



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:22 PM UTC

PDB ID : 4K64 / pdb_00004k64
Title : Structure of an avian influenza H5 hemagglutinin from the influenza virus complexed with human receptor analog LSTc
Authors : Zhang, W.; Shi, Y.; Lu, X.; Shu, Y.; Qi, J.; Gao, G.F.
Deposited on : 2013-04-15
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

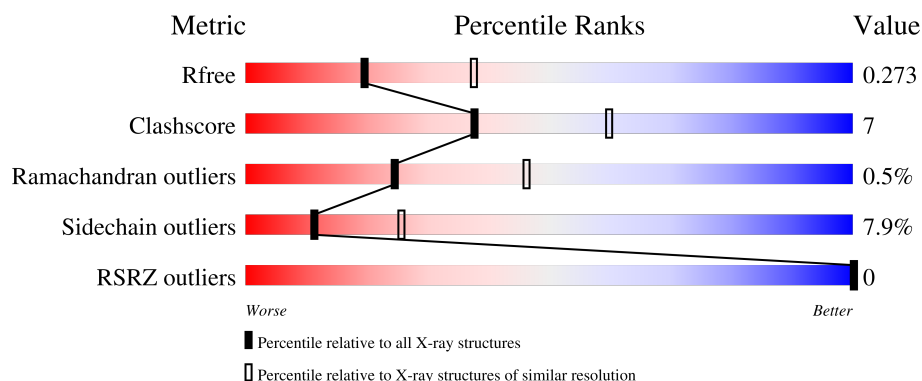
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



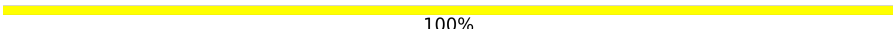
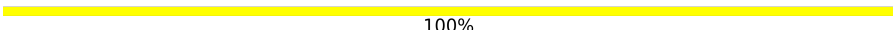
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	 80% 19% .
1	C	321	 79% 20% .
1	E	321	 75% 23% .
1	G	321	 72% 25% .
2	B	164	 84% 15% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	164	 78% 21% .
2	F	164	 71% 27% .
2	H	164	 75% 22% .
3	I	2	 100%
3	J	2	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15829 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	321	Total	C	N	O	S	0	0	0
			2541	1605	436	485	15			
1	C	321	Total	C	N	O	S	0	0	0
			2541	1605	436	485	15			
1	E	321	Total	C	N	O	S	0	0	0
			2541	1605	436	485	15			
1	G	321	Total	C	N	O	S	0	0	0
			2541	1605	436	485	15			

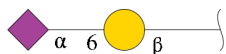
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLN	-	expression tag	UNP A8HWY8
C	4	GLN	-	expression tag	UNP A8HWY8
E	4	GLN	-	expression tag	UNP A8HWY8
G	4	GLN	-	expression tag	UNP A8HWY8

- Molecule 2 is a protein called Hemagglutinin.

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

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose.



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	86	Total	O	0	0
			86	86		

Continued on next page...

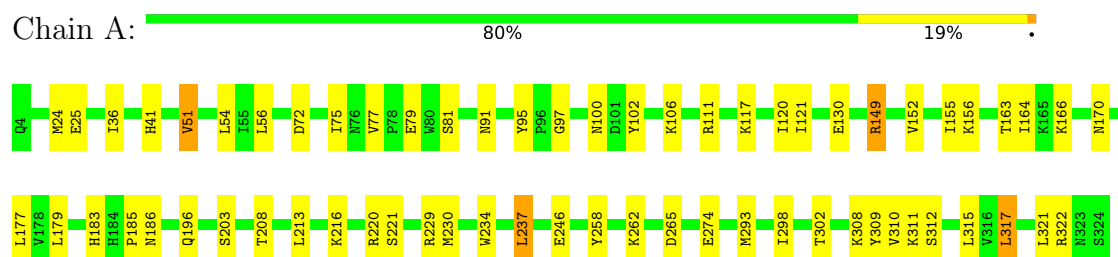
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	25	Total 25	O 25	0	0
5	C	81	Total 81	O 81	0	0
5	D	20	Total 20	O 20	0	0
5	E	8	Total 8	O 8	0	0
5	F	2	Total 2	O 2	0	0
5	G	9	Total 9	O 9	0	0
5	H	2	Total 2	O 2	0	0

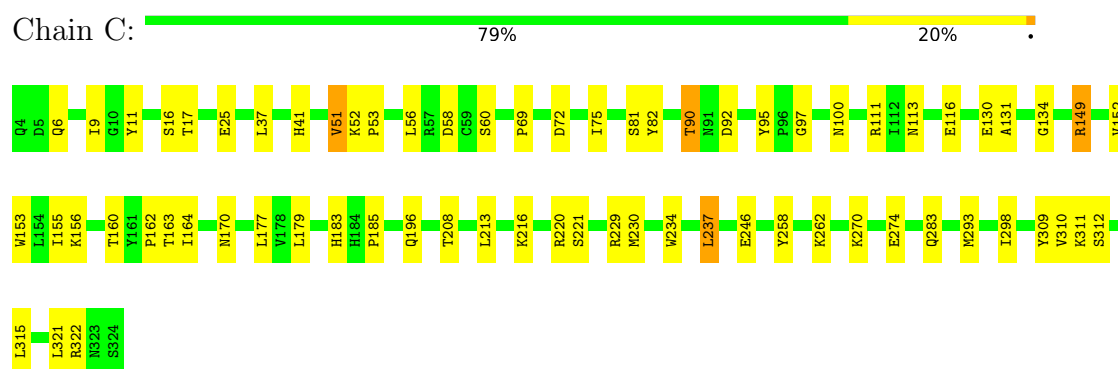
3 Residue-property plots

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.

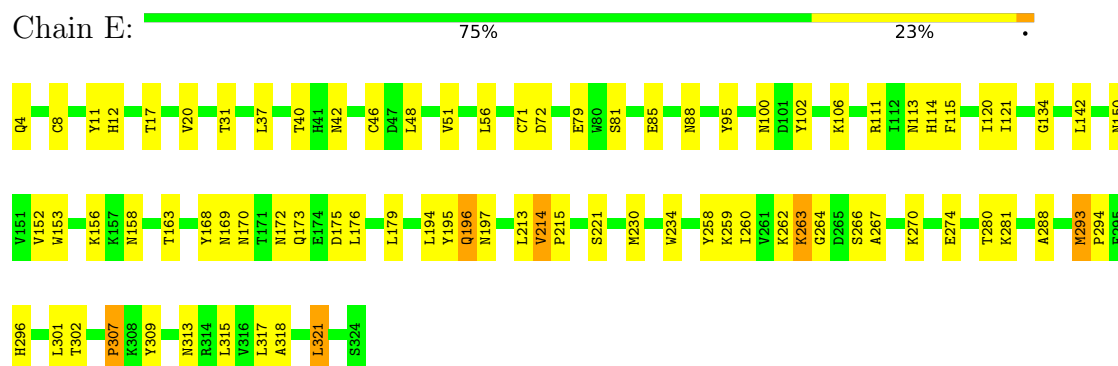
• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin



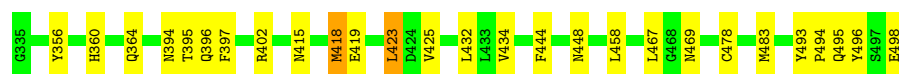
• Molecule 1: Hemagglutinin

Chain G:  72% 25%



• Molecule 2: Hemagglutinin

Chain B:  84% 15%



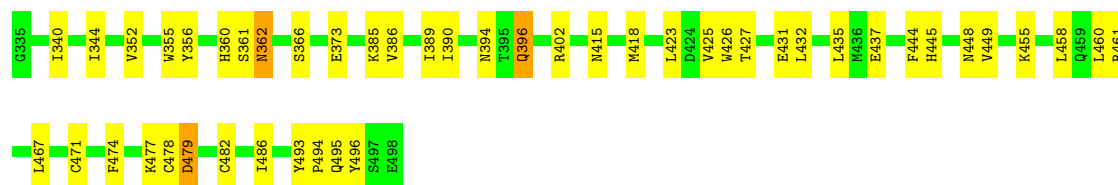
• Molecule 2: Hemagglutinin

Chain D:  78% 21%



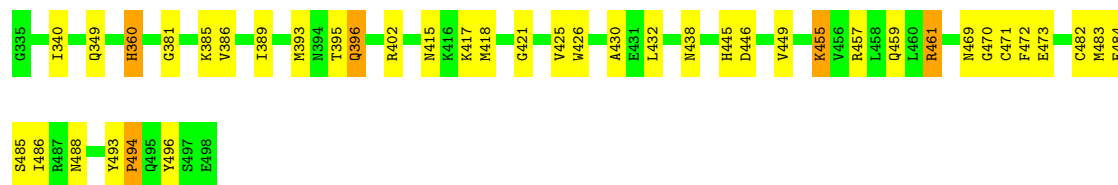
• Molecule 2: Hemagglutinin

Chain F:  71% 27%



• Molecule 2: Hemagglutinin

Chain H:  75% 22%



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose

Chain I:  100%

GAL1
SIA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose

Chain J:  100%

GAL1
SIA2

4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	70.34Å 70.34Å 491.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.04 – 2.60 36.04 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.5 (36.04-2.60) 92.5 (36.04-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.221 , 0.280 0.216 , 0.273	Depositor DCC
R_{free} test set	3864 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.437 for -h,-k,l 0.093 for h,-h-k,-l 0.087 for -k,-h,-l	Xtriage
Reported twinning fraction	0.391 for -h,-k,l	Depositor
Outliers	0 of 77142 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15829	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: NAG, GAL, 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	0.30	0/2603	0.71	0/3537
1	C	0.31	0/2603	0.72	0/3537
1	E	0.27	0/2603	0.73	0/3537
1	G	0.29	0/2603	0.73	0/3537
2	B	0.30	0/1355	0.71	0/1823
2	D	0.29	0/1355	0.69	0/1823
2	F	0.28	0/1355	0.73	2/1823 (0.1%)
2	H	0.27	0/1355	0.71	0/1823
All	All	0.29	0/15832	0.72	2/21440 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	460	LEU	CB-CA-C	7.09	124.29	110.67
2	F	461	ARG	CB-CA-C	-6.03	109.61	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2541	0	2478	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2541	0	2478	39	0
1	E	2541	0	2477	44	0
1	G	2541	0	2478	49	0
2	B	1328	0	1231	14	0
2	D	1328	0	1231	19	0
2	F	1328	0	1231	22	0
2	H	1328	0	1231	26	0
3	I	32	0	27	0	0
3	J	32	0	27	0	0
4	A	14	0	13	0	0
4	C	14	0	13	0	0
4	E	14	0	13	0	0
4	G	14	0	13	0	0
5	A	86	0	0	4	0
5	B	25	0	0	1	0
5	C	81	0	0	6	0
5	D	20	0	0	3	0
5	E	8	0	0	0	0
5	F	2	0	0	0	0
5	G	9	0	0	3	0
5	H	2	0	0	0	0
All	All	15829	0	14941	215	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (215) 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)
2:D:479:ASP:OD2	5:D:513:HOH:O	1.93	0.87
1:E:172:ASN:HD22	1:E:259:LYS:HD3	1.45	0.82
1:C:116:GLU:OE2	5:C:755:HOH:O	1.98	0.81
1:A:149:ARG:NH2	5:A:714:HOH:O	2.15	0.79
1:G:241:ASP:OD1	5:G:704:HOH:O	1.98	0.79
1:C:311:LYS:HE3	2:D:423:LEU:HD23	1.68	0.75
1:G:156:LYS:HD2	1:G:196:GLN:HG2	1.69	0.75
1:A:156:LYS:HD2	1:A:196:GLN:HG2	1.68	0.74
1:E:4:GLN:NE2	2:F:474:PHE:O	2.21	0.73
2:H:469:ASN:ND2	2:H:471:CYS:SG	2.64	0.71
1:C:131:ALA:O	5:C:706:HOH:O	2.09	0.70
1:G:20:VAL:HG21	1:G:318:ALA:HB2	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:TYR:HE2	2:B:423:LEU:HD21	1.57	0.69
2:H:455:LYS:O	2:H:459:GLN:NE2	2.26	0.69
1:C:69:PRO:O	5:C:728:HOH:O	2.11	0.69
1:C:156:LYS:HD2	1:C:196:GLN:HG2	1.75	0.68
1:E:51:VAL:HG23	1:E:81:SER:HB3	1.75	0.68
1:A:91:ASN:ND2	5:A:750:HOH:O	2.28	0.67
1:G:321:LEU:HB3	2:H:445:HIS:HD2	1.60	0.67
1:E:120:ILE:HG13	1:E:121:ILE:HG13	1.77	0.67
1:A:310:VAL:HG12	1:A:312:SER:H	1.60	0.67
1:G:51:VAL:HG13	1:G:81:SER:HB3	1.77	0.66
1:C:309:TYR:HE2	2:D:423:LEU:HD21	1.60	0.66
1:G:197:ASN:ND2	5:G:708:HOH:O	2.19	0.65
1:G:317:LEU:HD23	2:H:386:VAL:HG22	1.78	0.65
1:G:150:ASN:ND2	1:G:258:TYR:OH	2.30	0.64
1:C:149:ARG:NH2	5:C:710:HOH:O	2.32	0.63
1:C:310:VAL:HG12	1:C:312:SER:H	1.64	0.63
1:A:311:LYS:HE3	2:B:423:LEU:HD23	1.81	0.62
1:C:52:LYS:HG2	1:C:53:PRO:HD2	1.81	0.62
1:A:166:LYS:NZ	5:A:737:HOH:O	2.11	0.61
1:G:296:HIS:HD2	1:G:307:PRO:HB2	1.65	0.61
2:F:493:TYR:O	2:F:495:GLN:N	2.34	0.61
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.83	0.60
1:C:270:LYS:NZ	5:C:723:HOH:O	2.23	0.60
1:G:134:GLY:HA3	1:G:153:TRP:HB3	1.86	0.58
1:C:9:ILE:HD13	2:D:453:TYR:HA	1.85	0.58
1:C:41:HIS:HB3	1:C:298:ILE:HD13	1.85	0.58
2:D:396:GLN:HG3	2:D:426:TRP:CD2	2.39	0.58
1:G:55:ILE:HD12	1:G:275:TYR:HB2	1.86	0.57
1:E:120:ILE:HB	1:E:168:TYR:CZ	2.38	0.57
1:G:111:ARG:O	1:G:263:LYS:NZ	2.36	0.57
1:E:111:ARG:O	1:E:263:LYS:NZ	2.37	0.57
1:C:310:VAL:HG13	2:D:427:THR:HA	1.87	0.57
2:D:380:ASP:O	2:D:384:ASN:ND2	2.37	0.57
1:G:169:ASN:OD1	1:G:170:ASN:N	2.38	0.57
1:A:41:HIS:HB3	1:A:298:ILE:HD13	1.87	0.57
1:E:296:HIS:HD2	1:E:307:PRO:HB2	1.70	0.57
1:G:15:ASN:OD1	1:G:15:ASN:N	2.37	0.57
1:A:95:TYR:CD2	1:A:230:MET:HG2	2.40	0.56
1:E:317:LEU:HD23	2:F:386:VAL:HG22	1.88	0.56
1:C:25:GLU:OE2	1:C:322:ARG:NH2	2.39	0.56
2:F:444:PHE:O	2:F:448:ASN:ND2	2.32	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:396:GLN:HG3	2:F:426:TRP:CD2	2.41	0.55
1:E:169:ASN:OD1	1:E:170:ASN:N	2.38	0.55
1:E:266:SER:OG	1:E:267:ALA:N	2.40	0.55
1:G:321:LEU:HB3	2:H:445:HIS:CD2	2.41	0.55
1:A:120:ILE:HG13	1:A:121:ILE:HG13	1.89	0.55
2:F:479:ASP:OD2	2:F:479:ASP:N	2.36	0.55
1:A:164:ILE:O	1:A:246:GLU:HA	2.07	0.54
1:E:195:TYR:O	1:E:197:ASN:N	2.39	0.54
1:A:309:TYR:HD2	2:B:423:LEU:HD11	1.71	0.54
2:F:402:ARG:NH1	2:F:415:ASN:OD1	2.40	0.54
1:C:309:TYR:HD2	2:D:423:LEU:HD11	1.73	0.54
1:G:174:GLU:N	1:G:174:GLU:OE1	2.40	0.53
1:A:54:LEU:HD22	1:A:77:VAL:HG11	1.90	0.53
2:D:493:TYR:O	2:D:495:GLN:N	2.42	0.53
2:F:361:SER:HA	2:F:366:SER:HA	1.91	0.53
2:B:444:PHE:O	2:B:448:ASN:ND2	2.42	0.52
1:C:58:ASP:HB3	1:C:90:THR:HG23	1.91	0.52
1:E:150:ASN:ND2	1:E:258:TYR:OH	2.42	0.52
1:G:280:THR:OG1	1:G:281:LYS:N	2.40	0.52
2:B:498:GLU:OE1	5:B:508:HOH:O	2.19	0.52
1:G:37:LEU:HB2	1:G:315:LEU:HB2	1.90	0.52
1:E:156:LYS:HD2	1:E:196:GLN:HG2	1.92	0.52
1:C:309:TYR:CD2	2:D:423:LEU:HD11	2.45	0.52
1:E:280:THR:OG1	1:E:281:LYS:N	2.43	0.52
2:H:340:ILE:N	2:H:446:ASP:OD2	2.37	0.52
1:E:321:LEU:HB3	2:F:445:HIS:CD2	2.45	0.51
1:E:293:MET:HG3	1:E:294:PRO:HD2	1.92	0.51
1:C:164:ILE:O	1:C:246:GLU:HA	2.09	0.51
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.91	0.51
1:E:12:HIS:N	2:F:355:TRP:O	2.43	0.51
1:C:113:ASN:HB2	1:C:262:LYS:HG2	1.92	0.51
1:A:177:LEU:HB3	1:A:258:TYR:HB2	1.93	0.50
2:D:402:ARG:NH1	2:D:415:ASN:OD1	2.44	0.50
1:G:14:ASN:OD1	1:G:323:ASN:ND2	2.44	0.50
1:C:179:LEU:HD23	1:C:234:TRP:HB3	1.92	0.50
1:G:70:MET:HA	1:G:70:MET:HE2	1.93	0.50
1:C:315:LEU:HD22	2:D:434:VAL:HG21	1.93	0.50
1:G:179:LEU:HD23	1:G:234:TRP:HB3	1.93	0.50
1:G:14:ASN:O	1:G:323:ASN:ND2	2.41	0.50
1:G:120:ILE:HG12	1:G:121:ILE:HG13	1.94	0.50
2:B:418:MET:HG3	2:B:419:GLU:N	2.25	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:TYR:CE2	1:A:106:LYS:HD2	2.48	0.49
1:C:177:LEU:HB3	1:C:258:TYR:HB2	1.95	0.49
1:C:95:TYR:CD2	1:C:230:MET:HG2	2.48	0.49
1:G:317:LEU:HD21	2:H:389:ILE:HD12	1.94	0.49
2:H:402:ARG:NH1	2:H:415:ASN:OD1	2.46	0.49
1:G:280:THR:HG21	1:G:288:ALA:HB1	1.94	0.49
1:C:37:LEU:HB2	1:C:315:LEU:HB2	1.94	0.48
1:E:179:LEU:HD23	1:E:234:TRP:HB3	1.95	0.48
1:C:60:SER:OG	1:C:92:ASP:OD2	2.24	0.48
1:A:117:LYS:NZ	5:A:735:HOH:O	2.23	0.48
1:A:51:VAL:HG22	1:A:81:SER:HB3	1.96	0.48
2:B:493:TYR:O	2:B:495:GLN:N	2.47	0.48
1:C:216:LYS:O	1:C:220:ARG:NH2	2.46	0.48
1:C:160:THR:HG22	1:C:162:PRO:HD3	1.95	0.48
1:C:170:ASN:HB2	1:C:237:LEU:HD13	1.96	0.48
2:H:396:GLN:HG3	2:H:426:TRP:CD2	2.49	0.48
1:A:309:TYR:CD2	2:B:423:LEU:HD11	2.48	0.48
1:A:25:GLU:OE2	1:A:322:ARG:NH2	2.46	0.48
1:E:294:PRO:HB3	2:F:390:ILE:HG23	1.96	0.48
1:G:110:SER:HB2	1:G:111:ARG:HE	1.78	0.48
2:H:484:GLU:OE1	2:H:488:ASN:ND2	2.47	0.48
1:E:46:CYS:HB2	1:E:280:THR:HG22	1.95	0.47
1:E:309:TYR:HE2	2:F:423:LEU:HD21	1.79	0.47
1:C:6:GLN:NE2	5:C:746:HOH:O	2.39	0.47
1:G:14:ASN:H	1:G:323:ASN:HD21	1.62	0.47
1:E:317:LEU:HD21	2:F:389:ILE:HD12	1.97	0.47
1:A:183:HIS:O	1:A:185:PRO:HD3	2.14	0.47
1:G:284:THR:OG1	1:G:287:GLY:O	2.30	0.47
1:E:175:ASP:HB2	1:E:260:ILE:HD12	1.96	0.47
1:G:11:TYR:CZ	2:H:340:ILE:HG23	2.50	0.47
1:E:95:TYR:CD2	1:E:230:MET:HG2	2.50	0.47
1:G:4:GLN:HG2	1:G:5:ASP:H	1.80	0.46
1:G:120:ILE:HB	1:G:168:TYR:CZ	2.50	0.46
1:C:51:VAL:HG22	1:C:81:SER:HB3	1.97	0.46
1:E:113:ASN:ND2	1:E:264:GLY:HA3	2.31	0.46
2:H:482:CYS:HA	2:H:485:SER:HB3	1.98	0.46
1:G:203:SER:OG	1:G:246:GLU:HB3	2.15	0.46
1:E:102:TYR:CE2	1:E:106:LYS:HD2	2.50	0.46
1:G:146:SER:OG	1:G:147:PHE:N	2.48	0.46
2:B:396:GLN:HB3	2:B:397:PHE:H	1.58	0.46
1:G:293:MET:HG3	1:G:294:PRO:HD2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:GLY:HA3	1:A:230:MET:O	2.16	0.45
1:A:179:LEU:HD23	1:A:234:TRP:HB3	1.97	0.45
2:B:419:GLU:O	2:B:423:LEU:HB2	2.15	0.45
1:E:42:ASN:HD21	1:E:288:ALA:HB3	1.81	0.45
1:E:296:HIS:CD2	1:E:307:PRO:HB2	2.49	0.45
1:A:216:LYS:O	1:A:220:ARG:NH2	2.49	0.45
2:D:409:ARG:NH1	2:D:412:GLU:OE2	2.50	0.45
2:F:385:LYS:HD3	2:F:437:GLU:HB3	1.97	0.45
2:H:482:CYS:O	2:H:486:ILE:HG13	2.17	0.45
1:A:72:ASP:HA	1:A:75:ILE:HG13	1.98	0.45
2:D:393:MET:HE1	2:D:430:ALA:HB2	1.97	0.45
1:G:195:TYR:O	1:G:197:ASN:N	2.45	0.45
1:E:48:LEU:O	1:E:51:VAL:HG22	2.17	0.45
1:G:57:ARG:NH1	1:G:73:GLU:OE2	2.50	0.45
2:H:417:LYS:HE2	2:H:417:LYS:HB3	1.58	0.45
2:B:469:ASN:N	2:B:469:ASN:OD1	2.50	0.45
1:G:294:PRO:HG2	1:G:295:PHE:HD2	1.81	0.45
1:A:79:GLU:OE2	1:A:262:LYS:NZ	2.50	0.44
2:D:465:LYS:NZ	5:D:504:HOH:O	2.40	0.44
1:E:11:TYR:CZ	2:F:340:ILE:HG23	2.52	0.44
1:A:97:GLY:HA2	1:A:229:ARG:HD2	2.00	0.44
2:F:445:HIS:O	2:F:449:VAL:HG23	2.17	0.44
1:A:203:SER:OG	1:A:246:GLU:HB3	2.17	0.44
2:D:482:CYS:O	2:D:485:SER:OG	2.27	0.44
1:E:31:THR:OG1	1:E:321:LEU:N	2.46	0.43
2:H:461:ARG:HG3	2:H:493:TYR:CE2	2.52	0.43
1:G:65:LEU:O	1:G:150:ASN:ND2	2.39	0.43
1:E:79:GLU:HG3	1:E:114:HIS:HB2	1.99	0.43
1:E:313:ASN:OD1	1:E:313:ASN:N	2.50	0.43
1:G:95:TYR:CD2	1:G:230:MET:HG2	2.53	0.43
1:G:216:LYS:O	1:G:220:ARG:NH2	2.51	0.43
1:A:36:ILE:HD13	1:A:317:LEU:HD22	1.99	0.43
1:A:308:LYS:HA	1:A:308:LYS:HD3	1.85	0.43
2:B:478:CYS:HB3	2:B:483:MET:HE2	1.99	0.43
2:D:335:GLY:HA3	5:D:502:HOH:O	2.18	0.43
1:E:37:LEU:HB2	1:E:315:LEU:HB2	1.99	0.43
1:E:321:LEU:HB3	2:F:445:HIS:HD2	1.83	0.43
1:A:315:LEU:HD22	2:B:434:VAL:HG21	2.01	0.43
1:C:183:HIS:O	1:C:185:PRO:HD3	2.18	0.43
1:G:42:ASN:HD21	1:G:288:ALA:HB3	1.83	0.43
1:C:97:GLY:HA3	1:C:230:MET:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:183:HIS:O	1:G:185:PRO:HD3	2.19	0.43
1:G:251:PHE:N	5:G:701:HOH:O	2.52	0.42
1:C:97:GLY:HA2	1:C:229:ARG:HD2	2.00	0.42
1:C:82:TYR:CZ	1:C:283:GLN:HG2	2.54	0.42
1:C:11:TYR:CZ	2:D:340:ILE:HG23	2.55	0.42
1:C:72:ASP:HA	1:C:75:ILE:HG13	2.01	0.42
1:E:85:GLU:OE2	1:E:270:LYS:NZ	2.52	0.42
1:G:317:LEU:HD12	2:H:438:ASN:OD1	2.20	0.42
2:H:457:ARG:HA	2:H:472:PHE:HE2	1.85	0.42
1:A:121:ILE:HG23	1:A:166:LYS:HE2	2.02	0.42
1:A:130:GLU:HB2	1:A:155:ILE:HG13	2.02	0.42
1:E:172:ASN:ND2	1:E:259:LYS:HD3	2.25	0.42
2:H:393:MET:HE1	2:H:430:ALA:HB2	2.01	0.42
1:A:170:ASN:HB2	1:A:237:LEU:HD13	2.02	0.42
2:F:482:CYS:O	2:F:486:ILE:HG13	2.20	0.42
2:B:402:ARG:NH1	2:B:415:ASN:OD1	2.53	0.42
1:E:280:THR:HG21	1:E:288:ALA:HB1	2.01	0.42
1:G:8:CYS:HA	2:H:471:CYS:HA	2.01	0.42
2:H:445:HIS:O	2:H:449:VAL:HG23	2.20	0.42
1:C:315:LEU:HD23	1:C:315:LEU:HA	1.91	0.41
1:C:130:GLU:HB2	1:C:155:ILE:HG13	2.02	0.41
1:G:9:ILE:N	2:H:470:GLY:O	2.51	0.41
2:H:457:ARG:HA	2:H:472:PHE:CE2	2.55	0.41
1:E:20:VAL:HG21	1:E:318:ALA:HB2	2.02	0.41
2:H:360:HIS:HB2	2:H:483:MET:HE3	2.03	0.41
1:E:8:CYS:HA	2:F:471:CYS:HA	2.01	0.41
2:H:493:TYR:HB3	2:H:494:PRO:HD3	2.01	0.41
2:H:381:GLY:O	2:H:385:LYS:N	2.49	0.41
2:F:477:LYS:HD3	2:F:477:LYS:HA	1.85	0.41
1:G:53:PRO:HG3	1:G:82:TYR:CZ	2.56	0.41
2:H:421:GLY:O	2:H:425:VAL:HG13	2.20	0.41
2:D:478:CYS:HB3	2:D:483:MET:HE2	2.02	0.40
1:E:114:HIS:HB3	1:E:262:LYS:HB3	2.03	0.40
1:E:173:GLN:H	1:E:173:GLN:HG2	1.77	0.40
2:F:362:ASN:ND2	2:F:478:CYS:O	2.54	0.40
1:G:266:SER:OG	1:G:267:ALA:N	2.54	0.40
1:G:57:ARG:H	1:G:74:PHE:HZ	1.68	0.40
1:E:214:VAL:HA	1:E:215:PRO:HD3	1.89	0.40
2:F:431:GLU:O	2:F:435:LEU:HG	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/321 (99%)	307 (96%)	12 (4%)	0	100	100
1	C	319/321 (99%)	308 (97%)	11 (3%)	0	100	100
1	E	319/321 (99%)	291 (91%)	26 (8%)	2 (1%)	21	42
1	G	319/321 (99%)	298 (93%)	20 (6%)	1 (0%)	36	58
2	B	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	21	42
2	D	162/164 (99%)	152 (94%)	8 (5%)	2 (1%)	10	23
2	F	162/164 (99%)	145 (90%)	15 (9%)	2 (1%)	10	23
2	H	162/164 (99%)	142 (88%)	18 (11%)	2 (1%)	10	23
All	All	1924/1940 (99%)	1794 (93%)	120 (6%)	10 (0%)	24	46

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	396	GLN
2	F	494	PRO
2	H	396	GLN
1	E	307	PRO
2	F	396	GLN
2	B	494	PRO
2	D	494	PRO
1	G	307	PRO
1	E	196	GLN
2	H	494	PRO

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	288/288 (100%)	269 (93%)	19 (7%)	15	34
1	C	288/288 (100%)	271 (94%)	17 (6%)	18	38
1	E	288/288 (100%)	265 (92%)	23 (8%)	11	25
1	G	288/288 (100%)	259 (90%)	29 (10%)	7	15
2	B	140/140 (100%)	128 (91%)	12 (9%)	10	22
2	D	140/140 (100%)	129 (92%)	11 (8%)	11	26
2	F	140/140 (100%)	124 (89%)	16 (11%)	5	11
2	H	140/140 (100%)	131 (94%)	9 (6%)	16	35
All	All	1712/1712 (100%)	1576 (92%)	136 (8%)	11	26

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	MET
1	A	51	VAL
1	A	56	LEU
1	A	100	ASN
1	A	111	ARG
1	A	149	ARG
1	A	152	VAL
1	A	163	THR
1	A	186	ASN
1	A	208	THR
1	A	213	LEU
1	A	221	SER
1	A	237	LEU
1	A	265	ASP
1	A	274	GLU
1	A	293	MET
1	A	302	THR
1	A	317	LEU
1	A	321	LEU
2	B	356	TYR
2	B	360	HIS
2	B	364	GLN
2	B	394	ASN
2	B	395	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	418	MET
2	B	423	LEU
2	B	425	VAL
2	B	432	LEU
2	B	458	LEU
2	B	467	LEU
2	B	496	TYR
1	C	16	SER
1	C	17	THR
1	C	51	VAL
1	C	56	LEU
1	C	90	THR
1	C	100	ASN
1	C	111	ARG
1	C	149	ARG
1	C	152	VAL
1	C	163	THR
1	C	208	THR
1	C	213	LEU
1	C	221	SER
1	C	237	LEU
1	C	274	GLU
1	C	293	MET
1	C	321	LEU
2	D	351	MET
2	D	356	TYR
2	D	360	HIS
2	D	395	THR
2	D	398	GLU
2	D	418	MET
2	D	425	VAL
2	D	432	LEU
2	D	458	LEU
2	D	467	LEU
2	D	496	TYR
1	E	17	THR
1	E	40	THR
1	E	56	LEU
1	E	71	CYS
1	E	72	ASP
1	E	88	ASN
1	E	100	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	115	PHE
1	E	142	LEU
1	E	152	VAL
1	E	158	ASN
1	E	163	THR
1	E	176	LEU
1	E	194	LEU
1	E	213	LEU
1	E	214	VAL
1	E	221	SER
1	E	263	LYS
1	E	274	GLU
1	E	293	MET
1	E	301	LEU
1	E	302	THR
1	E	321	LEU
2	F	344	ILE
2	F	352	VAL
2	F	356	TYR
2	F	360	HIS
2	F	362	ASN
2	F	373	GLU
2	F	394	ASN
2	F	418	MET
2	F	425	VAL
2	F	427	THR
2	F	432	LEU
2	F	455	LYS
2	F	458	LEU
2	F	467	LEU
2	F	479	ASP
2	F	496	TYR
1	G	9	ILE
1	G	15	ASN
1	G	20	VAL
1	G	28	VAL
1	G	29	THR
1	G	40	THR
1	G	49	ASP
1	G	56	LEU
1	G	88	ASN
1	G	100	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	109	LEU
1	G	111	ARG
1	G	120	ILE
1	G	152	VAL
1	G	158	ASN
1	G	163	THR
1	G	176	LEU
1	G	194	LEU
1	G	213	LEU
1	G	214	VAL
1	G	237	LEU
1	G	263	LYS
1	G	274	GLU
1	G	278	CYS
1	G	293	MET
1	G	301	LEU
1	G	302	THR
1	G	310	VAL
1	G	321	LEU
2	H	349	GLN
2	H	360	HIS
2	H	395	THR
2	H	418	MET
2	H	432	LEU
2	H	455	LYS
2	H	461	ARG
2	H	473	GLU
2	H	496	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	19	GLN
1	A	76	ASN
1	A	186	ASN
1	A	244	ASN
2	B	480	ASN
2	B	492	ASN
1	C	6	GLN
1	C	91	ASN
1	C	299	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	448	ASN
1	E	19	GLN
1	E	91	ASN
1	E	150	ASN
1	E	172	ASN
1	E	296	HIS
1	E	323	ASN
2	F	394	ASN
1	G	119	GLN
1	G	197	ASN
1	G	296	HIS
2	H	492	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 ⓘ

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	0.55	0	17,17,17	0.91	2 (11%)
3	SIA	I	2	3	20,20,21	3.66	8 (40%)	21,28,31	3.46	6 (28%)
3	GAL	J	1	3	12,12,12	0.57	0	17,17,17	1.45	4 (23%)
3	SIA	J	2	3	20,20,21	3.71	7 (35%)	21,28,31	3.71	7 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GAL	I	1	3	-	2/2/22/22	0/1/1/1
3	SIA	I	2	3	-	4/18/34/38	0/1/1/1
3	GAL	J	1	3	-	2/2/22/22	0/1/1/1
3	SIA	J	2	3	-	5/18/34/38	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	2	SIA	C4-C5	-12.16	1.42	1.53
3	I	2	SIA	C4-C5	-11.90	1.42	1.53
3	I	2	SIA	C7-C6	-7.46	1.43	1.52
3	J	2	SIA	C7-C6	-7.18	1.44	1.52
3	J	2	SIA	O6-C6	4.94	1.51	1.44
3	I	2	SIA	C10-N5	4.72	1.49	1.34
3	J	2	SIA	C10-N5	4.64	1.49	1.34
3	I	2	SIA	O6-C6	4.12	1.50	1.44
3	J	2	SIA	C2-C1	-2.46	1.49	1.52
3	I	2	SIA	C2-C1	-2.39	1.49	1.52
3	J	2	SIA	O7-C7	-2.33	1.37	1.43
3	I	2	SIA	O7-C7	-2.33	1.37	1.43
3	I	2	SIA	C5-N5	2.12	1.49	1.45
3	I	2	SIA	O8-C8	-2.11	1.38	1.43
3	J	2	SIA	C3-C2	2.07	1.55	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	2	SIA	O6-C2-C3	-13.43	92.50	110.56
3	I	2	SIA	O6-C2-C3	-11.84	94.64	110.56
3	I	2	SIA	O6-C2-C1	8.00	122.82	107.72
3	J	2	SIA	O6-C2-C1	7.98	122.79	107.72
3	I	2	SIA	O1B-C1-C2	3.44	121.66	112.71
3	I	2	SIA	O9-C9-C8	3.04	117.54	111.16
3	J	2	SIA	O9-C9-C8	3.04	117.53	111.16
3	J	1	GAL	C4-C3-C2	2.96	116.03	110.83
3	J	1	GAL	O5-C5-C4	2.96	115.03	109.70
3	J	2	SIA	O1B-C1-C2	2.74	119.83	112.71
3	J	1	GAL	O5-C1-C2	-2.67	105.61	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	2	SIA	C11-C10-N5	2.62	120.46	116.12
3	J	2	SIA	O1B-C1-O1A	-2.29	118.89	124.08
3	I	2	SIA	C11-C10-N5	2.25	119.84	116.12
3	J	2	SIA	C8-C7-C6	-2.23	108.87	113.05
3	I	2	SIA	O1B-C1-O1A	-2.14	119.22	124.08
3	J	1	GAL	C3-C4-C5	2.11	114.06	110.23
3	I	1	GAL	O5-C1-C2	-2.10	106.61	110.30
3	I	1	GAL	C3-C4-C5	2.05	113.95	110.23

There are no chirality outliers.

All (13) torsion outliers are listed below:

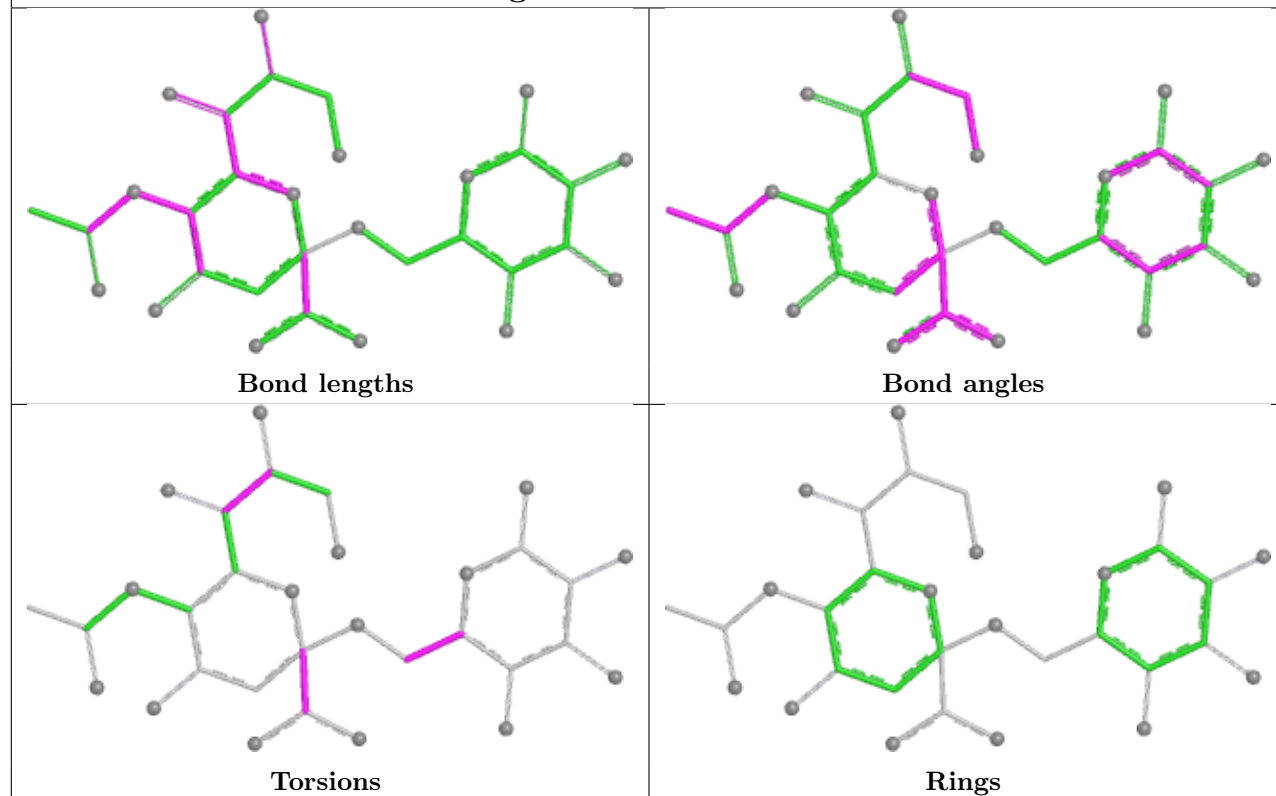
Mol	Chain	Res	Type	Atoms
3	I	1	GAL	O5-C5-C6-O6
3	J	1	GAL	O5-C5-C6-O6
3	I	1	GAL	C4-C5-C6-O6
3	J	1	GAL	C4-C5-C6-O6
3	J	2	SIA	O7-C7-C8-C9
3	J	2	SIA	O7-C7-C8-O8
3	J	2	SIA	C6-C7-C8-O8
3	I	2	SIA	O1A-C1-C2-O6
3	J	2	SIA	O1A-C1-C2-O6
3	J	2	SIA	C6-C7-C8-C9
3	I	2	SIA	O7-C7-C8-O8
3	I	2	SIA	O7-C7-C8-C9
3	I	2	SIA	C6-C7-C8-O8

There are no ring outliers.

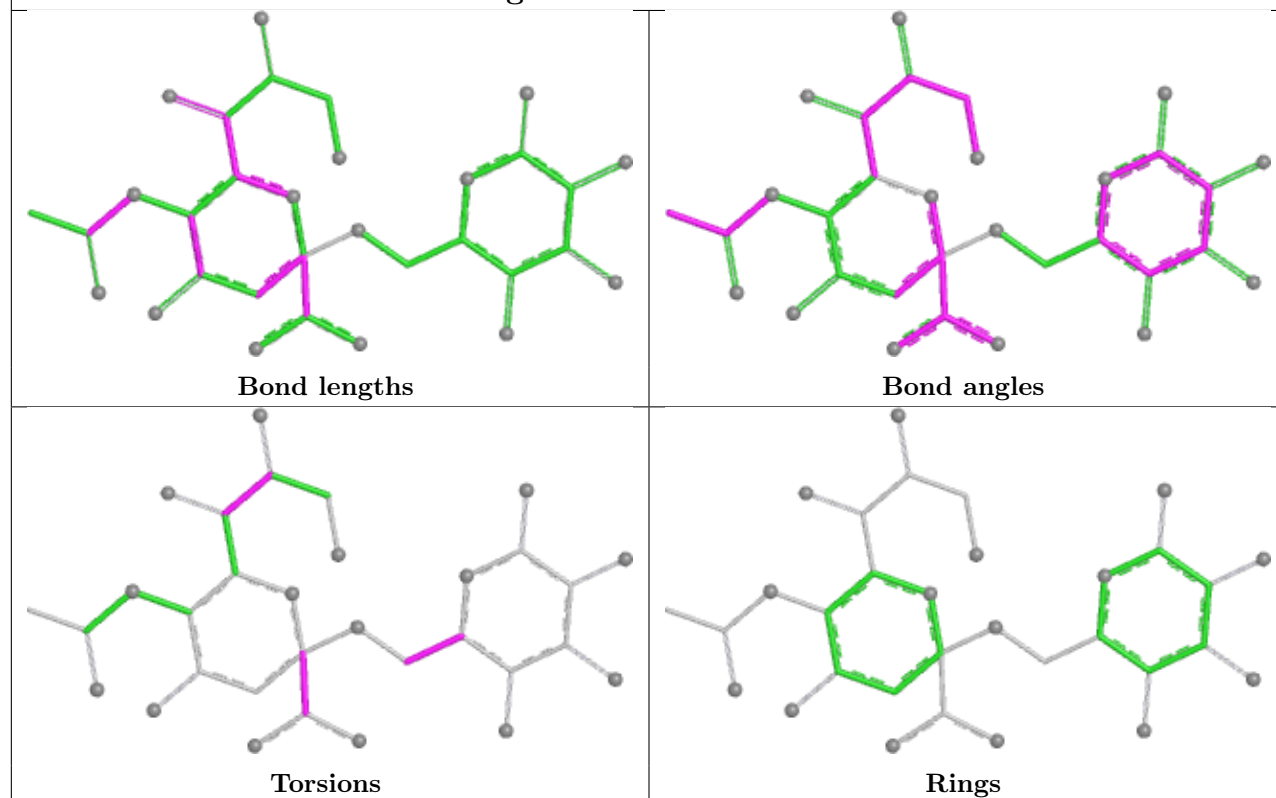
No monomer is involved in short contacts.

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

Oligosaccharide Chain I



Oligosaccharide Chain J



5.6 Ligand geometry

4 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	0.46	0	17,19,21	0.92	1 (5%)
4	NAG	E	601	1	14,14,15	0.46	0	17,19,21	1.05	1 (5%)
4	NAG	G	601	1	14,14,15	0.52	0	17,19,21	0.61	0
4	NAG	A	601	1	14,14,15	0.50	0	17,19,21	0.97	1 (5%)

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	-	0/6/23/26	0/1/1/1
4	NAG	E	601	1	-	4/6/23/26	0/1/1/1
4	NAG	G	601	1	-	2/6/23/26	0/1/1/1
4	NAG	A	601	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	NAG	C1-O5-C5	2.85	116.00	112.19
4	E	601	NAG	C1-O5-C5	2.48	115.51	112.19
4	A	601	NAG	C1-O5-C5	2.28	115.24	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	601	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	E	601	NAG	O7-C7-N2-C2
4	E	601	NAG	O5-C5-C6-O6
4	E	601	NAG	C4-C5-C6-O6
4	G	601	NAG	C8-C7-N2-C2
4	G	601	NAG	O7-C7-N2-C2
4	A	601	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-1.71	0 100 100	16, 37, 59, 83	0
1	C	321/321 (100%)	-1.70	0 100 100	14, 37, 58, 86	0
1	E	321/321 (100%)	-1.32	0 100 100	33, 72, 130, 180	0
1	G	321/321 (100%)	-1.32	0 100 100	29, 74, 131, 228	0
2	B	164/164 (100%)	-1.59	0 100 100	21, 51, 82, 114	0
2	D	164/164 (100%)	-1.59	0 100 100	18, 52, 84, 118	0
2	F	164/164 (100%)	-0.79	0 100 100	41, 123, 172, 198	0
2	H	164/164 (100%)	-0.79	0 100 100	40, 122, 175, 234	0
All	All	1940/1940 (100%)	-1.40	0 100 100	14, 56, 146, 234	0

There are no RSRZ outliers to report.

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

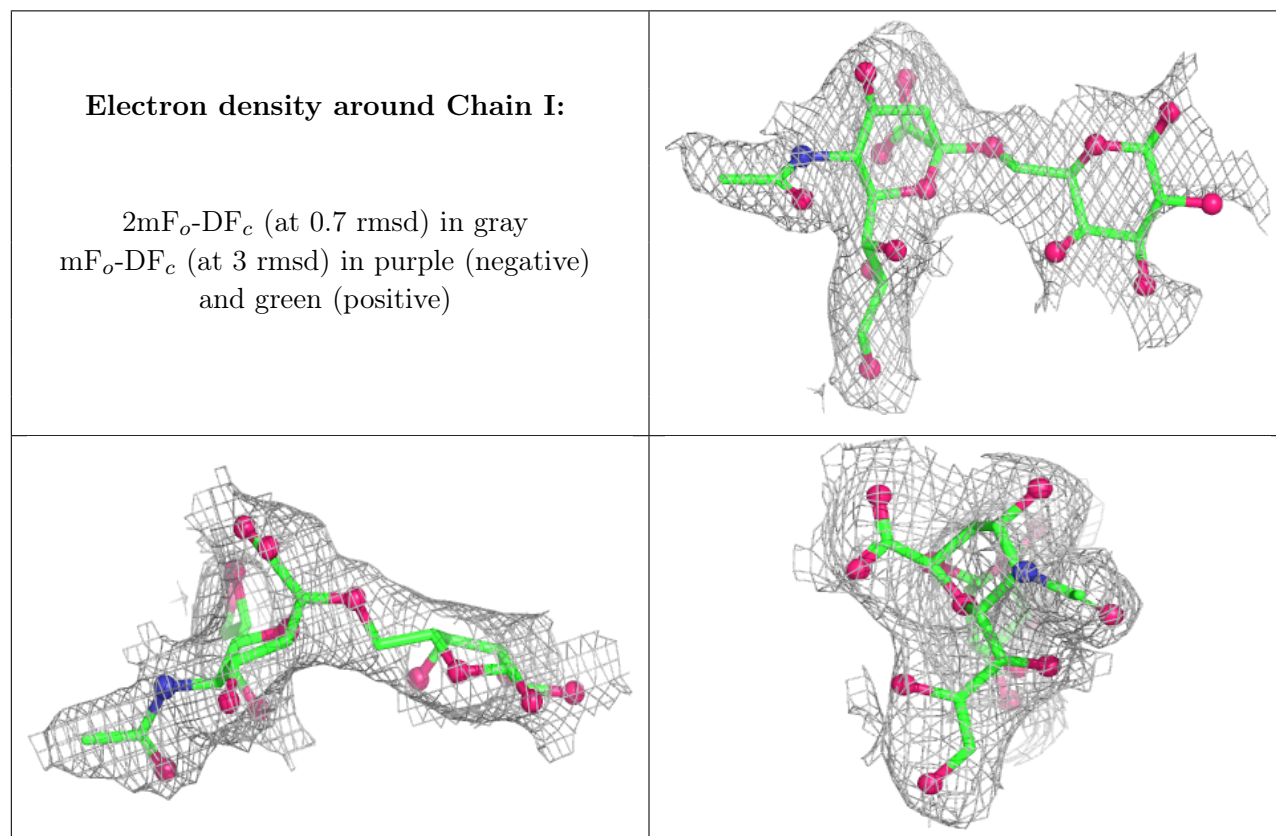
There are no non-standard protein/DNA/RNA residues in this entry.

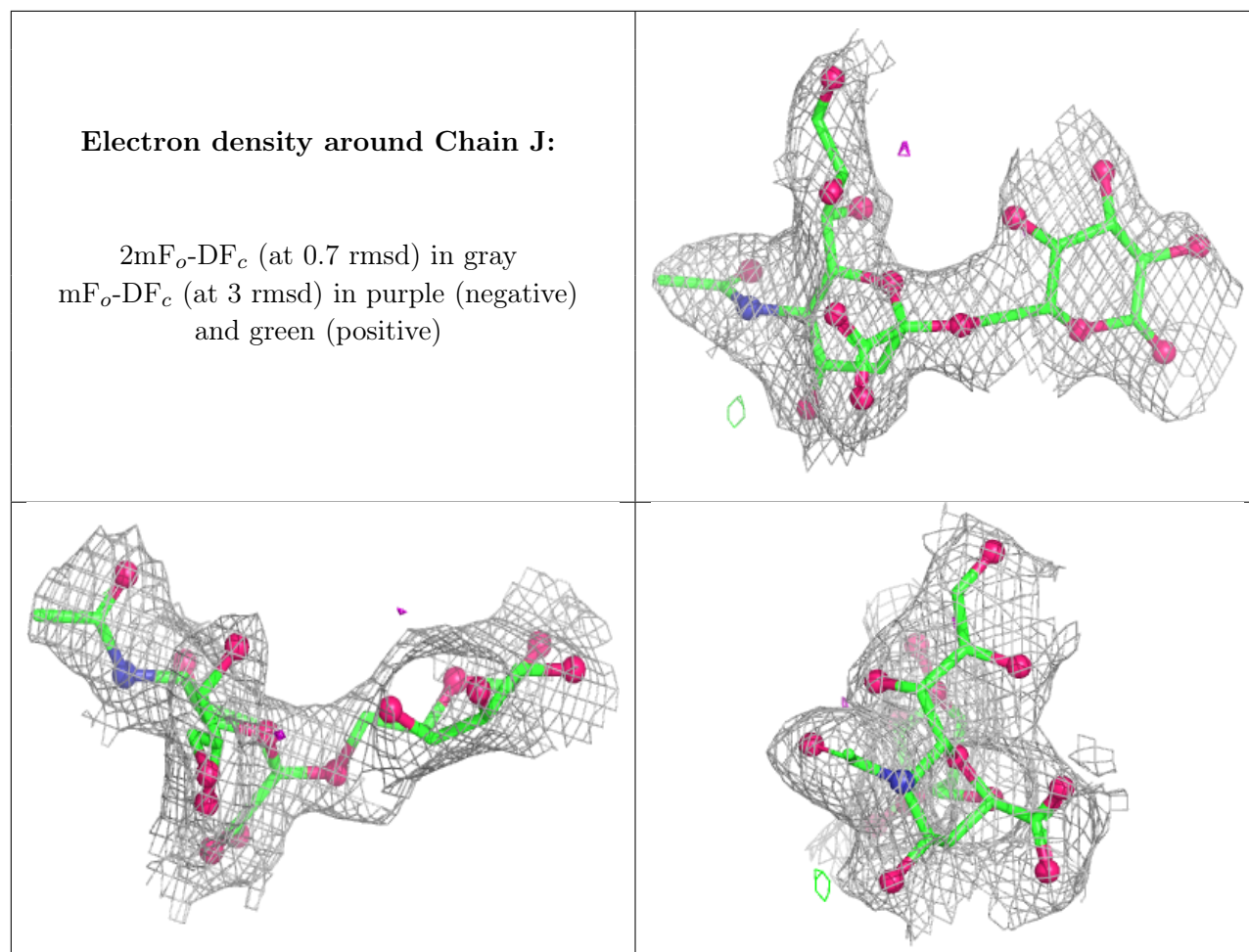
6.3 Carbohydrates [i](#)

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
3	GAL	J	1	12/12	0.98	0.04	52,69,82,83	0
3	SIA	I	2	20/21	0.99	0.03	26,39,46,50	0
3	GAL	I	1	12/12	0.99	0.04	52,71,84,95	0
3	SIA	J	2	20/21	0.99	0.03	28,40,47,48	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($\text{\AA}^2$)	Q<0.9
4	NAG	A	601	14/15	0.98	0.05	34,62,74,76	0
4	NAG	E	601	14/15	0.98	0.07	97,116,124,129	0
4	NAG	C	601	14/15	0.99	0.04	35,56,71,83	0
4	NAG	G	601	14/15	0.99	0.05	90,110,118,125	0

6.5 Other polymers [i](#)

There are no such residues in this entry.