Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 12:15 PM BST

PDB ID	:	2WR3
Title	:	structure of influenza H2 duck Ontario hemagglutinin with avian 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	:	2.50 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 following versions of software and data (see references ⓘ) were used in the production of this report:

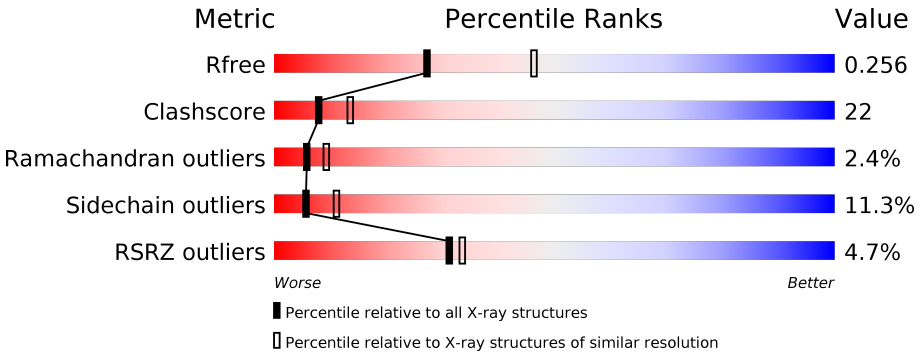
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	507	5% 61% 28% 6%
1	B	507	3% 66% 25% 5%
1	C	507	6% 61% 27% 7%
2	D	3	100%

2 Entry composition (i)

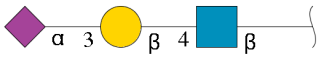
There are 3 unique types of molecules in this entry. The entry contains 11868 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	485	Total	C	N	O	S	0	0	0
			3806	2388	653	743	22			
1	B	486	Total	C	N	O	S	0	0	0
			3820	2399	655	744	22			
1	C	486	Total	C	N	O	S	0	0	0
			3820	2399	655	744	22			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			45	25	2	18			

- Molecule 3 is water.

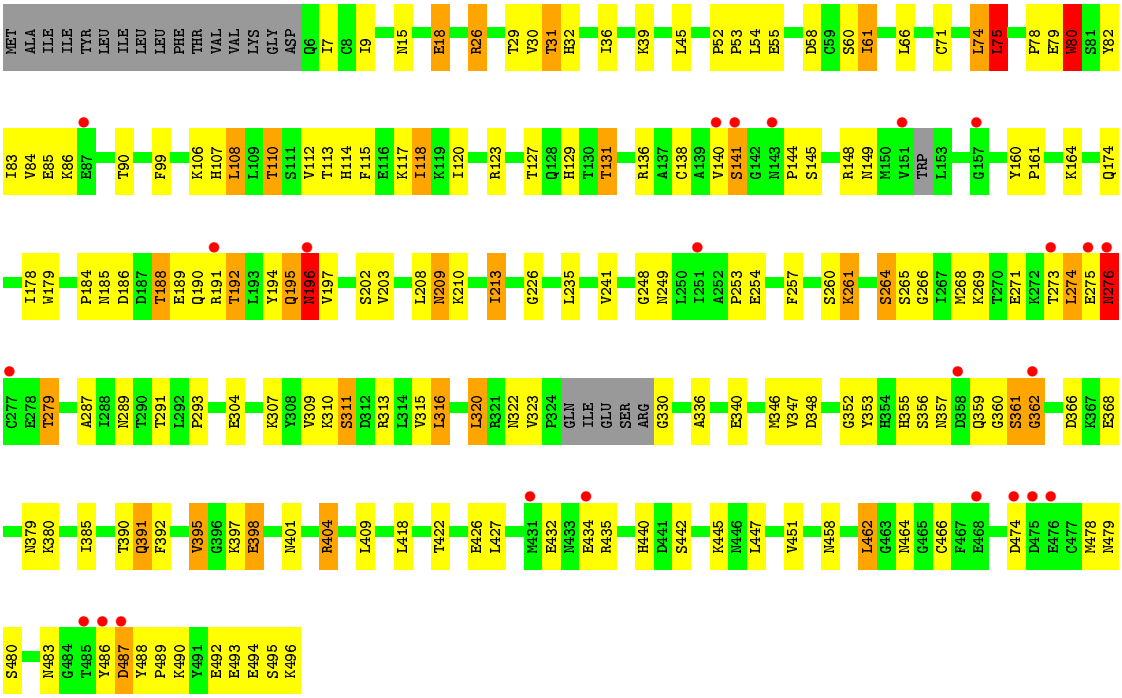
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	110	Total	O	0	0
			110	110		
3	B	166	Total	O	0	0
			166	166		
3	C	101	Total	O	0	0
			101	101		

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.

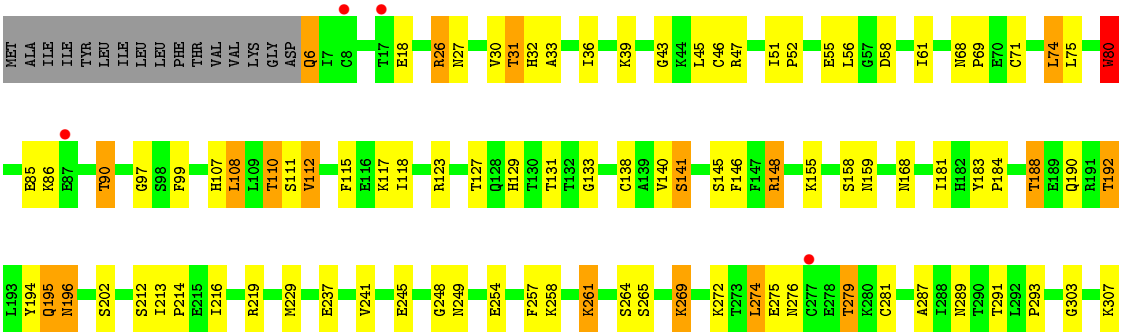
- Molecule 1: HEMAGGLUTININ

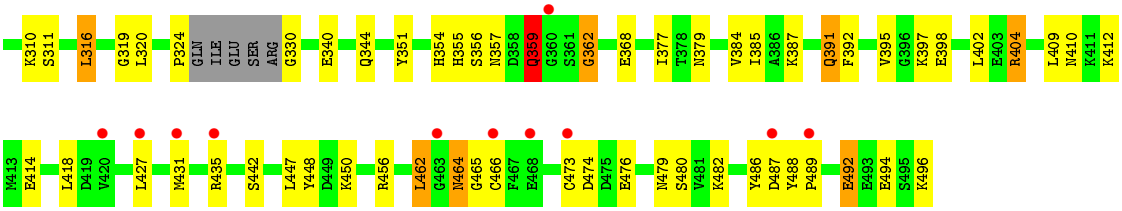
Chain A:



- Molecule 1: HEMAGGLUTININ

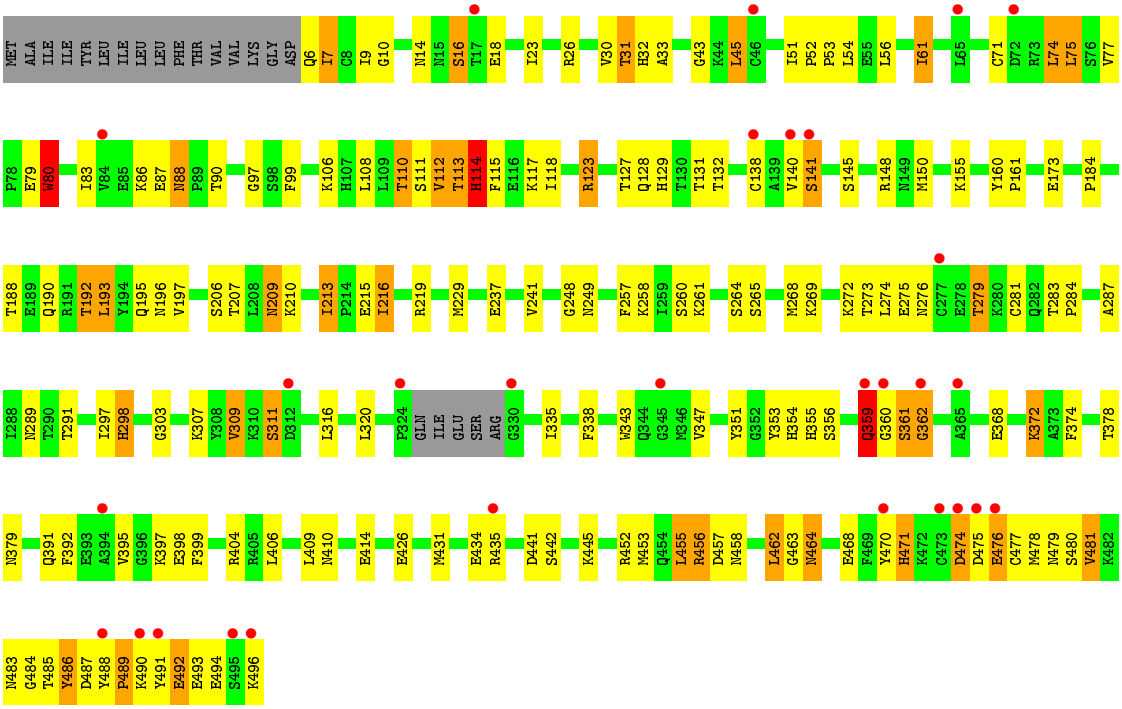
Chain B:





• Molecule 1: HEMAGGLUTININ

Chain C:



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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.69Å 148.83Å 195.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 2.50 29.91 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.4 (29.91-2.50) 99.8 (29.91-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.218 , 0.256 0.215 , 0.256	Depositor DCC
R_{free} test set	4429 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	65.7	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 54.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11868	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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	0.48	0/3889	0.62	0/5269
1	B	0.53	0/3906	0.65	0/5295
1	C	0.44	0/3906	0.62	2/5295 (0.0%)
All	All	0.48	0/11701	0.63	2/15859 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	114	HIS	N-CA-C	7.03	129.99	111.00
1	C	113	THR	C-N-CA	5.81	136.22	121.70

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	3806	0	3634	165	0
1	B	3820	0	3645	148	0
1	C	3820	0	3645	173	0
2	D	45	0	38	0	0
3	A	110	0	0	35	0
3	B	166	0	0	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	101	0	0	40	0
All	All	11868	0	10962	483	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 22.

All (483) 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:445:LYS:HE3	3:C:2085:HOH:O	1.49	1.12
1:B:324:PRO:HB3	1:B:344:GLN:HE22	1.19	1.05
1:A:496:LYS:HG2	3:A:2106:HOH:O	1.59	1.02
1:A:427:LEU:HD11	3:A:2090:HOH:O	1.60	1.01
1:C:298:HIS:HB3	3:C:2053:HOH:O	1.59	1.00
1:B:340:GLU:HG2	1:B:464:ASN:HD22	1.24	0.98
1:B:118:ILE:HD11	1:B:258:LYS:HD2	1.46	0.96
1:A:261:LYS:HZ3	1:A:261:LYS:HB2	1.32	0.95
1:C:6:GLN:HB3	1:C:356:SER:HB3	1.47	0.95
1:B:148:ARG:HH11	1:B:148:ARG:HG2	1.28	0.95
1:B:26:ARG:HH11	1:B:26:ARG:HG3	1.30	0.94
1:A:261:LYS:NZ	1:A:261:LYS:HB2	1.82	0.93
1:A:397:LYS:HE2	3:A:2088:HOH:O	1.68	0.93
1:B:397:LYS:HG2	3:B:2133:HOH:O	1.69	0.92
1:C:283:THR:HB	3:C:2053:HOH:O	1.69	0.91
1:C:452:ARG:HH11	1:C:452:ARG:HG2	1.32	0.91
1:C:279:THR:HG21	1:C:287:ALA:HB1	1.52	0.90
1:B:279:THR:HG21	1:B:287:ALA:HB1	1.53	0.89
1:B:324:PRO:HB3	1:B:344:GLN:NE2	1.86	0.88
3:A:2090:HOH:O	1:B:384:VAL:HA	1.74	0.87
1:A:123:ARG:HG2	1:A:254:GLU:OE2	1.74	0.87
1:C:483:ASN:ND2	3:C:2092:HOH:O	2.07	0.86
3:B:2145:HOH:O	1:C:435:ARG:HD3	1.75	0.85
1:C:492:GLU:HA	1:C:492:GLU:OE1	1.75	0.85
1:A:264:SER:HB3	3:C:2075:HOH:O	1.76	0.84
1:A:110:THR:HG21	1:A:265:SER:H	1.42	0.84
1:C:359:GLN:HE21	1:C:359:GLN:H	1.21	0.84
1:A:264:SER:CB	3:C:2075:HOH:O	2.25	0.83
1:C:128:GLN:HB3	1:C:161:PRO:HG2	1.61	0.82
1:C:110:THR:HG21	1:C:265:SER:H	1.43	0.82
1:C:455:LEU:O	1:C:456:ARG:HB2	1.80	0.82
1:A:86:LYS:HE2	1:A:271:GLU:HG3	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LYS:NZ	3:A:2050:HOH:O	2.12	0.80
1:B:496:LYS:HE3	3:B:2162:HOH:O	1.81	0.80
1:B:155:LYS:HD2	1:B:195:GLN:HG2	1.62	0.79
1:C:110:THR:CG2	1:C:265:SER:H	1.96	0.79
1:C:197:VAL:HG13	3:C:2033:HOH:O	1.81	0.78
1:C:279:THR:CG2	1:C:287:ALA:HB1	2.14	0.78
1:B:340:GLU:HG2	1:B:464:ASN:ND2	1.99	0.78
1:B:26:ARG:HH11	1:B:26:ARG:CG	1.97	0.77
1:C:261:LYS:HD2	3:C:2050:HOH:O	1.85	0.76
1:A:357:ASN:HD21	1:A:474:ASP:HA	1.51	0.76
1:A:492:GLU:HA	1:A:492:GLU:OE1	1.85	0.75
1:A:112:VAL:HG11	1:A:115:PHE:HB2	1.66	0.75
1:B:112:VAL:HG11	1:B:115:PHE:HB2	1.69	0.75
1:C:213:ILE:HD13	1:C:213:ILE:H	1.48	0.75
1:A:279:THR:HG21	1:A:287:ALA:HB1	1.67	0.75
1:A:279:THR:CG2	1:A:287:ALA:HB1	2.17	0.75
1:A:309:VAL:HG13	1:A:422:THR:HA	1.69	0.75
1:C:359:GLN:HE21	1:C:359:GLN:N	1.85	0.74
1:B:494:GLU:HG3	3:B:2161:HOH:O	1.86	0.74
1:A:110:THR:HG23	1:A:265:SER:HB3	1.69	0.74
1:C:53:PRO:HD2	1:C:274:LEU:HD12	1.69	0.73
1:C:216:ILE:H	1:C:216:ILE:HD12	1.53	0.73
1:A:174:GLN:NE2	1:A:235:LEU:HD13	2.04	0.72
1:A:26:ARG:CG	1:A:26:ARG:HH11	2.02	0.72
1:B:447:LEU:HG	3:B:2149:HOH:O	1.87	0.72
1:C:452:ARG:HG2	1:C:452:ARG:NH1	2.02	0.72
1:B:110:THR:CG2	1:B:265:SER:H	2.03	0.72
1:C:445:LYS:HG3	3:C:2084:HOH:O	1.90	0.72
1:B:397:LYS:HD3	3:B:2134:HOH:O	1.89	0.71
1:C:113:THR:OG1	1:C:260:SER:HB2	1.91	0.71
1:C:335:ILE:HD12	1:C:441:ASP:HA	1.72	0.71
1:B:123:ARG:HG3	1:B:254:GLU:OE2	1.91	0.71
1:C:188:THR:O	1:C:192:THR:HG23	1.91	0.71
1:B:58:ASP:HB3	1:B:86:LYS:HD2	1.73	0.71
1:C:488:TYR:N	1:C:489:PRO:HD2	2.05	0.71
1:B:75:LEU:HG	1:B:75:LEU:O	1.90	0.70
1:A:196:ASN:ND2	1:A:196:ASN:H	1.88	0.70
1:B:168:ASN:ND2	3:B:2069:HOH:O	2.24	0.70
1:B:148:ARG:HH11	1:B:148:ARG:CG	2.04	0.70
1:A:26:ARG:HH11	1:A:26:ARG:HG3	1.56	0.70
1:B:494:GLU:HG2	3:B:2162:HOH:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:LYS:HB2	1:C:261:LYS:HZ3	1.58	0.69
1:B:261:LYS:HB2	1:B:261:LYS:HZ3	1.56	0.69
1:C:494:GLU:HB3	3:C:2098:HOH:O	1.92	0.69
1:B:138:CYS:HB2	3:B:2064:HOH:O	1.93	0.69
1:C:455:LEU:O	1:C:456:ARG:CB	2.41	0.69
1:B:188:THR:O	1:B:192:THR:HG23	1.92	0.68
1:A:261:LYS:CB	1:A:261:LYS:NZ	2.54	0.68
1:C:43:GLY:O	1:C:272:LYS:HE2	1.92	0.68
1:B:431:MET:HB3	1:C:435:ARG:HH22	1.60	0.67
1:B:377:ILE:HB	3:B:2126:HOH:O	1.95	0.67
3:A:2011:HOH:O	1:B:379:ASN:HB3	1.94	0.67
1:A:466:CYS:HB2	3:A:2095:HOH:O	1.93	0.67
1:C:112:VAL:HG11	1:C:115:PHE:HB2	1.77	0.67
1:B:359:GLN:H	1:B:359:GLN:HE21	1.41	0.67
1:C:311:SER:HB2	1:C:426:GLU:OE2	1.95	0.67
1:A:113:THR:OG1	1:A:260:SER:HB2	1.95	0.66
1:B:279:THR:HG22	3:B:2106:HOH:O	1.95	0.66
1:B:184:PRO:HG2	1:B:190:GLN:NE2	2.11	0.66
1:C:279:THR:HB	1:C:281:CYS:H	1.61	0.66
1:C:269:LYS:HE2	1:C:398:GLU:OE1	1.95	0.65
1:C:184:PRO:HG2	1:C:190:GLN:NE2	2.11	0.65
1:C:184:PRO:HG2	1:C:190:GLN:HE21	1.62	0.65
1:A:86:LYS:HE3	3:A:2025:HOH:O	1.96	0.65
1:A:52:PRO:O	1:A:80:TRP:HA	1.97	0.65
1:A:313:ARG:HA	3:A:2015:HOH:O	1.96	0.65
1:C:6:GLN:HB3	1:C:356:SER:CB	2.24	0.65
1:C:118:ILE:HD11	1:C:258:LYS:CD	2.27	0.65
1:A:494:GLU:HA	3:A:2106:HOH:O	1.97	0.64
1:A:140:VAL:O	1:A:140:VAL:HG23	1.97	0.64
1:B:188:THR:O	1:B:192:THR:CG2	2.45	0.64
1:B:488:TYR:HB3	1:B:489:PRO:HD3	1.80	0.64
1:B:110:THR:HG21	1:B:265:SER:H	1.62	0.64
1:B:118:ILE:HD11	1:B:258:LYS:CD	2.26	0.64
1:B:31:THR:HG23	1:B:32:HIS:CE1	2.33	0.64
1:A:74:LEU:O	1:A:75:LEU:HB3	1.96	0.64
1:C:18:GLU:HG2	1:C:33:ALA:HB3	1.80	0.63
1:A:178:ILE:O	1:A:253:PRO:HG3	1.99	0.63
1:A:26:ARG:CZ	3:A:2011:HOH:O	2.45	0.63
1:A:189:GLU:HA	1:A:192:THR:HG23	1.78	0.63
1:B:110:THR:HG23	1:B:265:SER:HB3	1.80	0.63
1:C:155:LYS:NZ	1:C:195:GLN:HE21	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ARG:HH22	1:C:431:MET:HG2	1.64	0.63
1:A:434:GLU:OE1	3:A:2092:HOH:O	2.16	0.63
1:A:129:HIS:CE1	1:A:161:PRO:HD2	2.33	0.63
1:B:494:GLU:C	1:B:496:LYS:H	2.01	0.62
1:A:110:THR:CG2	1:A:265:SER:H	2.09	0.62
1:A:379:ASN:HB3	3:C:2007:HOH:O	1.98	0.62
1:B:158:SER:O	1:B:195:GLN:HG3	1.99	0.62
1:A:99:PHE:HZ	1:A:178:ILE:HD13	1.65	0.62
1:B:111:SER:HB2	1:B:265:SER:HB2	1.80	0.62
1:A:264:SER:HB2	3:C:2075:HOH:O	1.96	0.61
1:C:488:TYR:H	1:C:489:PRO:HD2	1.64	0.61
1:B:74:LEU:O	1:B:75:LEU:HB3	2.00	0.61
1:C:129:HIS:HD2	3:C:2019:HOH:O	1.81	0.61
1:C:274:LEU:HD23	1:C:275:GLU:N	2.15	0.61
1:B:18:GLU:HG2	1:B:33:ALA:HB3	1.83	0.61
1:B:279:THR:CG2	1:B:287:ALA:HB1	2.28	0.60
1:B:398:GLU:HB2	3:B:2047:HOH:O	2.00	0.60
1:C:118:ILE:HD11	1:C:258:LYS:HD3	1.83	0.60
1:B:129:HIS:HD2	3:B:2059:HOH:O	1.81	0.60
1:A:58:ASP:HB3	1:A:86:LYS:HD2	1.83	0.60
1:B:184:PRO:HG2	1:B:190:GLN:HE21	1.66	0.60
1:C:10:GLY:HA3	1:C:343:TRP:CH2	2.36	0.60
1:C:359:GLN:H	1:C:359:GLN:NE2	1.98	0.60
1:B:494:GLU:HA	3:B:2162:HOH:O	2.01	0.59
1:C:31:THR:HB	1:C:320:LEU:H	1.67	0.59
1:C:213:ILE:HD13	1:C:213:ILE:N	2.17	0.59
1:A:380:LYS:HE2	1:A:432:GLU:OE2	2.01	0.59
1:C:210:LYS:HG3	3:C:2040:HOH:O	2.01	0.59
1:C:487:ASP:OD1	1:C:490:LYS:HB2	2.03	0.59
1:C:470:TYR:O	1:C:471:HIS:HB3	2.02	0.59
1:B:248:GLY:C	1:B:249:ASN:HD22	2.04	0.59
1:B:138:CYS:O	1:B:145:SER:HB3	2.02	0.58
1:B:31:THR:CG2	1:B:32:HIS:ND1	2.66	0.58
1:C:471:HIS:CE1	1:C:491:TYR:CD1	2.91	0.58
1:B:377:ILE:CB	3:B:2126:HOH:O	2.51	0.58
1:C:71:CYS:O	1:C:74:LEU:HB2	2.02	0.58
1:C:303:GLY:HA2	1:C:392:PHE:CE1	2.38	0.58
1:A:31:THR:CG2	1:A:32:HIS:ND1	2.67	0.58
1:C:494:GLU:HG3	3:C:2100:HOH:O	2.02	0.58
1:A:31:THR:HG22	1:A:32:HIS:ND1	2.18	0.58
1:B:410:ASN:O	1:B:414:GLU:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:HIS:CD2	1:C:491:TYR:HB3	2.39	0.58
1:A:75:LEU:O	1:A:75:LEU:HG	2.02	0.58
1:C:53:PRO:HD2	1:C:274:LEU:CD1	2.31	0.58
1:A:15:ASN:ND2	3:A:2006:HOH:O	2.29	0.58
1:A:404:ARG:HH11	1:A:404:ARG:HG2	1.68	0.58
1:C:309:VAL:CG1	1:C:311:SER:HB3	2.33	0.58
1:B:307:LYS:HD2	3:B:2113:HOH:O	2.03	0.57
1:C:61:ILE:HD11	1:C:83:ILE:HD13	1.86	0.57
1:B:31:THR:HG22	1:B:319:GLY:HA3	1.86	0.57
1:C:410:ASN:O	1:C:414:GLU:HG2	2.04	0.57
1:A:61:ILE:HD13	1:A:106:LYS:HD2	1.87	0.57
1:C:452:ARG:HH12	1:C:453:MET:HG3	1.69	0.57
1:C:216:ILE:CD1	1:C:216:ILE:H	2.12	0.57
1:A:7:ILE:HD11	1:A:353:TYR:HB3	1.85	0.57
1:B:492:GLU:OE1	1:B:492:GLU:HA	2.04	0.57
1:A:275:GLU:O	1:A:276:ASN:HB3	2.03	0.57
1:A:26:ARG:CG	1:A:26:ARG:NH1	2.67	0.57
1:B:31:THR:HG23	1:B:32:HIS:ND1	2.19	0.57
1:A:110:THR:CG2	1:A:265:SER:N	2.67	0.57
1:C:274:LEU:HD23	1:C:276:ASN:H	1.69	0.56
1:A:36:ILE:HG21	1:A:316:LEU:HD22	1.86	0.56
1:A:346:MET:SD	1:A:352:GLY:HA3	2.45	0.56
1:A:45:LEU:HD21	1:A:84:VAL:HG21	1.86	0.56
1:B:310:LYS:HG3	1:B:418:LEU:HD21	1.86	0.56
1:A:269:LYS:NZ	3:A:2061:HOH:O	2.38	0.56
1:A:395:VAL:N	3:A:2084:HOH:O	2.37	0.56
1:B:140:VAL:HG23	1:B:140:VAL:O	2.06	0.56
1:B:494:GLU:HB2	3:B:2164:HOH:O	2.04	0.56
1:C:298:HIS:CB	3:C:2053:HOH:O	2.33	0.56
1:C:355:HIS:HB2	1:C:478:MET:CE	2.36	0.56
1:C:297:ILE:O	1:C:298:HIS:HB2	2.06	0.56
1:A:276:ASN:CG	1:A:276:ASN:O	2.43	0.56
1:A:404:ARG:HH11	1:A:404:ARG:CG	2.18	0.55
1:B:71:CYS:O	1:B:74:LEU:HB2	2.06	0.55
1:C:155:LYS:HD2	1:C:195:GLN:HG2	1.88	0.55
1:A:366:ASP:OD1	1:A:447:LEU:HD11	2.06	0.55
1:A:117:LYS:HG3	1:A:257:PHE:CE2	2.41	0.55
1:B:117:LYS:HG3	1:B:257:PHE:CE2	2.42	0.55
1:B:43:GLY:O	1:B:272:LYS:HE2	2.06	0.55
1:C:462:LEU:HD21	1:C:468:GLU:HB2	1.88	0.55
1:C:155:LYS:NZ	1:C:195:GLN:NE2	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:SER:O	1:B:261:LYS:CD	2.55	0.54
1:B:36:ILE:HG21	1:B:316:LEU:HD22	1.90	0.54
1:B:487:ASP:OD1	1:B:489:PRO:HD2	2.07	0.54
1:A:248:GLY:C	1:A:249:ASN:HD22	2.11	0.54
1:A:357:ASN:HD21	1:A:474:ASP:CA	2.21	0.54
1:A:480:SER:HA	1:A:483:ASN:OD1	2.06	0.54
1:B:330:GLY:N	3:B:2120:HOH:O	2.41	0.54
1:C:23:ILE:HD11	1:C:431:MET:HG3	1.89	0.54
1:A:26:ARG:NH2	3:A:2011:HOH:O	2.39	0.54
1:B:261:LYS:CB	1:B:261:LYS:HZ3	2.21	0.54
1:A:307:LYS:NZ	3:A:2072:HOH:O	2.41	0.53
1:B:107:HIS:O	1:B:110:THR:HB	2.09	0.53
1:B:494:GLU:C	1:B:496:LYS:N	2.61	0.53
1:B:26:ARG:N	1:B:26:ARG:HD3	2.23	0.53
1:A:495:SER:N	3:A:2106:HOH:O	2.42	0.53
1:A:7:ILE:O	1:A:7:ILE:HG23	2.07	0.53
1:C:303:GLY:HA2	1:C:392:PHE:CD1	2.43	0.53
1:A:136:ARG:NH1	1:A:144:PRO:HD3	2.23	0.53
1:C:6:GLN:N	3:C:2001:HOH:O	2.41	0.53
1:A:330:GLY:N	3:A:2076:HOH:O	2.41	0.53
1:B:450:LYS:NZ	3:B:2150:HOH:O	2.38	0.53
1:C:487:ASP:OD1	1:C:490:LYS:HE3	2.09	0.53
1:A:108:LEU:HD23	1:A:261:LYS:HE3	1.91	0.53
1:A:390:THR:HG22	3:A:2072:HOH:O	2.08	0.53
1:A:307:LYS:HD2	3:A:2072:HOH:O	2.09	0.52
1:C:75:LEU:HG	1:C:75:LEU:O	2.09	0.52
1:C:209:ASN:HB2	3:C:2036:HOH:O	2.09	0.52
1:B:27:ASN:ND2	3:B:2016:HOH:O	2.42	0.52
1:B:74:LEU:O	1:B:74:LEU:HD13	2.10	0.52
1:A:185:ASN:HD21	1:A:226:GLY:HA3	1.74	0.52
1:C:216:ILE:N	1:C:216:ILE:HD12	2.21	0.52
1:A:160:TYR:CZ	1:A:248:GLY:HA2	2.45	0.52
1:B:359:GLN:H	1:B:359:GLN:NE2	2.08	0.52
1:C:374:PHE:CB	3:C:2064:HOH:O	2.58	0.52
1:A:493:GLU:HB3	3:A:2105:HOH:O	2.10	0.52
1:B:148:ARG:NH1	1:B:148:ARG:HG2	2.09	0.52
1:C:397:LYS:NZ	3:C:2068:HOH:O	2.42	0.52
1:C:493:GLU:C	3:C:2097:HOH:O	2.47	0.52
1:B:480:SER:OG	1:B:486:TYR:HA	2.09	0.52
1:B:482:LYS:HE2	3:B:2157:HOH:O	2.10	0.51
1:C:155:LYS:HZ2	1:C:195:GLN:HE21	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PRO:HG3	1:A:82:TYR:CZ	2.45	0.51
1:C:470:TYR:O	1:C:471:HIS:CB	2.57	0.51
1:B:492:GLU:OE1	1:B:492:GLU:CA	2.59	0.51
1:A:194:TYR:O	1:A:195:GLN:HB2	2.09	0.51
1:A:30:VAL:HG13	1:A:31:THR:N	2.25	0.51
1:C:56:LEU:HD11	1:C:61:ILE:HG13	1.92	0.51
1:C:31:THR:CG2	1:C:32:HIS:CE1	2.94	0.51
1:C:355:HIS:HB2	1:C:478:MET:HE3	1.93	0.51
1:C:457:ASP:HB2	1:C:488:TYR:OH	2.10	0.51
1:A:129:HIS:HD2	3:A:2036:HOH:O	1.92	0.51
1:A:18:GLU:O	1:A:29:THR:HA	2.11	0.51
1:A:74:LEU:O	1:A:75:LEU:CB	2.59	0.51
1:C:173:GLU:HG3	1:C:258:LYS:HE3	1.92	0.51
1:A:107:HIS:O	1:A:110:THR:HB	2.11	0.51
1:B:357:ASN:OD1	1:B:473:CYS:O	2.29	0.51
1:C:188:THR:O	1:C:192:THR:CG2	2.58	0.51
1:B:140:VAL:O	1:B:141:SER:C	2.49	0.50
1:C:261:LYS:CD	3:C:2050:HOH:O	2.51	0.50
1:C:45:LEU:HD12	1:C:272:LYS:HB2	1.93	0.50
1:B:261:LYS:CB	1:B:261:LYS:NZ	2.72	0.50
1:B:448:TYR:CE1	1:B:465:GLY:HA2	2.46	0.50
1:C:9:ILE:N	1:C:9:ILE:HD13	2.26	0.50
1:A:75:LEU:O	1:A:75:LEU:CG	2.59	0.50
1:B:269:LYS:HE2	1:B:398:GLU:OE1	2.11	0.50
1:C:487:ASP:O	1:C:487:ASP:OD2	2.29	0.50
1:A:184:PRO:HG2	1:A:190:GLN:HE21	1.76	0.50
1:A:185:ASN:ND2	3:A:2045:HOH:O	2.40	0.50
1:C:490:LYS:HB3	1:C:491:TYR:CD2	2.46	0.50
1:C:9:ILE:HD12	1:C:353:TYR:CD2	2.47	0.50
1:C:372:LYS:O	1:C:372:LYS:HG2	2.11	0.50
1:A:213:ILE:HD13	1:A:213:ILE:H	1.75	0.50
1:C:106:LYS:NZ	1:C:398:GLU:OE2	2.40	0.50
1:B:6:GLN:CA	3:B:2002:HOH:O	2.60	0.50
1:C:10:GLY:HA3	1:C:343:TRP:CZ3	2.47	0.50
1:B:494:GLU:CB	3:B:2164:HOH:O	2.59	0.49
1:C:79:GLU:HG3	1:C:113:THR:O	2.12	0.49
1:C:478:MET:O	1:C:480:SER:N	2.45	0.49
1:A:140:VAL:O	1:A:141:SER:C	2.51	0.49
1:C:86:LYS:C	1:C:88:ASN:H	2.15	0.49
1:A:279:THR:HG22	3:A:2064:HOH:O	2.11	0.49
1:C:464:ASN:N	3:C:2087:HOH:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:CYS:O	1:A:145:SER:HB3	2.13	0.49
1:B:26:ARG:CG	1:B:26:ARG:NH1	2.65	0.49
1:C:434:GLU:HG2	3:C:2079:HOH:O	2.13	0.49
1:A:309:VAL:HG12	1:A:311:SER:H	1.78	0.49
1:A:427:LEU:HD21	3:A:2090:HOH:O	2.12	0.49
1:B:219:ARG:HD3	3:C:2036:HOH:O	2.13	0.49
1:B:261:LYS:NZ	1:B:261:LYS:HB2	2.26	0.49
1:C:474:ASP:O	1:C:476:GLU:N	2.46	0.49
1:A:188:THR:O	1:A:192:THR:HG22	2.13	0.49
1:A:268:MET:HE2	3:A:2071:HOH:O	2.12	0.49
1:A:464:ASN:N	3:A:2095:HOH:O	2.45	0.49
1:B:397:LYS:CG	3:B:2133:HOH:O	2.43	0.49
1:A:26:ARG:HA	1:A:26:ARG:HD3	1.45	0.49
1:C:87:GLU:HA	1:C:269:LYS:HG2	1.95	0.49
1:A:208:LEU:HG	1:A:209:ASN:N	2.28	0.48
1:B:148:ARG:NH1	1:B:148:ARG:CG	2.70	0.48
1:C:155:LYS:CD	1:C:195:GLN:HG2	2.43	0.48
1:B:303:GLY:HA2	1:B:392:PHE:CD1	2.48	0.48
1:B:462:LEU:HD23	1:B:462:LEU:HA	1.51	0.48
1:A:392:PHE:C	1:A:392:PHE:CD2	2.87	0.48
1:C:354:HIS:HA	1:C:362:GLY:O	2.14	0.48
1:C:97:GLY:HA3	1:C:229:MET:O	2.14	0.48
1:A:478:MET:C	1:A:480:SER:H	2.16	0.48
1:B:377:ILE:CG1	3:B:2126:HOH:O	2.62	0.48
1:B:354:HIS:HA	1:B:362:GLY:O	2.14	0.48
1:C:361:SER:HA	1:C:362:GLY:HA3	1.69	0.48
1:C:434:GLU:CG	3:C:2079:HOH:O	2.61	0.48
1:C:148:ARG:HG2	1:C:148:ARG:NH1	2.29	0.48
1:A:310:LYS:HE3	1:A:418:LEU:HD21	1.95	0.48
1:B:359:GLN:HE21	1:B:359:GLN:N	2.12	0.48
1:C:160:TYR:CZ	1:C:248:GLY:HA2	2.48	0.48
1:B:474:ASP:OD1	1:B:476:GLU:HB2	2.14	0.47
1:A:117:LYS:HG2	1:A:118:ILE:H	1.78	0.47
1:A:191:ARG:NH1	1:A:197:VAL:HG21	2.29	0.47
1:A:71:CYS:HB3	1:A:74:LEU:HD23	1.96	0.47
1:B:450:LYS:HE2	1:B:450:LYS:HB3	1.44	0.47
1:A:360:GLY:O	1:A:361:SER:HB3	2.13	0.47
1:A:458:ASN:OD1	1:A:488:TYR:CE1	2.67	0.47
1:C:148:ARG:HG2	1:C:148:ARG:HH11	1.79	0.47
1:A:184:PRO:HG2	1:A:190:GLN:NE2	2.29	0.47
1:B:26:ARG:HG3	1:B:26:ARG:NH1	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:THR:HG22	1:A:322:ASN:HB3	1.97	0.47
1:C:113:THR:OG1	1:C:260:SER:CB	2.61	0.47
1:C:54:LEU:HB2	1:C:80:TRP:CG	2.50	0.47
1:B:462:LEU:HB2	1:B:466:CYS:O	2.14	0.47
1:C:112:VAL:HG13	1:C:114:HIS:O	2.13	0.47
1:C:494:GLU:CB	3:C:2098:HOH:O	2.57	0.47
1:A:31:THR:HG23	1:A:32:HIS:CE1	2.50	0.47
1:B:111:SER:HB2	1:B:265:SER:CB	2.43	0.47
1:C:289:ASN:ND2	3:C:2056:HOH:O	2.47	0.47
1:C:309:VAL:HG12	1:C:311:SER:H	1.80	0.47
1:A:164:LYS:HD3	3:C:2042:HOH:O	2.15	0.47
1:C:480:SER:HB2	1:C:485:THR:O	2.15	0.47
1:C:488:TYR:N	1:C:489:PRO:CD	2.76	0.47
1:B:397:LYS:CD	3:B:2134:HOH:O	2.55	0.47
1:B:183:TYR:CE1	1:B:214:PRO:HA	2.49	0.46
1:A:9:ILE:HD11	1:A:451:VAL:HG21	1.96	0.46
1:C:492:GLU:OE1	1:C:492:GLU:CA	2.55	0.46
1:B:482:LYS:NZ	3:B:2157:HOH:O	2.47	0.46
1:C:464:ASN:O	1:C:464:ASN:OD1	2.34	0.46
1:A:110:THR:HG21	1:A:265:SER:N	2.19	0.46
1:A:55:GLU:CD	1:A:274:LEU:HB2	2.36	0.46
1:A:289:ASN:ND2	3:A:2065:HOH:O	2.46	0.46
1:B:56:LEU:HD11	1:B:61:ILE:HG13	1.97	0.46
1:A:30:VAL:CG1	1:A:31:THR:N	2.78	0.46
1:B:146:PHE:HD1	3:B:2064:HOH:O	1.98	0.46
1:B:45:LEU:C	1:B:45:LEU:HD23	2.36	0.46
1:C:298:HIS:CG	3:C:2053:HOH:O	2.63	0.46
1:A:108:LEU:HD11	1:A:235:LEU:HD11	1.97	0.46
1:A:113:THR:HG1	1:A:260:SER:HB2	1.81	0.46
1:A:74:LEU:O	1:A:74:LEU:HD12	2.15	0.46
1:B:45:LEU:HD23	1:B:46:CYS:N	2.31	0.46
1:C:7:ILE:HA	1:C:7:ILE:HD12	1.79	0.46
1:A:488:TYR:N	1:A:489:PRO:CD	2.79	0.45
1:C:86:LYS:C	1:C:88:ASN:N	2.69	0.45
1:C:140:VAL:O	1:C:141:SER:C	2.54	0.45
1:C:338:PHE:O	1:C:464:ASN:HA	2.17	0.45
1:C:138:CYS:O	1:C:145:SER:HB3	2.17	0.45
1:C:474:ASP:O	1:C:477:CYS:N	2.46	0.45
1:C:18:GLU:HG2	1:C:33:ALA:CB	2.46	0.45
1:A:293:PRO:HG3	1:A:385:ILE:HA	1.99	0.45
1:C:110:THR:CG2	1:C:265:SER:N	2.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:GLU:C	3:A:2106:HOH:O	2.55	0.45
1:C:207:THR:HG23	3:C:2035:HOH:O	2.16	0.45
1:A:404:ARG:HD2	1:A:404:ARG:HA	1.52	0.45
1:A:60:SER:HB2	3:A:2026:HOH:O	2.15	0.45
1:B:194:TYR:O	1:B:196:ASN:N	2.47	0.45
1:A:398:GLU:HG3	3:A:2030:HOH:O	2.17	0.45
1:C:51:ILE:HA	1:C:52:PRO:HD3	1.82	0.45
1:C:77:VAL:HG23	1:C:79:GLU:H	1.82	0.45
1:B:392:PHE:CD2	1:B:392:PHE:C	2.90	0.44
1:B:431:MET:O	1:B:435:ARG:HG3	2.18	0.44
1:A:320:LEU:HB3	1:A:440:HIS:CG	2.52	0.44
1:A:309:VAL:CG1	1:A:422:THR:HA	2.44	0.44
1:A:85:GLU:O	1:A:269:LYS:HA	2.17	0.44
1:C:248:GLY:O	1:C:249:ASN:HB2	2.17	0.44
1:B:111:SER:O	1:B:261:LYS:HD3	2.17	0.44
1:B:275:GLU:O	1:B:276:ASN:HB3	2.18	0.44
1:C:209:ASN:CB	3:C:2038:HOH:O	2.66	0.44
1:C:261:LYS:HB2	1:C:261:LYS:NZ	2.26	0.44
1:A:313:ARG:NH1	1:A:315:VAL:HG21	2.31	0.44
1:A:53:PRO:HD2	1:A:274:LEU:HG	2.00	0.44
1:B:479:ASN:N	3:B:2157:HOH:O	2.51	0.44
1:C:155:LYS:HZ3	1:C:195:GLN:NE2	2.15	0.44
1:C:399:PHE:CE1	1:C:406:LEU:HG	2.52	0.44
1:B:85:GLU:O	1:B:269:LYS:HA	2.17	0.44
1:A:426:GLU:HB3	1:B:387:LYS:HD2	1.99	0.44
1:C:490:LYS:HE3	1:C:490:LYS:HB2	1.85	0.44
1:B:279:THR:HB	1:B:281:CYS:H	1.83	0.44
1:B:391:GLN:H	1:B:391:GLN:HG2	1.54	0.44
1:A:118:ILE:O	1:A:118:ILE:HG22	2.16	0.44
1:A:462:LEU:HB2	1:A:466:CYS:HB2	1.99	0.44
1:B:97:GLY:HA3	1:B:229:MET:O	2.18	0.44
1:C:193:LEU:HD12	1:C:193:LEU:HA	1.66	0.44
1:C:458:ASN:O	1:C:470:TYR:HB2	2.17	0.44
1:B:216:ILE:HD12	1:B:216:ILE:H	1.83	0.44
1:B:272:LYS:HB3	1:B:272:LYS:HE3	1.83	0.43
1:B:55:GLU:CD	1:B:274:LEU:HB2	2.37	0.43
1:C:206:SER:HB2	3:C:2035:HOH:O	2.18	0.43
1:A:196:ASN:ND2	1:A:196:ASN:N	2.57	0.43
1:A:336:ALA:HB3	3:A:2077:HOH:O	2.17	0.43
1:A:361:SER:HA	1:A:362:GLY:HA3	1.82	0.43
1:A:445:LYS:O	1:A:445:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LEU:O	1:A:149:ASN:HB2	2.18	0.43
1:B:404:ARG:N	1:B:404:ARG:HD2	2.24	0.43
1:A:54:LEU:HD23	1:A:83:ILE:HG12	1.99	0.43
1:B:355:HIS:C	1:B:355:HIS:CD2	2.91	0.43
1:B:47:ARG:HG3	1:B:51:ILE:C	2.39	0.43
1:A:483:ASN:ND2	3:A:2101:HOH:O	2.50	0.43
1:C:30:VAL:HG13	1:C:31:THR:N	2.34	0.43
1:C:456:ARG:NH2	1:C:488:TYR:CD2	2.85	0.43
1:B:52:PRO:O	1:B:80:TRP:HA	2.18	0.43
1:A:478:MET:C	1:A:480:SER:N	2.71	0.43
1:C:112:VAL:HG11	1:C:115:PHE:CB	2.48	0.43
1:C:106:LYS:CE	1:C:398:GLU:OE2	2.67	0.43
1:C:452:ARG:NH1	1:C:453:MET:HG3	2.32	0.43
1:C:484:GLY:O	1:C:485:THR:HG23	2.19	0.43
1:A:355:HIS:CD2	1:A:361:SER:HA	2.54	0.43
1:C:215:GLU:O	1:C:219:ARG:NH2	2.52	0.43
1:A:174:GLN:HE22	1:A:235:LEU:HD13	1.81	0.43
1:A:488:TYR:HB3	1:A:489:PRO:HD3	2.01	0.43
1:B:293:PRO:HG3	1:B:385:ILE:HA	2.01	0.43
1:C:113:THR:HG23	1:C:261:LYS:HA	2.00	0.43
1:B:289:ASN:ND2	3:B:2107:HOH:O	2.51	0.42
1:B:402:LEU:HD23	1:B:402:LEU:HA	1.84	0.42
1:C:128:GLN:HB2	3:C:2019:HOH:O	2.18	0.42
1:A:203:VAL:HG12	1:A:208:LEU:HD23	2.01	0.42
1:A:265:SER:OG	1:A:266:GLY:N	2.50	0.42
1:C:486:TYR:CD2	1:C:486:TYR:O	2.72	0.42
1:B:482:LYS:CE	3:B:2157:HOH:O	2.67	0.42
1:B:51:ILE:HA	1:B:52:PRO:HD3	1.79	0.42
1:C:14:ASN:OD1	1:C:16:SER:HB3	2.19	0.42
1:A:348:ASP:OD1	1:A:348:ASP:N	2.53	0.42
1:A:320:LEU:HB3	1:A:440:HIS:CB	2.49	0.42
1:A:71:CYS:O	1:A:74:LEU:HB2	2.18	0.42
1:B:248:GLY:O	1:B:249:ASN:HB2	2.20	0.42
1:B:464:ASN:O	1:B:464:ASN:CG	2.58	0.42
1:C:360:GLY:O	1:C:361:SER:CB	2.67	0.42
1:C:483:ASN:ND2	3:C:2093:HOH:O	2.52	0.42
1:B:133:GLY:N	3:B:2062:HOH:O	2.46	0.42
1:A:391:GLN:H	1:A:391:GLN:HG2	1.56	0.42
1:A:79:GLU:O	1:A:80:TRP:O	2.38	0.42
1:C:463:GLY:N	3:C:2087:HOH:O	2.52	0.42
1:A:316:LEU:HD12	1:A:316:LEU:HA	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:ASP:OD2	1:A:490:LYS:HB3	2.20	0.42
1:A:140:VAL:HG11	1:A:148:ARG:HH22	1.85	0.42
1:A:186:ASP:N	1:A:186:ASP:OD2	2.53	0.42
1:C:478:MET:O	1:C:481:VAL:N	2.53	0.42
1:C:56:LEU:HD23	1:C:56:LEU:HA	1.84	0.42
1:B:202:SER:HB3	1:B:245:GLU:HB3	2.01	0.41
1:C:283:THR:CB	3:C:2053:HOH:O	2.44	0.41
1:C:355:HIS:CE1	1:C:362:GLY:HA3	2.55	0.41
1:B:110:THR:CG2	1:B:265:SER:N	2.78	0.41
1:C:268:MET:HE2	3:C:2058:HOH:O	2.19	0.41
1:C:309:VAL:HG13	1:C:311:SER:HB3	2.02	0.41
1:A:174:GLN:HE21	1:A:235:LEU:HB3	1.84	0.41
1:A:189:GLU:CA	1:A:192:THR:HG23	2.47	0.41
1:B:435:ARG:NE	3:B:2147:HOH:O	2.53	0.41
1:B:412:LYS:CE	3:C:2068:HOH:O	2.67	0.41
1:C:155:LYS:HZ2	1:C:195:GLN:NE2	2.18	0.41
1:A:131:THR:HG23	1:A:131:THR:O	2.21	0.41
1:B:216:ILE:HD12	1:B:216:ILE:N	2.34	0.41
1:C:284:PRO:HD2	3:C:2053:HOH:O	2.21	0.41
1:A:188:THR:O	1:A:192:THR:CG2	2.69	0.41
1:A:235:LEU:HD23	1:A:235:LEU:HA	1.88	0.41
1:C:123:ARG:NH2	1:C:150:MET:O	2.53	0.41
1:A:30:VAL:HG13	1:A:31:THR:H	1.85	0.41
1:C:118:ILE:HD11	1:C:258:LYS:HD2	2.00	0.41
1:A:78:PRO:O	1:A:114:HIS:HA	2.20	0.41
1:B:181:ILE:HD12	1:B:212:SER:HB2	2.03	0.41
1:B:58:ASP:OD2	1:B:90:THR:HG23	2.20	0.41
1:B:68:ASN:HA	1:B:69:PRO:HD3	1.94	0.41
1:B:6:GLN:CB	3:B:2002:HOH:O	2.68	0.41
1:C:86:LYS:O	1:C:88:ASN:N	2.54	0.41
1:A:261:LYS:HD3	3:A:2060:HOH:O	2.19	0.41
1:C:117:LYS:HG3	1:C:257:PHE:CE2	2.55	0.41
1:B:6:GLN:HA	3:B:2002:HOH:O	2.21	0.41
1:A:108:LEU:HD21	1:A:261:LYS:HZ1	1.87	0.40
1:A:118:ILE:CG2	1:A:120:ILE:HG23	2.51	0.40
1:A:179:TRP:CE2	1:A:203:VAL:HG21	2.55	0.40
1:B:248:GLY:C	1:B:249:ASN:ND2	2.74	0.40
1:B:108:LEU:HD23	1:B:261:LYS:NZ	2.36	0.40
1:C:108:LEU:O	1:C:261:LYS:HD3	2.21	0.40
1:C:110:THR:HG23	1:C:265:SER:N	2.35	0.40
1:B:74:LEU:HA	1:B:74:LEU:HD22	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	479/507 (94%)	431 (90%)	37 (8%)	11 (2%)	6 10
1	B	482/507 (95%)	447 (93%)	28 (6%)	7 (2%)	10 18
1	C	482/507 (95%)	429 (89%)	36 (8%)	17 (4%)	3 4
All	All	1443/1521 (95%)	1307 (91%)	101 (7%)	35 (2%)	6 9

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	TRP
1	B	80	TRP
1	B	311	SER
1	B	359	GLN
1	C	80	TRP
1	C	361	SER
1	C	455	LEU
1	C	456	ARG
1	A	141	SER
1	A	196	ASN
1	A	276	ASN
1	A	361	SER
1	B	141	SER
1	B	362	GLY
1	C	141	SER
1	C	471	HIS
1	C	475	ASP
1	C	479	ASN
1	A	479	ASN
1	B	195	GLN
1	A	311	SER

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Mol	Chain	Res	Type
1	A	362	GLY
1	A	395	VAL
1	C	489	PRO
1	A	75	LEU
1	A	195	GLN
1	C	75	LEU
1	C	114	HIS
1	C	359	GLN
1	C	464	ASN
1	B	395	VAL
1	C	298	HIS
1	C	395	VAL
1	C	481	VAL
1	C	362	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	415/445 (93%)	369 (89%)	46 (11%)	6 11
1	B	416/445 (94%)	373 (90%)	43 (10%)	7 14
1	C	416/445 (94%)	364 (88%)	52 (12%)	4 8
All	All	1247/1335 (93%)	1106 (89%)	141 (11%)	6 11

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	26	ARG
1	A	31	THR
1	A	39	LYS
1	A	61	ILE
1	A	74	LEU
1	A	75	LEU
1	A	80	TRP

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Mol	Chain	Res	Type
1	A	90	THR
1	A	108	LEU
1	A	110	THR
1	A	118	ILE
1	A	127	THR
1	A	131	THR
1	A	188	THR
1	A	192	THR
1	A	196	ASN
1	A	202	SER
1	A	209	ASN
1	A	213	ILE
1	A	241	VAL
1	A	261	LYS
1	A	264	SER
1	A	273	THR
1	A	274	LEU
1	A	276	ASN
1	A	279	THR
1	A	291	THR
1	A	304	GLU
1	A	316	LEU
1	A	320	LEU
1	A	323	VAL
1	A	340	GLU
1	A	347	VAL
1	A	356	SER
1	A	359	GLN
1	A	368	GLU
1	A	391	GLN
1	A	398	GLU
1	A	401	ASN
1	A	404	ARG
1	A	409	LEU
1	A	442	SER
1	A	462	LEU
1	A	486	TYR
1	A	487	ASP
1	B	6	GLN
1	B	26	ARG
1	B	30	VAL
1	B	31	THR

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Mol	Chain	Res	Type
1	B	39	LYS
1	B	74	LEU
1	B	80	TRP
1	B	90	THR
1	B	99	PHE
1	B	108	LEU
1	B	110	THR
1	B	112	VAL
1	B	127	THR
1	B	131	THR
1	B	148	ARG
1	B	159	ASN
1	B	188	THR
1	B	192	THR
1	B	196	ASN
1	B	213	ILE
1	B	237	GLU
1	B	241	VAL
1	B	261	LYS
1	B	264	SER
1	B	269	LYS
1	B	274	LEU
1	B	279	THR
1	B	291	THR
1	B	316	LEU
1	B	320	LEU
1	B	351	TYR
1	B	356	SER
1	B	359	GLN
1	B	368	GLU
1	B	391	GLN
1	B	404	ARG
1	B	409	LEU
1	B	427	LEU
1	B	442	SER
1	B	456	ARG
1	B	462	LEU
1	B	464	ASN
1	B	492	GLU
1	C	7	ILE
1	C	16	SER
1	C	26	ARG

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Mol	Chain	Res	Type
1	C	31	THR
1	C	45	LEU
1	C	61	ILE
1	C	74	LEU
1	C	80	TRP
1	C	88	ASN
1	C	90	THR
1	C	99	PHE
1	C	110	THR
1	C	111	SER
1	C	112	VAL
1	C	114	HIS
1	C	123	ARG
1	C	127	THR
1	C	131	THR
1	C	132	THR
1	C	192	THR
1	C	193	LEU
1	C	196	ASN
1	C	209	ASN
1	C	213	ILE
1	C	216	ILE
1	C	237	GLU
1	C	241	VAL
1	C	264	SER
1	C	273	THR
1	C	279	THR
1	C	291	THR
1	C	307	LYS
1	C	309	VAL
1	C	311	SER
1	C	316	LEU
1	C	347	VAL
1	C	351	TYR
1	C	359	GLN
1	C	368	GLU
1	C	372	LYS
1	C	378	THR
1	C	379	ASN
1	C	391	GLN
1	C	404	ARG
1	C	409	LEU

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Mol	Chain	Res	Type
1	C	442	SER
1	C	462	LEU
1	C	474	ASP
1	C	476	GLU
1	C	486	TYR
1	C	492	GLU
1	C	496	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	129	HIS
1	A	159	ASN
1	A	174	GLN
1	A	185	ASN
1	A	190	GLN
1	A	196	ASN
1	A	249	ASN
1	A	355	HIS
1	A	357	ASN
1	B	27	ASN
1	B	129	HIS
1	B	190	GLN
1	B	196	ASN
1	B	249	ASN
1	B	344	GLN
1	B	355	HIS
1	B	357	ASN
1	B	391	GLN
1	B	464	ASN
1	C	129	HIS
1	C	159	ASN
1	C	190	GLN
1	C	195	GLN
1	C	249	ASN
1	C	359	GLN
1	C	391	GLN

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

3 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	$\#\|Z\| > 2$
2	NAG	D	1	2	14,14,15	0.53	0	17,19,21	2.04	5 (29%)
2	GAL	D	2	2	11,11,12	0.32	0	15,15,17	1.23	2 (13%)
2	SIA	D	3	2	17,20,21	0.36	0	21,28,31	1.06	1 (4%)

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	D	1	2	-	0/6/23/26	0/1/1/1
2	GAL	D	2	2	-	2/2/19/22	0/1/1/1
2	SIA	D	3	2	-	0/14/34/38	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	NAG	C1-C2-N2	-3.96	103.72	110.49
2	D	1	NAG	O5-C1-C2	3.90	117.44	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	NAG	C3-C4-C5	-3.66	103.72	110.24
2	D	1	NAG	O5-C5-C6	3.28	112.34	107.20
2	D	3	SIA	C4-C5-N5	-2.21	105.99	110.38
2	D	2	GAL	C1-C2-C3	2.20	112.37	109.67
2	D	2	GAL	O3-C3-C2	-2.18	105.81	109.99
2	D	1	NAG	C1-O5-C5	2.17	115.13	112.19

There are no chirality outliers.

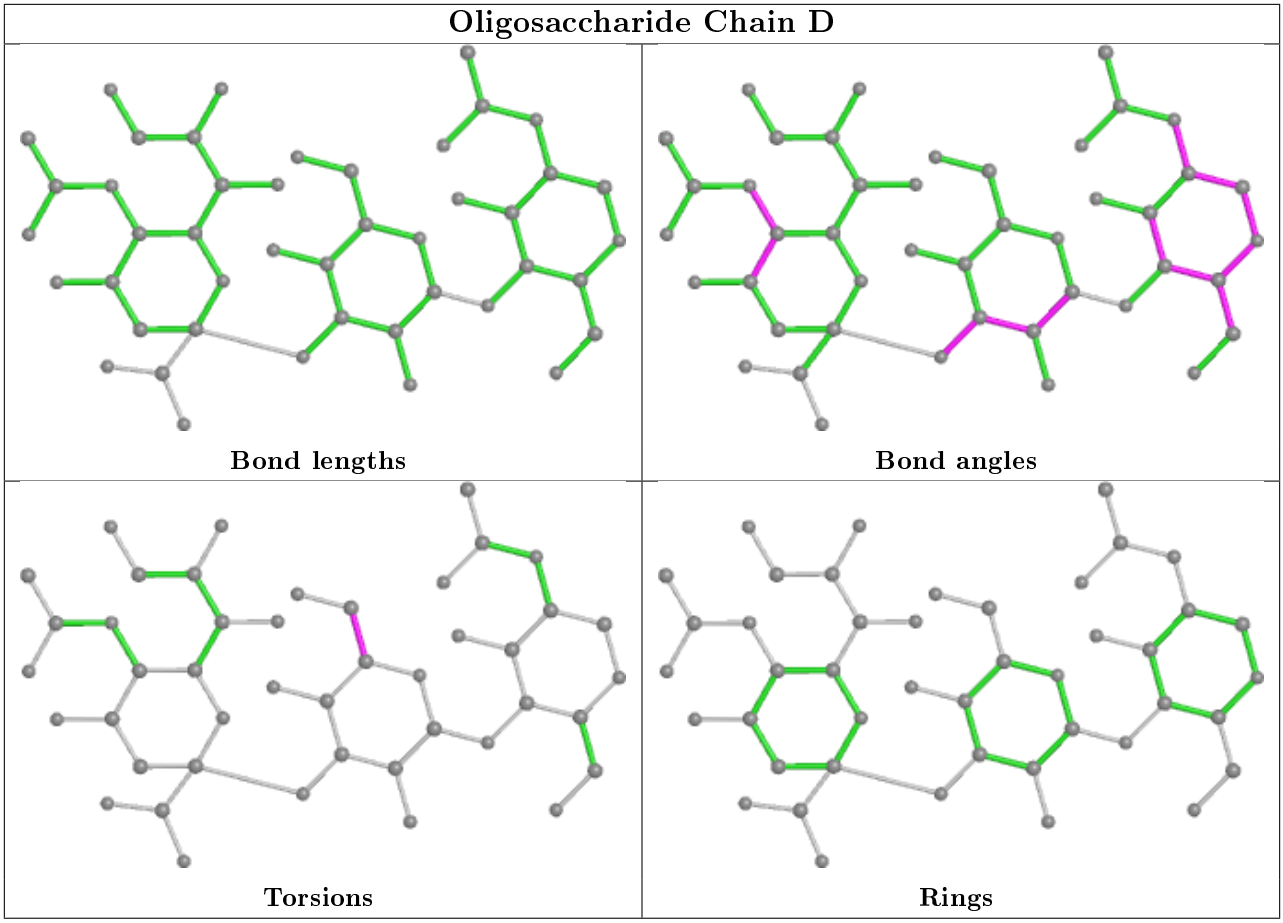
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	GAL	O5-C5-C6-O6
2	D	2	GAL	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	485/507 (95%)	0.25	24 (4%)	29	31	45, 76, 139, 259	0
1	B	486/507 (95%)	0.09	15 (3%)	49	52	40, 65, 117, 222	0
1	C	486/507 (95%)	0.28	29 (5%)	21	22	47, 78, 142, 239	0
All	All	1457/1521 (95%)	0.21	68 (4%)	31	33	40, 73, 137, 259	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	360	GLY	6.0
1	C	360	GLY	5.1
1	C	324	PRO	4.9
1	A	276	ASN	4.6
1	C	277	CYS	4.6
1	A	151	VAL	4.5
1	A	141	SER	4.4
1	C	470	TYR	4.0
1	A	476	GLU	4.0
1	C	488	TYR	3.8
1	C	141	SER	3.8
1	C	473	CYS	3.8
1	A	431	MET	3.8
1	A	277	CYS	3.7
1	A	275	GLU	3.6
1	B	463	GLY	3.6
1	A	475	ASP	3.5
1	C	140	VAL	3.4
1	C	476	GLU	3.4
1	C	490	LYS	3.4
1	A	434	GLU	3.3
1	C	474	ASP	3.3
1	A	362	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	358	ASP	3.3
1	C	475	ASP	3.3
1	C	46	CYS	3.2
1	A	140	VAL	3.1
1	B	431	MET	3.0
1	C	491	TYR	3.0
1	A	143	ASN	3.0
1	B	468	GLU	3.0
1	A	157	GLY	2.9
1	C	359	GLN	2.8
1	A	485	THR	2.6
1	C	394	ALA	2.6
1	A	486	TYR	2.6
1	A	474	ASP	2.6
1	C	435	ARG	2.6
1	C	72	ASP	2.5
1	B	473	CYS	2.5
1	C	362	GLY	2.5
1	B	87	GLU	2.5
1	B	277	CYS	2.4
1	C	345	GLY	2.4
1	B	489	PRO	2.4
1	A	87	GLU	2.4
1	C	138	CYS	2.4
1	A	273	THR	2.4
1	B	8	CYS	2.3
1	C	65	LEU	2.3
1	B	466	CYS	2.3
1	B	427	LEU	2.3
1	C	84	VAL	2.3
1	B	487	ASP	2.2
1	C	496	LYS	2.2
1	B	435	ARG	2.1
1	C	495	SER	2.1
1	C	365	ALA	2.1
1	B	17	THR	2.1
1	C	17	THR	2.1
1	A	191	ARG	2.1
1	A	468	GLU	2.1
1	C	330	GLY	2.1
1	A	196	ASN	2.1
1	C	312	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	420	VAL	2.0
1	A	251	ILE	2.0
1	A	487	ASP	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)

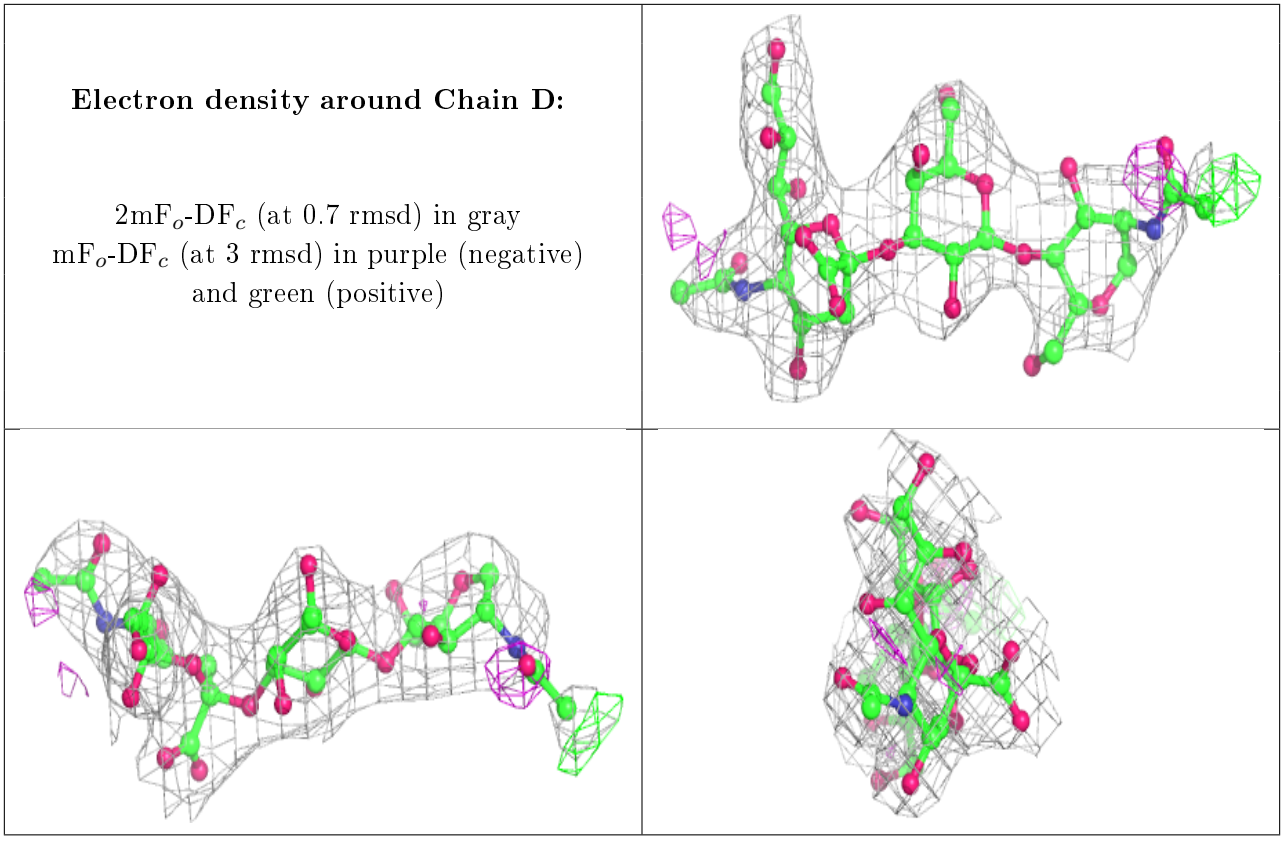
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	D	1	14/15	0.83	0.38	101,105,107,108	0
2	SIA	D	3	20/21	0.94	0.14	83,85,88,88	0
2	GAL	D	2	11/12	0.95	0.09	91,97,98,99	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 D:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.