHE:CZ	1:A:253:ALA:HA	2.55	0.42
1:C:296:GLN:O	1:C:309:TYR:HA	2.20	0.42
1:A:152:VAL:CG2	1:A:253:ALA:HB3	2.50	0.42
2:B:109:ASP:C	6:B:206:HOH:O	2.24	0.42
1:A:267:ARG:NH1	2:B:67:ARG:HD3	2.34	0.42
2:B:48:ILE:O	2:B:52:ILE:HD13	2.20	0.42
2:B:71:ASN:OD1	2:B:74:GLU:HG2	2.20	0.42
2:B:166:SER:N	6:B:208:HOH:O	2.52	0.42
2:D:71:ASN:OD1	2:D:74:GLU:HG2	2.20	0.42
2:B:32:THR:HA	2:B:33:GLY:HA3	1.82	0.41
2:D:9:PHE:HB3	2:F:124:ARG:CZ	2.50	0.41
1:E:54:PRO:HG2	1:E:275:MET:HE3	2.02	0.41
1:E:79:ARG:HA	1:E:116:PHE:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:VAL:HA	1:E:191:THR:CG2	2.49	0.41
2:F:25:GLN:HG3	2:F:33:GLY:O	2.20	0.41
1:A:188:VAL:HA	1:A:191:THR:CG2	2.49	0.41
2:B:25:GLN:HG3	2:B:33:GLY:O	2.20	0.41
1:C:284:THR:C	1:C:286:VAL:H	2.26	0.41
1:E:272:ARG:H	1:E:272:ARG:CD	2.21	0.41
2:B:5:ALA:HB3	2:B:112:ASP:OD2	2.19	0.41
2:D:5:ALA:HB3	2:D:112:ASP:OD2	2.20	0.41
1:E:227:ARG:HH11	1:E:227:ARG:CG	2.27	0.41
1:A:179:LEU:HD23	1:A:234:TRP:HB3	2.03	0.41
1:A:296:GLN:O	1:A:309:TYR:HA	2.20	0.41
2:D:25:GLN:HG3	2:D:33:GLY:O	2.20	0.41
1:E:152:VAL:CG2	1:E:253:ALA:HB3	2.50	0.41
1:E:324:VAL:HA	1:E:325:PRO:HD3	1.90	0.41
1:A:324:VAL:HA	1:A:325:PRO:HD3	1.90	0.41
1:E:24:LEU:HD22	2:F:102:LEU:CD2	2.49	0.41
1:E:292:ASN:HD22	1:E:292:ASN:HA	1.70	0.41
1:E:296:GLN:O	1:E:309:TYR:HA	2.21	0.41
2:F:30:GLN:HE21	2:F:30:GLN:HB2	1.65	0.41
2:F:48:ILE:O	2:F:52:ILE:HD13	2.21	0.41
1:A:123:PRO:HA	1:A:124:PRO:HD3	1.80	0.41
2:B:22:TYR:CD1	2:B:115:VAL:HG12	2.56	0.41
1:A:184:HIS:O	1:A:228:SER:HB2	2.21	0.40
1:C:251:PHE:CZ	1:C:253:ALA:HA	2.56	0.40
1:C:316:LYS:CG	6:C:412:HOH:O	2.30	0.40
1:E:69:ASN:HA	1:E:70:PRO:HD3	1.96	0.40
2:F:22:TYR:CD1	2:F:115:VAL:HG12	2.56	0.40
2:F:44:ALA:HA	6:F:201:HOH:O	2.19	0.40
1:A:292:ASN:HD22	1:A:292:ASN:HA	1.70	0.40
1:C:202:THR:HG21	1:C:251:PHE:CD1	2.57	0.40
1:E:179:LEU:HD23	1:E:234:TRP:HB3	2.03	0.40
2:F:71:ASN:OD1	2:F:74:GLU:HG2	2.22	0.40
1:C:179:LEU:HD23	1:C:234:TRP:HB3	2.03	0.40
2:D:25:GLN:HG3	2:D:34:ILE:HG23	2.04	0.40
1:E:111:SER:HB2	1:E:267:ARG:N	2.36	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	322/324 (99%)	304 (94%)	16 (5%)	2 (1%)	21	39
1	C	322/324 (99%)	307 (95%)	15 (5%)	0	100	100
1	E	322/324 (99%)	306 (95%)	15 (5%)	1 (0%)	36	56
2	B	163/165 (99%)	153 (94%)	8 (5%)	2 (1%)	10	22
2	D	163/165 (99%)	152 (93%)	9 (6%)	2 (1%)	10	22
2	F	163/165 (99%)	153 (94%)	8 (5%)	2 (1%)	10	22
All	All	1455/1467 (99%)	1375 (94%)	71 (5%)	9 (1%)	21	39

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ASN
2	B	145	ASN
2	D	145	ASN
2	F	145	ASN
2	B	33	GLY
2	D	33	GLY
2	F	33	GLY
1	A	225	GLY
1	E	222	GLY

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	285/285 (100%)	257 (90%)	28 (10%)	7	16
1	C	285/285 (100%)	261 (92%)	24 (8%)	10	22
1	E	285/285 (100%)	256 (90%)	29 (10%)	7	14
2	B	140/140 (100%)	127 (91%)	13 (9%)	8	18
2	D	140/140 (100%)	127 (91%)	13 (9%)	8	18
2	F	140/140 (100%)	128 (91%)	12 (9%)	10	21
All	All	1275/1275 (100%)	1156 (91%)	119 (9%)	8	18

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	18	SER
1	A	19	GLU
1	A	73	THR
1	A	79	ARG
1	A	119	THR
1	A	121	LEU
1	A	125	THR
1	A	141	ASN
1	A	166	LYS
1	A	167	THR
1	A	190	GLU
1	A	191	THR
1	A	192	LYS
1	A	214	LYS
1	A	224	ASN
1	A	227	ARG
1	A	248	ASN
1	A	271	SER
1	A	272	ARG
1	A	286	VAL
1	A	290	ASN
1	A	296	GLN
1	A	300	LYS
1	A	317	LEU
1	A	321	LEU
1	A	324	VAL
1	A	327	ILE
2	B	11	GLU
2	B	17	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	22	TYR
2	B	30	GLN
2	B	34	ILE
2	B	72	GLN
2	B	73	VAL
2	B	98	LEU
2	B	115	VAL
2	B	116	LYS
2	B	123	ARG
2	B	144	CYS
2	B	146	ASP
1	C	14	SER
1	C	18	SER
1	C	73	THR
1	C	79	ARG
1	C	119	THR
1	C	121	LEU
1	C	125	THR
1	C	166	LYS
1	C	167	THR
1	C	190	GLU
1	C	191	THR
1	C	192	LYS
1	C	214	LYS
1	C	227	ARG
1	C	248	ASN
1	C	271	SER
1	C	272	ARG
1	C	286	VAL
1	C	290	ASN
1	C	296	GLN
1	C	317	LEU
1	C	321	LEU
1	C	324	VAL
1	C	327	ILE
2	D	17	LEU
2	D	22	TYR
2	D	30	GLN
2	D	34	ILE
2	D	72	GLN
2	D	73	VAL
2	D	74	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	98	LEU
2	D	115	VAL
2	D	116	LYS
2	D	123	ARG
2	D	144	CYS
2	D	146	ASP
1	E	7	ARG
1	E	14	SER
1	E	17	SER
1	E	18	SER
1	E	73	THR
1	E	79	ARG
1	E	119	THR
1	E	121	LEU
1	E	125	THR
1	E	139	ARG
1	E	166	LYS
1	E	167	THR
1	E	190	GLU
1	E	191	THR
1	E	192	LYS
1	E	214	LYS
1	E	224	ASN
1	E	227	ARG
1	E	248	ASN
1	E	271	SER
1	E	272	ARG
1	E	274	ARG
1	E	286	VAL
1	E	290	ASN
1	E	296	GLN
1	E	317	LEU
1	E	321	LEU
1	E	324	VAL
1	E	327	ILE
2	F	17	LEU
2	F	22	TYR
2	F	30	GLN
2	F	34	ILE
2	F	72	GLN
2	F	73	VAL
2	F	98	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	115	VAL
2	F	116	LYS
2	F	123	ARG
2	F	144	CYS
2	F	146	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	50	ASN
1	A	141	ASN
1	A	150	ASN
1	A	170	ASN
1	A	197	ASN
1	A	224	ASN
1	A	226	GLN
1	A	248	ASN
1	A	279	ASN
1	A	292	ASN
2	B	25	GLN
2	B	30	GLN
2	B	54	ASN
2	B	117	ASN
2	B	119	HIS
2	B	121	GLN
1	C	42	HIS
1	C	50	ASN
1	C	141	ASN
1	C	150	ASN
1	C	169	ASN
1	C	170	ASN
1	C	197	ASN
1	C	224	ASN
1	C	248	ASN
1	C	270	GLN
1	C	279	ASN
1	C	292	ASN
2	D	25	GLN
2	D	30	GLN
2	D	54	ASN
2	D	117	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	119	HIS
1	E	42	HIS
1	E	50	ASN
1	E	141	ASN
1	E	150	ASN
1	E	170	ASN
1	E	197	ASN
1	E	224	ASN
1	E	226	GLN
1	E	238	HIS
1	E	248	ASN
1	E	279	ASN
1	E	292	ASN
2	F	25	GLN
2	F	30	GLN
2	F	54	ASN
2	F	117	ASN
2	F	119	HIS
2	F	121	GLN

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](#)

5 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GAL	G	1	3	12,12,12	0.51	0	17,17,17	1.50	3 (17%)
3	SIA	G	2	3	20,20,21	3.83	8 (40%)	21,28,31	3.58	6 (28%)
4	NAG	H	1	4	15,15,15	0.44	0	21,21,21	0.85	0
4	GAL	H	2	4	11,11,12	0.62	0	15,15,17	1.39	2 (13%)
4	SIA	H	3	4	20,20,21	3.75	8 (40%)	21,28,31	3.92	7 (33%)

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	GAL	G	1	3	-	1/2/22/22	0/1/1/1
3	SIA	G	2	3	-	1/18/34/38	0/1/1/1
4	NAG	H	1	4	-	2/6/26/26	0/1/1/1
4	GAL	H	2	4	-	2/2/19/22	0/1/1/1
4	SIA	H	3	4	-	2/18/34/38	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2	SIA	C4-C5	-14.16	1.40	1.53
4	H	3	SIA	C4-C5	-13.87	1.40	1.53
3	G	2	SIA	C7-C6	-4.61	1.47	1.52
4	H	3	SIA	C7-C6	-4.11	1.47	1.52
4	H	3	SIA	O6-C6	3.94	1.50	1.44
4	H	3	SIA	O8-C8	-3.58	1.35	1.43
3	G	2	SIA	O8-C8	-3.42	1.36	1.43
4	H	3	SIA	C10-N5	3.38	1.45	1.34
3	G	2	SIA	C10-N5	3.37	1.45	1.34
3	G	2	SIA	O6-C6	3.27	1.49	1.44
4	H	3	SIA	C5-N5	2.99	1.50	1.45
3	G	2	SIA	C5-N5	2.99	1.50	1.45
3	G	2	SIA	C6-C5	-2.71	1.48	1.53
4	H	3	SIA	C6-C5	-2.66	1.48	1.53
3	G	2	SIA	O1A-C1	2.24	1.28	1.22
4	H	3	SIA	O1A-C1	2.05	1.28	1.22

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	3	SIA	O6-C2-C3	-14.65	90.87	110.56
3	G	2	SIA	O6-C2-C3	-13.03	93.04	110.56
4	H	3	SIA	O6-C2-C1	7.75	122.34	107.72
3	G	2	SIA	O6-C2-C1	7.68	122.22	107.72
4	H	2	GAL	C1-C2-C3	4.12	115.64	109.64
3	G	1	GAL	C4-C3-C2	-3.86	104.05	110.83
4	H	3	SIA	O1B-C1-C2	3.11	120.80	112.71
4	H	3	SIA	O9-C9-C8	2.78	117.00	111.16
4	H	3	SIA	C11-C10-N5	2.77	120.72	116.12
4	H	3	SIA	O1B-C1-O1A	-2.72	117.91	124.08
4	H	2	GAL	O3-C3-C2	-2.70	104.54	110.05
3	G	2	SIA	O1B-C1-C2	2.63	119.55	112.71
3	G	2	SIA	O9-C9-C8	2.63	116.67	111.16
3	G	2	SIA	C11-C10-N5	2.60	120.44	116.12
3	G	1	GAL	O4-C4-C3	-2.31	104.92	110.38
3	G	2	SIA	C8-C7-C6	-2.23	108.86	113.05
3	G	1	GAL	O2-C2-C3	2.15	115.44	110.38
4	H	3	SIA	C5-N5-C10	-2.09	118.22	123.11

There are no chirality outliers.

All (8) torsion outliers are listed below:

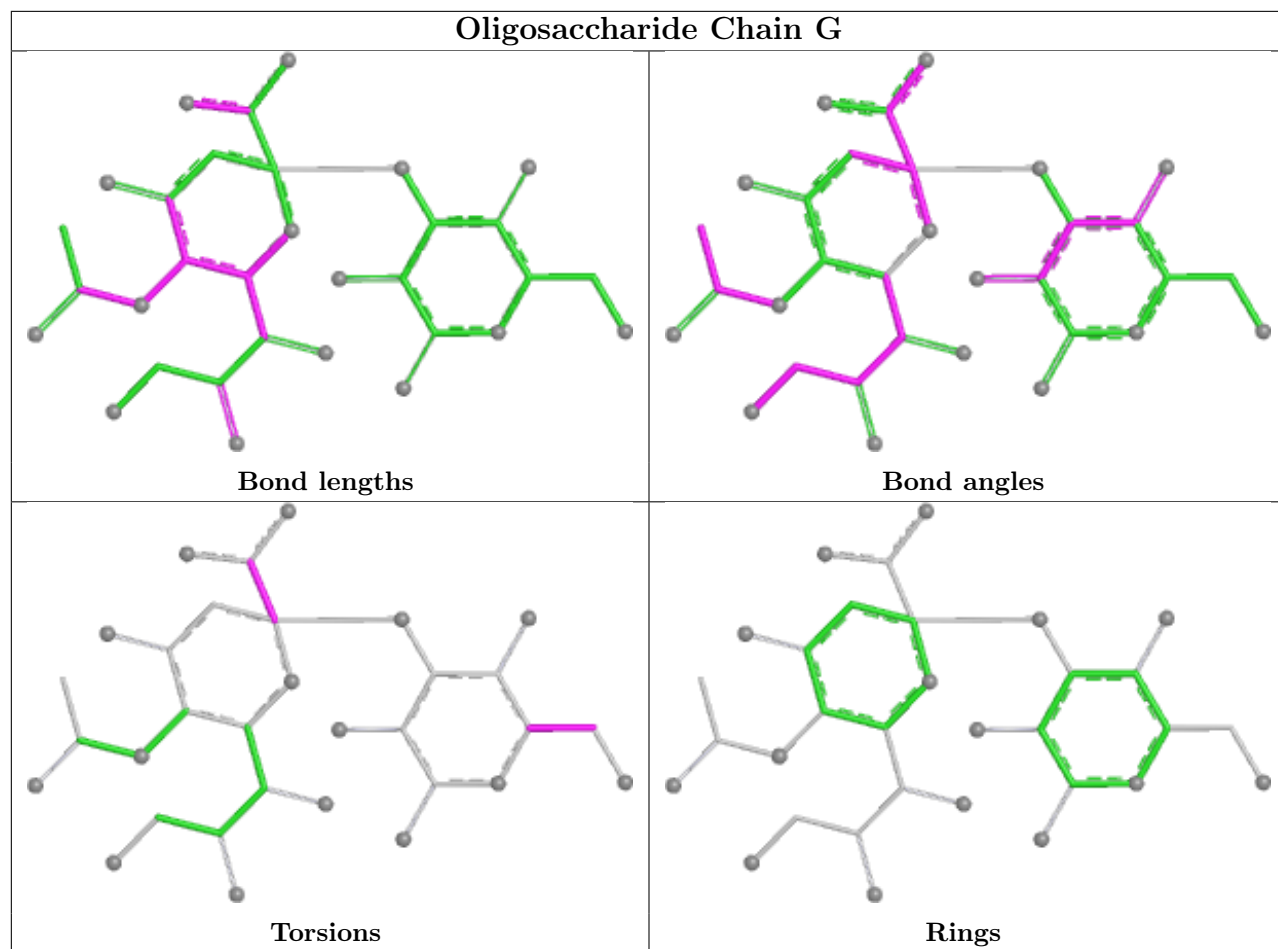
Mol	Chain	Res	Type	Atoms
4	H	2	GAL	O5-C5-C6-O6
3	G	1	GAL	O5-C5-C6-O6
3	G	2	SIA	O1A-C1-C2-O6
4	H	3	SIA	C7-C8-C9-O9
4	H	2	GAL	C4-C5-C6-O6
4	H	1	NAG	C8-C7-N2-C2
4	H	3	SIA	O8-C8-C9-O9
4	H	1	NAG	O7-C7-N2-C2

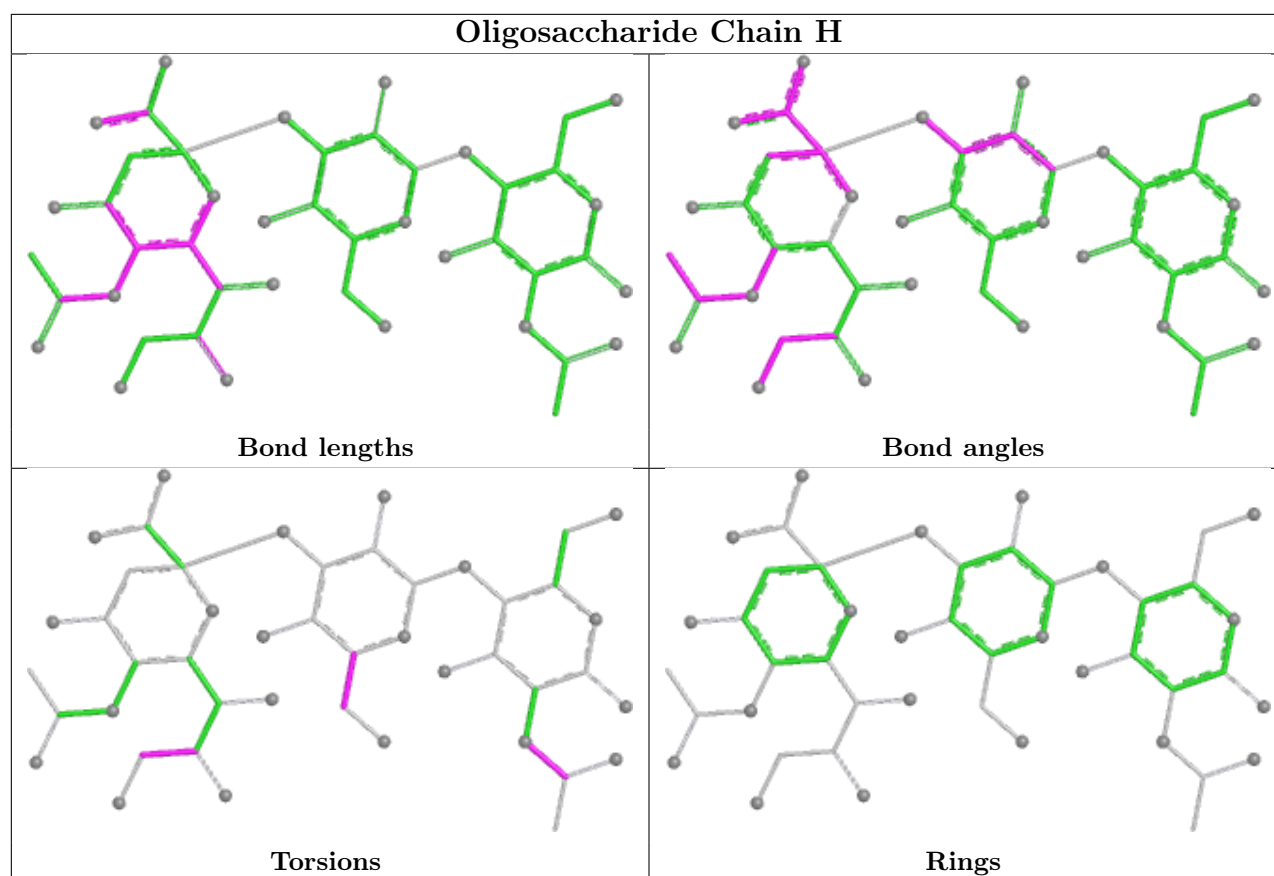
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	3	SIA	2	0
3	G	2	SIA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





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	E	601	1	14,14,15	0.29	0	17,19,21	0.56	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	601	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	601	NAG	O5-C5-C6-O6
5	E	601	NAG	C4-C5-C6-O6
5	E	601	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	324/324 (100%)	0.52	12 (3%) 45 40	38, 70, 111, 147	0
1	C	324/324 (100%)	0.67	15 (4%) 37 33	43, 80, 115, 156	0
1	E	324/324 (100%)	0.54	12 (3%) 45 40	41, 71, 107, 181	0
2	B	165/165 (100%)	0.56	7 (4%) 40 36	35, 61, 106, 280	0
2	D	165/165 (100%)	0.60	10 (6%) 27 22	38, 67, 119, 189	0
2	F	165/165 (100%)	0.72	11 (6%) 24 20	36, 72, 148, 211	0
All	All	1467/1467 (100%)	0.60	67 (4%) 37 33	35, 72, 118, 280	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	142	THR	4.4
2	F	146	ASP	4.0
1	A	72	CYS	4.0
2	B	147	SER	3.8
1	E	141	ASN	3.5
1	C	242	MET	3.3
2	B	163	ALA	3.1
1	A	278	CYS	3.1
1	E	278	CYS	3.1
1	E	72	CYS	3.1
2	D	19	ASN	2.9
2	F	162	TYR	2.9
2	F	105	ASP	2.9
1	C	198	SER	2.9
1	C	142	THR	2.8
2	B	105	ASP	2.8
2	D	145	ASN	2.7
2	F	30	GLN	2.7
2	F	32	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	78	ILE	2.7
1	E	95	CYS	2.6
1	C	57	LEU	2.5
1	C	326	ALA	2.5
1	C	244	THR	2.5
1	A	138	CYS	2.5
2	D	166	SER	2.5
2	D	85	ASP	2.4
2	D	17	LEU	2.4
2	F	17	LEU	2.4
2	F	25	GLN	2.4
1	A	47	CYS	2.4
1	C	4	ILE	2.4
1	E	244	THR	2.4
1	C	89	ALA	2.4
1	E	327	ILE	2.3
1	E	36	ASP	2.3
1	C	257	GLY	2.3
1	C	298	ILE	2.3
1	C	327	ILE	2.3
1	E	32	THR	2.3
2	D	147	SER	2.3
1	A	154	PHE	2.3
1	C	190	GLU	2.3
1	A	5	GLN	2.2
1	A	327	ILE	2.2
2	F	33	GLY	2.2
2	D	29	GLU	2.2
2	B	2	LEU	2.2
1	A	6	ASP	2.2
2	B	150	GLU	2.2
2	F	36	ALA	2.1
1	C	152	VAL	2.1
1	C	188	VAL	2.1
2	D	36	ALA	2.1
1	E	4	ILE	2.1
1	A	92	HIS	2.1
1	A	152	VAL	2.1
2	D	2	LEU	2.1
1	E	11	GLY	2.1
2	F	34	ILE	2.1
2	B	33	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	20	GLY	2.0
1	C	36	ASP	2.0
2	B	146	ASP	2.0
1	A	275	MET	2.0
1	A	306	CYS	2.0
2	F	145	ASN	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](#)

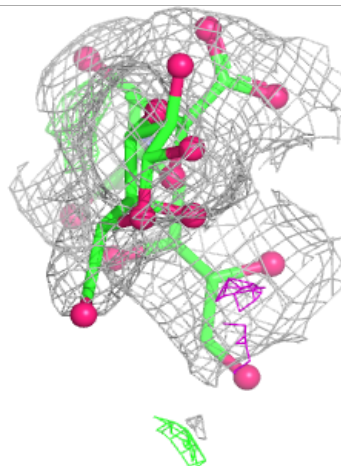
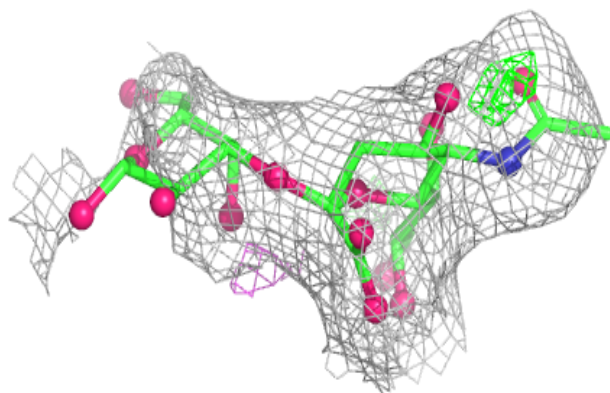
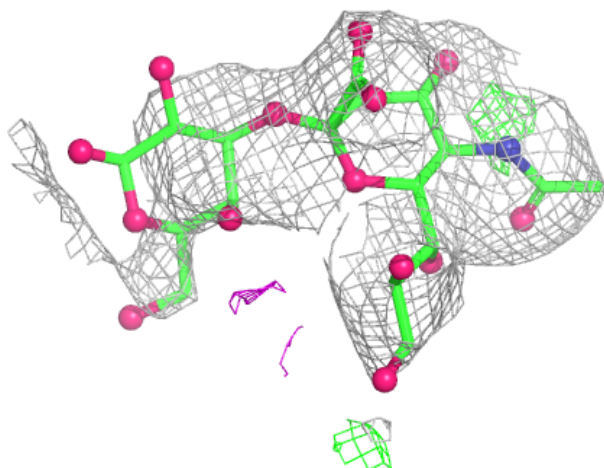
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

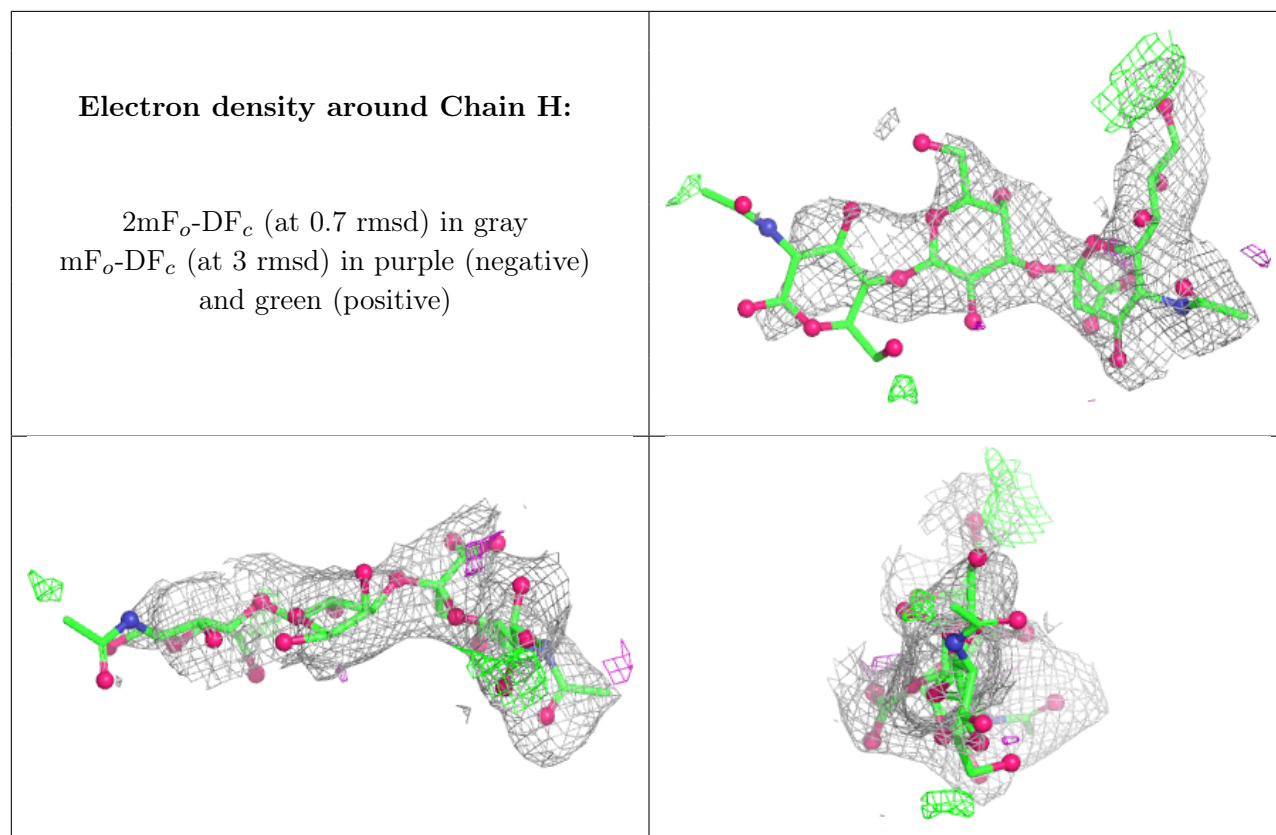
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	H	1	15/15	0.42	0.16	163,175,183,185	0
3	GAL	G	1	12/12	0.65	0.21	132,146,159,163	0
4	GAL	H	2	11/12	0.72	0.15	121,134,150,152	0
4	SIA	H	3	20/21	0.87	0.11	72,85,96,96	0
3	SIA	G	2	20/21	0.89	0.11	90,102,109,111	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	E	601	14/15	0.57	0.17	137,145,151,152	0

6.5 Other polymers [i](#)

There are no such residues in this entry.