



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2022 – 12:15 AM EDT

PDB ID : 4K66
Title : Structure of an airborne transmissible avian influenza H5 hemagglutinin mutant from the influenza virus A/Indonesia/5/2005 complexed with avian receptor analog LSTa
Authors : Zhang, W.; Shi, Y.; Lu, X.; Shu, Y.; Qi, J.; Gao, G.F.
Deposited on : 2013-04-15
Resolution : 3.00 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
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) : 2.29

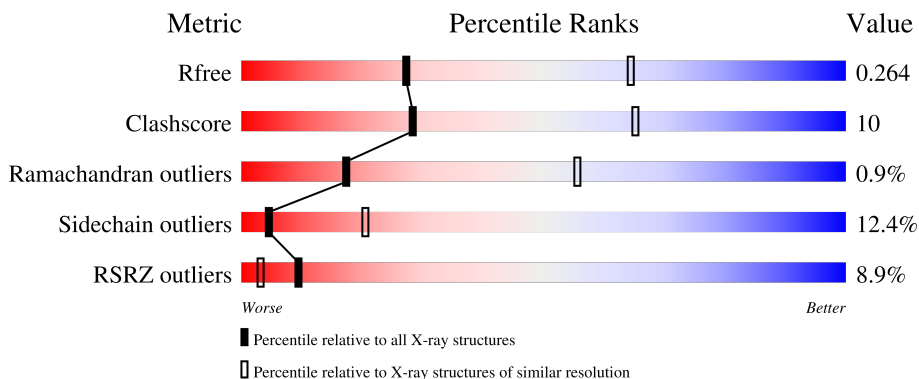
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	321	
1	C	321	
1	E	321	
1	G	321	
2	B	164	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	164	<p>%</p> <p>71% 26%</p> <p>..</p>
2	F	164	<p>33% 64% 31%</p> <p>..</p>
2	H	164	<p>27% 63% 32%</p> <p>..</p>
3	I	2	<p>100%</p>
3	J	2	<p>100%</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15572 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
			Total	C	N	O	S			
1	A	321	2542	1609	433	485	15	0	0	0
1	C	321	2542	1609	433	485	15	0	0	0
1	E	321	2542	1609	433	485	15	0	0	0
1	G	321	2542	1609	433	485	15	0	0	0

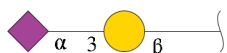
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLN	-	expression tag	UNP A8HWY8
A	107	TYR	HIS	engineered mutation	UNP A8HWY8
A	160	ALA	THR	engineered mutation	UNP A8HWY8
A	226	LEU	GLN	engineered mutation	UNP A8HWY8
A	228	SER	GLY	engineered mutation	UNP A8HWY8
C	4	GLN	-	expression tag	UNP A8HWY8
C	107	TYR	HIS	engineered mutation	UNP A8HWY8
C	160	ALA	THR	engineered mutation	UNP A8HWY8
C	226	LEU	GLN	engineered mutation	UNP A8HWY8
C	228	SER	GLY	engineered mutation	UNP A8HWY8
E	4	GLN	-	expression tag	UNP A8HWY8
E	107	TYR	HIS	engineered mutation	UNP A8HWY8
E	160	ALA	THR	engineered mutation	UNP A8HWY8
E	226	LEU	GLN	engineered mutation	UNP A8HWY8
E	228	SER	GLY	engineered mutation	UNP A8HWY8
G	4	GLN	-	expression tag	UNP A8HWY8
G	107	TYR	HIS	engineered mutation	UNP A8HWY8
G	160	ALA	THR	engineered mutation	UNP A8HWY8
G	226	LEU	GLN	engineered mutation	UNP A8HWY8
G	228	SER	GLY	engineered mutation	UNP A8HWY8

- Molecule 2 is a protein called Hemagglutinin.

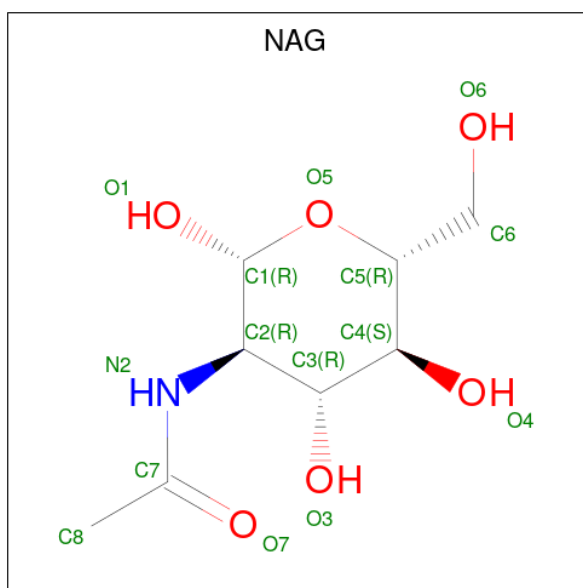
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	164	Total 1328	C 828	N 229	O 263	S 8	0	0	0
2	D	164	Total 1328	C 828	N 229	O 263	S 8	0	0	0
2	F	164	Total 1328	C 828	N 229	O 263	S 8	0	0	0
2	H	164	Total 1328	C 828	N 229	O 263	S 8	0	0	0

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



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

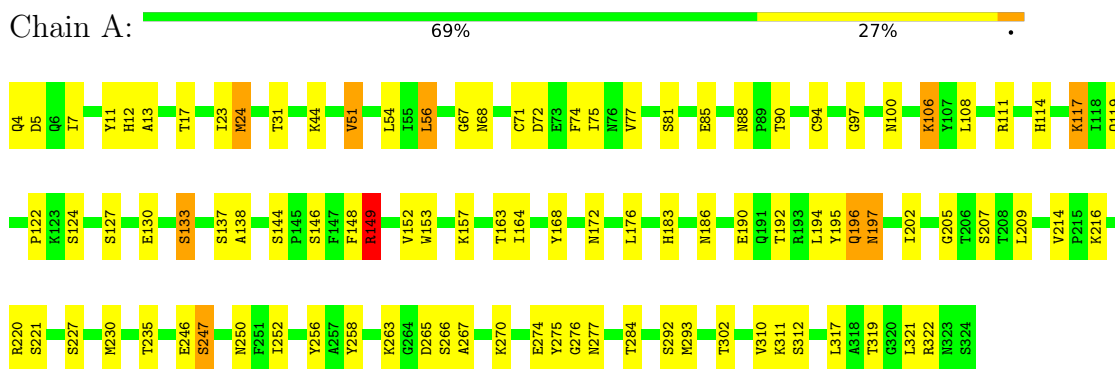


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

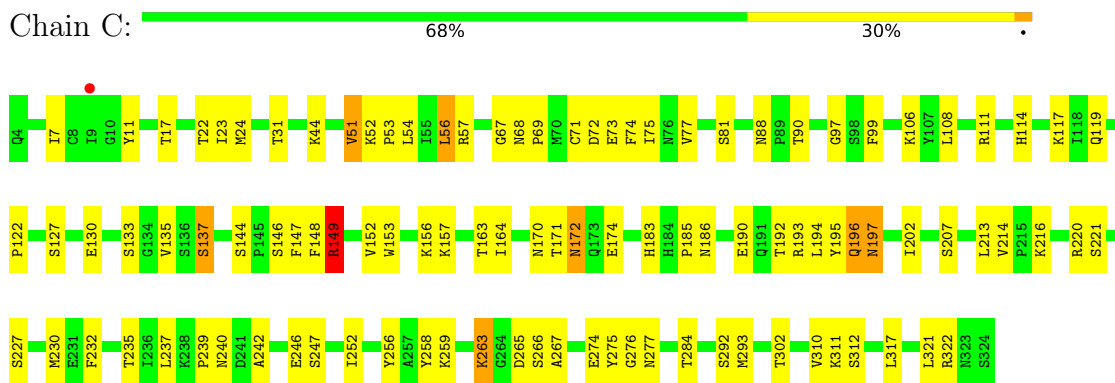
3 Residue-property plots [i](#)

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

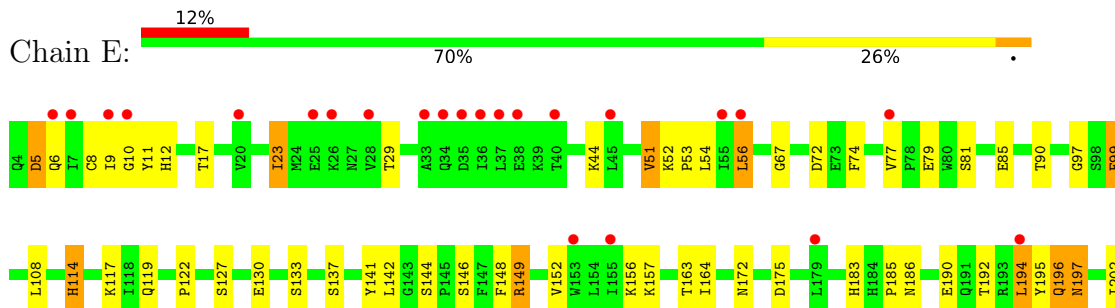
- Molecule 1: Hemagglutinin

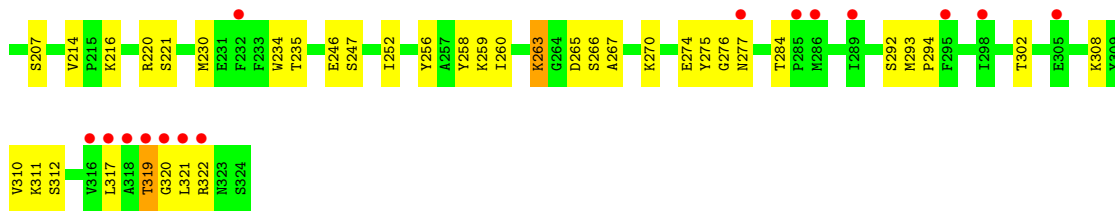


- Molecule 1: Hemagglutinin

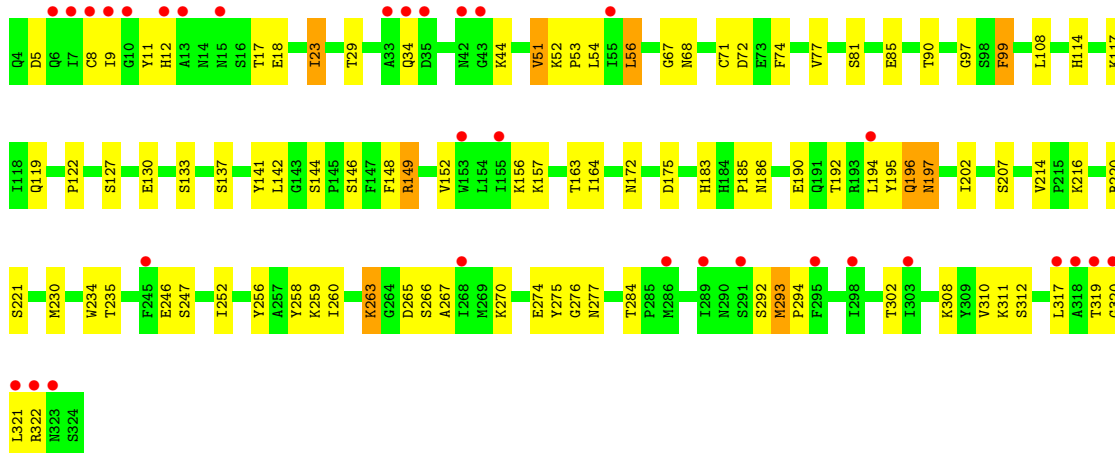


- Molecule 1: Hemagglutinin





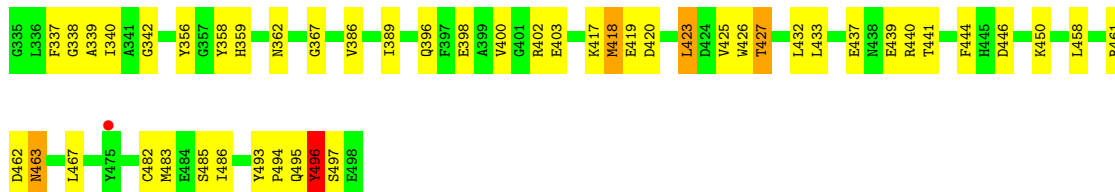
• Molecule 1: Hemagglutinin



• Molecule 2: Hemagglutinin

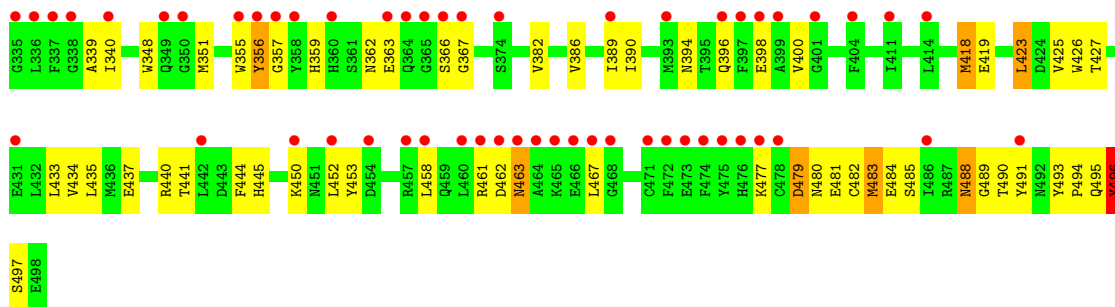


• Molecule 2: Hemagglutinin

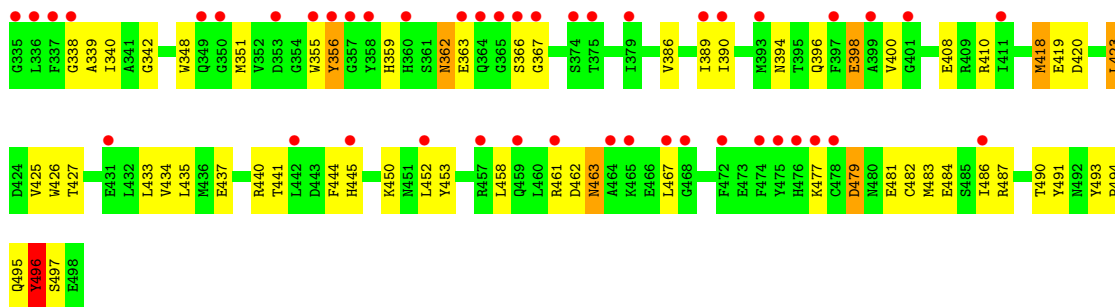


• Molecule 2: Hemagglutinin

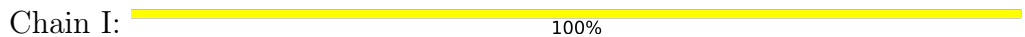




• Molecule 2: Hemagglutinin



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



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



4 Data and refinement statistics i

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	70.61Å 70.61Å 490.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.01 – 3.00 49.01 – 3.01	Depositor EDS
% Data completeness (in resolution range)	91.7 (49.01-3.00) 91.7 (49.01-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.219 , 0.262 0.221 , 0.264	Depositor DCC
R_{free} test set	2545 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.398 for -h,-k,l 0.073 for h,-h-k,-l 0.065 for -k,-h,-l	Xtriage
Reported twinning fraction	0.255 for -h,-k,l	Depositor
Outliers	0 of 50058 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15572	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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 i

5.1 Standard geometry i

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	0.90	2/2604 (0.1%)	0.87	1/3539 (0.0%)
1	C	0.90	1/2604 (0.0%)	0.86	1/3539 (0.0%)
1	E	0.52	0/2604	0.69	1/3539 (0.0%)
1	G	0.49	0/2604	0.66	0/3539
2	B	0.72	0/1355	0.78	1/1823 (0.1%)
2	D	0.71	0/1355	0.97	3/1823 (0.2%)
2	F	0.50	0/1355	0.64	1/1823 (0.1%)
2	H	0.48	0/1355	0.65	1/1823 (0.1%)
All	All	0.69	3/15836 (0.0%)	0.78	9/21448 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	ASN	CG-ND2	6.13	1.48	1.32
1	A	100	ASN	CG-OD1	5.83	1.36	1.24
1	C	232	PHE	CE1-CZ	-5.06	1.27	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	440	ARG	NE-CZ-NH1	-18.17	111.22	120.30
2	D	440	ARG	NE-CZ-NH2	17.40	129.00	120.30
1	E	5	ASP	N-CA-CB	-9.89	92.79	110.60
1	C	149	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	A	149	ARG	NE-CZ-NH2	-8.31	116.15	120.30
2	D	440	ARG	CD-NE-CZ	8.17	135.04	123.60
2	F	440	ARG	NE-CZ-NH2	-5.11	117.75	120.30
2	H	440	ARG	NE-CZ-NH2	-5.09	117.76	120.30
2	B	440	ARG	NE-CZ-NH2	-5.01	117.80	120.30

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	2542	0	2483	48	0
1	C	2542	0	2483	52	0
1	E	2542	0	2484	67	0
1	G	2542	0	2484	60	0
2	B	1328	0	1231	24	0
2	D	1328	0	1231	25	0
2	F	1328	0	1231	45	0
2	H	1328	0	1231	43	1
3	I	32	0	28	2	0
3	J	32	0	28	3	0
4	A	14	0	13	0	0
4	C	14	0	13	2	0
All	All	15572	0	14940	300	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (300) 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:E:12:HIS:HB2	2:F:355:TRP:HA	1.36	1.08
1:G:12:HIS:HB2	2:H:355:TRP:HA	1.46	0.97
1:E:9:ILE:HG23	2:F:452:LEU:HD23	1.53	0.90
1:E:12:HIS:N	2:F:355:TRP:O	2.07	0.88
1:G:9:ILE:HG23	2:H:452:LEU:HD23	1.58	0.86
1:E:11:TYR:HA	2:F:356:TYR:HA	1.61	0.80
1:G:12:HIS:N	2:H:355:TRP:O	2.16	0.78
1:E:294:PRO:HG3	2:F:390:ILE:HG12	1.64	0.77
2:H:483:MET:HA	2:H:486:ILE:HD12	1.66	0.77
1:E:294:PRO:HB3	2:F:390:ILE:HG23	1.67	0.75
1:G:294:PRO:HG3	2:H:390:ILE:HG12	1.71	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:359:HIS:CE1	2:H:366:SER:HB3	2.24	0.71
1:C:216:LYS:O	1:C:220:ARG:NH2	2.24	0.71
1:E:308:LYS:HD2	2:F:396:GLN:HB3	1.73	0.69
1:G:11:TYR:HA	2:H:356:TYR:HA	1.73	0.69
1:G:294:PRO:HB3	2:H:390:ILE:HG23	1.76	0.67
1:A:216:LYS:O	1:A:220:ARG:NH2	2.27	0.67
2:D:483:MET:HA	2:D:486:ILE:HG13	1.78	0.66
1:A:311:LYS:H	2:B:427:THR:HG1	1.42	0.66
1:C:311:LYS:HG3	2:D:423:LEU:HD11	1.77	0.66
1:G:216:LYS:O	1:G:220:ARG:NH2	2.29	0.66
2:F:481:GLU:O	2:F:484:GLU:HB2	1.96	0.66
1:G:308:LYS:HD2	2:H:396:GLN:HB3	1.76	0.65
1:A:44:LYS:HD3	1:A:276:GLY:HA3	1.78	0.65
2:D:418:MET:HG3	2:D:419:GLU:N	2.10	0.65
2:H:481:GLU:O	2:H:484:GLU:HB3	1.96	0.65
1:C:311:LYS:H	2:D:427:THR:HG1	1.45	0.64
2:B:418:MET:HG3	2:B:419:GLU:N	2.13	0.64
2:D:389:ILE:HG12	2:D:433:LEU:HD21	1.79	0.64
1:E:216:LYS:O	1:E:220:ARG:NH2	2.30	0.64
2:F:389:ILE:HG12	2:F:433:LEU:HD21	1.80	0.64
1:C:54:LEU:HD22	1:C:77:VAL:HG11	1.80	0.63
1:C:172:ASN:HD22	1:C:172:ASN:N	1.96	0.63
2:B:389:ILE:HG12	2:B:433:LEU:HD21	1.79	0.63
1:E:317:LEU:HD23	2:F:386:VAL:HG22	1.80	0.63
1:G:317:LEU:HD23	2:H:386:VAL:HG22	1.79	0.63
1:C:72:ASP:OD1	1:C:149:ARG:NH1	2.32	0.62
1:C:153:TRP:CH2	3:J:2:SIA:H112	2.34	0.62
2:H:418:MET:HG3	2:H:419:GLU:N	2.13	0.62
1:A:67:GLY:O	1:A:148:PHE:HA	2.00	0.61
1:E:172:ASN:OD1	1:E:259:LYS:HD3	2.00	0.61
1:E:311:LYS:HE3	2:F:423:LEU:HD21	1.82	0.61
2:F:418:MET:HG3	2:F:419:GLU:N	2.14	0.61
2:B:493:TYR:O	2:B:495:GLN:N	2.32	0.61
2:H:493:TYR:O	2:H:495:GLN:N	2.33	0.61
2:F:479:ASP:OD1	2:F:479:ASP:N	2.34	0.60
2:F:493:TYR:O	2:F:495:GLN:N	2.34	0.60
1:E:44:LYS:HD3	1:E:276:GLY:HA3	1.81	0.60
2:D:493:TYR:O	2:D:495:GLN:N	2.34	0.60
1:G:311:LYS:HE3	2:H:423:LEU:HD21	1.84	0.60
1:C:311:LYS:HE3	2:D:423:LEU:HD21	1.83	0.60
1:G:44:LYS:HD3	1:G:276:GLY:HA3	1.81	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HD22	1:A:77:VAL:HG11	1.85	0.59
1:E:17:THR:HA	1:E:29:THR:HG23	1.84	0.59
1:G:54:LEU:HD22	1:G:77:VAL:HG11	1.85	0.59
1:G:172:ASN:OD1	1:G:259:LYS:HD3	2.03	0.58
2:H:389:ILE:HG12	2:H:433:LEU:HD21	1.84	0.58
1:C:67:GLY:O	1:C:148:PHE:HA	2.03	0.58
1:E:308:LYS:HZ2	2:F:396:GLN:H	1.51	0.58
1:G:17:THR:HA	1:G:29:THR:HG23	1.85	0.58
1:C:44:LYS:HD3	1:C:276:GLY:HA3	1.84	0.58
2:H:462:ASP:OD1	2:H:493:TYR:OH	2.21	0.58
1:A:311:LYS:HG3	2:B:423:LEU:HD11	1.86	0.57
1:C:172:ASN:OD1	1:C:259:LYS:HD3	2.04	0.57
1:A:72:ASP:OD1	1:A:149:ARG:NH1	2.37	0.57
1:E:266:SER:OG	1:E:267:ALA:N	2.37	0.57
1:C:186:ASN:HB3	1:C:190:GLU:OE1	2.05	0.57
2:F:462:ASP:OD1	2:F:493:TYR:OH	2.22	0.57
1:E:72:ASP:OD1	1:E:149:ARG:NH1	2.37	0.57
1:A:119:GLN:NE2	1:A:122:PRO:HA	2.20	0.56
1:A:311:LYS:HE3	2:B:423:LEU:HD21	1.86	0.56
2:B:485:SER:OG	2:B:491:TYR:HA	2.05	0.56
1:E:54:LEU:HD22	1:E:77:VAL:HG11	1.86	0.56
2:B:462:ASP:OD1	2:B:493:TYR:OH	2.24	0.56
1:C:11:TYR:CZ	2:D:340:ILE:HG23	2.41	0.55
2:D:359:HIS:HA	2:D:367:GLY:O	2.07	0.55
1:G:186:ASN:HB3	1:G:190:GLU:OE1	2.07	0.55
1:E:10:GLY:O	2:F:357:GLY:N	2.35	0.55
1:G:11:TYR:CZ	2:H:340:ILE:HG23	2.42	0.55
1:G:72:ASP:OD1	1:G:149:ARG:NH1	2.40	0.55
1:G:130:GLU:HG2	1:G:157:LYS:HB2	1.90	0.54
2:H:359:HIS:HE1	2:H:366:SER:HB3	1.73	0.54
1:C:130:GLU:HG2	1:C:157:LYS:HB2	1.89	0.54
2:D:462:ASP:OD1	2:D:493:TYR:OH	2.25	0.54
1:A:11:TYR:CZ	2:B:340:ILE:HG23	2.43	0.54
1:C:164:ILE:O	1:C:246:GLU:HA	2.08	0.54
1:E:141:TYR:CE2	1:E:142:LEU:HD12	2.42	0.54
2:D:496:TYR:CG	2:D:497:SER:N	2.75	0.54
1:E:321:LEU:HB3	2:F:445:HIS:CG	2.43	0.54
2:H:496:TYR:CG	2:H:497:SER:N	2.76	0.54
1:C:266:SER:OG	1:C:267:ALA:N	2.41	0.53
1:A:7:ILE:HD12	2:B:483:MET:SD	2.49	0.53
1:A:186:ASN:HB3	1:A:190:GLU:OE1	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:ASN:HB3	1:E:190:GLU:OE1	2.08	0.53
1:E:311:LYS:HG3	2:F:423:LEU:HD11	1.90	0.53
1:E:119:GLN:HB2	1:E:256:TYR:CE1	2.44	0.52
1:A:56:LEU:HA	1:A:74:PHE:CZ	2.44	0.52
2:B:359:HIS:HA	2:B:367:GLY:O	2.08	0.52
1:E:51:VAL:HG22	1:E:81:SER:HB3	1.91	0.52
1:G:311:LYS:HG3	2:H:423:LEU:HD11	1.91	0.52
1:G:119:GLN:HB2	1:G:256:TYR:CE1	2.45	0.52
1:G:266:SER:OG	1:G:267:ALA:N	2.40	0.52
2:F:482:CYS:C	2:F:484:GLU:H	2.14	0.52
1:E:130:GLU:HG2	1:E:157:LYS:HB2	1.92	0.51
1:G:119:GLN:NE2	1:G:122:PRO:HA	2.26	0.51
1:A:266:SER:OG	1:A:267:ALA:N	2.43	0.51
1:G:141:TYR:CE2	1:G:142:LEU:HD12	2.44	0.51
1:A:51:VAL:HG22	1:A:81:SER:HB3	1.93	0.51
1:E:119:GLN:NE2	1:E:122:PRO:HA	2.26	0.51
1:E:320:GLY:HA2	2:F:355:TRP:CZ2	2.46	0.51
2:F:496:TYR:CG	2:F:497:SER:N	2.76	0.51
1:E:17:THR:HG22	1:E:29:THR:HG21	1.92	0.51
1:E:67:GLY:O	1:E:148:PHE:HA	2.10	0.51
1:C:119:GLN:HB2	1:C:256:TYR:CE1	2.46	0.50
1:C:242:ALA:H	4:C:601:NAG:H82	1.75	0.50
1:A:164:ILE:O	1:A:246:GLU:HA	2.12	0.50
1:A:11:TYR:O	2:B:348:TRP:N	2.25	0.50
1:E:9:ILE:HD13	2:F:453:TYR:HA	1.94	0.50
1:G:51:VAL:HG22	1:G:81:SER:HB3	1.94	0.50
1:G:97:GLY:HA3	1:G:230:MET:O	2.12	0.50
2:B:496:TYR:CG	2:B:497:SER:N	2.77	0.49
2:D:339:ALA:HB2	2:D:450:LYS:HB2	1.94	0.49
1:E:56:LEU:HA	1:E:74:PHE:CZ	2.47	0.49
1:E:172:ASN:N	1:E:172:ASN:HD22	2.09	0.49
1:G:317:LEU:HD13	2:H:434:VAL:HG22	1.92	0.49
1:A:68:ASN:HB3	1:A:71:CYS:SG	2.52	0.49
1:C:56:LEU:HA	1:C:74:PHE:CZ	2.47	0.49
1:G:9:ILE:HD13	2:H:453:TYR:HA	1.95	0.49
1:E:317:LEU:HD13	2:F:434:VAL:HG22	1.95	0.49
1:A:172:ASN:N	1:A:172:ASN:HD22	2.09	0.49
2:D:482:CYS:O	2:D:485:SER:OG	2.18	0.49
2:B:417:LYS:HB3	2:B:417:LYS:HE3	1.60	0.49
2:H:486:ILE:HA	2:H:491:TYR:HB2	1.94	0.49
1:E:97:GLY:HA3	1:E:230:MET:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLN:HB2	1:A:256:TYR:CE1	2.47	0.48
1:A:130:GLU:HG2	1:A:157:LYS:HB2	1.95	0.48
1:A:274:GLU:HG3	1:A:275:TYR:H	1.78	0.48
1:G:274:GLU:HG3	1:G:275:TYR:H	1.79	0.48
1:E:8:CYS:HB3	2:F:348:TRP:HH2	1.79	0.48
2:F:359:HIS:CE1	2:F:366:SER:HB3	2.48	0.48
1:G:67:GLY:O	1:G:148:PHE:HA	2.13	0.48
2:H:463:ASN:N	2:H:463:ASN:OD1	2.47	0.48
2:B:339:ALA:HB2	2:B:450:LYS:HB2	1.96	0.48
1:C:52:LYS:HG2	1:C:53:PRO:HD2	1.96	0.48
1:C:68:ASN:HB3	1:C:71:CYS:SG	2.54	0.48
1:A:97:GLY:HA3	1:A:230:MET:O	2.12	0.48
1:G:172:ASN:N	1:G:172:ASN:HD22	2.11	0.48
1:A:317:LEU:HD23	2:B:386:VAL:HG22	1.96	0.47
1:E:12:HIS:HB2	2:F:355:TRP:CA	2.24	0.47
1:G:192:THR:HG22	1:G:196:GLN:O	2.13	0.47
2:B:338:GLY:O	2:B:342:GLY:HA3	2.14	0.47
2:H:339:ALA:HB2	2:H:450:LYS:HB2	1.96	0.47
1:C:106:LYS:NZ	2:D:403:GLU:OE2	2.41	0.47
1:E:308:LYS:HE3	2:F:394:ASN:O	2.14	0.47
1:C:7:ILE:HD12	2:D:483:MET:SD	2.54	0.47
1:C:195:TYR:O	1:C:197:ASN:N	2.47	0.47
1:E:9:ILE:CG2	2:F:452:LEU:HD23	2.37	0.47
1:E:11:TYR:CZ	2:F:340:ILE:HG23	2.50	0.47
2:F:339:ALA:HB2	2:F:450:LYS:HB2	1.97	0.47
1:G:34:GLN:OE1	2:H:386:VAL:HG21	2.15	0.47
1:A:202:ILE:HA	1:A:247:SER:HB2	1.96	0.47
2:B:362:ASN:ND2	2:B:479:ASP:HA	2.29	0.47
1:C:51:VAL:HG22	1:C:81:SER:HB3	1.95	0.47
1:C:317:LEU:HD23	2:D:386:VAL:HG22	1.96	0.47
1:G:196:GLN:HE21	1:G:196:GLN:HA	1.79	0.47
2:H:359:HIS:HA	2:H:367:GLY:O	2.14	0.47
1:G:56:LEU:HA	1:G:74:PHE:CZ	2.50	0.47
1:G:321:LEU:HB3	2:H:445:HIS:CG	2.50	0.47
1:C:119:GLN:NE2	1:C:122:PRO:HA	2.30	0.46
1:C:156:LYS:HD2	1:C:196:GLN:HG2	1.96	0.46
1:C:69:PRO:HG3	1:C:147:PHE:O	2.14	0.46
1:E:195:TYR:O	1:E:197:ASN:N	2.48	0.46
1:C:137:SER:OG	3:J:2:SIA:O1A	2.32	0.46
2:F:463:ASN:OD1	2:F:463:ASN:N	2.49	0.46
1:E:12:HIS:HB3	2:F:355:TRP:HD1	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ASP:OD2	1:A:149:ARG:HD2	2.15	0.46
1:C:97:GLY:HA3	1:C:230:MET:O	2.15	0.46
2:F:359:HIS:HA	2:F:367:GLY:O	2.15	0.46
2:F:348:TRP:HE3	2:F:351:MET:HE2	1.81	0.46
1:A:133:SER:O	3:I:2:SIA:H113	2.15	0.46
1:E:99:PHE:HE2	1:E:234:TRP:CD1	2.34	0.46
1:E:52:LYS:HG2	1:E:53:PRO:HD2	1.97	0.45
1:A:44:LYS:HD3	1:A:276:GLY:CA	2.45	0.45
2:B:396:GLN:HG3	2:B:426:TRP:CD2	2.52	0.45
1:C:171:THR:C	1:C:172:ASN:HD22	2.20	0.45
2:D:337:PHE:HB2	2:D:446:ASP:OD2	2.16	0.45
1:C:274:GLU:HG3	1:C:275:TYR:H	1.81	0.45
2:D:463:ASN:OD1	2:D:463:ASN:N	2.50	0.45
1:E:6:GLN:O	2:F:483:MET:HE1	2.17	0.45
1:G:23:ILE:HA	2:H:435:LEU:HD13	1.98	0.45
1:C:183:HIS:O	1:C:185:PRO:HD3	2.16	0.45
1:G:183:HIS:HB2	1:G:252:ILE:HD11	1.98	0.45
1:G:308:LYS:HZ2	2:H:396:GLN:H	1.65	0.45
1:C:220:ARG:HD2	1:C:227:SER:O	2.17	0.45
2:D:441:THR:O	2:D:444:PHE:HB3	2.16	0.45
1:G:263:LYS:H	1:G:263:LYS:HG2	1.44	0.45
1:A:153:TRP:CH2	3:I:2:SIA:H112	2.52	0.45
2:B:463:ASN:OD1	2:B:463:ASN:N	2.49	0.45
1:A:195:TYR:O	1:A:197:ASN:N	2.50	0.45
1:E:164:ILE:O	1:E:246:GLU:HA	2.17	0.45
1:E:319:THR:O	2:F:382:VAL:HG11	2.17	0.45
1:E:321:LEU:HB3	2:F:445:HIS:ND1	2.32	0.44
1:A:106:LYS:NZ	2:B:403:GLU:OE2	2.43	0.44
1:C:183:HIS:HB2	1:C:252:ILE:HD11	1.99	0.44
1:E:192:THR:HG22	1:E:196:GLN:O	2.16	0.44
1:E:274:GLU:HG3	1:E:275:TYR:H	1.82	0.44
1:C:44:LYS:HD3	1:C:276:GLY:CA	2.47	0.44
1:C:75:ILE:HD13	1:C:75:ILE:HG21	1.65	0.44
1:E:119:GLN:HE21	1:E:122:PRO:HA	1.82	0.44
1:E:156:LYS:HD2	1:E:196:GLN:HG2	1.98	0.44
1:A:117:LYS:HD3	1:A:258:TYR:CE1	2.52	0.44
1:A:220:ARG:HD2	1:A:227:SER:O	2.17	0.44
1:C:202:ILE:HA	1:C:247:SER:HB2	2.00	0.44
1:E:79:GLU:HB2	1:E:114:HIS:CD2	2.52	0.44
2:F:488:ASN:HB2	2:F:489:GLY:H	1.62	0.44
1:G:195:TYR:O	1:G:197:ASN:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:52:LYS:HG2	1:G:53:PRO:HD2	1.98	0.44
2:H:398:GLU:H	2:H:398:GLU:HG2	1.64	0.44
2:H:441:THR:O	2:H:444:PHE:HB3	2.17	0.44
1:A:119:GLN:HE21	1:A:122:PRO:HA	1.81	0.44
1:E:23:ILE:HA	2:F:435:LEU:HD13	2.00	0.44
2:D:396:GLN:HG3	2:D:426:TRP:CD2	2.52	0.44
2:B:441:THR:O	2:B:444:PHE:HB3	2.17	0.44
1:E:85:GLU:O	1:E:270:LYS:HA	2.18	0.43
1:E:263:LYS:H	1:E:263:LYS:HG2	1.43	0.43
2:F:441:THR:O	2:F:444:PHE:HB3	2.17	0.43
1:C:174:GLU:OE1	1:C:259:LYS:HD2	2.18	0.43
1:E:44:LYS:HD3	1:E:276:GLY:CA	2.48	0.43
1:G:183:HIS:O	1:G:185:PRO:HD3	2.19	0.43
1:G:8:CYS:HB3	2:H:348:TRP:HH2	1.84	0.43
1:A:4:GLN:HG2	1:A:5:ASP:H	1.84	0.43
1:A:205:GLY:HA2	1:A:209:LEU:O	2.19	0.43
1:C:192:THR:HG22	1:C:196:GLN:O	2.18	0.43
2:D:423:LEU:O	2:D:423:LEU:HD12	2.18	0.43
1:G:119:GLN:HE21	1:G:122:PRO:HA	1.82	0.43
2:D:417:LYS:HB3	2:D:417:LYS:HE3	1.61	0.43
1:E:196:GLN:HA	1:E:196:GLN:HE21	1.83	0.43
1:G:99:PHE:HE2	1:G:234:TRP:CD1	2.37	0.43
1:A:176:LEU:HD23	1:A:176:LEU:HA	1.78	0.43
1:A:196:GLN:HE21	1:A:196:GLN:HA	1.83	0.43
1:C:170:ASN:HB2	1:C:237:LEU:HD13	2.01	0.43
1:C:242:ALA:N	4:C:601:NAG:H82	2.33	0.43
1:G:44:LYS:HD3	1:G:276:GLY:CA	2.49	0.43
2:H:362:ASN:ND2	2:H:479:ASP:HA	2.34	0.43
2:F:485:SER:O	2:F:491:TYR:N	2.52	0.43
1:A:24:MET:HE2	1:A:24:MET:HB2	1.83	0.42
1:C:22:THR:HB	2:D:439:GLU:HB2	2.00	0.42
1:G:164:ILE:O	1:G:246:GLU:HA	2.19	0.42
1:A:12:HIS:HD2	1:A:13:ALA:O	2.02	0.42
1:E:72:ASP:OD2	1:E:149:ARG:HD2	2.19	0.42
2:F:396:GLN:HG3	2:F:426:TRP:CD2	2.54	0.42
2:B:402:ARG:HH11	2:B:402:ARG:HD2	1.69	0.42
1:A:85:GLU:O	1:A:270:LYS:HA	2.20	0.42
1:C:72:ASP:OD2	1:C:149:ARG:HD2	2.20	0.42
2:H:362:ASN:HB2	2:H:363:GLU:H	1.57	0.42
2:F:479:ASP:HB2	2:F:480:ASN:H	1.72	0.42
1:C:57:ARG:HD2	1:C:73:GLU:OE1	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:202:ILE:HG23	1:G:247:SER:HB2	2.01	0.42
2:D:338:GLY:O	2:D:342:GLY:HA3	2.20	0.42
1:E:17:THR:HA	1:E:29:THR:CG2	2.48	0.42
1:G:293:MET:HG3	1:G:294:PRO:HD2	2.02	0.42
1:E:311:LYS:CG	2:F:423:LEU:HD11	2.50	0.42
1:G:12:HIS:HB3	2:H:355:TRP:HD1	1.84	0.42
1:G:321:LEU:HD12	1:G:322:ARG:O	2.19	0.42
2:H:396:GLN:HG3	2:H:426:TRP:CD2	2.55	0.41
2:H:482:CYS:C	2:H:484:GLU:H	2.21	0.41
1:A:183:HIS:HB2	1:A:252:ILE:HD11	2.03	0.41
2:H:348:TRP:HE3	2:H:351:MET:HE2	1.85	0.41
2:H:482:CYS:O	2:H:486:ILE:HG13	2.21	0.41
1:E:117:LYS:HD3	1:E:258:TYR:CE1	2.55	0.41
1:C:156:LYS:HE2	1:C:193:ARG:O	2.20	0.41
1:C:263:LYS:H	1:C:263:LYS:HG2	1.48	0.41
1:E:183:HIS:O	1:E:185:PRO:HD3	2.20	0.41
1:G:202:ILE:HA	1:G:247:SER:HB2	2.02	0.41
1:A:31:THR:HG23	1:A:321:LEU:O	2.20	0.41
1:A:168:TYR:CD2	1:A:168:TYR:C	2.90	0.41
1:C:117:LYS:HD3	1:C:258:TYR:CE1	2.55	0.41
1:C:153:TRP:CZ3	3:J:2:SIA:H112	2.54	0.41
1:G:85:GLU:O	1:G:270:LYS:HA	2.20	0.41
1:G:156:LYS:HD2	1:G:196:GLN:HG2	2.02	0.41
1:A:75:ILE:HG21	1:A:75:ILE:HD13	1.64	0.41
2:B:358:TYR:O	2:B:368:TYR:HA	2.21	0.41
1:E:175:ASP:HB2	1:E:260:ILE:HD12	2.02	0.41
1:E:194:LEU:HB3	1:E:195:TYR:CE1	2.56	0.41
1:E:202:ILE:HA	1:E:247:SER:HB2	2.03	0.41
1:G:68:ASN:HB3	1:G:71:CYS:SG	2.61	0.41
1:G:175:ASP:HB2	1:G:260:ILE:HD12	2.03	0.41
1:A:94:CYS:HB2	1:A:138:ALA:O	2.21	0.41
1:A:192:THR:HG22	1:A:196:GLN:O	2.21	0.41
1:C:239:PRO:O	1:C:240:ASN:HB2	2.21	0.41
1:E:321:LEU:HD12	1:E:322:ARG:O	2.20	0.40
1:G:117:LYS:HD3	1:G:258:TYR:CE1	2.55	0.40
2:H:338:GLY:O	2:H:342:GLY:HA3	2.21	0.40
1:G:17:THR:HA	1:G:29:THR:CG2	2.48	0.40
1:G:308:LYS:HE3	2:H:394:ASN:O	2.21	0.40
1:G:320:GLY:HA2	2:H:355:TRP:CZ2	2.56	0.40
1:A:274:GLU:HG3	1:A:275:TYR:N	2.36	0.40
1:C:31:THR:HG23	1:C:321:LEU:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:402:ARG:HH11	2:D:402:ARG:HD2	1.71	0.40
1:E:183:HIS:HB2	1:E:252:ILE:HD11	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:408:GLU:OE2	2:H:410:ARG:NH2[2_665]	2.15	0.05

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	319/321 (99%)	294 (92%)	24 (8%)	1 (0%)	41 76
1	C	319/321 (99%)	296 (93%)	22 (7%)	1 (0%)	41 76
1	E	319/321 (99%)	293 (92%)	25 (8%)	1 (0%)	41 76
1	G	319/321 (99%)	294 (92%)	23 (7%)	2 (1%)	25 64
2	B	162/164 (99%)	142 (88%)	17 (10%)	3 (2%)	8 36
2	D	162/164 (99%)	140 (86%)	20 (12%)	2 (1%)	13 48
2	F	162/164 (99%)	134 (83%)	24 (15%)	4 (2%)	5 28
2	H	162/164 (99%)	137 (85%)	22 (14%)	3 (2%)	8 36
All	All	1924/1940 (99%)	1730 (90%)	177 (9%)	17 (1%)	17 55

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
2	B	494	PRO
2	B	496	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	196	GLN
2	D	494	PRO
2	D	496	TYR
1	E	196	GLN
2	F	494	PRO
2	F	496	TYR
1	G	196	GLN
2	H	494	PRO
2	H	496	TYR
2	F	483	MET
2	B	341	ALA
2	F	461	ARG
2	H	461	ARG
1	G	18	GLU

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	288/288 (100%)	248 (86%)	40 (14%)	3	16
1	C	288/288 (100%)	250 (87%)	38 (13%)	4	18
1	E	288/288 (100%)	256 (89%)	32 (11%)	6	25
1	G	288/288 (100%)	256 (89%)	32 (11%)	6	25
2	B	140/140 (100%)	122 (87%)	18 (13%)	4	19
2	D	140/140 (100%)	123 (88%)	17 (12%)	5	21
2	F	140/140 (100%)	122 (87%)	18 (13%)	4	19
2	H	140/140 (100%)	122 (87%)	18 (13%)	4	19
All	All	1712/1712 (100%)	1499 (88%)	213 (12%)	4	20

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	23	ILE
1	A	24	MET
1	A	51	VAL
1	A	56	LEU
1	A	88	ASN
1	A	90	THR
1	A	106	LYS
1	A	108	LEU
1	A	111	ARG
1	A	114	HIS
1	A	117	LYS
1	A	124	SER
1	A	127	SER
1	A	133	SER
1	A	137	SER
1	A	144	SER
1	A	146	SER
1	A	149	ARG
1	A	152	VAL
1	A	163	THR
1	A	194	LEU
1	A	197	ASN
1	A	207	SER
1	A	214	VAL
1	A	221	SER
1	A	235	THR
1	A	247	SER
1	A	250	ASN
1	A	263	LYS
1	A	265	ASP
1	A	277	ASN
1	A	284	THR
1	A	292	SER
1	A	293	MET
1	A	302	THR
1	A	310	VAL
1	A	312	SER
1	A	319	THR
1	A	322	ARG
2	B	356	TYR
2	B	358	TYR
2	B	362	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	398	GLU
2	B	400	VAL
2	B	418	MET
2	B	420	ASP
2	B	423	LEU
2	B	425	VAL
2	B	427	THR
2	B	432	LEU
2	B	437	GLU
2	B	458	LEU
2	B	461	ARG
2	B	463	ASN
2	B	467	LEU
2	B	490	THR
2	B	496	TYR
1	C	17	THR
1	C	23	ILE
1	C	24	MET
1	C	51	VAL
1	C	56	LEU
1	C	88	ASN
1	C	90	THR
1	C	99	PHE
1	C	108	LEU
1	C	111	ARG
1	C	114	HIS
1	C	127	SER
1	C	133	SER
1	C	135	VAL
1	C	137	SER
1	C	144	SER
1	C	146	SER
1	C	149	ARG
1	C	152	VAL
1	C	163	THR
1	C	172	ASN
1	C	194	LEU
1	C	197	ASN
1	C	207	SER
1	C	213	LEU
1	C	214	VAL
1	C	221	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	235	THR
1	C	263	LYS
1	C	265	ASP
1	C	277	ASN
1	C	284	THR
1	C	292	SER
1	C	293	MET
1	C	302	THR
1	C	310	VAL
1	C	312	SER
1	C	322	ARG
2	D	356	TYR
2	D	358	TYR
2	D	362	ASN
2	D	398	GLU
2	D	400	VAL
2	D	418	MET
2	D	420	ASP
2	D	423	LEU
2	D	425	VAL
2	D	427	THR
2	D	432	LEU
2	D	437	GLU
2	D	458	LEU
2	D	461	ARG
2	D	463	ASN
2	D	467	LEU
2	D	496	TYR
1	E	5	ASP
1	E	23	ILE
1	E	51	VAL
1	E	56	LEU
1	E	90	THR
1	E	99	PHE
1	E	108	LEU
1	E	114	HIS
1	E	127	SER
1	E	133	SER
1	E	137	SER
1	E	144	SER
1	E	146	SER
1	E	149	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	152	VAL
1	E	163	THR
1	E	194	LEU
1	E	197	ASN
1	E	207	SER
1	E	214	VAL
1	E	221	SER
1	E	235	THR
1	E	263	LYS
1	E	265	ASP
1	E	277	ASN
1	E	284	THR
1	E	292	SER
1	E	293	MET
1	E	302	THR
1	E	310	VAL
1	E	312	SER
1	E	319	THR
2	F	356	TYR
2	F	362	ASN
2	F	363	GLU
2	F	398	GLU
2	F	400	VAL
2	F	418	MET
2	F	423	LEU
2	F	425	VAL
2	F	427	THR
2	F	437	GLU
2	F	458	LEU
2	F	463	ASN
2	F	467	LEU
2	F	477	LYS
2	F	479	ASP
2	F	488	ASN
2	F	490	THR
2	F	496	TYR
1	G	5	ASP
1	G	23	ILE
1	G	51	VAL
1	G	56	LEU
1	G	90	THR
1	G	99	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	108	LEU
1	G	114	HIS
1	G	127	SER
1	G	133	SER
1	G	137	SER
1	G	144	SER
1	G	146	SER
1	G	149	ARG
1	G	152	VAL
1	G	163	THR
1	G	194	LEU
1	G	197	ASN
1	G	207	SER
1	G	214	VAL
1	G	221	SER
1	G	235	THR
1	G	263	LYS
1	G	265	ASP
1	G	277	ASN
1	G	284	THR
1	G	292	SER
1	G	293	MET
1	G	302	THR
1	G	310	VAL
1	G	312	SER
1	G	319	THR
2	H	356	TYR
2	H	362	ASN
2	H	398	GLU
2	H	400	VAL
2	H	418	MET
2	H	420	ASP
2	H	423	LEU
2	H	425	VAL
2	H	427	THR
2	H	437	GLU
2	H	458	LEU
2	H	463	ASN
2	H	467	LEU
2	H	477	LYS
2	H	479	ASP
2	H	487	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	490	THR
2	H	496	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	186	ASN
1	A	196	GLN
2	B	362	ASN
1	C	12	HIS
1	C	119	GLN
1	C	196	GLN
1	E	12	HIS
1	E	119	GLN
1	E	196	GLN
2	F	362	ASN
1	G	12	HIS
1	G	119	GLN
1	G	196	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GAL	I	1	3	12,12,12	1.04	0	17,17,17	2.37	7 (41%)
3	SIA	I	2	3	20,20,21	0.61	0	24,28,31	0.72	0
3	GAL	J	1	3	12,12,12	1.02	0	17,17,17	1.88	6 (35%)
3	SIA	J	2	3	20,20,21	0.60	0	24,28,31	0.72	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	GAL	I	1	3	-	2/2/22/22	0/1/1/1
3	SIA	I	2	3	-	2/18/34/38	0/1/1/1
3	GAL	J	1	3	-	2/2/22/22	0/1/1/1
3	SIA	J	2	3	-	2/18/34/38	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1	GAL	O2-C2-C3	-5.81	96.92	110.35
3	J	1	GAL	O3-C3-C4	3.54	118.54	110.35
3	I	1	GAL	O5-C5-C6	3.24	114.49	106.44
3	I	1	GAL	C4-C3-C2	3.22	116.44	110.82
3	J	1	GAL	O1-C1-C2	3.18	117.99	109.03
3	I	1	GAL	C1-C2-C3	3.04	116.62	110.31
3	I	1	GAL	O3-C3-C4	2.81	116.85	110.35
3	J	1	GAL	O5-C5-C4	-2.68	104.83	109.69
3	J	1	GAL	O1-C1-O5	-2.64	102.44	110.38
3	I	1	GAL	C1-O5-C5	2.49	118.36	113.66
3	I	1	GAL	O2-C2-C1	2.49	114.94	109.16
3	J	1	GAL	O2-C2-C1	2.47	114.88	109.16
3	J	1	GAL	C1-O5-C5	-2.05	109.79	113.66

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	2	SIA	O8-C8-C9-O9
3	J	1	GAL	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

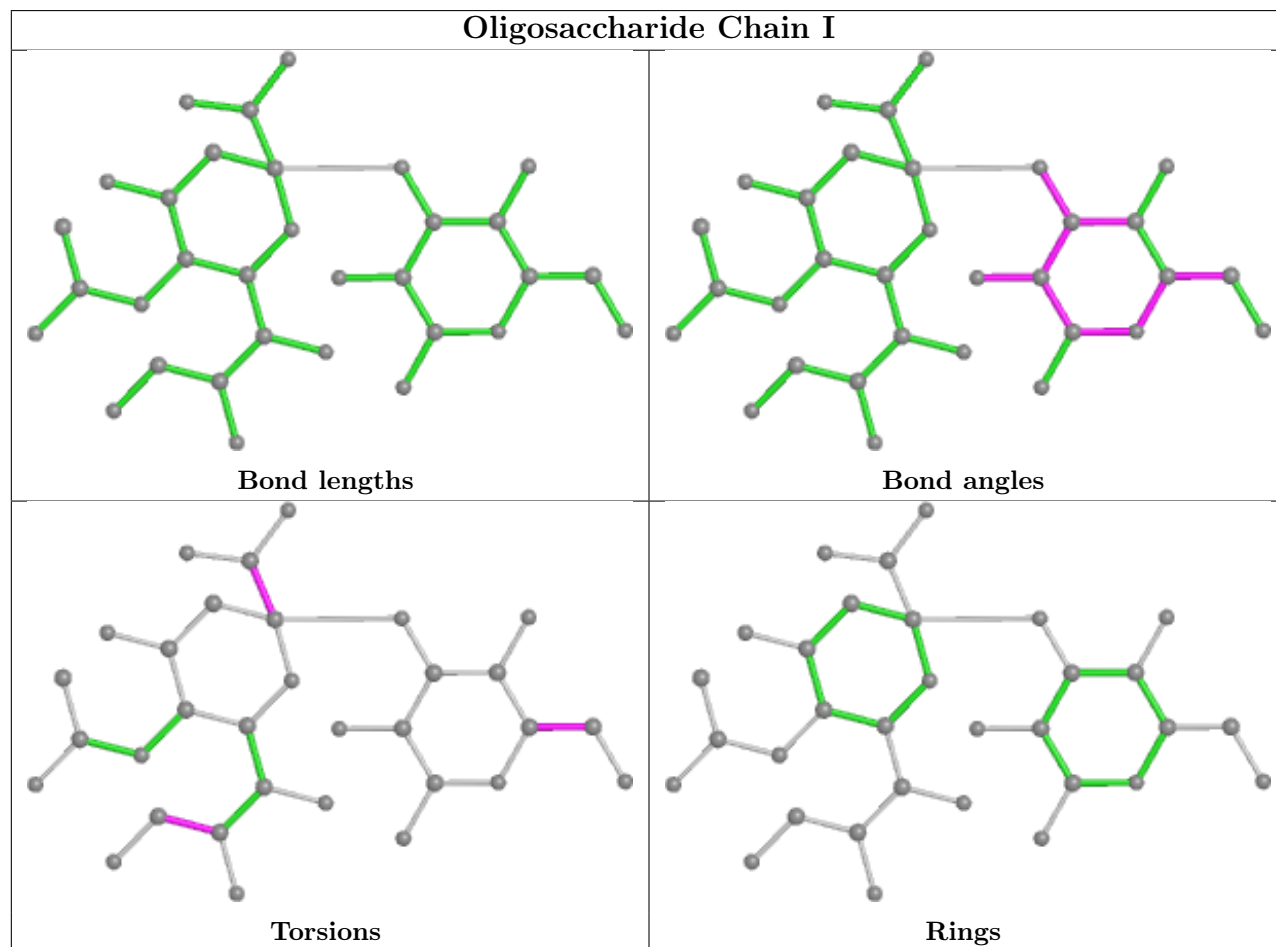
Mol	Chain	Res	Type	Atoms
3	I	1	GAL	C4-C5-C6-O6
3	J	2	SIA	C7-C8-C9-O9
3	I	1	GAL	O5-C5-C6-O6
3	J	1	GAL	C4-C5-C6-O6
3	I	2	SIA	O1A-C1-C2-O6
3	I	2	SIA	O8-C8-C9-O9

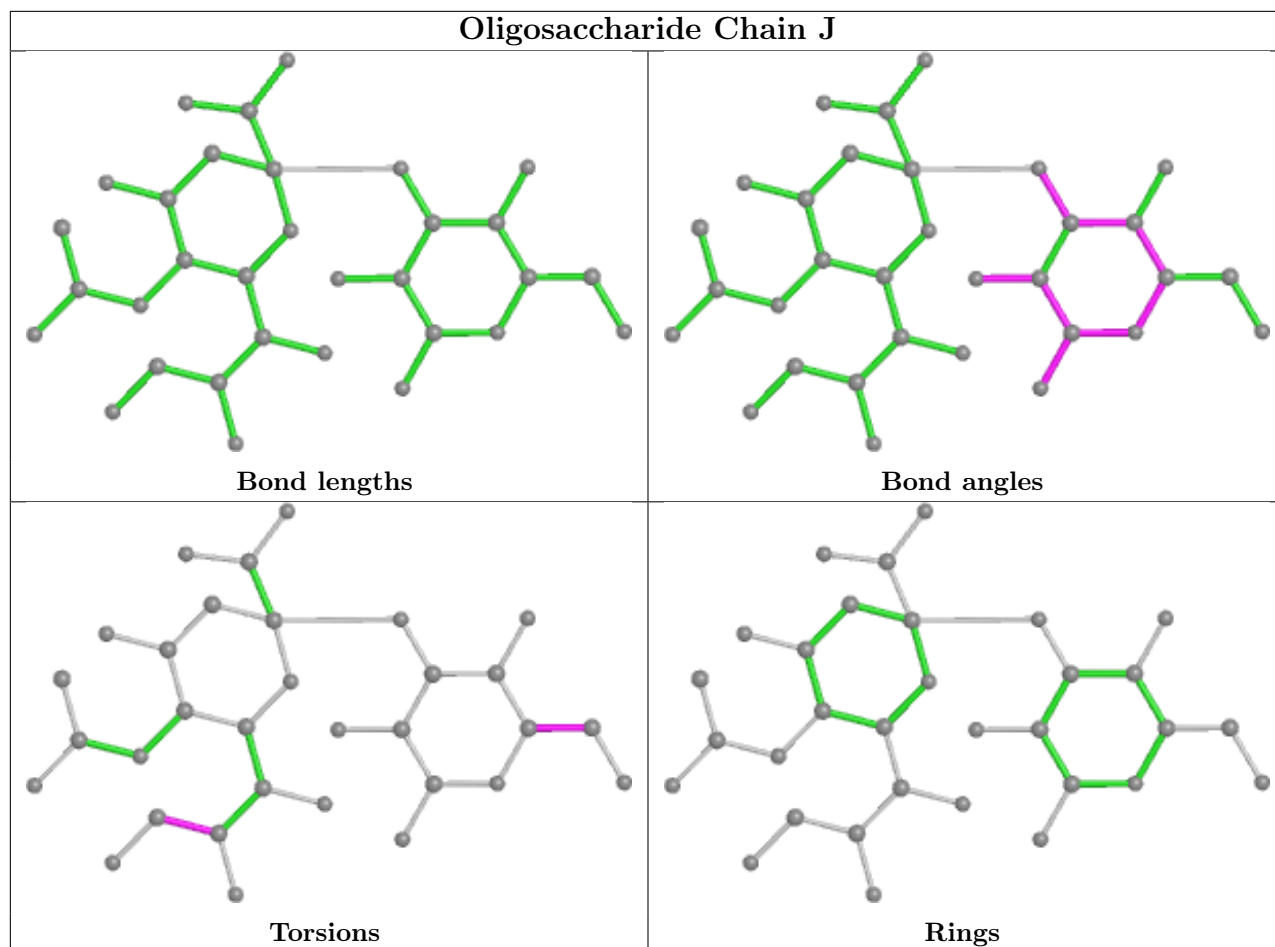
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	2	SIA	3	0
3	I	2	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 [i](#)

2 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
4	NAG	C	601	1	14,14,15	1.20	1 (7%)	17,19,21	2.24	8 (47%)
4	NAG	A	601	1	14,14,15	0.72	0	17,19,21	1.67	5 (29%)

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
4	NAG	C	601	1	-	2/6/23/26	0/1/1/1
4	NAG	A	601	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	NAG	O5-C1	-2.71	1.39	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	NAG	C2-N2-C7	-4.93	115.89	122.90
4	C	601	NAG	C1-O5-C5	3.61	117.09	112.19
4	C	601	NAG	O5-C1-C2	3.41	116.67	111.29
4	A	601	NAG	O4-C4-C5	3.12	117.03	109.30
4	A	601	NAG	C3-C4-C5	-2.86	105.14	110.24
4	C	601	NAG	C3-C4-C5	-2.77	105.30	110.24
4	C	601	NAG	C4-C3-C2	-2.75	106.99	111.02
4	C	601	NAG	O3-C3-C4	2.68	116.55	110.35
4	A	601	NAG	C1-C2-N2	-2.53	106.16	110.49
4	C	601	NAG	C1-C2-N2	-2.48	106.25	110.49
4	A	601	NAG	C2-N2-C7	-2.13	119.87	122.90
4	A	601	NAG	C1-O5-C5	2.11	115.05	112.19
4	C	601	NAG	O3-C3-C2	2.11	113.83	109.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	601	NAG	O5-C5-C6-O6
4	C	601	NAG	C4-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6
4	A	601	NAG	O5-C5-C6-O6
4	A	601	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	NAG	2	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	321/321 (100%)	-0.20	0 100 100	17, 41, 84, 122	0
1	C	321/321 (100%)	-0.24	1 (0%) 94 84	16, 41, 87, 131	0
1	E	321/321 (100%)	0.53	38 (11%) 4 1	65, 120, 189, 261	0
1	G	321/321 (100%)	0.48	32 (9%) 7 2	58, 117, 187, 236	0
2	B	164/164 (100%)	0.00	1 (0%) 89 72	22, 85, 126, 140	0
2	D	164/164 (100%)	-0.01	1 (0%) 89 72	23, 84, 127, 150	0
2	F	164/164 (100%)	1.29	54 (32%) 0 0	85, 165, 241, 300	0
2	H	164/164 (100%)	1.23	45 (27%) 0 0	82, 161, 228, 304	0
All	All	1940/1940 (100%)	0.31	172 (8%) 9 3	16, 94, 193, 304	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	474	PHE	9.4
1	E	319	THR	9.0
1	G	9	ILE	9.0
1	E	318	ALA	8.7
2	F	366	SER	7.7
2	H	367	GLY	7.2
2	H	475	TYR	6.6
2	F	475	TYR	6.6
2	F	467	LEU	6.6
2	F	363	GLU	6.5
2	H	467	LEU	6.3
1	E	10	GLY	5.9
2	F	472	PHE	5.9
2	H	477	LYS	5.7
1	E	9	ILE	5.7
2	H	366	SER	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	468	GLY	5.5
2	F	356	TYR	5.5
2	F	399	ALA	5.4
2	H	486	ILE	5.1
2	F	365	GLY	5.1
2	H	350	GLY	5.0
2	F	474	PHE	4.9
2	H	356	TYR	4.9
1	G	33	ALA	4.8
2	F	367	GLY	4.7
2	H	374	SER	4.7
1	G	295	PHE	4.7
1	E	322	ARG	4.7
2	H	431	GLU	4.7
1	G	319	THR	4.7
2	H	476	HIS	4.5
1	G	10	GLY	4.5
2	H	338	GLY	4.5
1	E	6	GLN	4.4
1	G	322	ARG	4.4
2	F	397	PHE	4.4
2	F	478	CYS	4.4
1	G	318	ALA	4.3
2	F	389	ILE	4.3
1	E	317	LEU	4.3
2	F	364	GLN	4.2
1	E	33	ALA	4.1
2	F	401	GLY	4.1
2	H	468	GLY	4.0
1	E	285	PRO	4.0
2	F	335	GLY	3.9
2	F	355	TRP	3.8
1	G	155	ILE	3.8
2	H	389	ILE	3.8
1	E	153	TRP	3.8
2	H	363	GLU	3.7
1	E	55	ILE	3.7
2	F	476	HIS	3.7
2	F	357	GLY	3.7
1	E	320	GLY	3.6
1	G	15	ASN	3.6
1	G	43	GLY	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	393	MET	3.6
1	E	194	LEU	3.6
2	H	355	TRP	3.6
1	E	321	LEU	3.6
2	F	393	MET	3.5
2	F	358	TYR	3.5
1	G	321	LEU	3.5
2	F	454	ASP	3.5
2	H	364	GLN	3.5
1	G	7	ILE	3.4
2	F	411	ILE	3.4
2	F	338	GLY	3.4
2	F	452	LEU	3.4
1	E	35	ASP	3.3
1	E	37	LEU	3.3
1	G	35	ASP	3.3
1	E	56	LEU	3.3
2	H	472	PHE	3.3
1	E	289	ILE	3.2
2	H	452	LEU	3.2
1	E	34	GLN	3.2
1	E	295	PHE	3.2
1	E	26	LYS	3.2
2	B	355	TRP	3.2
2	H	461	ARG	3.1
2	F	336	LEU	3.1
1	G	320	GLY	3.1
2	F	486	ILE	3.1
2	F	465	LYS	3.1
2	H	442	LEU	3.1
1	G	303	ILE	3.1
2	F	398	GLU	3.0
2	H	397	PHE	3.0
2	H	379	ILE	3.0
2	H	365	GLY	2.9
2	F	431	GLU	2.9
1	G	13	ALA	2.9
2	H	399	ALA	2.9
2	F	473	GLU	2.9
1	G	286	MET	2.8
2	F	374	SER	2.8
2	H	358	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	289	ILE	2.8
1	E	28	VAL	2.8
2	H	464	ALA	2.8
2	F	404	PHE	2.7
2	H	459	GLN	2.7
1	E	36	ILE	2.7
2	F	442	LEU	2.7
2	F	349	GLN	2.7
2	H	445	HIS	2.7
2	H	349	GLN	2.7
1	E	155	ILE	2.7
1	G	42	ASN	2.6
1	E	45	LEU	2.6
1	G	153	TRP	2.6
2	H	360	HIS	2.6
2	H	357	GLY	2.6
1	E	20	VAL	2.6
1	G	34	GLN	2.6
1	E	298	ILE	2.5
2	F	477	LYS	2.5
2	H	411	ILE	2.5
1	E	25	GLU	2.5
2	F	457	ARG	2.5
1	E	179	LEU	2.4
1	E	277	ASN	2.4
2	F	463	ASN	2.4
2	F	460	LEU	2.4
2	H	457	ARG	2.4
1	G	298	ILE	2.4
1	G	8	CYS	2.4
2	H	336	LEU	2.4
2	F	491	TYR	2.4
2	H	465	LYS	2.4
1	E	40	THR	2.4
2	F	414	LEU	2.3
2	F	458	LEU	2.3
2	H	401	GLY	2.3
2	F	461	ARG	2.3
1	E	7	ILE	2.3
2	F	340	ILE	2.3
1	G	194	LEU	2.3
1	G	317	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	337	PHE	2.3
1	G	291	SER	2.3
2	D	475	TYR	2.3
1	G	323	ASN	2.3
2	F	350	GLY	2.3
1	G	55	ILE	2.2
1	E	38	GLU	2.2
1	G	268	ILE	2.2
1	G	6	GLN	2.2
1	G	12	HIS	2.2
1	G	245	PHE	2.2
1	E	305	GLU	2.2
2	F	360	HIS	2.2
2	F	464	ALA	2.1
2	F	471	CYS	2.1
2	H	375	THR	2.1
2	H	353	ASP	2.1
2	H	390	ILE	2.1
1	E	286	MET	2.1
1	C	9	ILE	2.1
2	H	478	CYS	2.1
1	E	232	PHE	2.1
2	F	450	LYS	2.1
2	F	466	GLU	2.1
2	H	337	PHE	2.1
2	H	335	GLY	2.1
2	F	396	GLN	2.0
2	F	462	ASP	2.1
1	E	316	VAL	2.0
1	E	77	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

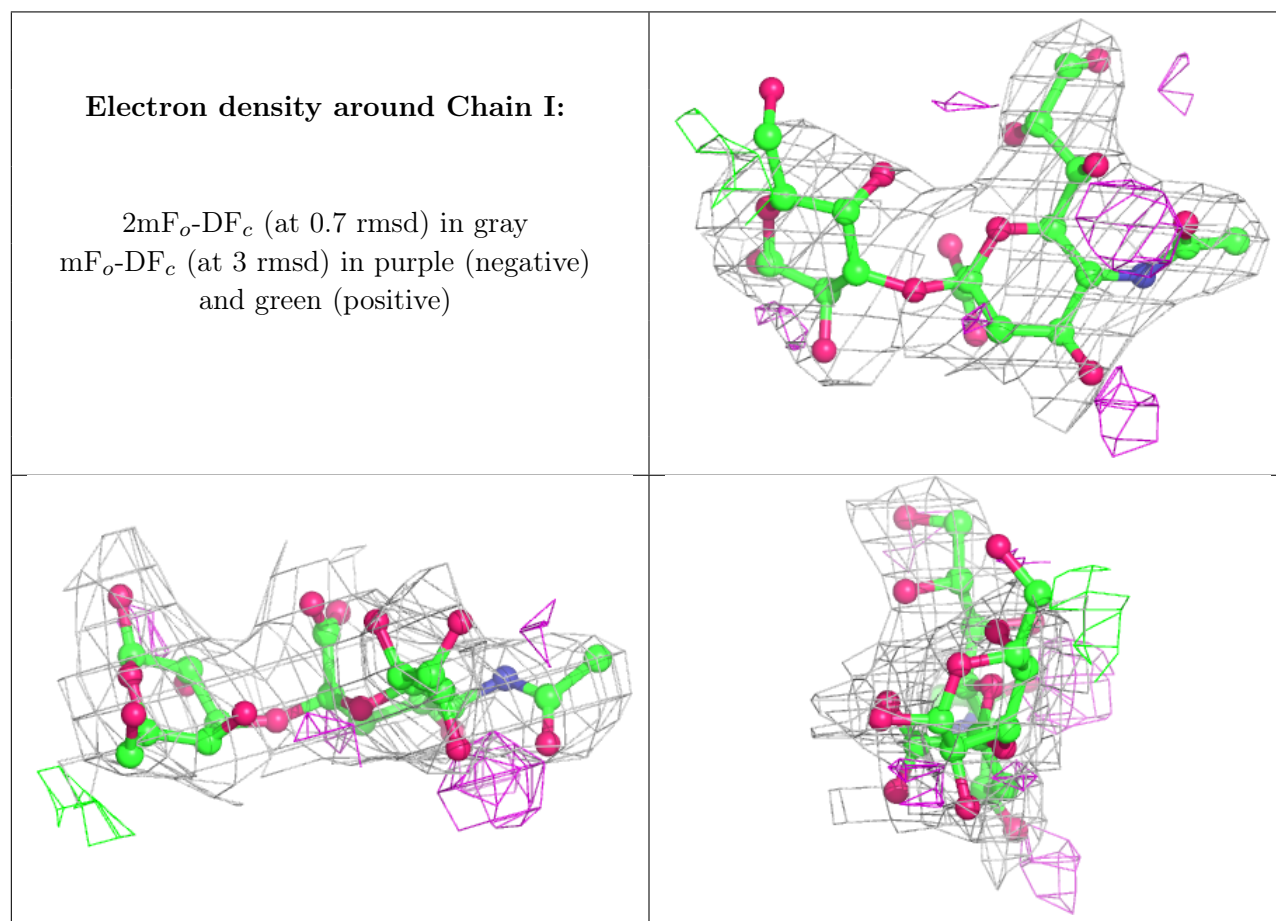
There are no non-standard protein/DNA/RNA residues in this entry.

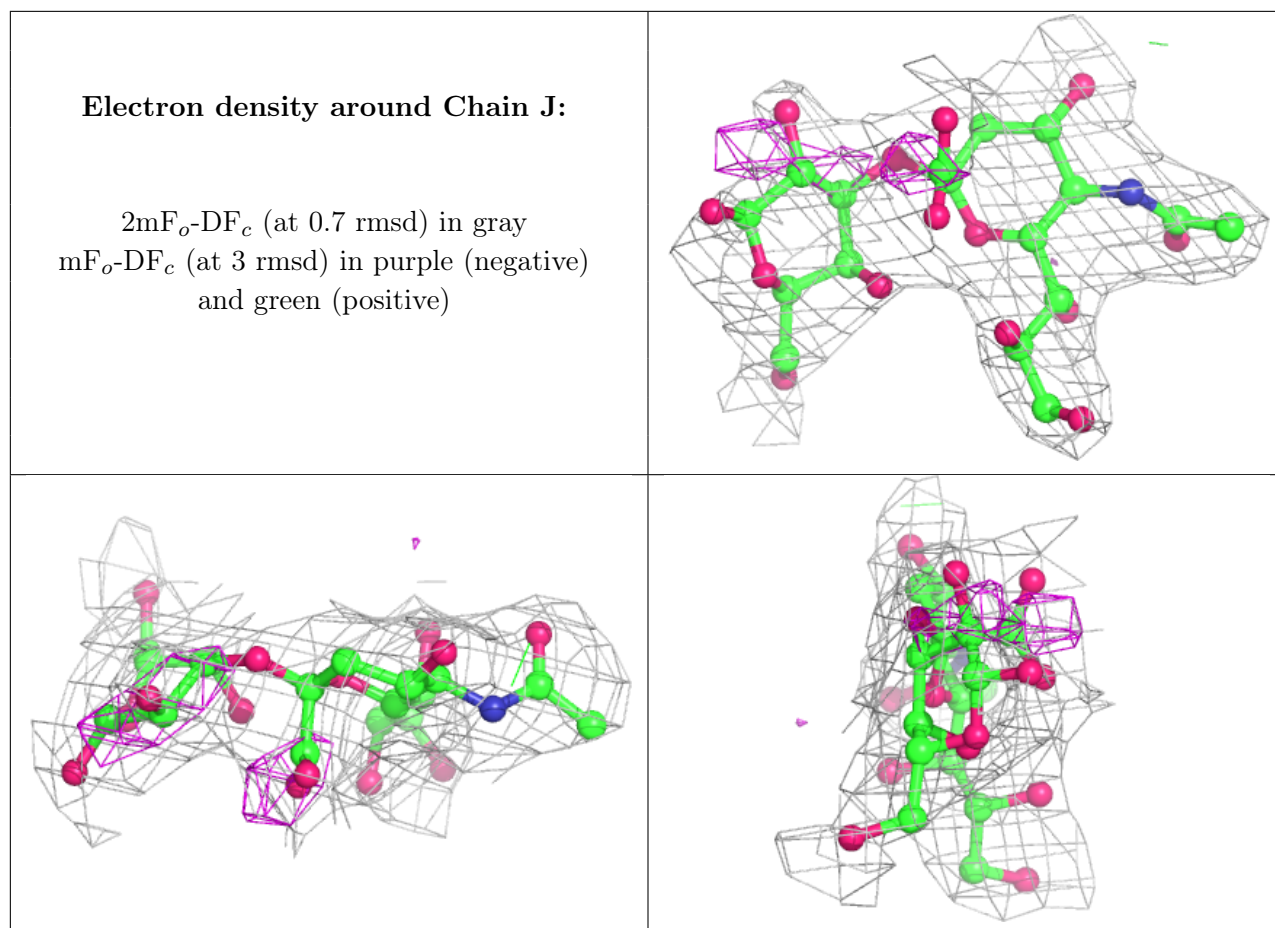
6.3 Carbohydrates [i](#)

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(\AA^2)	Q<0.9
3	GAL	J	1	12/12	0.83	0.27	62,69,85,92	0
3	GAL	I	1	12/12	0.89	0.22	60,64,85,87	0
3	SIA	J	2	20/21	0.94	0.19	32,45,56,58	0
3	SIA	I	2	20/21	0.96	0.22	31,45,55,55	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.





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(Å ²)	Q<0.9
4	NAG	C	601	14/15	0.90	0.21	37,51,67,71	0
4	NAG	A	601	14/15	0.93	0.16	39,55,63,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.