



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:46 PM EDT

PDB ID : 2WR2 / pdb_00002wr2
Title : structure of influenza H2 avian 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 : 2.40 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:

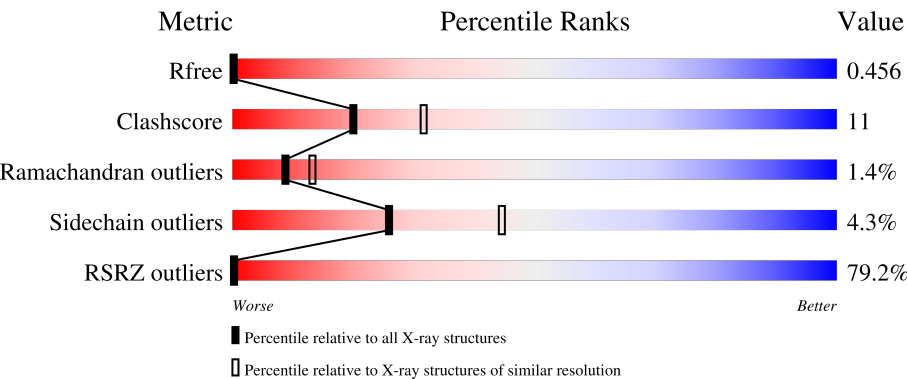
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	509	85% 76% 18% ...
1	B	509	61% 71% 22% ...
1	C	509	82% 75% 17% 5%
2	D	3	33% 33% 33%
2	E	3	100%

2 Entry composition [i](#)

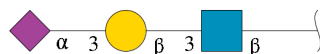
There are 4 unique types of molecules in this entry. The entry contains 12274 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1	0
			3887	2438	672	755	22			
1	C	485	Total	C	N	O	S	0	0	0
			3844	2413	664	745	22			

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



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

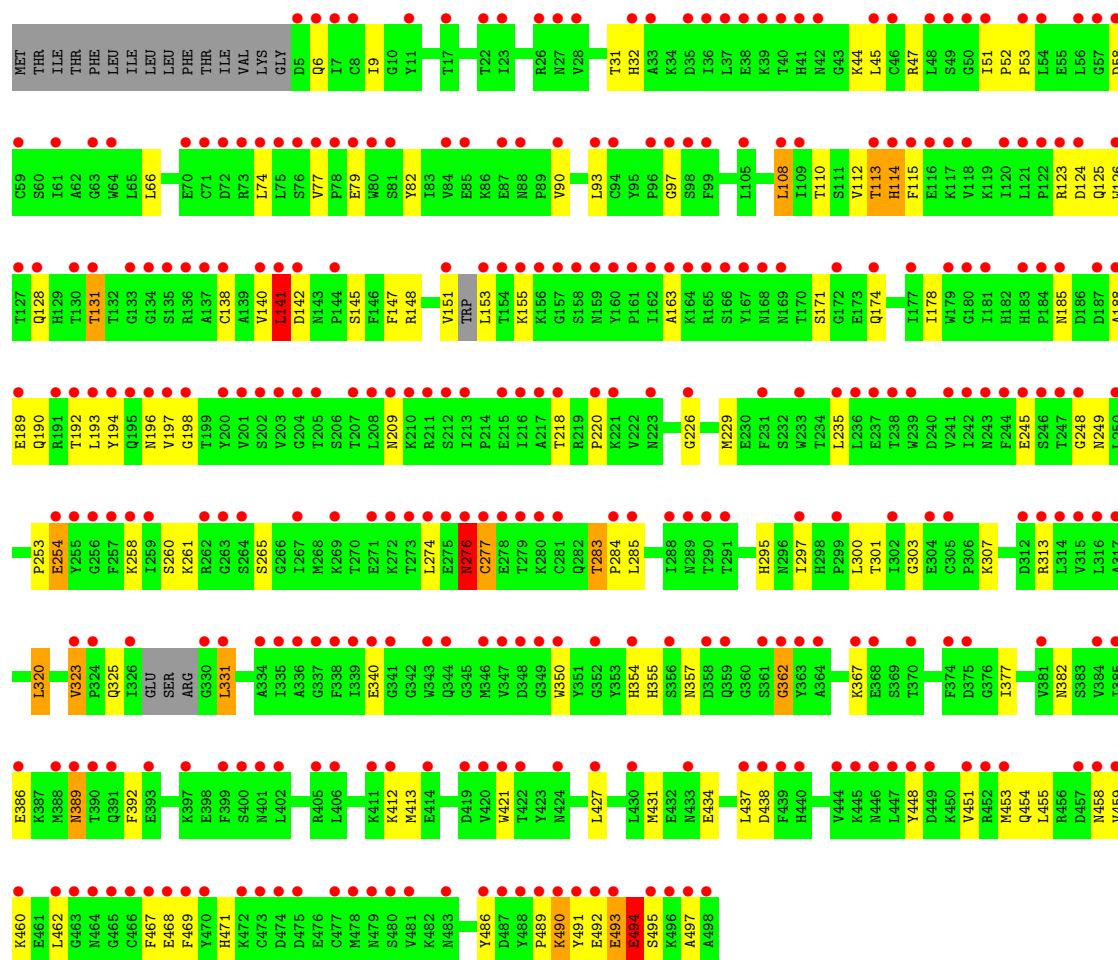
- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



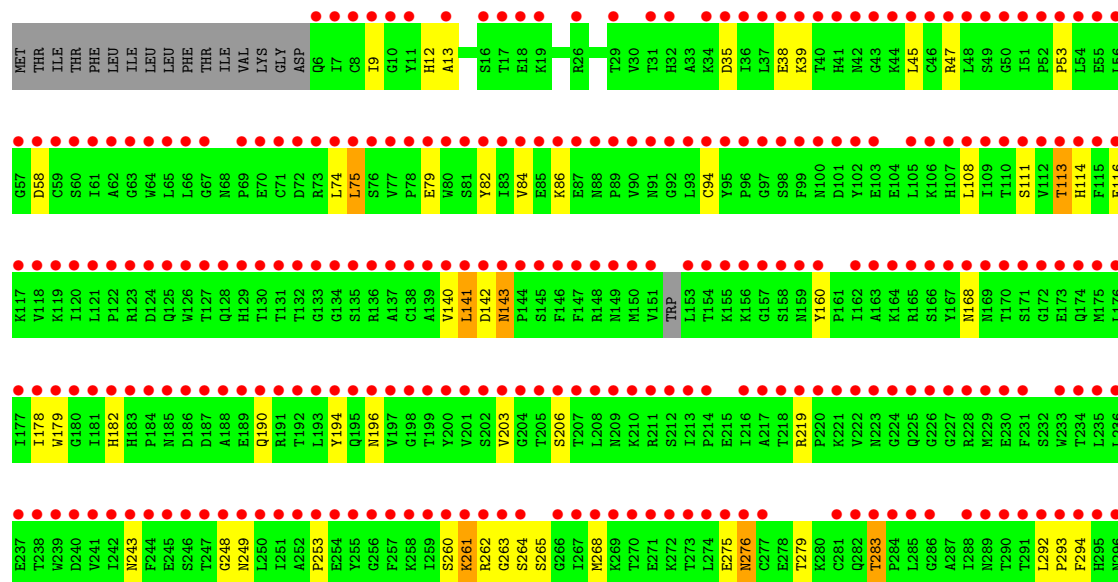
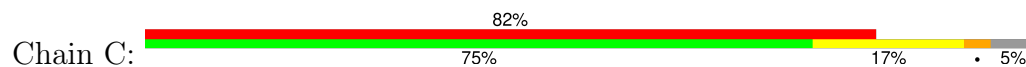
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			13	8	1	4		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

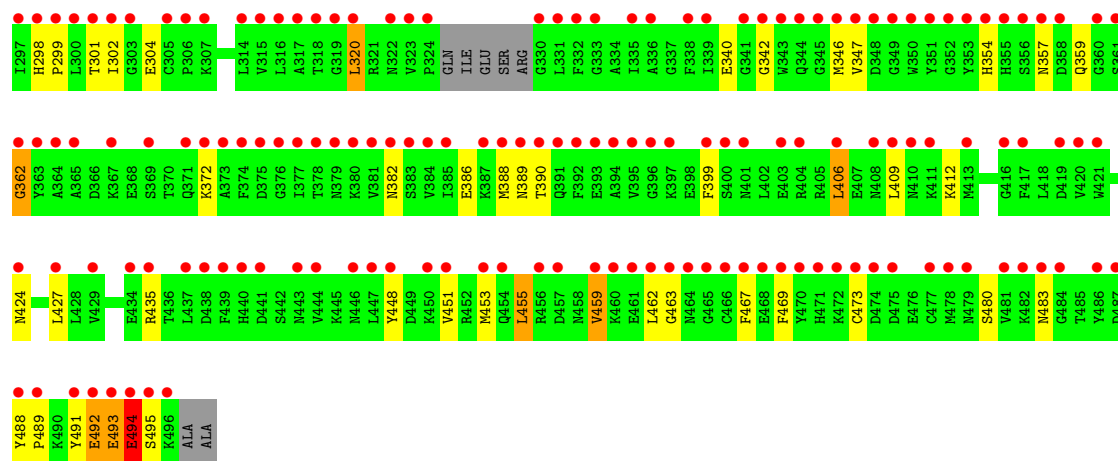
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	185	Total	O	0	0
			185	185		
4	B	169	Total	O	0	0
			169	169		
4	C	174	Total	O	0	0
			174	174		

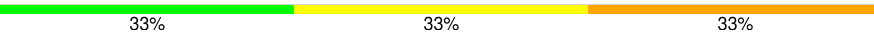


• Molecule 1: HEMAGGLUTININ



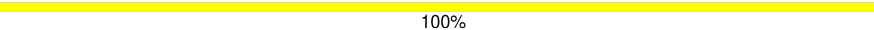


- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  33%



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

Chain E:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.88Å 142.72Å 199.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 2.40 29.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.94-2.40) 99.8 (29.94-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.210 , 0.248 0.447 , 0.456	Depositor DCC
R_{free} test set	3956 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	12274	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: GAL, NAG, SIA

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	0.41	0/3968	0.79	2/5372 (0.0%)
1	B	0.40	0/3970	0.80	5/5372 (0.1%)
1	C	0.40	0/3927	0.78	2/5313 (0.0%)
All	All	0.40	0/11865	0.79	9/16057 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	THR	N-CA-C	6.24	120.72	111.04
1	B	113	THR	CA-C-N	5.98	132.46	121.70
1	B	113	THR	C-N-CA	5.98	132.46	121.70
1	A	109	ILE	CB-CA-C	-5.57	105.79	112.19
1	B	340	GLU	N-CA-C	5.40	118.08	111.82
1	B	254	GLU	N-CA-C	-5.39	106.83	113.41
1	C	340	GLU	N-CA-C	5.38	117.90	111.71
1	A	497	ALA	N-CA-C	-5.26	106.80	113.43
1	C	141	LEU	N-CA-C	5.14	120.96	113.40

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	3882	0	3742	89	2
1	B	3887	0	3756	112	2
1	C	3844	0	3718	72	0
2	D	46	0	40	2	0
2	E	46	0	40	0	0
3	A	27	0	25	7	0
3	C	14	0	13	3	0
4	A	185	0	0	5	0
4	B	169	0	0	10	0
4	C	174	0	0	2	0
All	All	12274	0	11334	263	2

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 11.

All (263) 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:B:325:GLN:NE2	4:B:2109:HOH:O	1.62	1.27
1:A:283:THR:HG22	1:A:285:LEU:H	1.18	1.05
1:A:148:ARG:HG2	1:A:148:ARG:HH11	1.32	0.94
1:B:325:GLN:HB3	4:B:2110:HOH:O	1.65	0.93
1:A:361:SER:HB3	1:A:362:GLY:HA3	1.49	0.92
1:C:114:HIS:H	1:C:260:SER:HB2	1.35	0.91
1:B:140:VAL:O	1:B:141:LEU:HB2	1.72	0.89
1:B:459:VAL:HG22	1:B:469:PHE:HA	1.55	0.89
1:B:276:ASN:HA	1:B:277:CYS:O	1.73	0.89
1:A:110:THR:CG2	1:A:265:SER:H	1.86	0.88
1:B:459:VAL:HG11	1:B:467:PHE:HB3	1.54	0.88
1:A:463:GLY:HA2	1:C:453:MET:HE2	1.57	0.84
1:C:168:ASN:HD21	3:C:1500:NAG:C1	1.89	0.84
1:B:47:ARG:HE	1:B:276:ASN:HB2	1.42	0.84
1:C:141:LEU:N	1:C:142:ASP:HA	1.95	0.82
1:A:110:THR:HG21	1:A:265:SER:H	1.44	0.82
1:B:141:LEU:N	1:B:142:ASP:HA	1.97	0.79
1:A:114:HIS:H	1:A:260:SER:HB2	1.45	0.79
1:B:32:HIS:CD2	4:B:2124:HOH:O	2.37	0.78
1:B:110:THR:CG2	1:B:265:SER:H	1.95	0.78
1:C:114:HIS:N	1:C:260:SER:HB2	1.98	0.77
1:A:479:ASN:HB3	3:A:1499:NAG:H81	1.64	0.77
1:A:168:ASN:HD21	3:A:1500:NAG:C5	1.97	0.77
1:B:113:THR:HB	1:B:114:HIS:HB3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLN:HE22	1:A:249:ASN:HD21	1.33	0.77
1:A:174:GLN:HE21	1:A:235:LEU:HD13	1.51	0.76
1:B:455:LEU:HD13	1:B:459:VAL:HG21	1.66	0.75
1:B:458:ASN:OD1	1:B:494:GLU:HG2	1.86	0.74
1:A:493:GLU:O	1:A:494:GLU:HB3	1.88	0.73
1:A:174:GLN:NE2	1:A:235:LEU:HD13	2.04	0.73
1:C:190:GLN:HE22	1:C:249:ASN:HD21	1.36	0.73
1:A:283:THR:HG22	1:A:285:LEU:N	1.99	0.73
1:A:320:LEU:HD23	1:A:320:LEU:H	1.53	0.72
1:A:166:SER:HB3	1:A:243:ASN:ND2	2.05	0.72
1:A:283:THR:HB	1:A:286:GLY:O	1.89	0.72
1:B:354:HIS:HA	1:B:362:GLY:O	1.90	0.72
1:B:140:VAL:HG12	1:B:141:LEU:HD23	1.73	0.70
1:C:74:LEU:O	1:C:75:LEU:HB2	1.90	0.70
1:B:453:MET:HE2	1:C:463:GLY:HA2	1.73	0.70
1:B:110:THR:HG23	1:B:265:SER:H	1.57	0.69
1:A:313:ARG:HA	4:A:2015:HOH:O	1.93	0.69
1:A:380:LYS:HE3	1:A:432:GLU:OE1	1.93	0.68
1:C:320:LEU:H	1:C:320:LEU:HD23	1.58	0.68
1:A:493:GLU:O	1:A:494:GLU:CB	2.43	0.67
1:A:168:ASN:ND2	3:A:1500:NAG:C1	2.58	0.66
1:A:248:GLY:C	1:A:249:ASN:HD22	2.04	0.66
1:B:490:LYS:O	1:B:490:LYS:HG2	1.93	0.66
1:B:188:ALA:O	1:B:192:THR:HG22	1.95	0.66
1:B:295:HIS:HD2	1:B:297:ILE:H	1.44	0.66
1:C:354:HIS:HA	1:C:362:GLY:O	1.94	0.66
1:A:114:HIS:N	1:A:260:SER:HB2	2.09	0.65
1:C:275:GLU:O	1:C:276:ASN:HB3	1.96	0.65
1:B:459:VAL:HG13	1:B:468:GLU:O	1.96	0.65
1:C:79:GLU:HG3	1:C:113:THR:HB	1.78	0.64
1:C:357:ASN:HB3	1:C:359:GLN:H	1.62	0.64
1:C:262:ARG:HG3	1:C:263:GLY:H	1.63	0.64
1:C:168:ASN:ND2	3:C:1500:NAG:C1	2.59	0.63
1:A:168:ASN:HD21	3:A:1500:NAG:C1	2.12	0.63
1:B:492:GLU:HA	1:B:493:GLU:C	2.23	0.62
1:C:459:VAL:HG23	1:C:469:PHE:HA	1.80	0.62
1:A:283:THR:CG2	1:A:285:LEU:H	2.05	0.62
1:B:350:TRP:NE1	4:B:2124:HOH:O	2.27	0.62
1:B:113:THR:HB	1:B:114:HIS:CB	2.29	0.61
1:A:140:VAL:HG23	1:A:145:SER:HB2	1.81	0.61
1:A:455:LEU:HD23	1:A:459:VAL:HG21	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLY:HA2	1:A:278:GLU:OE2	2.00	0.61
1:C:111:SER:HB2	1:C:265:SER:HB2	1.83	0.61
1:B:413:MET:HE1	1:C:412:LYS:HG2	1.83	0.61
1:A:191:ARG:HD2	4:A:2085:HOH:O	2.00	0.61
1:B:140:VAL:C	1:B:142:ASP:HA	2.25	0.60
1:A:470:TYR:HB3	1:A:495:SER:HA	1.83	0.60
1:A:353:TYR:OH	1:A:447:LEU:HD11	2.01	0.60
1:B:320:LEU:HD23	1:B:320:LEU:H	1.66	0.60
1:A:435:ARG:NH1	1:C:435:ARG:NH1	2.49	0.60
1:C:459:VAL:HG21	1:C:467:PHE:HB3	1.84	0.59
1:B:190:GLN:HE22	1:B:249:ASN:HD21	1.49	0.59
1:B:454:GLN:NE2	1:B:486:TYR:H	2.00	0.58
1:A:72:ASP:OD1	1:A:73:ARG:N	2.36	0.58
1:C:493:GLU:C	1:C:494:GLU:HG3	2.27	0.58
1:B:123:ARG:HB2	1:B:254:GLU:OE2	2.03	0.58
1:B:171:SER:HB2	1:B:258:LYS:HD2	1.85	0.58
1:B:325:GLN:CB	4:B:2110:HOH:O	2.38	0.57
1:C:58:ASP:HB3	1:C:86:LYS:HD2	1.85	0.57
1:B:110:THR:HG21	1:B:265:SER:H	1.68	0.57
1:A:111:SER:HB2	1:A:265:SER:HB2	1.85	0.57
1:B:492:GLU:CD	1:B:495:SER:H	2.12	0.57
1:C:113:THR:HG23	1:C:113:THR:O	2.03	0.57
1:A:148:ARG:HH11	1:A:148:ARG:CG	2.10	0.56
1:C:488:TYR:HB3	1:C:489:PRO:HD3	1.87	0.56
1:C:53:PRO:HG3	1:C:82:TYR:CZ	2.41	0.56
1:B:112:VAL:HG11	1:B:115:PHE:HB2	1.86	0.56
1:B:493:GLU:O	1:B:494:GLU:HB2	2.05	0.56
1:A:298:HIS:ND1	1:A:299:PRO:HD2	2.20	0.56
1:A:9:ILE:HD11	1:A:451:VAL:HG21	1.88	0.56
1:B:44:LYS:HD3	1:B:277:CYS:SG	2.46	0.56
1:C:179:TRP:CE2	1:C:203:VAL:HG21	2.41	0.56
1:B:490:LYS:C	1:B:492:GLU:N	2.63	0.56
1:A:11:TYR:HB2	1:A:320:LEU:HD11	1.87	0.55
1:C:283:THR:HG22	1:C:301:THR:HG22	1.87	0.55
1:B:492:GLU:OE2	1:B:495:SER:N	2.39	0.55
1:C:47:ARG:O	1:C:279:THR:HG22	2.06	0.55
1:B:193:LEU:HD21	2:D:3:SIA:O10	2.06	0.55
1:B:490:LYS:C	1:B:492:GLU:H	2.13	0.55
1:A:413:MET:HE1	1:B:412:LYS:HE3	1.89	0.55
1:C:114:HIS:H	1:C:260:SER:CB	2.14	0.55
1:C:45:LEU:HD21	1:C:84:VAL:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ASP:OD2	1:A:148:ARG:HD2	2.07	0.54
1:B:283:THR:HG22	1:B:301:THR:HG22	1.89	0.54
1:B:9:ILE:HD11	1:B:451:VAL:HG21	1.89	0.54
1:B:382:ASN:O	1:B:386:GLU:HG2	2.07	0.54
1:A:148:ARG:HG2	1:A:148:ARG:NH1	2.11	0.54
1:B:31:THR:C	1:B:32:HIS:CD2	2.86	0.54
1:B:495:SER:C	1:B:497:ALA:N	2.65	0.54
1:A:110:THR:HG23	1:A:265:SER:HB3	1.90	0.54
1:B:138:CYS:O	1:B:145:SER:HB3	2.08	0.53
1:C:114:HIS:CE1	1:C:116:GLU:HB2	2.43	0.53
1:B:124:ASP:OD1	1:B:125:GLN:HG3	2.08	0.53
1:C:424:ASN:ND2	4:C:2149:HOH:O	2.42	0.53
1:C:113:THR:C	1:C:260:SER:HB2	2.34	0.52
1:A:110:THR:CG2	1:A:265:SER:N	2.66	0.52
1:B:53:PRO:HG3	1:B:82:TYR:CZ	2.45	0.52
1:B:355:HIS:CE1	1:B:362:GLY:HA2	2.44	0.52
1:C:357:ASN:OD1	1:C:473:CYS:O	2.28	0.52
1:B:490:LYS:HB2	4:B:2167:HOH:O	2.09	0.52
1:C:262:ARG:HG3	1:C:263:GLY:N	2.24	0.52
1:A:495:SER:HB2	4:A:2177:HOH:O	2.10	0.52
1:C:304:GLU:HB3	1:C:390:THR:HG22	1.90	0.51
1:A:361:SER:CB	1:A:362:GLY:HA3	2.29	0.51
1:B:491:TYR:O	1:B:494:GLU:HB2	2.09	0.51
1:A:19:LYS:O	1:A:313:ARG:NH2	2.44	0.51
1:B:126:TRP:HZ3	1:B:163:ALA:HB1	1.76	0.51
1:A:113:THR:HG23	1:A:113:THR:O	2.10	0.51
1:B:491:TYR:C	1:B:494:GLU:HB2	2.36	0.50
1:A:355:HIS:CE1	1:A:361:SER:HB2	2.46	0.50
1:B:492:GLU:HA	1:B:492:GLU:OE1	2.11	0.50
1:C:143:ASN:N	1:C:143:ASN:HD22	2.10	0.50
1:C:492:GLU:O	1:C:492:GLU:HG2	2.11	0.50
1:C:262:ARG:NH1	4:C:2029:HOH:O	2.44	0.50
1:A:213:ILE:HD12	1:A:214:PRO:O	2.12	0.50
1:A:141:LEU:HG	1:A:141:LEU:O	2.12	0.49
1:B:276:ASN:HA	1:B:277:CYS:C	2.35	0.49
1:B:53:PRO:HD2	1:B:274:LEU:HD22	1.94	0.49
1:A:498:ALA:C	4:A:2177:HOH:O	2.55	0.49
1:B:491:TYR:O	1:B:494:GLU:CB	2.61	0.49
1:B:357:ASN:HB2	4:B:2126:HOH:O	2.12	0.49
1:A:140:VAL:HG12	1:A:141:LEU:HD22	1.93	0.49
1:A:479:ASN:O	1:A:483:ASN:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:TRP:CZ3	1:B:163:ALA:HB1	2.48	0.49
1:C:140:VAL:C	1:C:142:ASP:HA	2.38	0.49
1:B:113:THR:HG22	1:B:114:HIS:HB2	1.96	0.48
1:C:248:GLY:O	1:C:249:ASN:HB2	2.13	0.48
1:B:123:ARG:HG2	1:B:131:THR:HG21	1.94	0.48
1:C:160:TYR:CZ	1:C:248:GLY:HA2	2.48	0.48
1:C:168:ASN:HD21	3:C:1500:NAG:C2	2.26	0.48
1:A:361:SER:HB3	1:A:362:GLY:CA	2.33	0.48
1:B:185[B]:ASN:OD1	1:B:226:GLY:C	2.56	0.47
1:A:51:ILE:HB	1:A:81:SER:HB3	1.96	0.47
1:A:112:VAL:C	1:A:113:THR:HG22	2.39	0.47
1:B:31:THR:OG1	1:B:32:HIS:HD2	1.98	0.47
1:A:354:HIS:O	1:A:355:HIS:CD2	2.67	0.47
1:B:471:HIS:HD2	1:B:494:GLU:OE2	1.98	0.47
1:A:102:TYR:CZ	1:A:106:LYS:HD3	2.50	0.47
1:B:331:LEU:HD22	1:B:438:ASP:OD2	2.14	0.47
1:B:459:VAL:CG1	1:B:460:LYS:N	2.77	0.47
1:B:218:THR:HA	4:B:2072:HOH:O	2.14	0.46
1:A:248:GLY:O	1:A:249:ASN:HB2	2.16	0.46
1:B:459:VAL:HG13	1:B:468:GLU:C	2.39	0.46
1:A:399:PHE:CE1	1:A:406:LEU:HG	2.51	0.46
1:B:189:GLU:HA	1:B:192:THR:HG22	1.97	0.46
1:B:459:VAL:HG12	1:B:460:LYS:N	2.30	0.46
1:C:13:ALA:HB2	1:C:342:GLY:HA3	1.96	0.46
2:D:3:SIA:O1A	2:D:3:SIA:H6	2.16	0.46
1:C:480:SER:HA	1:C:483:ASN:OD1	2.16	0.46
1:B:155:LYS:HE2	1:B:192:THR:O	2.16	0.45
1:C:9:ILE:HG13	1:C:448:TYR:HA	1.98	0.45
3:A:1500:NAG:C5	3:A:1500:NAG:C1	2.95	0.45
1:A:220:PRO:HD3	1:C:243:ASN:HD22	1.81	0.45
1:C:12:HIS:HD2	1:C:346:MET:O	1.99	0.45
1:C:455:LEU:HD23	1:C:459:VAL:HG11	1.99	0.45
1:B:51:ILE:HG23	1:B:79:GLU:HG2	1.99	0.45
1:B:389:ASN:CG	4:B:2130:HOH:O	2.60	0.45
1:A:9:ILE:HG13	1:A:448:TYR:HA	1.98	0.45
1:B:114:HIS:HB3	1:B:260:SER:HB2	1.98	0.45
1:A:103:GLU:H	1:A:103:GLU:CD	2.26	0.44
1:B:459:VAL:CG1	1:B:467:PHE:HB3	2.38	0.44
1:B:495:SER:C	1:B:497:ALA:H	2.24	0.44
1:B:197:VAL:HG22	1:B:198:GLY:H	1.82	0.44
1:B:248:GLY:O	1:B:249:ASN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:GLN:OE1	1:B:235:LEU:HD13	2.18	0.44
1:B:178:ILE:O	1:B:253:PRO:HG3	2.18	0.44
1:C:182:HIS:CD2	1:C:194:TYR:OH	2.70	0.44
1:C:491:TYR:C	1:C:493:GLU:H	2.25	0.44
1:A:128:GLN:HB3	1:A:161:PRO:HG2	1.99	0.44
1:B:108:LEU:HD11	1:B:261:LYS:HE2	1.99	0.44
1:C:390:THR:HG22	1:C:390:THR:O	2.17	0.44
1:B:131:THR:O	1:B:131:THR:HG23	2.18	0.44
1:C:38:GLU:HB2	1:C:292:LEU:HD12	2.00	0.44
1:A:99:PHE:HB3	1:A:102:TYR:HB2	1.99	0.44
1:B:303:GLY:HA2	1:B:392:PHE:CE1	2.53	0.44
1:A:423:TYR:CE1	1:C:388:MET:HE2	2.53	0.43
1:C:276:ASN:CG	1:C:276:ASN:O	2.60	0.43
1:B:295:HIS:CD2	1:B:297:ILE:H	2.32	0.43
1:A:123:ARG:HG2	1:A:131:THR:HG21	2.00	0.43
1:A:220:PRO:HD3	1:C:243:ASN:ND2	2.34	0.43
1:B:66:LEU:O	1:B:147:PHE:HB3	2.18	0.43
1:B:113:THR:HB	1:B:260:SER:HB2	2.00	0.43
1:B:151:VAL:HG12	1:B:153:LEU:HD12	1.99	0.43
1:B:389:ASN:HD22	1:B:389:ASN:HA	1.68	0.43
1:A:71:CYS:O	1:A:74:LEU:HB2	2.18	0.43
1:B:9:ILE:HG13	1:B:448:TYR:HA	2.01	0.43
1:B:112:VAL:CG1	1:B:115:PHE:HB2	2.48	0.43
1:B:493:GLU:O	1:B:494:GLU:CB	2.66	0.43
1:C:9:ILE:HD11	1:C:451:VAL:HG21	2.00	0.43
1:A:74:LEU:HD13	1:A:74:LEU:O	2.18	0.43
1:A:480:SER:HA	1:A:483:ASN:HB3	2.01	0.43
1:B:458:ASN:OD1	1:B:491:TYR:HA	2.19	0.43
1:C:494:GLU:OE2	1:C:495:SER:N	2.42	0.43
1:A:23:ILE:HG23	1:A:24:LEU:HG	2.01	0.43
1:B:194:TYR:O	1:B:196:ASN:N	2.47	0.43
1:C:268:MET:HE3	1:C:302:ILE:HD12	1.99	0.43
1:B:209:ASN:OD1	1:C:219:ARG:NH1	2.50	0.42
1:B:307:LYS:HD3	1:B:307:LYS:HA	1.90	0.42
1:C:320:LEU:HD23	1:C:320:LEU:N	2.30	0.42
1:A:110:THR:HG23	1:A:265:SER:H	1.77	0.42
1:A:197:VAL:HG12	1:A:198:GLY:N	2.33	0.42
1:B:189:GLU:HA	1:B:192:THR:CG2	2.48	0.42
1:A:492:GLU:O	4:A:2177:HOH:O	2.22	0.42
1:B:320:LEU:HD23	1:B:320:LEU:N	2.33	0.42
1:A:140:VAL:HG23	1:A:145:SER:CB	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:LEU:O	1:C:261:LYS:HD2	2.18	0.42
1:B:471:HIS:CD2	1:B:494:GLU:OE2	2.72	0.42
1:C:178:ILE:O	1:C:253:PRO:HG3	2.19	0.42
1:C:399:PHE:CE1	1:C:406:LEU:HG	2.55	0.42
1:A:311:SER:HB3	1:A:426:GLU:OE1	2.20	0.42
1:C:293:PRO:HG2	1:C:294:PHE:CD2	2.55	0.42
1:A:53:PRO:HB3	1:A:82:TYR:CE2	2.55	0.42
1:A:213:ILE:HD12	1:A:213:ILE:C	2.45	0.42
1:B:307:LYS:HE2	1:B:421:TRP:NE1	2.35	0.42
1:B:458:ASN:HA	1:B:494:GLU:CG	2.49	0.41
1:A:409:LEU:HD21	1:C:409:LEU:HD22	2.02	0.41
1:A:488:TYR:N	1:A:489:PRO:CD	2.83	0.41
1:B:367:LYS:HD3	1:B:367:LYS:HA	1.64	0.41
1:A:459:VAL:HG12	1:A:469:PHE:HA	2.02	0.41
1:B:52:PRO:HA	1:B:53:PRO:HD3	1.86	0.41
1:C:298:HIS:ND1	1:C:299:PRO:HD2	2.35	0.41
1:A:141:LEU:O	1:A:141:LEU:CG	2.68	0.41
1:B:163:ALA:O	1:B:245:GLU:HA	2.21	0.41
1:A:79:GLU:HG3	1:A:113:THR:HA	2.02	0.41
1:A:113:THR:C	1:A:260:SER:HB2	2.45	0.41
1:A:241:VAL:HG23	3:A:1500:NAG:H61	2.03	0.41
1:B:97:GLY:HA3	1:B:229:MET:O	2.21	0.41
1:B:113:THR:CB	1:B:114:HIS:CB	2.98	0.41
1:B:323:VAL:HG12	4:B:2108:HOH:O	2.21	0.41
1:B:427:LEU:O	1:B:431:MET:HG3	2.20	0.41
1:C:143:ASN:N	1:C:143:ASN:ND2	2.69	0.41
1:C:382:ASN:O	1:C:386:GLU:HB2	2.21	0.41
1:A:222:VAL:HG22	1:C:206:SER:HB2	2.03	0.41
1:C:35:ASP:OD2	1:C:39:LYS:NZ	2.54	0.40
1:A:241:VAL:HB	1:B:220:PRO:HG3	2.03	0.40
1:C:372:LYS:HA	1:C:372:LYS:HD2	1.91	0.40
1:A:168:ASN:ND2	3:A:1500:NAG:C5	2.75	0.40
1:B:6:GLN:HB2	1:B:467:PHE:O	2.22	0.40
1:B:284:PRO:HD3	1:B:300:LEU:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:CD2	1:B:128:GLN:OE1[1_655]	1.82	0.38
1:A:141:LEU:CD1	1:B:128:GLN:OE1[1_655]	2.03	0.17

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%)	459 (94%)	21 (4%)	6 (1%)	10	16
1	B	485/509 (95%)	456 (94%)	20 (4%)	9 (2%)	6	8
1	C	479/509 (94%)	457 (95%)	16 (3%)	6 (1%)	9	14
All	All	1450/1527 (95%)	1372 (95%)	57 (4%)	21 (1%)	9	13

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	THR
1	A	494	GLU
1	B	277	CYS
1	B	490	LYS
1	B	494	GLU
1	C	113	THR
1	B	114	HIS
1	B	141	LEU
1	B	276	ASN
1	C	276	ASN
1	B	362	GLY
1	C	362	GLY
1	C	492	GLU
1	C	494	GLU
1	A	496	LYS
1	B	489	PRO
1	C	75	LEU
1	A	140	VAL
1	B	313	ARG
1	A	74	LEU
1	A	355	HIS

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%)	411 (96%)	16 (4%)	30	51
1	B	429/447 (96%)	406 (95%)	23 (5%)	20	35
1	C	425/447 (95%)	409 (96%)	16 (4%)	29	49
All	All	1281/1341 (96%)	1226 (96%)	55 (4%)	26	44

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	74	LEU
1	A	94	CYS
1	A	110	THR
1	A	113	THR
1	A	131	THR
1	A	148	ARG
1	A	202	SER
1	A	275	GLU
1	A	278	GLU
1	A	283	THR
1	A	320	LEU
1	A	351	TYR
1	A	355	HIS
1	A	404	ARG
1	A	437	LEU
1	B	45	LEU
1	B	58	ASP
1	B	74	LEU
1	B	77	VAL
1	B	90	VAL
1	B	93	LEU
1	B	108	LEU
1	B	131	THR
1	B	141	LEU
1	B	148	ARG

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Mol	Chain	Res	Type
1	B	276	ASN
1	B	283	THR
1	B	285	LEU
1	B	320	LEU
1	B	323	VAL
1	B	331	LEU
1	B	377	ILE
1	B	389	ASN
1	B	434	GLU
1	B	437	LEU
1	B	462	LEU
1	B	493	GLU
1	B	494	GLU
1	C	94	CYS
1	C	143	ASN
1	C	196	ASN
1	C	261	LYS
1	C	264	SER
1	C	283	THR
1	C	320	LEU
1	C	347	VAL
1	C	389	ASN
1	C	406	LEU
1	C	427	LEU
1	C	455	LEU
1	C	459	VAL
1	C	462	LEU
1	C	493	GLU
1	C	494	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	A	168	ASN
1	A	174	GLN
1	A	182	HIS
1	A	195	GLN
1	A	243	ASN
1	A	249	ASN
1	A	295	HIS
1	A	344	GLN

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Mol	Chain	Res	Type
1	A	479	ASN
1	B	27	ASN
1	B	32	HIS
1	B	114	HIS
1	B	128	GLN
1	B	182	HIS
1	B	225	GLN
1	B	249	ASN
1	B	295	HIS
1	B	325	GLN
1	B	371	GLN
1	B	382	ASN
1	B	391	GLN
1	B	408	ASN
1	B	424	ASN
1	B	454	GLN
1	C	12	HIS
1	C	15	ASN
1	C	91	ASN
1	C	100	ASN
1	C	114	HIS
1	C	125	GLN
1	C	143	ASN
1	C	168	ASN
1	C	174	GLN
1	C	182	HIS
1	C	243	ASN
1	C	249	ASN
1	C	357	ASN
1	C	382	ASN
1	C	389	ASN
1	C	408	ASN
1	C	424	ASN
1	C	454	GLN
1	C	479	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 ⓘ

6 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	15,15,15	0.91	1 (6%)	21,21,21	0.74	0
2	GAL	D	2	2	11,11,12	0.74	0	15,15,17	0.67	0
2	SIA	D	3	2	20,20,21	0.90	0	21,28,31	0.92	1 (4%)
2	NAG	E	1	2	15,15,15	0.89	0	21,21,21	1.10	2 (9%)
2	GAL	E	2	2	11,11,12	0.60	0	15,15,17	0.99	1 (6%)
2	SIA	E	3	2	20,20,21	0.98	1 (5%)	21,28,31	0.90	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
2	NAG	D	1	2	-	2/6/26/26	0/1/1/1
2	GAL	D	2	2	-	2/2/19/22	0/1/1/1
2	SIA	D	3	2	-	0/18/34/38	0/1/1/1
2	NAG	E	1	2	-	1/6/26/26	0/1/1/1
2	GAL	E	2	2	-	0/2/19/22	0/1/1/1
2	SIA	E	3	2	-	0/18/34/38	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	SIA	C4-C5	2.17	1.55	1.53
2	D	1	NAG	C1-C2	2.04	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	GAL	C1-C2-C3	3.02	114.05	109.64
2	E	1	NAG	C3-C4-C5	2.72	115.16	110.23
2	D	3	SIA	O1B-C1-C2	2.28	118.64	112.71
2	E	1	NAG	O5-C5-C4	2.06	113.41	109.70

There are no chirality outliers.

All (5) torsion outliers are listed below:

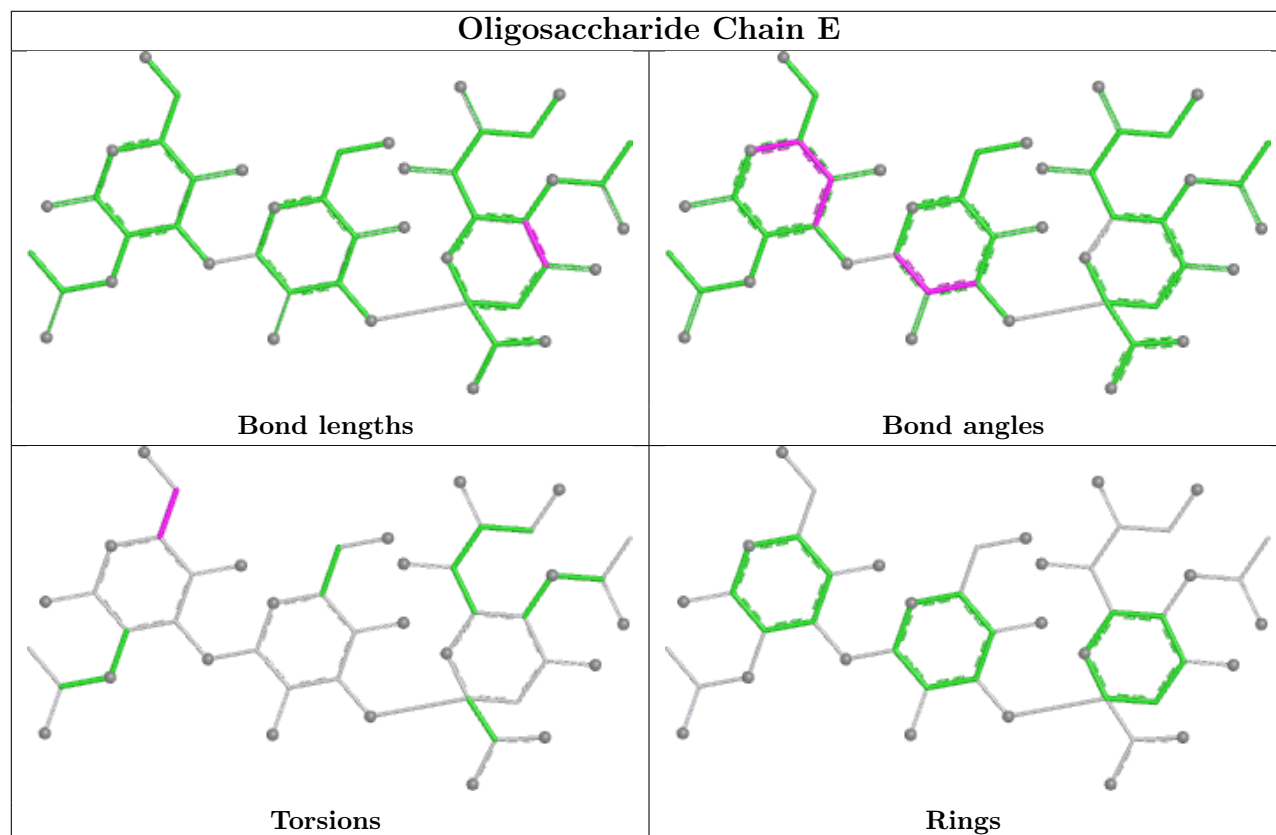
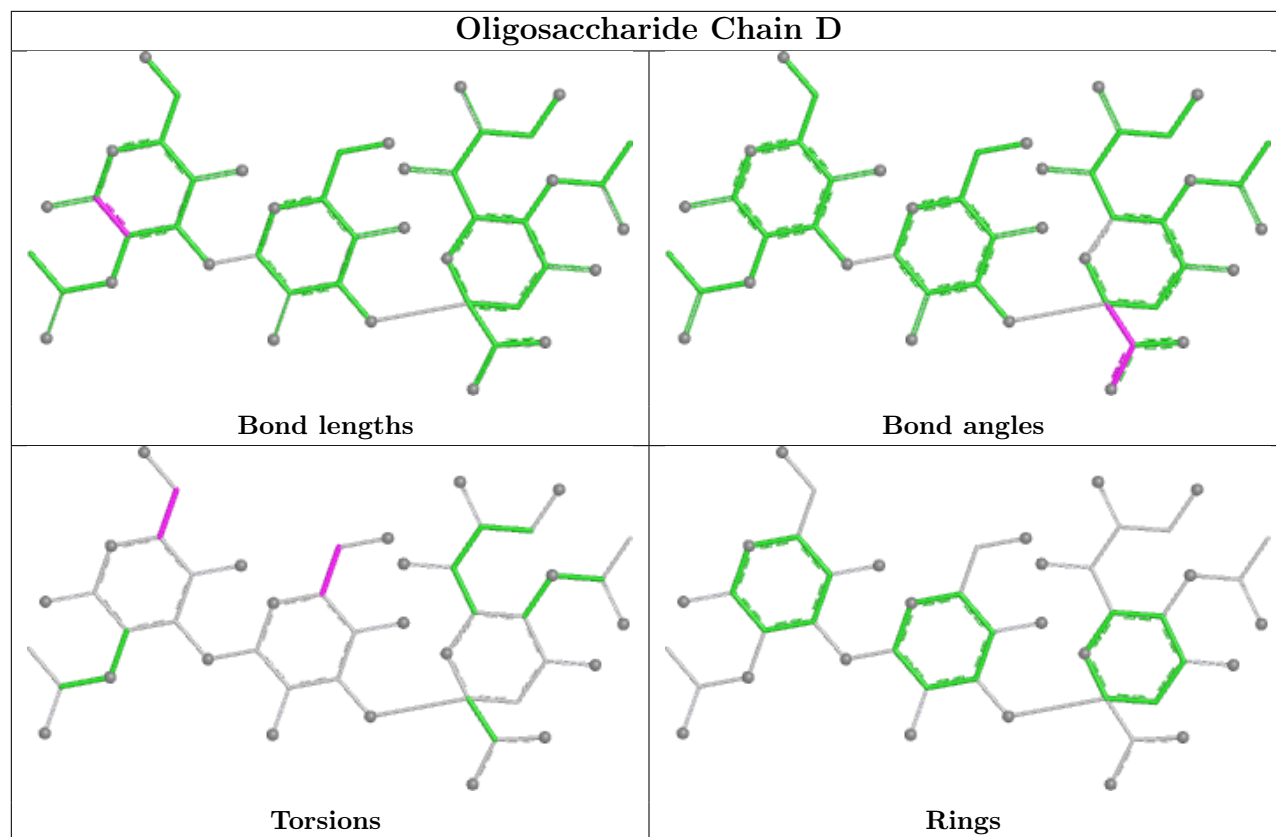
Mol	Chain	Res	Type	Atoms
2	D	2	GAL	C4-C5-C6-O6
2	D	2	GAL	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	SIA	2	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

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
3	NAG	A	1499	-	14,14,15	0.46	0	17,19,21	0.75	0
3	NAG	A	1500	-	12,12,15	0.45	0	14,15,21	0.88	0
3	NAG	C	1500	-	14,14,15	0.56	0	17,19,21	0.90	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
3	NAG	A	1499	-	-	4/6/23/26	0/1/1/1
3	NAG	A	1500	-	-	6/15/15/26	-
3	NAG	C	1500	-	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1499	NAG	C1-C2-N2-C7
3	A	1500	NAG	C1-C2-N2-C7
3	A	1500	NAG	O4-C4-C5-C6
3	A	1500	NAG	C8-C7-N2-C2
3	A	1500	NAG	O7-C7-N2-C2
3	A	1499	NAG	C8-C7-N2-C2
3	A	1499	NAG	O7-C7-N2-C2
3	C	1500	NAG	O5-C5-C6-O6
3	A	1500	NAG	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	C	1500	NAG	C4-C5-C6-O6
3	A	1499	NAG	O5-C5-C6-O6
3	A	1500	NAG	C4-C5-C6-O6
3	C	1500	NAG	C8-C7-N2-C2
3	C	1500	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1499	NAG	1	0
3	A	1500	NAG	6	0
3	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%)	3.37	431 (87%)  	29, 54, 94, 134	1 (0%)
1	B	490/509 (96%)	2.52	311 (63%)  	30, 55, 95, 159	1 (0%)
1	C	485/509 (95%)	3.35	418 (86%)  	36, 55, 87, 134	0
All	All	1465/1527 (95%)	3.08	1160 (79%)  	29, 55, 92, 159	2 (0%)

All (1160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	196	ASN	8.8
1	C	206	SER	7.8
1	A	9	ILE	7.8
1	C	66	LEU	7.6
1	C	120	ILE	7.5
1	C	198	GLY	7.4
1	C	197	VAL	7.2
1	B	213	ILE	7.2
1	A	153	LEU	6.9
1	C	253	PRO	6.9
1	C	151	VAL	6.8
1	A	463	GLY	6.7
1	C	141	LEU	6.7
1	A	90	VAL	6.5
1	C	157	GLY	6.5
1	C	9	ILE	6.5
1	C	166	SER	6.5
1	A	316	LEU	6.5
1	A	109	ILE	6.5
1	C	140	VAL	6.5
1	C	288	ILE	6.4
1	C	153	LEU	6.4
1	B	162	ILE	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	323	VAL	6.4
1	B	277	CYS	6.4
1	C	194	TYR	6.3
1	A	224	GLY	6.3
1	A	350	TRP	6.3
1	A	354	HIS	6.3
1	C	154	THR	6.3
1	C	44	LYS	6.2
1	C	147	PHE	6.1
1	B	498	ALA	6.1
1	C	138	CYS	6.1
1	A	42	ASN	6.1
1	C	222	VAL	6.1
1	A	364	ALA	6.0
1	C	85	GLU	6.0
1	C	235	LEU	6.0
1	A	247	THR	6.0
1	A	459	VAL	5.9
1	C	93	LEU	5.9
1	C	126	TRP	5.9
1	A	45	LEU	5.9
1	A	95	TYR	5.8
1	A	219	ARG	5.8
1	C	128	GLN	5.8
1	A	8	CYS	5.8
1	C	131	THR	5.8
1	A	138	CYS	5.7
1	A	302	ILE	5.7
1	C	272	LYS	5.7
1	C	180	GLY	5.7
1	C	463	GLY	5.7
1	B	491	TYR	5.7
1	A	451	VAL	5.7
1	A	89	PRO	5.7
1	A	189	GLU	5.6
1	C	95	TYR	5.6
1	C	160	TYR	5.6
1	A	49	SER	5.6
1	A	80	TRP	5.6
1	B	51	ILE	5.6
1	C	121	LEU	5.6
1	B	167	TYR	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	120	ILE	5.5
1	C	127	THR	5.5
1	A	56	LEU	5.5
1	C	65	LEU	5.5
1	A	287	ALA	5.5
1	C	187	ASP	5.5
1	C	376	GLY	5.5
1	C	387	LYS	5.5
1	B	140	VAL	5.4
1	A	356	SER	5.4
1	A	134	GLY	5.4
1	C	274	LEU	5.4
1	B	163	ALA	5.4
1	A	214	PRO	5.4
1	A	74	LEU	5.4
1	A	97	GLY	5.3
1	A	422	THR	5.3
1	B	235	LEU	5.3
1	B	462	LEU	5.3
1	C	223	ASN	5.3
1	A	210	LYS	5.3
1	C	118	VAL	5.3
1	A	137	ALA	5.3
1	B	204	GLY	5.3
1	A	93	LEU	5.3
1	B	159	ASN	5.3
1	C	352	GLY	5.3
1	C	113	THR	5.3
1	A	469	PHE	5.2
1	C	184	PRO	5.2
1	A	181	ILE	5.2
1	C	129	HIS	5.2
1	B	226	GLY	5.2
1	B	390	THR	5.2
1	A	353	TYR	5.2
1	C	53	PRO	5.2
1	A	362	GLY	5.2
1	C	51	ILE	5.2
1	C	64	TRP	5.2
1	C	363	TYR	5.2
1	A	462	LEU	5.2
1	C	258	LYS	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	57	GLY	5.1
1	C	251	ILE	5.1
1	A	91	ASN	5.1
1	A	157	GLY	5.1
1	A	61	ILE	5.1
1	C	191	ARG	5.1
1	C	130	THR	5.1
1	C	264	SER	5.1
1	A	140	VAL	5.1
1	C	96	PRO	5.1
1	C	109	ILE	5.1
1	A	324	PRO	5.0
1	C	89	PRO	5.0
1	A	78	PRO	5.0
1	A	177	ILE	5.0
1	A	225	GLN	5.0
1	A	335	ILE	5.0
1	B	244	PHE	5.0
1	A	296	ASN	4.9
1	C	82	TYR	4.9
1	A	347	VAL	4.9
1	C	243	ASN	4.9
1	C	473	CYS	4.9
1	A	265	SER	4.9
1	C	115	PHE	4.9
1	C	297	ILE	4.9
1	A	142	ASP	4.9
1	C	62	ALA	4.8
1	A	184	PRO	4.8
1	A	414	GLU	4.8
1	A	357	ASN	4.8
1	A	497	ALA	4.8
1	C	252	ALA	4.8
1	A	470	TYR	4.8
1	C	133	GLY	4.8
1	A	85	GLU	4.8
1	C	397	LYS	4.8
1	A	229	MET	4.8
1	A	58	ASP	4.8
1	B	264	SER	4.8
1	A	195	GLN	4.7
1	A	417	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	98	SER	4.7
1	C	87	GLU	4.7
1	A	77	VAL	4.7
1	A	84	VAL	4.7
1	B	495	SER	4.7
1	A	14	ASN	4.7
1	B	157	GLY	4.7
1	C	204	GLY	4.7
1	A	131	THR	4.7
1	B	118	VAL	4.7
1	A	319	GLY	4.7
1	C	302	ILE	4.7
1	A	346	MET	4.7
1	C	356	SER	4.6
1	B	242	ILE	4.6
1	B	262	ARG	4.6
1	B	121	LEU	4.6
1	A	146	PHE	4.6
1	A	36	ILE	4.6
1	B	326	ILE	4.6
1	C	178	ILE	4.6
1	A	18	GLU	4.6
1	C	45	LEU	4.6
1	B	203	VAL	4.6
1	C	256	GLY	4.6
1	C	177	ILE	4.6
1	A	299	PRO	4.6
1	C	144	PRO	4.6
1	B	126	TRP	4.6
1	A	301	THR	4.6
1	A	197	VAL	4.6
1	C	263	GLY	4.6
1	C	324	PRO	4.6
1	A	277	CYS	4.6
1	A	5	ASP	4.6
1	A	482	LYS	4.6
1	C	244	PHE	4.5
1	C	257	PHE	4.5
1	C	384	VAL	4.5
1	A	53	PRO	4.5
1	C	143	ASN	4.5
1	C	250	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	79	GLU	4.5
1	C	43	GLY	4.5
1	C	241	VAL	4.5
1	C	78	PRO	4.5
1	C	306	PRO	4.5
1	A	6	GLN	4.5
1	A	13	ALA	4.5
1	C	150	MET	4.5
1	B	75	LEU	4.5
1	C	262	ARG	4.5
1	A	115	PHE	4.5
1	A	481	VAL	4.5
1	C	434	GLU	4.5
1	A	59	CYS	4.4
1	A	218	THR	4.4
1	A	256	GLY	4.4
1	C	465	GLY	4.4
1	B	459	VAL	4.4
1	C	269	LYS	4.4
1	A	136	ARG	4.4
1	A	300	LEU	4.4
1	C	237	GLU	4.4
1	B	77	VAL	4.4
1	A	196	ASN	4.4
1	A	260	SER	4.4
1	B	76	SER	4.4
1	C	163	ALA	4.4
1	A	69	PRO	4.4
1	A	144	PRO	4.4
1	B	160	TYR	4.4
1	B	313	ARG	4.4
1	C	193	LEU	4.4
1	B	79	GLU	4.4
1	C	318	THR	4.4
1	A	213	ILE	4.4
1	B	216	ILE	4.4
1	A	94	CYS	4.4
1	A	264	SER	4.4
1	A	394	ALA	4.4
1	B	38	GLU	4.4
1	A	67	GLY	4.3
1	A	284	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	73	ARG	4.3
1	C	236	LEU	4.3
1	A	297	ILE	4.3
1	A	55	GLU	4.3
1	B	411	LYS	4.3
1	A	331	LEU	4.3
1	C	54	LEU	4.3
1	C	176	LEU	4.3
1	A	92	GLY	4.3
1	A	360	GLY	4.3
1	A	216	ILE	4.3
1	A	222	VAL	4.3
1	B	451	VAL	4.3
1	C	420	VAL	4.3
1	C	156	LYS	4.3
1	A	278	GLU	4.3
1	A	351	TYR	4.3
1	B	200	TYR	4.3
1	A	455	LEU	4.3
1	A	71	CYS	4.3
1	C	171	SER	4.3
1	B	5	ASP	4.3
1	B	291	THR	4.3
1	B	48	LEU	4.3
1	A	73	ARG	4.3
1	B	53	PRO	4.2
1	A	29	THR	4.2
1	B	241	VAL	4.2
1	B	141	LEU	4.2
1	A	389	ASN	4.2
1	B	142	ASP	4.2
1	C	67	GLY	4.2
1	C	242	ILE	4.2
1	C	481	VAL	4.2
1	B	209	ASN	4.2
1	C	209	ASN	4.2
1	B	114	HIS	4.2
1	A	72	ASP	4.2
1	C	155	LYS	4.2
1	A	217	ALA	4.2
1	C	394	ALA	4.2
1	C	361	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	459	VAL	4.2
1	A	425	ALA	4.2
1	C	139	ALA	4.2
1	A	133	GLY	4.1
1	C	40	THR	4.1
1	C	291	THR	4.1
1	C	108	LEU	4.1
1	A	272	LYS	4.1
1	A	68	ASN	4.1
1	C	91	ASN	4.1
1	A	454	GLN	4.1
1	A	112	VAL	4.1
1	A	201	VAL	4.1
1	B	258	LYS	4.1
1	A	295	HIS	4.1
1	C	116	GLU	4.1
1	A	309	VAL	4.1
1	A	315	VAL	4.1
1	B	315	VAL	4.1
1	A	373	ALA	4.1
1	A	483	ASN	4.1
1	C	18	GLU	4.1
1	A	361	SER	4.1
1	C	212	SER	4.1
1	A	40	THR	4.1
1	C	170	THR	4.1
1	A	121	LEU	4.1
1	C	105	LEU	4.1
1	C	32	HIS	4.1
1	A	124	ASP	4.0
1	A	465	GLY	4.0
1	C	438	ASP	4.0
1	B	137	ALA	4.0
1	B	42	ASN	4.0
1	C	179	TRP	4.0
1	C	367	LYS	4.0
1	A	76	SER	4.0
1	A	255	TYR	4.0
1	C	167	TYR	4.0
1	C	417	PHE	4.0
1	A	70	GLU	4.0
1	C	59	CYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	217	ALA	4.0
1	A	280	LYS	4.0
1	A	330	GLY	4.0
1	C	416	GLY	4.0
1	A	126	TRP	4.0
1	C	238	THR	4.0
1	C	270	THR	4.0
1	A	429	VAL	4.0
1	C	395	VAL	4.0
1	B	257	PHE	4.0
1	C	496	LYS	4.0
1	A	182	HIS	4.0
1	A	113	THR	4.0
1	C	488	TYR	4.0
1	C	299	PRO	4.0
1	A	41	HIS	3.9
1	C	29	THR	3.9
1	A	194	TYR	3.9
1	C	173	GLU	3.9
1	C	245	GLU	3.9
1	A	43	GLY	3.9
1	C	330	GLY	3.9
1	A	474	ASP	3.9
1	A	477	CYS	3.9
1	A	12	HIS	3.9
1	B	259	ILE	3.9
1	B	361	SER	3.9
1	C	74	LEU	3.9
1	B	381	VAL	3.9
1	A	11	TYR	3.9
1	B	169	ASN	3.9
1	C	7	ILE	3.9
1	B	437	LEU	3.9
1	C	255	TYR	3.9
1	C	231	PHE	3.9
1	B	362	GLY	3.9
1	C	61	ILE	3.9
1	C	216	ILE	3.9
1	A	320	LEU	3.9
1	B	138	CYS	3.9
1	A	111	SER	3.9
1	B	275	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	279	THR	3.9
1	C	218	THR	3.9
1	A	231	PHE	3.8
1	A	392	PHE	3.8
1	A	467	PHE	3.8
1	A	298	HIS	3.8
1	C	482	LYS	3.8
1	B	250	LEU	3.8
1	C	225	GLN	3.8
1	B	239	TRP	3.8
1	C	364	ALA	3.8
1	A	160	TYR	3.8
1	B	211	ARG	3.8
1	C	450	LYS	3.8
1	C	406	LEU	3.8
1	B	305	CYS	3.8
1	C	175	MET	3.8
1	A	491	TYR	3.8
1	A	50	GLY	3.8
1	A	464	ASN	3.8
1	B	207	THR	3.8
1	A	114	HIS	3.8
1	C	317	ALA	3.8
1	A	10	GLY	3.8
1	C	172	GLY	3.8
1	C	224	GLY	3.8
1	A	423	TYR	3.8
1	A	162	ILE	3.8
1	A	480	SER	3.7
1	C	110	THR	3.7
1	A	172	GLY	3.7
1	B	198	GLY	3.7
1	B	256	GLY	3.7
1	A	486	TYR	3.7
1	B	343	TRP	3.7
1	C	83	ILE	3.7
1	C	300	LEU	3.7
1	A	186	ASP	3.7
1	B	475	ASP	3.7
1	C	444	VAL	3.7
1	B	27	ASN	3.7
1	C	159	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	348	ASP	3.7
1	B	80	TRP	3.7
1	C	348	ASP	3.7
1	B	324	PRO	3.7
1	A	228	ARG	3.7
1	A	262	ARG	3.7
1	A	38	GLU	3.7
1	A	473	CYS	3.7
1	C	94	CYS	3.7
1	A	48	LEU	3.7
1	C	162	ILE	3.7
1	C	320	LEU	3.7
1	B	124	ASP	3.7
1	B	358	ASP	3.7
1	A	363	TYR	3.7
1	C	207	THR	3.7
1	B	87	GLU	3.7
1	C	92	GLY	3.7
1	C	374	PHE	3.7
1	A	325	GLN	3.7
1	A	370	THR	3.6
1	A	420	VAL	3.6
1	A	248	GLY	3.6
1	C	56	LEU	3.6
1	A	51	ILE	3.6
1	C	86	LYS	3.6
1	A	308	TYR	3.6
1	A	64	TRP	3.6
1	A	421	TRP	3.6
1	A	158	SER	3.6
1	B	158	SER	3.6
1	C	49	SER	3.6
1	C	135	SER	3.6
1	B	336	ALA	3.6
1	B	115	PHE	3.6
1	A	132	THR	3.6
1	A	270	THR	3.6
1	A	436	THR	3.6
1	A	444	VAL	3.6
1	C	158	SER	3.6
1	C	219	ARG	3.6
1	C	268	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	338	PHE	3.6
1	A	7	ILE	3.6
1	C	213	ILE	3.6
1	C	385	ILE	3.6
1	A	407	GLU	3.6
1	A	448	TYR	3.6
1	A	318	THR	3.6
1	A	343	TRP	3.6
1	C	239	TRP	3.6
1	A	311	SER	3.6
1	A	120	ILE	3.6
1	C	69	PRO	3.6
1	C	332	PHE	3.6
1	A	159	ASN	3.6
1	C	483	ASN	3.6
1	C	41	HIS	3.5
1	A	156	LYS	3.5
1	A	221	LYS	3.5
1	B	481	VAL	3.5
1	A	391	GLN	3.5
1	A	400	SER	3.5
1	A	478	MET	3.5
1	B	478	MET	3.5
1	B	6	GLN	3.5
1	C	6	GLN	3.5
1	C	202	SER	3.5
1	A	487	ASP	3.5
1	C	58	ASP	3.5
1	C	354	HIS	3.5
1	C	277	CYS	3.5
1	C	165	ARG	3.5
1	C	200	TYR	3.5
1	A	141	LEU	3.5
1	A	285	LEU	3.5
1	C	345	GLY	3.5
1	B	161	PRO	3.5
1	A	310	LYS	3.5
1	C	117	LYS	3.5
1	C	119	LYS	3.5
1	B	127	THR	3.5
1	C	190	GLN	3.5
1	A	418	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	52	PRO	3.5
1	A	267	ILE	3.5
1	C	80	TRP	3.5
1	B	467	PHE	3.5
1	A	88	ASN	3.5
1	C	124	ASP	3.5
1	C	169	ASN	3.5
1	A	215	GLU	3.5
1	B	215	GLU	3.5
1	C	90	VAL	3.5
1	C	347	VAL	3.5
1	C	8	CYS	3.5
1	A	250	LEU	3.5
1	A	82	TYR	3.5
1	B	49	SER	3.5
1	C	137	ALA	3.5
1	C	383	SER	3.5
1	C	267	ILE	3.5
1	A	183	HIS	3.5
1	A	20	VAL	3.4
1	C	112	VAL	3.4
1	A	37	LEU	3.4
1	B	153	LEU	3.4
1	A	349	GLY	3.4
1	B	341	GLY	3.4
1	A	460	LYS	3.4
1	B	364	ALA	3.4
1	C	221	LYS	3.4
1	A	471	HIS	3.4
1	A	453	MET	3.4
1	A	344	GLN	3.4
1	A	86	LYS	3.4
1	B	144	PRO	3.4
1	C	122	PRO	3.4
1	A	305	CYS	3.4
1	C	351	TYR	3.4
1	C	493	GLU	3.4
1	A	375	ASP	3.4
1	C	375	ASP	3.4
1	A	168	ASN	3.4
1	C	125	GLN	3.4
1	B	331	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	198	GLY	3.4
1	A	263	GLY	3.4
1	A	334	ALA	3.4
1	B	202	SER	3.4
1	C	470	TYR	3.4
1	C	392	PHE	3.4
1	A	366	ASP	3.4
1	A	239	TRP	3.4
1	A	193	LEU	3.4
1	A	274	LEU	3.4
1	A	279	THR	3.4
1	B	430	LEU	3.4
1	C	201	VAL	3.4
1	C	284	PRO	3.4
1	B	385	ILE	3.4
1	A	461	GLU	3.4
1	A	244	PHE	3.3
1	B	453	MET	3.3
1	B	312	ASP	3.3
1	C	487	ASP	3.3
1	A	130	THR	3.3
1	C	63	GLY	3.3
1	C	211	ARG	3.3
1	A	275	GLU	3.3
1	A	377	ILE	3.3
1	B	217	ALA	3.3
1	C	55	GLU	3.3
1	C	336	ALA	3.3
1	C	229	MET	3.3
1	C	469	PHE	3.3
1	B	473	CYS	3.3
1	A	475	ASP	3.3
1	B	58	ASP	3.3
1	C	437	LEU	3.3
1	B	151	VAL	3.3
1	B	191	ARG	3.3
1	B	238	THR	3.3
1	C	123	ARG	3.3
1	A	341	GLY	3.3
1	B	246	SER	3.3
1	A	457	ASP	3.3
1	C	72	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	479	ASN	3.3
1	B	401	ASN	3.3
1	C	289	ASN	3.3
1	C	315	VAL	3.3
1	A	468	GLU	3.3
1	B	131	THR	3.3
1	C	273	THR	3.3
1	C	396	GLY	3.3
1	A	106	LYS	3.3
1	A	450	LYS	3.3
1	C	145	SER	3.3
1	A	332	PHE	3.3
1	B	128	GLN	3.3
1	B	187	ASP	3.3
1	C	195	GLN	3.3
1	C	11	TYR	3.3
1	A	110	THR	3.3
1	A	226	GLY	3.3
1	A	268	MET	3.3
1	B	134	GLY	3.3
1	A	339	ILE	3.3
1	C	188	ALA	3.3
1	A	16	SER	3.2
1	A	135	SER	3.2
1	B	99	PHE	3.2
1	A	21	ASP	3.2
1	B	26	ARG	3.2
1	C	100	ASN	3.2
1	C	102	TYR	3.2
1	B	254	GLU	3.2
1	B	278	GLU	3.2
1	B	468	GLU	3.2
1	C	471	HIS	3.2
1	A	395	VAL	3.2
1	A	412	LYS	3.2
1	A	496	LYS	3.2
1	C	34	LYS	3.2
1	C	106	LYS	3.2
1	C	210	LYS	3.2
1	C	472	LYS	3.2
1	C	335	ILE	3.2
1	A	60	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	187	ASP	3.2
1	C	393	GLU	3.2
1	C	403	GLU	3.2
1	C	453	MET	3.2
1	B	197	VAL	3.2
1	B	347	VAL	3.2
1	C	203	VAL	3.2
1	A	83	ILE	3.2
1	A	212	SER	3.2
1	A	437	LEU	3.2
1	B	243	ASN	3.2
1	C	382	ASN	3.2
1	C	489	PRO	3.2
1	B	346	MET	3.2
1	B	263	GLY	3.2
1	C	466	CYS	3.2
1	B	218	THR	3.2
1	A	62	ALA	3.2
1	A	188	ALA	3.2
1	A	122	PRO	3.2
1	A	27	ASN	3.2
1	A	314	LEU	3.2
1	A	340	GLU	3.2
1	A	386	GLU	3.2
1	B	223	ASN	3.2
1	B	276	ASN	3.2
1	B	304	GLU	3.2
1	B	340	GLU	3.2
1	C	316	LEU	3.2
1	C	448	TYR	3.2
1	B	57	GLY	3.2
1	C	77	VAL	3.2
1	A	273	THR	3.2
1	B	71	CYS	3.2
1	A	495	SER	3.1
1	C	76	SER	3.1
1	B	35	ASP	3.1
1	A	355	HIS	3.1
1	A	492	GLU	3.1
1	C	220	PRO	3.1
1	C	285	LEU	3.1
1	C	341	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	17	THR	3.1
1	C	373	ALA	3.1
1	A	119	LYS	3.1
1	A	99	PHE	3.1
1	C	88	ASN	3.1
1	A	28	VAL	3.1
1	A	313	ARG	3.1
1	B	297	ILE	3.1
1	C	390	THR	3.1
1	C	174	GLN	3.1
1	B	280	LYS	3.1
1	A	104	GLU	3.1
1	B	492	GLU	3.1
1	C	146	PHE	3.1
1	B	421	TRP	3.1
1	C	479	ASN	3.1
1	A	381	VAL	3.1
1	A	238	THR	3.1
1	A	259	ILE	3.1
1	B	194	TYR	3.1
1	B	470	TYR	3.1
1	A	19	LYS	3.1
1	C	271	GLU	3.1
1	B	184	PRO	3.1
1	B	74	LEU	3.1
1	C	331	LEU	3.1
1	B	212	SER	3.1
1	A	443	ASN	3.1
1	C	389	ASN	3.1
1	C	381	VAL	3.1
1	A	155	LYS	3.0
1	A	390	THR	3.0
1	B	247	THR	3.0
1	C	372	LYS	3.0
1	C	353	TYR	3.0
1	B	393	GLU	3.0
1	C	230	GLU	3.0
1	C	275	GLU	3.0
1	A	24	LEU	3.0
1	A	294	PHE	3.0
1	B	374	PHE	3.0
1	B	98	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	401	ASN	3.0
1	A	352	GLY	3.0
1	B	472	LYS	3.0
1	A	23	ILE	3.0
1	B	61	ILE	3.0
1	C	84	VAL	3.0
1	B	40	THR	3.0
1	A	271	GLU	3.0
1	B	116	GLU	3.0
1	A	402	LEU	3.0
1	B	45	LEU	3.0
1	B	59	CYS	3.0
1	B	487	ASP	3.0
1	A	269	LYS	3.0
1	A	288	ILE	3.0
1	C	343	TRP	3.0
1	A	22	THR	3.0
1	A	31	THR	3.0
1	C	132	THR	3.0
1	C	254	GLU	3.0
1	C	461	GLU	3.0
1	C	355	HIS	3.0
1	A	161	PRO	3.0
1	B	208	LEU	3.0
1	C	462	LEU	3.0
1	A	321	ARG	3.0
1	A	281	CYS	3.0
1	B	466	CYS	3.0
1	A	117	LYS	3.0
1	A	367	LYS	3.0
1	A	322	ASN	3.0
1	A	227	GLY	3.0
1	C	349	GLY	3.0
1	C	36	ILE	3.0
1	A	485	THR	3.0
1	B	493	GLU	3.0
1	C	114	HIS	3.0
1	A	235	LEU	3.0
1	B	274	LEU	3.0
1	A	399	PHE	3.0
1	C	475	ASP	3.0
1	B	479	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	248	GLY	3.0
1	C	226	GLY	3.0
1	A	87	GLU	2.9
1	A	150	MET	2.9
1	A	151	VAL	2.9
1	B	245	GLU	2.9
1	A	154	THR	2.9
1	C	298	HIS	2.9
1	A	66	LEU	2.9
1	A	372	LYS	2.9
1	C	427	LEU	2.9
1	B	81	SER	2.9
1	A	209	ASN	2.9
1	A	382	ASN	2.9
1	A	466	CYS	2.9
1	C	149	ASN	2.9
1	A	431	MET	2.9
1	B	177	ILE	2.9
1	C	181	ILE	2.9
1	C	205	THR	2.9
1	A	33	ALA	2.9
1	C	293	PRO	2.9
1	C	380	LYS	2.9
1	B	236	LEU	2.9
1	C	314	LEU	2.9
1	A	167	TYR	2.9
1	C	240	ASP	2.9
1	A	15	ASN	2.9
1	A	249	ASN	2.9
1	A	424	ASN	2.9
1	C	410	ASN	2.9
1	A	25	GLU	2.9
1	A	398	GLU	2.9
1	C	103	GLU	2.9
1	A	290	THR	2.9
1	C	247	THR	2.9
1	A	445	LYS	2.9
1	A	406	LEU	2.9
1	A	430	LEU	2.9
1	C	409	LEU	2.9
1	C	186	ASP	2.9
1	A	337	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	181	ILE	2.9
1	C	107	HIS	2.9
1	C	136	ARG	2.9
1	C	323	VAL	2.9
1	C	451	VAL	2.9
1	A	17	THR	2.9
1	A	220	PRO	2.9
1	B	154	THR	2.9
1	C	199	THR	2.9
1	A	65	LEU	2.9
1	C	75	LEU	2.9
1	A	312	ASP	2.9
1	A	180	GLY	2.9
1	A	410	ASN	2.8
1	B	123	ARG	2.8
1	C	260	SER	2.8
1	C	464	ASN	2.8
1	B	90	VAL	2.8
1	B	22	THR	2.8
1	A	317	ALA	2.8
1	A	498	ALA	2.8
1	B	188	ALA	2.8
1	A	174	GLN	2.8
1	A	358	ASP	2.8
1	C	350	TRP	2.8
1	C	413	MET	2.8
1	C	338	PHE	2.8
1	B	255	TYR	2.8
1	C	261	LYS	2.8
1	C	484	GLY	2.8
1	A	171	SER	2.8
1	A	178	ILE	2.8
1	C	440	HIS	2.8
1	B	78	PRO	2.8
1	A	163	ALA	2.8
1	B	474	ASP	2.8
1	A	34	LYS	2.8
1	A	211	ARG	2.8
1	C	439	PHE	2.8
1	A	63	GLY	2.8
1	C	10	GLY	2.8
1	A	242	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	385	ILE	2.8
1	B	166	SER	2.8
1	B	289	ASN	2.8
1	B	483	ASN	2.8
1	C	81	SER	2.8
1	C	495	SER	2.8
1	C	283	THR	2.8
1	B	189	GLU	2.8
1	B	391	GLN	2.8
1	C	344	GLN	2.8
1	B	375	ASP	2.8
1	C	457	ASP	2.8
1	A	257	PHE	2.8
1	C	467	PHE	2.8
1	B	465	GLY	2.8
1	A	488	TYR	2.8
1	A	202	SER	2.8
1	A	96	PRO	2.8
1	B	84	VAL	2.8
1	B	323	VAL	2.8
1	B	37	LEU	2.8
1	B	130	THR	2.8
1	C	307	LYS	2.8
1	A	190	GLN	2.8
1	A	371	GLN	2.8
1	C	474	ASP	2.8
1	B	231	PHE	2.8
1	C	286	GLY	2.7
1	A	143	ASN	2.7
1	A	233	TRP	2.7
1	B	168	ASN	2.7
1	B	448	TYR	2.7
1	C	379	ASN	2.7
1	C	246	SER	2.7
1	B	56	LEU	2.7
1	A	44	LYS	2.7
1	C	19	LYS	2.7
1	A	123	ARG	2.7
1	B	271	GLU	2.7
1	C	391	GLN	2.7
1	C	322	ASN	2.7
1	B	444	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	37	LEU	2.7
1	C	292	LEU	2.7
1	C	447	LEU	2.7
1	A	127	THR	2.7
1	B	317	ALA	2.7
1	B	195	GLN	2.7
1	B	344	GLN	2.7
1	B	359	GLN	2.7
1	B	8	CYS	2.7
1	C	214	PRO	2.7
1	B	196	ASN	2.7
1	A	102	TYR	2.7
1	A	442	SER	2.7
1	B	105	LEU	2.7
1	A	456	ARG	2.7
1	B	205	THR	2.7
1	B	405	ARG	2.7
1	A	440	HIS	2.7
1	C	182	HIS	2.7
1	C	358	ASP	2.7
1	A	46	CYS	2.7
1	B	50	GLY	2.7
1	B	172	GLY	2.7
1	B	330	GLY	2.7
1	A	490	LYS	2.7
1	B	185[A]	ASN	2.7
1	B	412	LYS	2.7
1	A	145	SER	2.7
1	B	201	VAL	2.7
1	C	16	SER	2.7
1	C	404	ARG	2.7
1	B	113	THR	2.7
1	B	192	THR	2.7
1	C	492	GLU	2.7
1	A	129	HIS	2.7
1	A	416	GLY	2.6
1	C	342	GLY	2.6
1	C	360	GLY	2.6
1	B	23	ILE	2.6
1	B	469	PHE	2.6
1	A	458	ASN	2.6
1	C	446	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	108	LEU	2.6
1	B	193	LEU	2.6
1	B	384	VAL	2.6
1	A	283	THR	2.6
1	C	282	GLN	2.6
1	B	41	HIS	2.6
1	A	380	LYS	2.6
1	B	164	LYS	2.6
1	B	463	GLY	2.6
1	B	302	ILE	2.6
1	C	148	ARG	2.6
1	A	243	ASN	2.6
1	C	249	ASN	2.6
1	B	368	GLU	2.6
1	B	420	VAL	2.6
1	C	17	THR	2.6
1	C	371	GLN	2.6
1	B	354	HIS	2.6
1	B	440	HIS	2.6
1	C	295	HIS	2.6
1	B	367	LYS	2.6
1	A	57	GLY	2.6
1	B	180	GLY	2.6
1	A	191	ARG	2.6
1	B	285	LEU	2.6
1	A	81	SER	2.6
1	C	400	SER	2.6
1	A	261	LYS	2.6
1	A	404	ARG	2.6
1	C	73	ARG	2.6
1	C	227	GLY	2.6
1	C	419	ASP	2.6
1	C	99	PHE	2.6
1	C	208	LEU	2.6
1	A	169	ASN	2.6
1	A	223	ASN	2.6
1	B	28	VAL	2.6
1	A	246	SER	2.6
1	A	192	THR	2.6
1	B	183	HIS	2.6
1	B	210	LYS	2.6
1	B	445	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	496	LYS	2.6
1	B	11	TYR	2.6
1	B	64	TRP	2.5
1	B	233	TRP	2.5
1	A	286	GLY	2.5
1	B	133	GLY	2.5
1	C	50	GLY	2.5
1	A	427	LEU	2.5
1	B	93	LEU	2.5
1	B	402	LEU	2.5
1	A	100	ASN	2.5
1	A	472	LYS	2.5
1	B	221	LYS	2.5
1	B	179	TRP	2.5
1	C	35	ASP	2.5
1	C	421	TRP	2.5
1	A	173	GLU	2.5
1	B	108	LEU	2.5
1	C	294	PHE	2.5
1	C	357	ASN	2.5
1	B	497	ALA	2.5
1	C	378	THR	2.5
1	B	165	ARG	2.5
1	C	228	ARG	2.5
1	C	478	MET	2.5
1	B	352	GLY	2.5
1	C	134	GLY	2.5
1	A	409	LEU	2.5
1	B	54	LEU	2.5
1	C	296	ASN	2.5
1	A	26	ARG	2.5
1	B	334	ALA	2.5
1	C	47	ARG	2.5
1	B	135	SER	2.5
1	C	31	THR	2.5
1	B	46	CYS	2.5
1	A	476	GLU	2.5
1	B	7	ILE	2.5
1	B	174	GLN	2.5
1	A	32	HIS	2.5
1	C	185	ASN	2.5
1	A	207	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	111	SER	2.5
1	B	299	PRO	2.4
1	B	363	TYR	2.4
1	C	339	ILE	2.4
1	B	338	PHE	2.4
1	B	350	TRP	2.4
1	C	369	SER	2.4
1	B	269	LYS	2.4
1	C	281	CYS	2.4
1	B	109	ILE	2.4
1	C	142	ASP	2.4
1	B	464	ASN	2.4
1	A	365	ALA	2.4
1	C	13	ALA	2.4
1	B	85	GLU	2.4
1	B	490	LYS	2.4
1	B	337	GLY	2.4
1	B	72	ASP	2.4
1	C	441	ASP	2.4
1	B	427	LEU	2.4
1	C	486	TYR	2.4
1	A	185	ASN	2.4
1	B	70	GLU	2.4
1	B	156	LYS	2.4
1	C	192	THR	2.4
1	C	234	THR	2.4
1	B	284	PRO	2.4
1	C	494	GLU	2.4
1	B	356	SER	2.4
1	C	333	GLY	2.4
1	B	449	ASP	2.4
1	C	435	ARG	2.4
1	C	454	GLN	2.4
1	C	46	CYS	2.4
1	C	276	ASN	2.4
1	A	139	ALA	2.4
1	B	397	LYS	2.4
1	A	403	GLU	2.4
1	C	52	PRO	2.3
1	C	233	TRP	2.4
1	A	206	SER	2.3
1	A	251	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	491	TYR	2.3
1	A	118	VAL	2.3
1	B	117	LYS	2.3
1	B	389	ASN	2.3
1	B	122	PRO	2.3
1	A	179	TRP	2.3
1	A	397	LYS	2.3
1	B	439	PHE	2.3
1	C	71	CYS	2.3
1	C	305	CYS	2.3
1	C	70	GLU	2.3
1	C	168	ASN	2.3
1	C	365	ALA	2.3
1	C	362	GLY	2.3
1	A	236	LEU	2.3
1	B	36	ILE	2.3
1	A	35	ASP	2.3
1	A	415	ASP	2.3
1	A	419	ASP	2.3
1	C	399	PHE	2.3
1	A	293	PRO	2.3
1	B	220	PRO	2.3
1	C	42	ASN	2.3
1	C	290	THR	2.3
1	A	342	GLY	2.3
1	B	63	GLY	2.3
1	C	248	GLY	2.3
1	B	400	SER	2.3
1	A	447	LEU	2.3
1	B	447	LEU	2.3
1	C	259	ILE	2.3
1	A	39	LYS	2.3
1	B	155	LYS	2.3
1	A	434	GLU	2.3
1	A	439	PHE	2.3
1	B	414	GLU	2.3
1	A	148	ARG	2.3
1	A	452	ARG	2.3
1	B	33	ALA	2.2
1	B	88	ASN	2.2
1	B	94	CYS	2.3
1	B	136	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	489	PRO	2.3
1	C	26	ARG	2.3
1	C	183	HIS	2.2
1	C	266	GLY	2.2
1	C	319	GLY	2.2
1	B	39	LYS	2.2
1	B	386	GLU	2.2
1	B	433	ASN	2.2
1	B	446	ASN	2.2
1	A	234	THR	2.2
1	A	378	THR	2.2
1	B	370	THR	2.2
1	C	301	THR	2.2
1	B	272	LYS	2.2
1	B	460	LYS	2.2
1	B	316	LEU	2.2
1	A	103	GLU	2.2
1	A	165	ARG	2.2
1	B	458	ASN	2.2
1	A	282	GLN	2.2
1	C	164	LYS	2.2
1	A	484	GLY	2.2
1	B	335	ILE	2.2
1	B	348	ASP	2.2
1	B	438	ASP	2.2
1	A	493	GLU	2.2
1	B	237	GLU	2.2
1	B	399	PHE	2.2
1	C	39	LYS	2.2
1	C	388	MET	2.2
1	B	422	THR	2.2
1	A	345	GLY	2.2
1	B	488	TYR	2.2
1	B	281	CYS	2.2
1	B	477	CYS	2.2
1	A	266	GLY	2.1
1	B	273	THR	2.1
1	C	97	GLY	2.1
1	C	377	ILE	2.1
1	C	477	CYS	2.1
1	C	98	SER	2.1
1	C	411	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	388	MET	2.1
1	A	446	ASN	2.1
1	C	443	ASN	2.1
1	A	369	SER	2.1
1	A	438	ASP	2.1
1	A	441	ASP	2.1
1	A	152	TRP	2.1
1	B	424	ASN	2.1
1	A	292	LEU	2.1
1	B	267	ILE	2.1
1	B	339	ILE	2.1
1	C	189	GLU	2.1
1	B	419	ASP	2.1
1	B	96	PRO	2.1
1	A	374	PHE	2.1
1	A	276	ASN	2.1
1	C	424	ASN	2.1
1	A	47	ARG	2.1
1	B	349	GLY	2.1
1	B	290	THR	2.1
1	C	38	GLU	2.1
1	B	486	TYR	2.1
1	C	101	ASP	2.1
1	C	60	SER	2.1
1	C	346	MET	2.1
1	B	452	ARG	2.0
1	C	456	ARG	2.0
1	A	208	LEU	2.0
1	B	406	LEU	2.0
1	C	48	LEU	2.0
1	C	408	ASN	2.0
1	A	79	GLU	2.0
1	A	204	GLY	2.0
1	B	97	GLY	2.0
1	C	303	GLY	2.0
1	C	468	GLU	2.0
1	A	205	THR	2.0
1	C	460	LYS	2.0
1	B	457	ASP	2.0
1	C	429	VAL	2.0
1	B	314	LEU	2.0
1	A	411	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	288	ILE	2.0
1	B	32	HIS	2.0
1	B	480	SER	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](#)

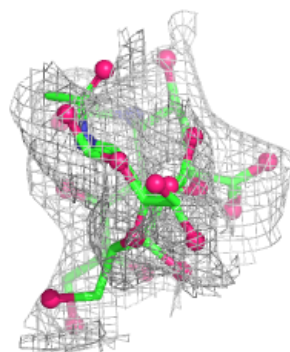
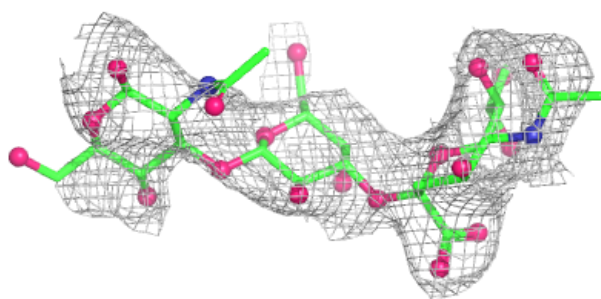
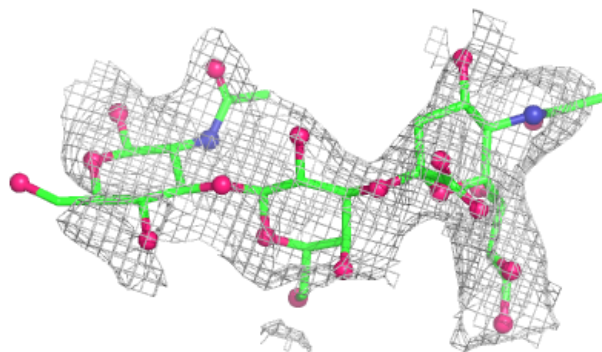
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GAL	D	2	11/12	0.55	0.18	82,84,85,85	0
2	NAG	E	1	15/15	0.56	0.20	70,74,74,75	0
2	NAG	D	1	15/15	0.60	0.19	86,89,89,90	0
2	SIA	E	3	20/21	0.63	0.24	54,58,60,61	0
2	GAL	E	2	11/12	0.73	0.25	63,66,67,68	0
2	SIA	D	3	20/21	0.76	0.15	77,79,81,81	0

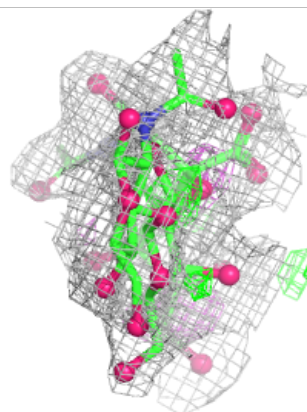
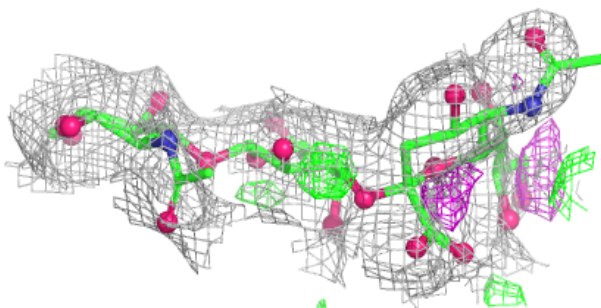
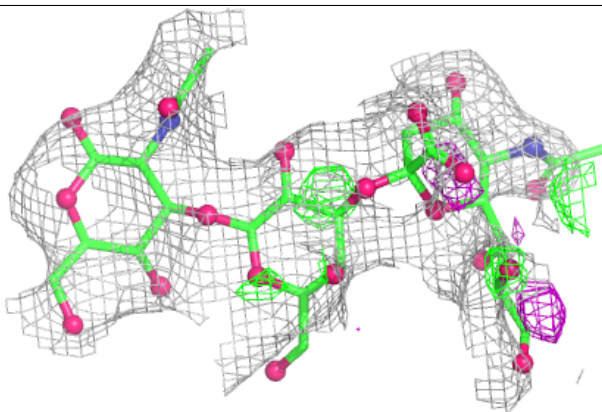
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

**Electron density around Chain E:**

$2mF_o-DF_c$ (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
3	NAG	A	1499	14/15	0.43	0.26	111,114,114,115	0
3	NAG	C	1500	14/15	0.47	0.26	78,79,80,80	0
3	NAG	A	1500	13/15	0.68	0.19	69,70,71,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.