Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 09:39 AM EDT

PDB ID	:	4KDN
Title	:	Crystal structure of the hemagglutinin of ferret-transmissible H5N1 virus in complex with avian receptor analog LSTa
Authors	:	Lu, X.; Shi, Y.; Zhang, W.; Zhang, Y.; Qi, J.; Gao, G.F.
Deposited on	:	2013-04-25
Resolution	:	2.48 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:

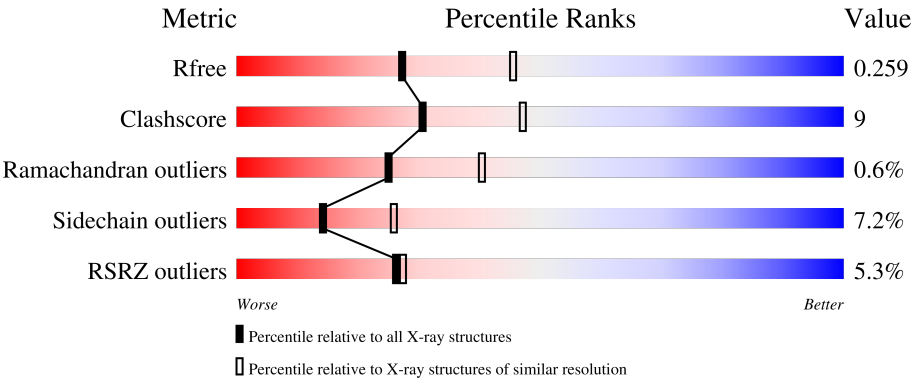
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.48 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 <=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	322	% 74% 21% 5%
1	C	322	% 72% 23% 5%
1	E	322	3% 74% 22% 5%
2	B	175	6% 85% 13%
2	D	175	17% 79% 19%

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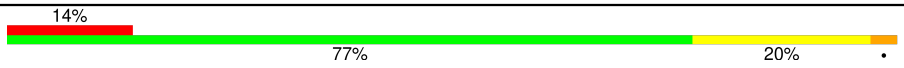
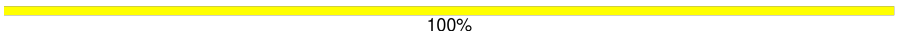
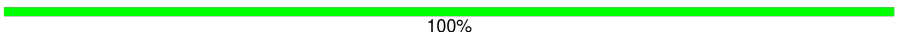
Mol	Chain	Length	Quality of chain
2	F	175	
3	G	2	
3	H	2	
3	I	2	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12269 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	322	Total	C	N	O	S	0	0	0
			2559	1621	440	483	15			
1	C	322	Total	C	N	O	S	0	0	0
			2559	1621	440	483	15			
1	E	322	Total	C	N	O	S	0	0	0
			2559	1621	440	483	15			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLN	-	expression tag	UNP Q6DQ33
A	158	ASP	ASN	engineered mutation	UNP Q6DQ33
A	224	LYS	ASN	engineered mutation	UNP Q6DQ33
A	226	LEU	GLN	engineered mutation	UNP Q6DQ33
A	319	ILE	THR	engineered mutation	UNP Q6DQ33
C	4	GLN	-	expression tag	UNP Q6DQ33
C	158	ASP	ASN	engineered mutation	UNP Q6DQ33
C	224	LYS	ASN	engineered mutation	UNP Q6DQ33
C	226	LEU	GLN	engineered mutation	UNP Q6DQ33
C	319	ILE	THR	engineered mutation	UNP Q6DQ33
E	4	GLN	-	expression tag	UNP Q6DQ33
E	158	ASP	ASN	engineered mutation	UNP Q6DQ33
E	224	LYS	ASN	engineered mutation	UNP Q6DQ33
E	226	LEU	GLN	engineered mutation	UNP Q6DQ33
E	319	ILE	THR	engineered mutation	UNP Q6DQ33

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			

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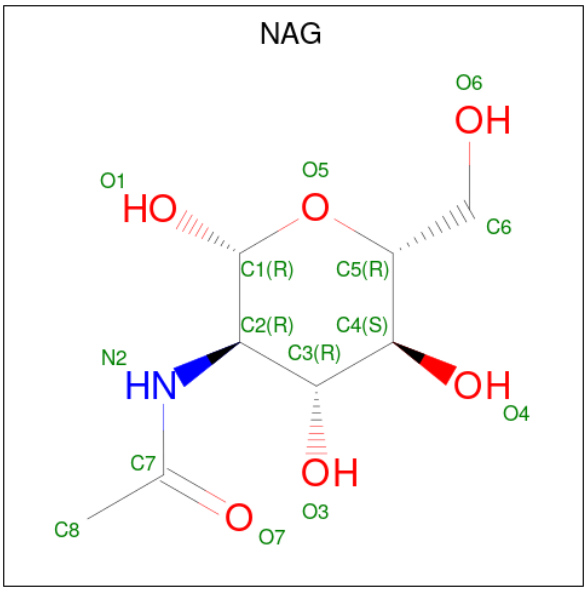
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	F	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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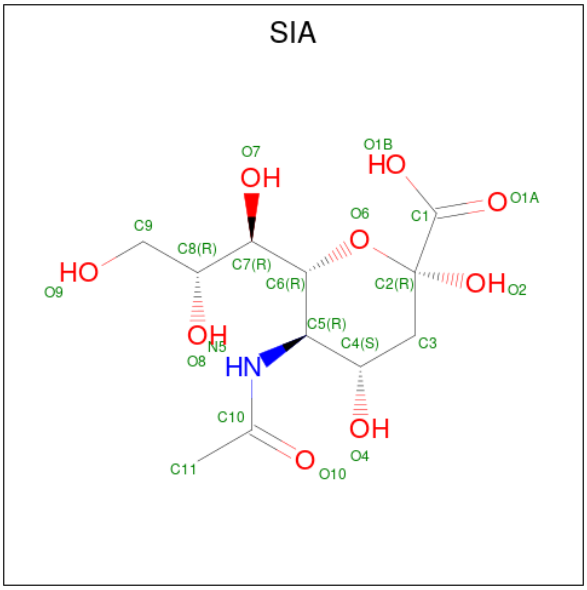
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 21 11 1 9	0	0
5	C	1	Total C N O 21 11 1 9	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	66	Total O 66 66	0	0
6	B	20	Total O 20 20	0	0
6	C	37	Total O 37 37	0	0
6	D	13	Total O 13 13	0	0
6	E	30	Total O 30 30	0	0

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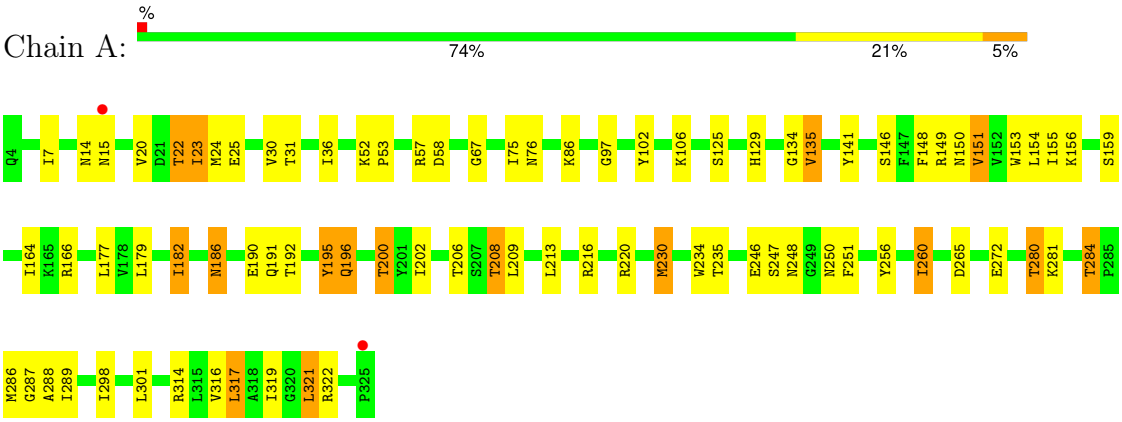
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	10	Total O 10 10	0	0

3 Residue-property plots (i)

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

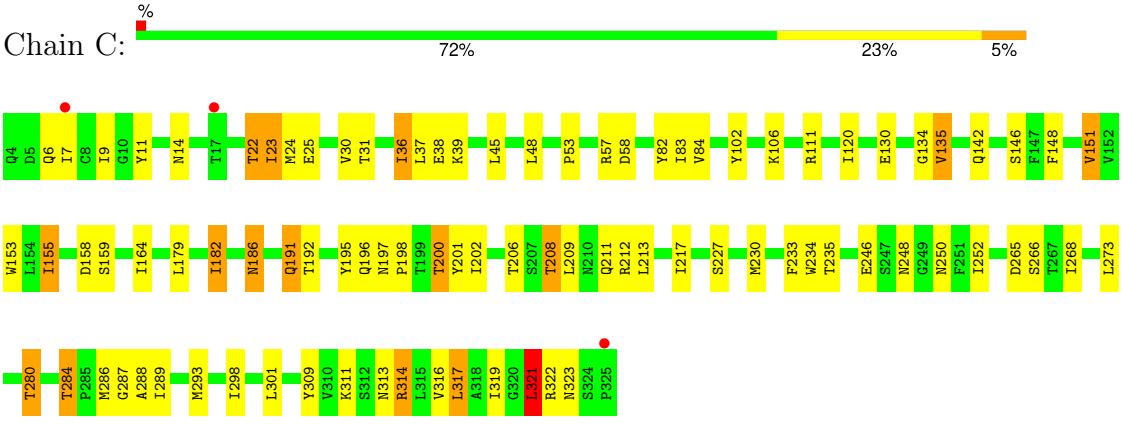
• Molecule 1: Hemagglutinin

Chain A:



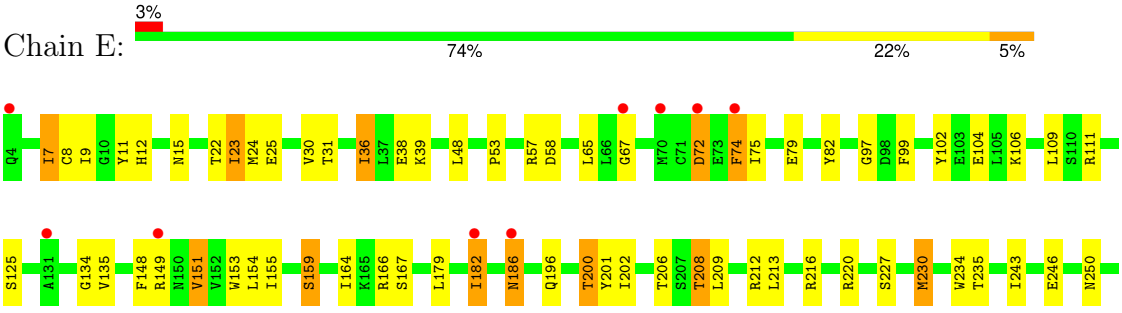
• Molecule 1: Hemagglutinin

Chain C:



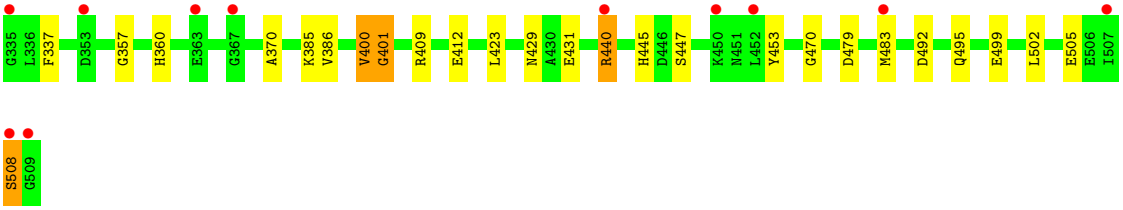
• Molecule 1: Hemagglutinin

Chain E:



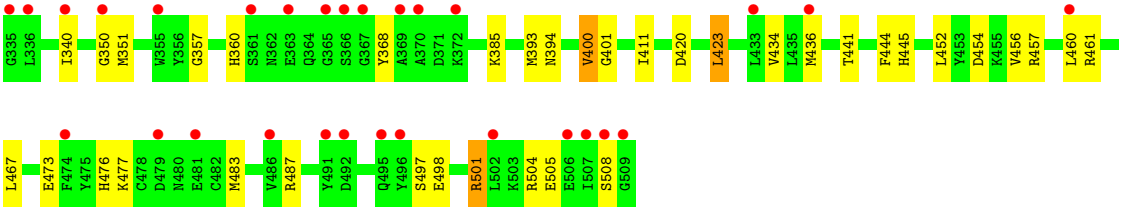
• Molecule 2: Hemagglutinin

Chain B:



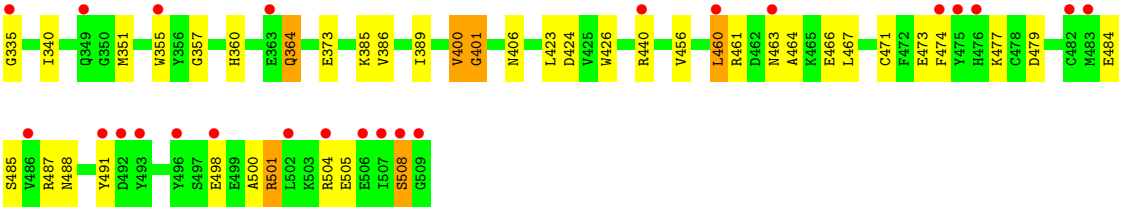
• Molecule 2: Hemagglutinin

Chain D:



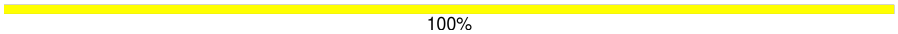
• Molecule 2: Hemagglutinin

Chain F:



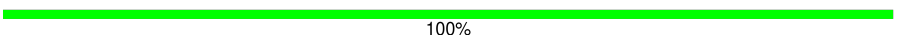
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.68Å 245.16Å 68.56Å 90.00° 113.75° 90.00°	Depositor
Resolution (Å)	35.37 – 2.48 35.37 – 2.48	Depositor EDS
% Data completeness (in resolution range)	97.1 (35.37-2.48) 97.1 (35.37-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.223 , 0.259 0.224 , 0.259	Depositor DCC
R_{free} test set	3468 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12269	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, 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	0.34	0/2621	0.58	1/3558 (0.0%)
1	C	0.31	0/2621	0.58	2/3558 (0.1%)
1	E	0.29	0/2621	0.54	0/3558
2	B	0.30	0/1443	0.47	0/1939
2	D	0.29	0/1443	0.47	0/1939
2	F	0.30	0/1443	0.49	1/1939 (0.1%)
All	All	0.31	0/12192	0.54	4/16491 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	158	ASP	N-CA-C	-5.55	96.01	111.00
2	F	460	LEU	CB-CA-C	5.45	120.56	110.20
1	A	195	TYR	N-CA-C	-5.33	96.62	111.00
1	C	321	LEU	CA-CB-CG	5.04	126.90	115.30

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	2559	0	2513	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2559	0	2513	55	0
1	E	2559	0	2513	62	0
2	B	1416	0	1319	20	0
2	D	1416	0	1319	28	0
2	F	1416	0	1319	30	0
3	G	28	0	25	1	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
4	A	14	0	13	0	0
4	C	14	0	13	0	0
4	E	14	0	13	0	0
5	A	21	0	17	3	0
5	C	21	0	17	1	0
6	A	66	0	0	11	0
6	B	20	0	0	4	0
6	C	37	0	0	4	0
6	D	13	0	0	2	0
6	E	30	0	0	6	0
6	F	10	0	0	4	0
All	All	12269	0	11644	218	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 9.

All (218) 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:504:ARG:NH2	6:D:611:HOH:O	1.94	0.99
1:C:192:THR:O	1:C:195:TYR:O	1.91	0.89
1:A:272:GLU:OE1	6:A:737:HOH:O	1.95	0.83
1:A:206:THR:O	6:A:706:HOH:O	1.96	0.82
2:B:412:GLU:OE1	6:B:617:HOH:O	1.97	0.81
1:E:206:THR:HG22	1:E:208:THR:H	1.46	0.81
1:A:206:THR:HG22	1:A:208:THR:H	1.46	0.79
1:E:79:GLU:OE2	6:E:729:HOH:O	2.00	0.77
1:E:104:GLU:O	6:E:708:HOH:O	2.02	0.76
2:D:393:MET:SD	6:F:603:HOH:O	2.44	0.75
1:A:284:THR:HG22	1:A:286:MET:H	1.51	0.74
1:E:284:THR:HG22	1:E:286:MET:H	1.52	0.74
1:E:256:TYR:O	6:E:707:HOH:O	2.04	0.74
2:F:406:ASN:O	6:F:609:HOH:O	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:VAL:HG22	1:C:146:SER:HA	1.71	0.72
2:B:447:SER:OG	6:B:608:HOH:O	2.07	0.71
1:A:25:GLU:OE2	1:A:322:ARG:NH2	2.21	0.70
1:A:76:ASN:OD1	6:A:738:HOH:O	2.08	0.70
1:C:284:THR:HG22	1:C:286:MET:H	1.57	0.69
1:A:22:THR:HG22	1:A:24:MET:H	1.56	0.68
1:E:209:LEU:O	6:E:703:HOH:O	2.10	0.67
1:E:280:THR:HG21	1:E:288:ALA:HB1	1.75	0.67
1:A:192:THR:O	1:A:195:TYR:O	2.12	0.67
1:E:182:ILE:HG23	1:E:202:ILE:HD12	1.76	0.67
1:A:280:THR:HG21	1:A:288:ALA:HB1	1.77	0.66
1:C:25:GLU:OE2	1:C:322:ARG:NH2	2.24	0.66
1:A:31:THR:HB	1:A:321:LEU:H	1.59	0.66
1:C:22:THR:HG22	1:C:24:MET:H	1.61	0.66
1:E:22:THR:HG22	1:E:24:MET:H	1.59	0.65
1:A:190:GLU:OE1	6:A:718:HOH:O	2.15	0.65
1:A:206:THR:HG21	6:A:743:HOH:O	1.95	0.65
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.78	0.65
1:C:186:ASN:OD1	1:C:186:ASN:N	2.31	0.64
1:C:289:ILE:HD11	1:C:298:ILE:HG13	1.80	0.64
1:C:206:THR:HG22	1:C:208:THR:H	1.63	0.63
1:E:212:ARG:NE	6:E:724:HOH:O	2.02	0.63
1:C:134:GLY:N	1:C:155:ILE:HD11	2.14	0.62
1:E:31:THR:HB	1:E:321:LEU:H	1.65	0.62
2:D:360:HIS:HD2	2:D:487:ARG:HH21	1.46	0.62
2:D:461:ARG:NH2	2:F:466:GLU:O	2.32	0.62
1:E:186:ASN:ND2	1:E:227:SER:HB2	2.15	0.62
1:E:317:LEU:HD21	2:F:389:ILE:HD12	1.81	0.61
1:C:31:THR:HB	1:C:321:LEU:H	1.66	0.61
5:A:604:SIA:O9	6:A:718:HOH:O	2.17	0.60
1:E:186:ASN:OD1	1:E:186:ASN:N	2.34	0.60
1:C:301:LEU:HA	2:D:400:VAL:HG22	1.84	0.60
1:A:52:LYS:HG2	1:A:53:PRO:HD2	1.83	0.60
1:E:39:LYS:NZ	1:E:313:ASN:O	2.27	0.60
1:E:25:GLU:OE2	1:E:322:ARG:NH2	2.35	0.60
1:A:182:ILE:HG23	1:A:202:ILE:HD12	1.84	0.59
1:C:200:THR:HA	1:C:248:ASN:HD21	1.67	0.59
1:C:212:ARG:NH1	6:C:721:HOH:O	2.08	0.59
1:E:301:LEU:HA	2:F:400:VAL:HG22	1.83	0.59
2:D:385:LYS:HG3	1:E:23:ILE:HD12	1.84	0.59
1:C:314:ARG:HG3	1:C:316:VAL:HG23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:THR:HB	1:A:209:LEU:HB3	1.85	0.58
1:A:148:PHE:HB2	1:A:151:VAL:HG12	1.84	0.58
2:F:463:ASN:ND2	2:F:491:TYR:OH	2.21	0.58
1:A:281:LYS:NZ	6:A:739:HOH:O	2.31	0.58
1:A:135:VAL:HG22	1:A:146:SER:HA	1.84	0.58
1:C:309:TYR:O	6:C:703:HOH:O	2.17	0.58
1:E:284:THR:HB	1:E:287:GLY:O	2.03	0.58
1:A:301:LEU:HA	2:B:400:VAL:HG22	1.85	0.58
2:F:460:LEU:HD13	2:F:464:ALA:HB3	1.85	0.57
2:D:360:HIS:CD2	2:D:487:ARG:HH21	2.21	0.57
1:E:148:PHE:HB2	1:E:151:VAL:HG12	1.86	0.57
2:B:385:LYS:HG3	1:C:23:ILE:HD12	1.86	0.57
1:A:186:ASN:N	1:A:186:ASN:OD1	2.37	0.56
1:A:129:HIS:O	6:A:760:HOH:O	2.17	0.56
1:C:39:LYS:NZ	1:C:313:ASN:O	2.28	0.56
2:F:505:GLU:HA	2:F:508:SER:HB3	1.88	0.56
1:C:182:ILE:HG23	1:C:202:ILE:HD12	1.87	0.56
1:C:201:TYR:OH	1:C:246:GLU:OE1	2.22	0.56
1:E:179:LEU:HD23	1:E:234:TRP:HB3	1.88	0.56
1:E:206:THR:HB	1:E:209:LEU:HB3	1.87	0.56
1:C:211:GLN:OE1	1:C:213:LEU:HD11	2.06	0.56
1:C:182:ILE:HD11	1:C:233:PHE:CE1	2.40	0.55
1:C:182:ILE:CD1	1:C:213:LEU:HD13	2.36	0.55
2:F:401:GLY:HA3	6:F:601:HOH:O	2.06	0.55
1:A:289:ILE:HD11	1:A:298:ILE:HG13	1.90	0.54
2:B:440:ARG:HH22	2:D:436:MET:HB3	1.72	0.54
1:C:280:THR:HG21	1:C:288:ALA:HB1	1.89	0.54
1:C:11:TYR:CZ	2:D:340:ILE:HG23	2.42	0.54
2:F:484:GLU:O	2:F:488:ASN:N	2.30	0.54
1:E:12:HIS:HB2	2:F:355:TRP:HA	1.90	0.54
1:E:38:GLU:HB2	1:E:293:MET:HB2	1.90	0.53
1:E:9:ILE:HD11	2:F:456:VAL:HG21	1.90	0.53
1:E:317:LEU:HD23	2:F:386:VAL:HG22	1.90	0.53
1:A:179:LEU:HD23	1:A:234:TRP:HB3	1.89	0.52
5:C:604:SIA:O6	5:C:604:SIA:O8	2.20	0.52
1:E:200:THR:HG21	1:E:250:ASN:OD1	2.09	0.52
1:C:9:ILE:HD11	2:D:456:VAL:HG21	1.91	0.52
2:B:505:GLU:HA	2:B:508:SER:HB3	1.92	0.52
1:C:6:GLN:HG2	2:D:473:GLU:HA	1.91	0.51
1:A:57:ARG:HH21	1:A:86:LYS:NZ	2.07	0.51
2:D:394:ASN:ND2	2:F:424:ASP:OD1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:705:HOH:O	3:G:1:NAG:O3	2.19	0.51
1:E:216:ARG:O	1:E:220:ARG:NH2	2.43	0.51
1:A:284:THR:HB	1:A:287:GLY:O	2.10	0.51
1:C:200:THR:HG21	1:C:250:ASN:OD1	2.10	0.50
1:E:74:PHE:HZ	1:E:149:ARG:HD3	1.75	0.50
1:A:314:ARG:HG2	1:A:316:VAL:HG23	1.92	0.50
1:E:72:ASP:C	1:E:74:PHE:H	2.14	0.50
1:E:53:PRO:HB3	1:E:82:TYR:CE2	2.46	0.50
1:E:102:TYR:CE2	1:E:106:LYS:HD2	2.47	0.50
1:E:31:THR:N	1:E:321:LEU:O	2.42	0.50
1:A:156:LYS:HD2	1:A:196:GLN:HG2	1.93	0.49
1:C:6:GLN:NE2	2:D:467:LEU:HD11	2.27	0.49
2:D:360:HIS:HB2	2:D:483:MET:SD	2.52	0.49
1:A:150:ASN:HB3	1:A:256:TYR:HB2	1.94	0.49
1:E:111:ARG:HH11	1:E:266:SER:HB3	1.77	0.49
2:F:467:LEU:HD21	2:F:473:GLU:HB2	1.94	0.49
1:C:37:LEU:HD23	1:C:39:LYS:HE2	1.93	0.49
1:E:74:PHE:CZ	1:E:149:ARG:HD3	2.47	0.49
1:A:125:SER:OG	1:A:166:ARG:NH2	2.46	0.49
1:A:200:THR:HG21	1:A:250:ASN:OD1	2.13	0.49
1:C:321:LEU:HB3	2:D:445:HIS:CD2	2.48	0.49
1:C:179:LEU:HD23	1:C:234:TRP:HB3	1.95	0.48
2:F:485:SER:HA	2:F:488:ASN:HB2	1.94	0.48
2:B:431:GLU:HA	6:B:609:HOH:O	2.13	0.48
1:E:25:GLU:CD	1:E:322:ARG:HH22	2.16	0.48
1:E:99:PHE:HB3	1:E:102:TYR:HB2	1.94	0.48
1:A:102:TYR:CE2	1:A:106:LYS:HD2	2.49	0.48
1:E:164:ILE:O	1:E:246:GLU:HA	2.13	0.48
2:B:492:ASP:OD1	2:B:495:GLN:HB2	2.14	0.48
1:E:125:SER:HB2	1:E:166:ARG:HH22	1.79	0.48
1:C:6:GLN:HE21	2:D:473:GLU:HG3	1.78	0.48
2:D:501:ARG:NE	2:D:505:GLU:OE2	2.47	0.48
1:C:148:PHE:HB2	1:C:151:VAL:HG12	1.96	0.48
2:D:454:ASP:OD1	2:D:457:ARG:NH1	2.46	0.47
2:D:350:GLY:HA3	2:D:368:TYR:CE1	2.49	0.47
6:A:708:HOH:O	2:D:411:ILE:HG13	2.14	0.47
1:C:164:ILE:O	1:C:246:GLU:HA	2.14	0.47
1:C:130:GLU:O	1:C:155:ILE:HD12	2.15	0.47
2:F:360:HIS:CD2	2:F:487:ARG:HH21	2.32	0.47
1:C:111:ARG:HH11	1:C:266:SER:HB3	1.80	0.47
2:B:360:HIS:HB2	2:B:483:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:SER:CB	1:E:166:ARG:HH22	2.28	0.47
1:E:36:ILE:HD13	1:E:36:ILE:HA	1.74	0.47
1:C:53:PRO:HB3	1:C:82:TYR:CE2	2.51	0.46
1:A:177:LEU:HB2	1:A:260:ILE:HD13	1.97	0.46
1:A:14:ASN:ND2	6:A:730:HOH:O	2.16	0.46
1:C:142:GLN:N	6:C:710:HOH:O	2.46	0.46
2:D:497:SER:O	2:D:501:ARG:HB2	2.15	0.46
2:B:337:PHE:CE1	2:B:447:SER:HB2	2.51	0.46
2:B:357:GLY:HA3	2:B:370:ALA:HA	1.97	0.46
1:C:36:ILE:HD13	1:C:36:ILE:HA	1.68	0.46
2:D:420:ASP:OD1	6:D:604:HOH:O	2.20	0.46
1:A:67:GLY:O	1:A:149:ARG:HG3	2.16	0.46
2:B:453:TYR:CE1	2:B:470:GLY:HA2	2.51	0.46
1:C:186:ASN:ND2	1:C:227:SER:HB2	2.30	0.46
1:E:65:LEU:HD11	1:E:109:LEU:HD11	1.98	0.46
2:D:351:MET:SD	2:D:357:GLY:HA3	2.56	0.46
2:B:499:GLU:O	2:B:502:LEU:HB2	2.17	0.45
1:E:67:GLY:HA3	1:E:149:ARG:H	1.81	0.45
2:B:409:ARG:NE	6:B:610:HOH:O	2.50	0.45
2:D:476:HIS:ND1	2:D:477:LYS:O	2.43	0.45
1:E:308:LYS:HD2	2:F:426:TRP:CE2	2.51	0.45
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.98	0.45
2:F:351:MET:SD	2:F:357:GLY:HA3	2.57	0.45
2:F:364:GLN:HE22	2:F:479:ASP:HA	1.82	0.45
1:A:164:ILE:O	1:A:246:GLU:HA	2.16	0.45
1:A:182:ILE:HG12	1:A:213:LEU:HD13	1.97	0.45
1:E:15:ASN:OD1	1:E:15:ASN:N	2.34	0.45
2:B:400:VAL:HA	2:B:401:GLY:HA3	1.71	0.45
1:C:206:THR:HB	1:C:209:LEU:HB3	1.99	0.44
1:A:317:LEU:HD23	2:B:386:VAL:HG22	1.99	0.44
1:C:273:LEU:HD11	1:C:286:MET:C	2.38	0.44
1:C:200:THR:HA	1:C:248:ASN:ND2	2.30	0.44
1:E:7:ILE:HB	2:F:474:PHE:CE1	2.52	0.44
2:F:400:VAL:HA	2:F:401:GLY:HA3	1.67	0.44
1:A:23:ILE:HD12	2:F:385:LYS:HG3	1.99	0.44
2:F:335:GLY:O	6:F:604:HOH:O	2.21	0.44
2:F:500:ALA:O	2:F:504:ARG:N	2.50	0.44
2:B:479:ASP:OD1	2:B:479:ASP:N	2.44	0.44
1:C:102:TYR:CE2	1:C:106:LYS:HD2	2.53	0.44
1:A:97:GLY:HA3	1:A:230:MET:O	2.17	0.44
1:A:321:LEU:HB3	2:B:445:HIS:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:THR:OG1	1:A:248:ASN:HB3	2.19	0.43
1:E:11:TYR:CZ	2:F:340:ILE:HG23	2.54	0.43
1:A:317:LEU:HD12	1:A:317:LEU:HA	1.84	0.43
1:C:45:LEU:HD13	1:C:84:VAL:HG21	2.01	0.43
2:D:441:THR:O	2:D:444:PHE:HB3	2.19	0.43
1:C:191:GLN:HG2	1:C:217:ILE:HD11	2.00	0.43
1:A:247:SER:OG	1:A:251:PHE:HB2	2.19	0.42
1:E:97:GLY:HA3	1:E:230:MET:O	2.19	0.42
1:E:201:TYR:OH	1:E:246:GLU:OE1	2.30	0.42
2:B:429:ASN:N	2:B:429:ASN:HD22	2.17	0.42
1:C:197:ASN:OD1	6:C:735:HOH:O	2.22	0.42
1:C:317:LEU:HD13	2:D:434:VAL:HG22	2.00	0.42
1:C:48:LEU:HD23	1:C:48:LEU:HA	1.88	0.42
1:C:284:THR:HB	1:C:287:GLY:O	2.20	0.42
1:A:155:ILE:HG12	5:A:604:SIA:H111	2.02	0.41
1:E:167:SER:HA	1:E:243:ILE:O	2.19	0.41
1:C:14:ASN:OD1	1:C:323:ASN:ND2	2.53	0.41
1:C:83:ILE:HB	1:C:268:ILE:HG13	2.03	0.41
1:E:159:SER:O	1:E:196:GLN:HG3	2.20	0.41
1:A:134:GLY:HA2	5:A:604:SIA:H113	2.03	0.41
1:A:154:LEU:C	1:A:155:ILE:HD12	2.40	0.41
1:A:216:ARG:O	1:A:220:ARG:NH2	2.53	0.41
2:D:452:LEU:HD12	2:D:452:LEU:HA	1.85	0.41
2:B:508:SER:O	2:F:501:ARG:NH1	2.54	0.41
1:E:8:CYS:HA	2:F:471:CYS:HA	2.03	0.41
1:A:15:ASN:OD1	1:A:15:ASN:N	2.37	0.41
1:E:72:ASP:C	1:E:74:PHE:N	2.74	0.41
1:E:206:THR:HG22	1:E:208:THR:N	2.25	0.41
1:C:311:LYS:HB2	2:D:423:LEU:HD21	2.03	0.41
1:E:154:LEU:O	6:E:701:HOH:O	2.22	0.41
1:E:182:ILE:HG12	1:E:213:LEU:HD13	2.02	0.41
2:F:479:ASP:OD1	2:F:479:ASP:N	2.46	0.41
1:C:38:GLU:HB2	1:C:293:MET:HB2	2.03	0.41
1:E:12:HIS:N	2:F:355:TRP:O	2.47	0.40
1:E:266:SER:OG	1:E:267:THR:N	2.54	0.40
1:E:48:LEU:HD23	1:E:48:LEU:HA	1.93	0.40
1:C:134:GLY:HA3	1:C:153:TRP:HB3	2.03	0.40
1:A:150:ASN:HA	1:A:256:TYR:HD1	1.86	0.40
1:E:7:ILE:HD13	1:E:7:ILE:HA	1.85	0.40
1:E:308:LYS:HD2	2:F:426:TRP:NE1	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	320/322 (99%)	300 (94%)	20 (6%)	0	100	100
1	C	320/322 (99%)	300 (94%)	19 (6%)	1 (0%)	41	59
1	E	320/322 (99%)	296 (92%)	22 (7%)	2 (1%)	25	40
2	B	173/175 (99%)	166 (96%)	5 (3%)	2 (1%)	13	22
2	D	173/175 (99%)	165 (95%)	6 (4%)	2 (1%)	13	22
2	F	173/175 (99%)	164 (95%)	7 (4%)	2 (1%)	13	22
All	All	1479/1491 (99%)	1391 (94%)	79 (5%)	9 (1%)	25	40

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	72	ASP
2	D	508	SER
1	E	74	PHE
2	F	508	SER
2	B	508	SER
2	B	401	GLY
2	D	401	GLY
2	F	401	GLY
1	C	198	PRO

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	290/290 (100%)	263 (91%)	27 (9%)	9 15
1	C	290/290 (100%)	262 (90%)	28 (10%)	8 14
1	E	290/290 (100%)	267 (92%)	23 (8%)	12 22
2	B	149/149 (100%)	146 (98%)	3 (2%)	55 77
2	D	149/149 (100%)	144 (97%)	5 (3%)	37 61
2	F	149/149 (100%)	140 (94%)	9 (6%)	19 34
All	All	1317/1317 (100%)	1222 (93%)	95 (7%)	14 26

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	20	VAL
1	A	22	THR
1	A	23	ILE
1	A	30	VAL
1	A	36	ILE
1	A	58	ASP
1	A	75	ILE
1	A	135	VAL
1	A	141	TYR
1	A	151	VAL
1	A	159	SER
1	A	182	ILE
1	A	186	ASN
1	A	191	GLN
1	A	196	GLN
1	A	200	THR
1	A	208	THR
1	A	230	MET
1	A	235	THR
1	A	260	ILE
1	A	265	ASP
1	A	280	THR
1	A	284	THR
1	A	317	LEU
1	A	319	ILE
1	A	321	LEU
2	B	400	VAL
2	B	423	LEU
2	B	440	ARG

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Mol	Chain	Res	Type
1	C	7	ILE
1	C	22	THR
1	C	23	ILE
1	C	30	VAL
1	C	36	ILE
1	C	57	ARG
1	C	58	ASP
1	C	120	ILE
1	C	135	VAL
1	C	151	VAL
1	C	155	ILE
1	C	159	SER
1	C	182	ILE
1	C	186	ASN
1	C	191	GLN
1	C	196	GLN
1	C	200	THR
1	C	208	THR
1	C	230	MET
1	C	235	THR
1	C	252	ILE
1	C	265	ASP
1	C	280	THR
1	C	284	THR
1	C	314	ARG
1	C	317	LEU
1	C	319	ILE
1	C	321	LEU
2	D	400	VAL
2	D	423	LEU
2	D	460	LEU
2	D	498	GLU
2	D	501	ARG
1	E	7	ILE
1	E	23	ILE
1	E	30	VAL
1	E	36	ILE
1	E	57	ARG
1	E	58	ASP
1	E	75	ILE
1	E	135	VAL
1	E	151	VAL

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Mol	Chain	Res	Type
1	E	155	ILE
1	E	159	SER
1	E	182	ILE
1	E	186	ASN
1	E	200	THR
1	E	208	THR
1	E	230	MET
1	E	235	THR
1	E	265	ASP
1	E	280	THR
1	E	314	ARG
1	E	317	LEU
1	E	319	ILE
1	E	321	LEU
2	F	364	GLN
2	F	373	GLU
2	F	400	VAL
2	F	423	LEU
2	F	440	ARG
2	F	461	ARG
2	F	477	LYS
2	F	498	GLU
2	F	501	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
2	B	429	ASN
1	C	6	GLN
2	D	360	HIS
2	D	429	ASN
2	F	429	ASN

5.3.3 RNA

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)

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	$\#\|Z\| > 2$
3	NAG	G	1	1,3	14,14,15	0.47	0	17,19,21	0.78	0
3	NAG	G	2	3	14,14,15	0.44	0	17,19,21	1.04	1 (5%)
3	NAG	H	1	1,3	14,14,15	0.57	0	17,19,21	0.64	0
3	NAG	H	2	3	14,14,15	0.58	0	17,19,21	0.67	0
3	NAG	I	1	1,3	14,14,15	0.59	0	17,19,21	1.19	2 (11%)
3	NAG	I	2	3	14,14,15	0.45	0	17,19,21	0.94	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	G	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	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(^{o})	Ideal(^{o})
3	I	1	NAG	C1-O5-C5	3.31	116.63	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	2	NAG	C2-N2-C7	-2.28	119.85	122.90
3	I	1	NAG	C3-C4-C5	2.08	114.01	110.23

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	I	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	I	2	NAG	C1-C2-N2-C7
3	G	1	NAG	O5-C5-C6-O6

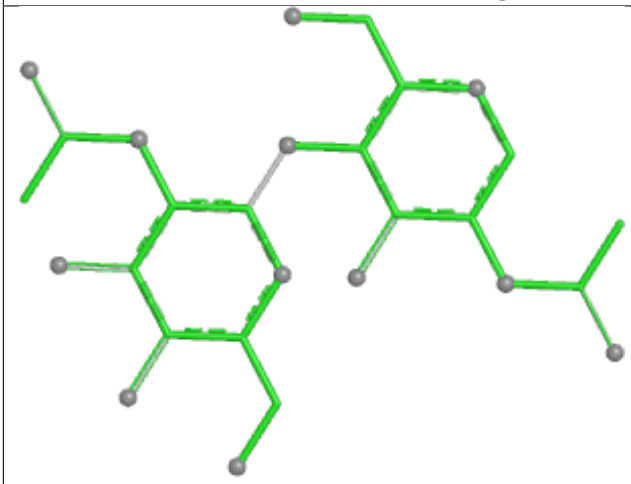
There are no ring outliers.

1 monomer is involved in 1 short contact:

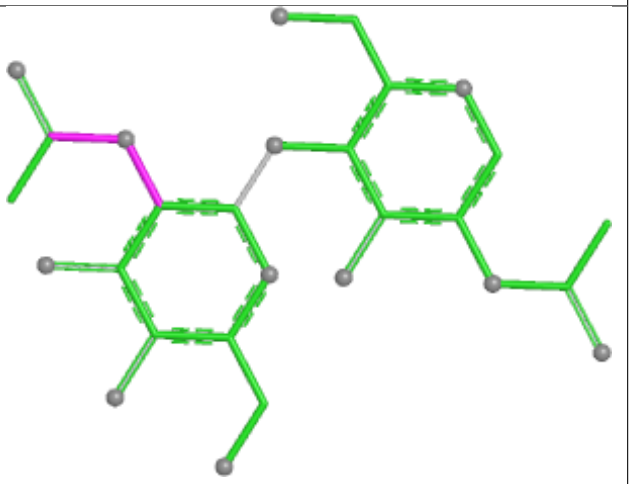
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0

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

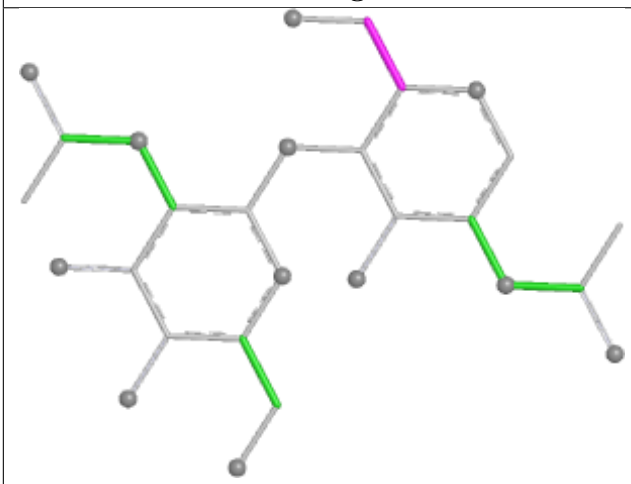
Oligosaccharide Chain G



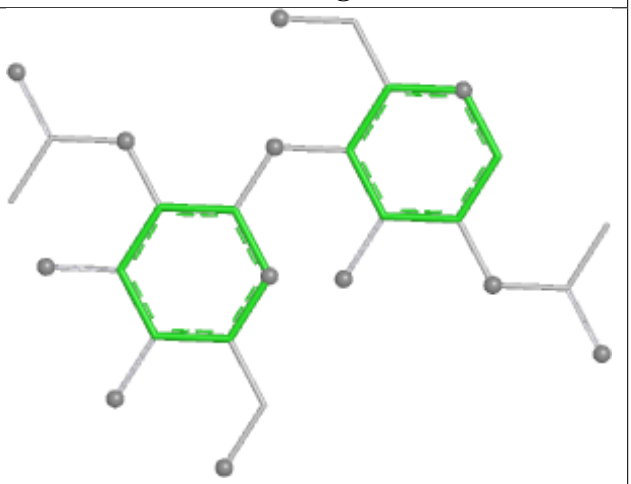
Bond lengths



Bond angles

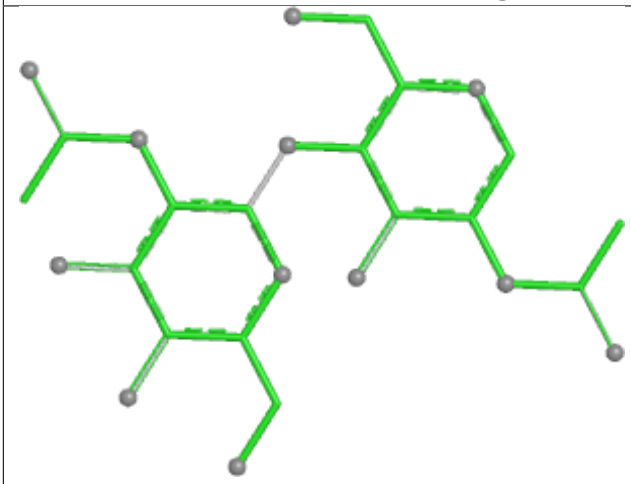


Torsions

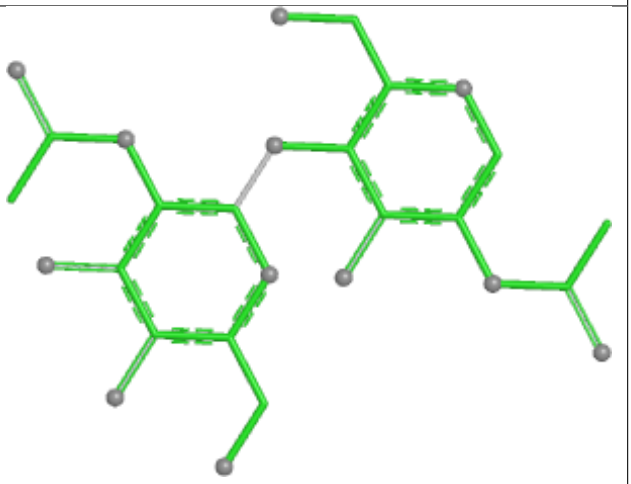


Rings

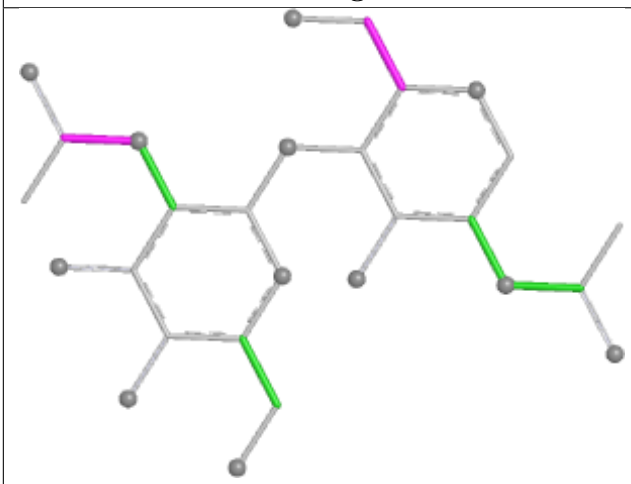
Oligosaccharide Chain H



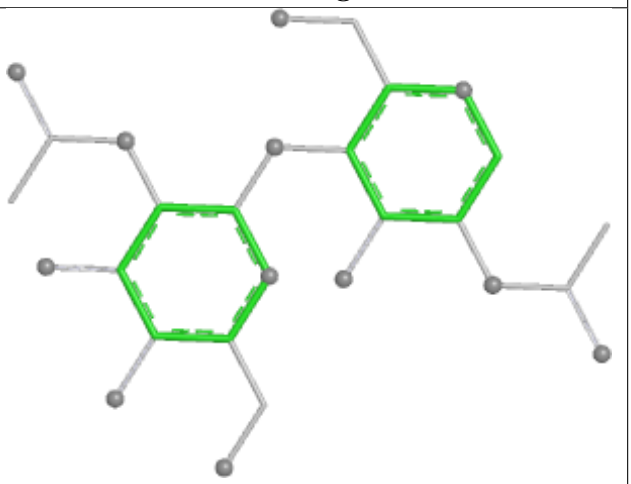
Bond lengths



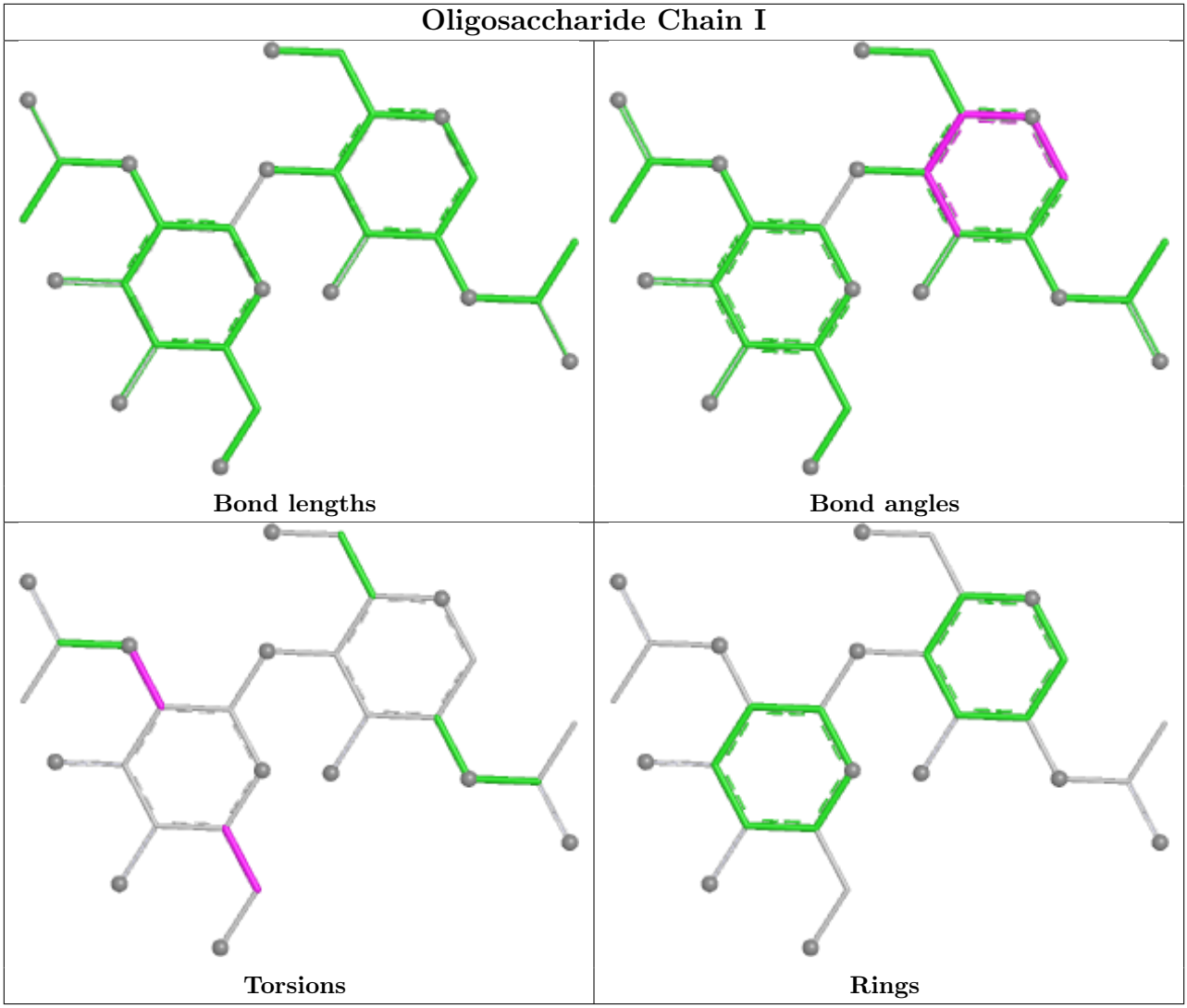
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

5 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	A	601	1	14,14,15	0.55	0	17,19,21	0.80	0
4	NAG	E	601	1	14,14,15	0.56	0	17,19,21	0.93	1 (5%)
5	SIA	C	604	-	21,21,21	3.93	9 (42%)	24,31,31	1.66	6 (25%)

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	0.44	0	17,19,21	1.06	1 (5%)
5	SIA	A	604	-	21,21,21	4.00	8 (38%)	24,31,31	1.68	6 (25%)

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	A	601	1	-	0/6/23/26	0/1/1/1
4	NAG	E	601	1	-	2/6/23/26	0/1/1/1
5	SIA	C	604	-	-	7/20/38/38	0/1/1/1
4	NAG	C	601	1	-	1/6/23/26	0/1/1/1
5	SIA	A	604	-	-	6/20/38/38	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	604	SIA	C7-C6	-10.11	1.40	1.52
5	C	604	SIA	C7-C6	-9.97	1.40	1.52
5	A	604	SIA	C3-C4	-8.69	1.40	1.53
5	C	604	SIA	C3-C4	-8.36	1.40	1.53
5	A	604	SIA	C4-C5	-6.33	1.47	1.53
5	C	604	SIA	C4-C5	-5.70	1.48	1.53
5	A	604	SIA	C3-C2	-5.57	1.44	1.51
5	C	604	SIA	O6-C6	5.57	1.52	1.44
5	A	604	SIA	O6-C6	5.41	1.52	1.44
5	C	604	SIA	C3-C2	-5.39	1.44	1.51
5	C	604	SIA	C10-N5	4.37	1.48	1.34
5	A	604	SIA	C10-N5	4.19	1.47	1.34
5	A	604	SIA	O6-C2	4.09	1.47	1.43
5	C	604	SIA	O6-C2	4.02	1.47	1.43
5	C	604	SIA	O4-C4	2.68	1.48	1.43
5	A	604	SIA	O4-C4	2.46	1.48	1.43
5	C	604	SIA	C6-C5	2.09	1.56	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	604	SIA	O6-C6-C7	3.67	112.38	106.65
5	C	604	SIA	O9-C9-C8	3.31	118.11	111.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	604	SIA	O9-C9-C8	3.07	117.61	111.16
4	C	601	NAG	C1-O5-C5	2.98	116.18	112.19
5	C	604	SIA	C11-C10-N5	2.86	120.87	116.12
5	C	604	SIA	O6-C6-C7	2.72	110.90	106.65
5	A	604	SIA	C8-C7-C6	-2.68	108.01	113.05
5	C	604	SIA	O6-C6-C5	-2.55	107.51	109.84
5	A	604	SIA	O1A-C1-C2	-2.50	119.69	123.85
5	C	604	SIA	O1A-C1-C2	-2.47	119.73	123.85
5	A	604	SIA	C3-C4-C5	2.28	113.25	109.72
5	C	604	SIA	C3-C4-C5	2.23	113.17	109.72
4	E	601	NAG	C1-O5-C5	2.07	114.96	112.19
5	A	604	SIA	C11-C10-N5	2.06	119.54	116.12

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	601	NAG	C8-C7-N2-C2
4	E	601	NAG	O7-C7-N2-C2
5	C	604	SIA	C6-C7-C8-O8
5	C	604	SIA	O7-C7-C8-O8
5	C	604	SIA	O7-C7-C8-C9
5	C	604	SIA	C6-C7-C8-C9
5	A	604	SIA	C6-C7-C8-O8
5	A	604	SIA	O7-C7-C8-O8
5	A	604	SIA	C6-C7-C8-C9
5	C	604	SIA	O1A-C1-C2-O2
5	A	604	SIA	O7-C7-C8-C9
4	C	601	NAG	O5-C5-C6-O6
5	A	604	SIA	O1A-C1-C2-C3
5	A	604	SIA	O1B-C1-C2-C3
5	C	604	SIA	O1A-C1-C2-C3
5	C	604	SIA	O1B-C1-C2-C3

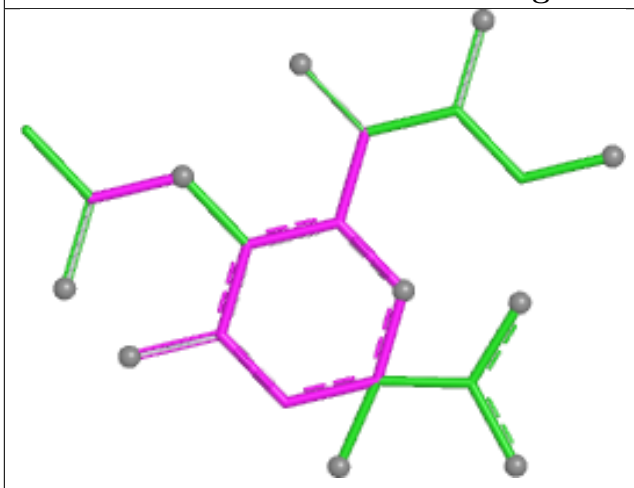
There are no ring outliers.

2 monomers are involved in 4 short contacts:

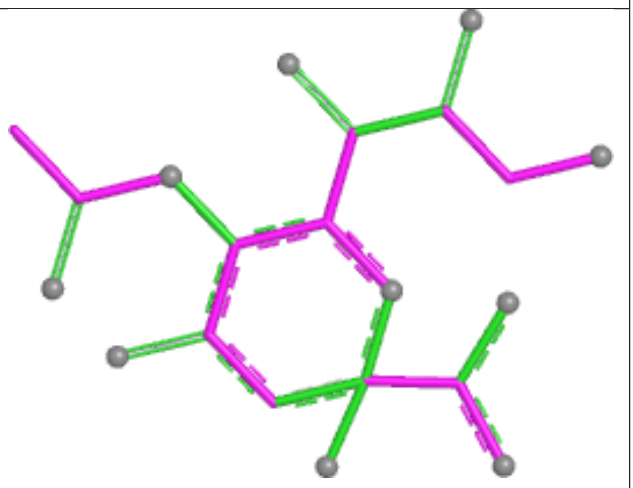
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	604	SIA	1	0
5	A	604	SIA	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

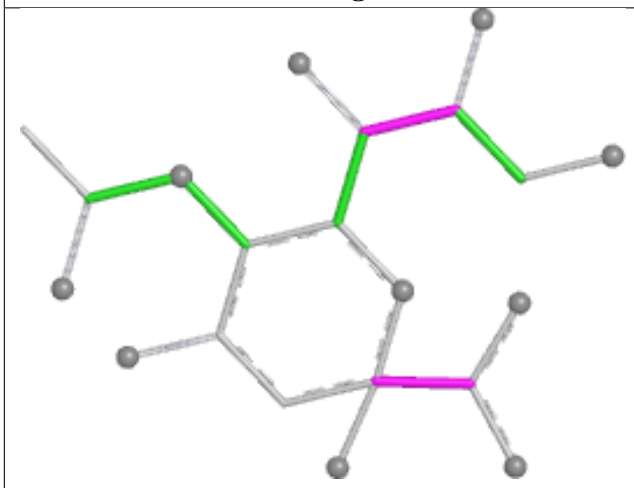
Ligand SIA C 604



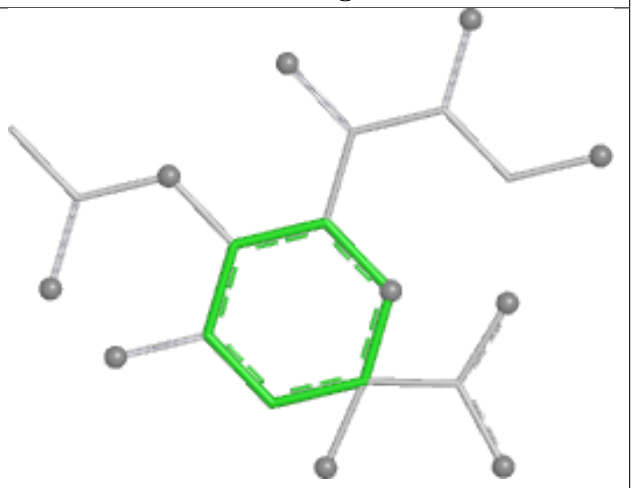
Bond lengths



Bond angles

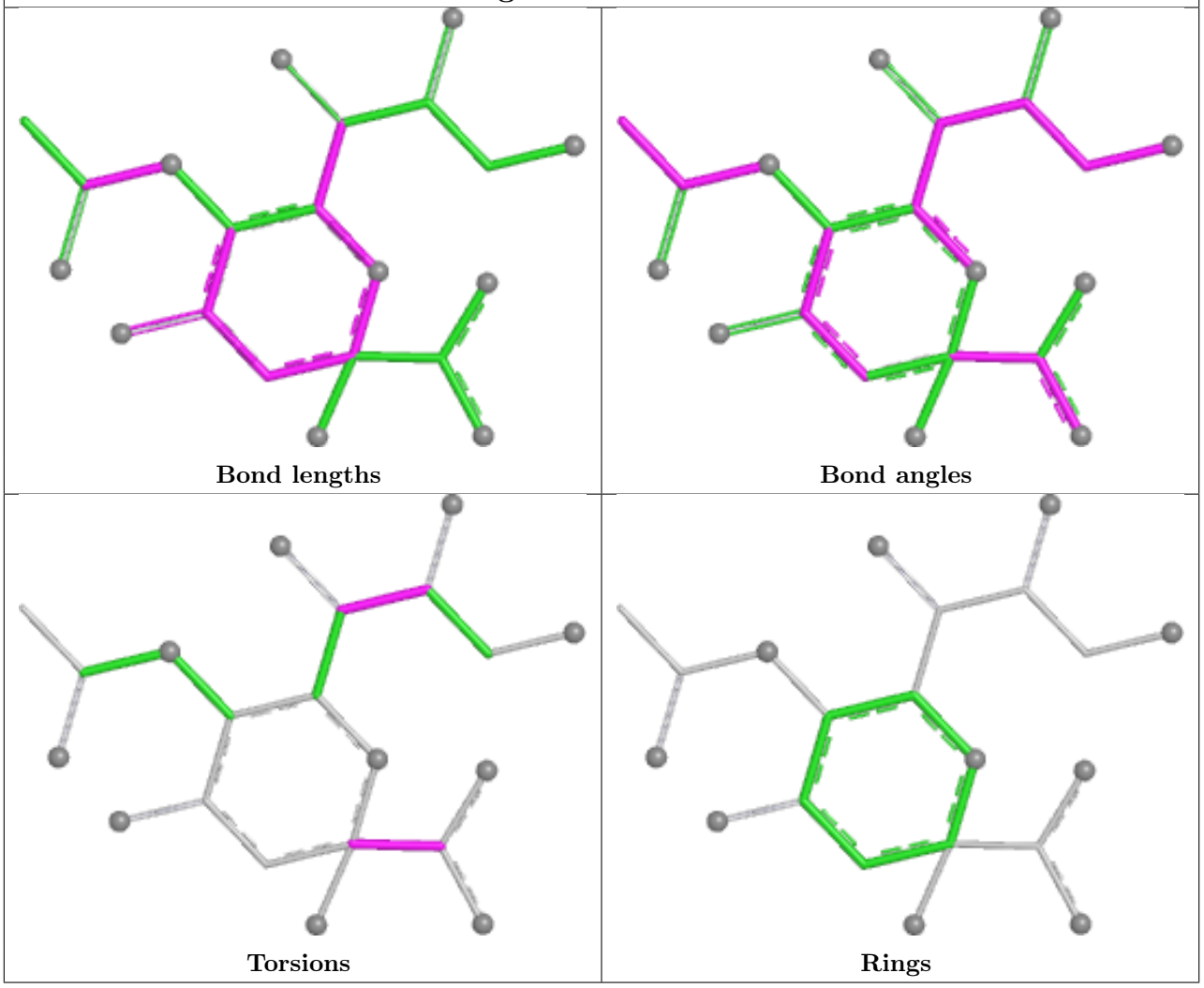


Torsions



Rings

Ligand SIA A 604



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	322/322 (100%)	0.02	2 (0%) 89 90	25, 48, 75, 112	0
1	C	322/322 (100%)	0.05	3 (0%) 84 86	29, 56, 85, 146	0
1	E	322/322 (100%)	0.18	10 (3%) 49 51	28, 55, 92, 140	0
2	B	175/175 (100%)	0.51	11 (6%) 20 20	28, 62, 97, 143	0
2	D	175/175 (100%)	0.98	29 (16%) 1 1	28, 76, 120, 165	0
2	F	175/175 (100%)	0.87	24 (13%) 3 2	29, 79, 137, 198	0
All	All	1491/1491 (100%)	0.33	79 (5%) 26 27	25, 56, 107, 198	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	507	ILE	10.0
2	F	502	LEU	9.3
2	F	507	ILE	8.4
1	C	325	PRO	6.5
1	E	325	PRO	6.2
2	F	474	PHE	6.2
2	F	508	SER	5.9
2	B	509	GLY	5.7
2	F	475	TYR	5.6
2	B	508	SER	5.6
2	D	508	SER	5.4
2	D	460	LEU	5.1
1	E	4	GLN	4.4
2	F	509	GLY	4.3
2	F	483	MET	4.2
2	D	491	TYR	3.9
2	D	335	GLY	3.8
2	D	492	ASP	3.8
2	D	369	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	481	GLU	3.7
2	D	363	GLU	3.7
2	D	367	GLY	3.7
2	F	498	GLU	3.6
2	D	474	PHE	3.5
2	D	509	GLY	3.4
2	F	491	TYR	3.4
2	D	486	VAL	3.3
1	E	67	GLY	3.3
1	E	74	PHE	3.2
2	D	496	TYR	3.2
2	D	365	GLY	3.2
2	F	506	GLU	3.0
2	F	493	TYR	3.0
2	B	353	ASP	2.9
1	E	72	ASP	2.9
2	B	335	GLY	2.9
2	D	495	GLN	2.8
2	D	340	ILE	2.8
2	F	504	ARG	2.8
2	D	350	GLY	2.8
2	B	507	ILE	2.7
1	C	17	THR	2.7
2	D	366	SER	2.7
2	F	492	ASP	2.6
2	B	363	GLU	2.6
1	A	15	ASN	2.6
2	D	370	ALA	2.5
2	F	496	TYR	2.5
1	E	149	ARG	2.5
1	E	186	ASN	2.4
1	C	7	ILE	2.4
2	F	460	LEU	2.4
1	A	325	PRO	2.4
2	D	355	TRP	2.4
2	F	355	TRP	2.4
2	F	335	GLY	2.4
2	D	433	LEU	2.4
2	B	367	GLY	2.4
1	E	70	MET	2.3
1	E	131	ALA	2.3
2	F	349	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	476	HIS	2.3
2	F	363	GLU	2.3
2	D	336	LEU	2.2
2	D	372	LYS	2.2
2	D	506	GLU	2.2
2	D	436	MET	2.2
1	E	182	ILE	2.2
2	B	450	LYS	2.2
2	F	486	VAL	2.2
2	B	440	ARG	2.1
2	F	482	CYS	2.1
2	D	479	ASP	2.1
2	B	452	LEU	2.1
2	D	502	LEU	2.1
2	D	361	SER	2.1
2	F	440	ARG	2.0
2	F	463	ASN	2.0
2	B	483	MET	2.0

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

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

6.3 Carbohydrates (i)

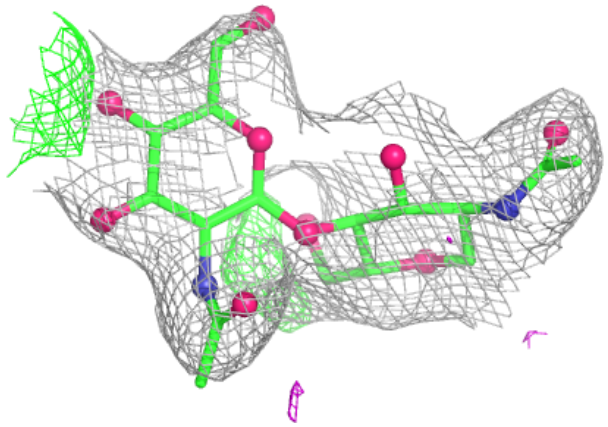
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

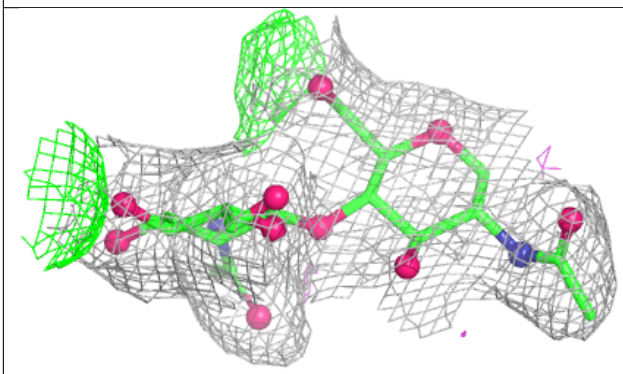
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	I	2	14/15	0.82	0.25	86,100,106,111	0
3	NAG	H	2	14/15	0.85	0.37	111,116,120,121	0
3	NAG	G	2	14/15	0.89	0.13	58,72,76,82	0
3	NAG	H	1	14/15	0.90	0.18	72,87,95,100	0
3	NAG	I	1	14/15	0.93	0.15	57,73,84,90	0
3	NAG	G	1	14/15	0.94	0.12	38,50,60,62	0

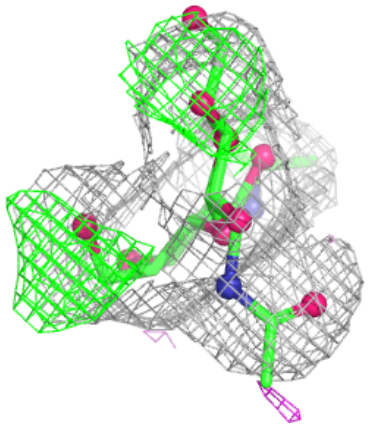
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

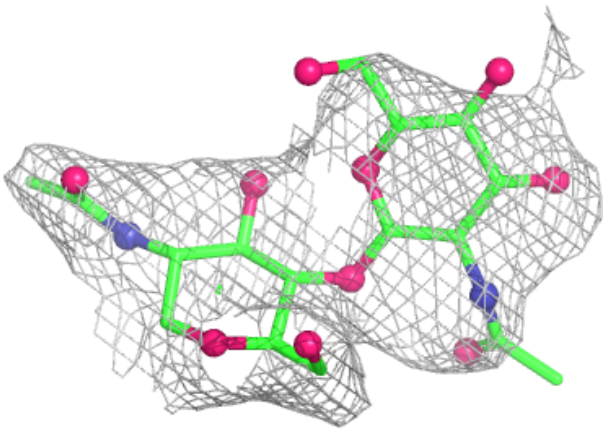


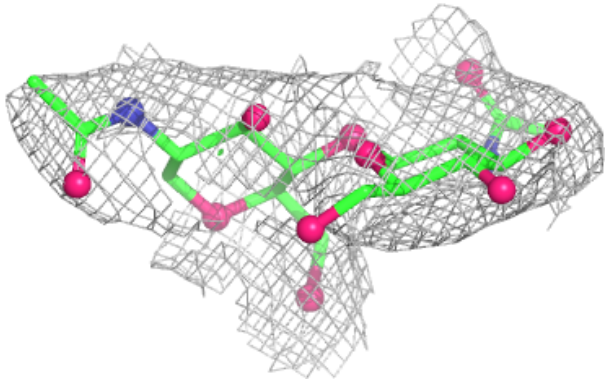


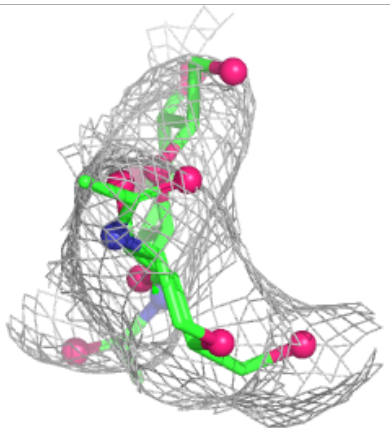


Electron density around Chain H:

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

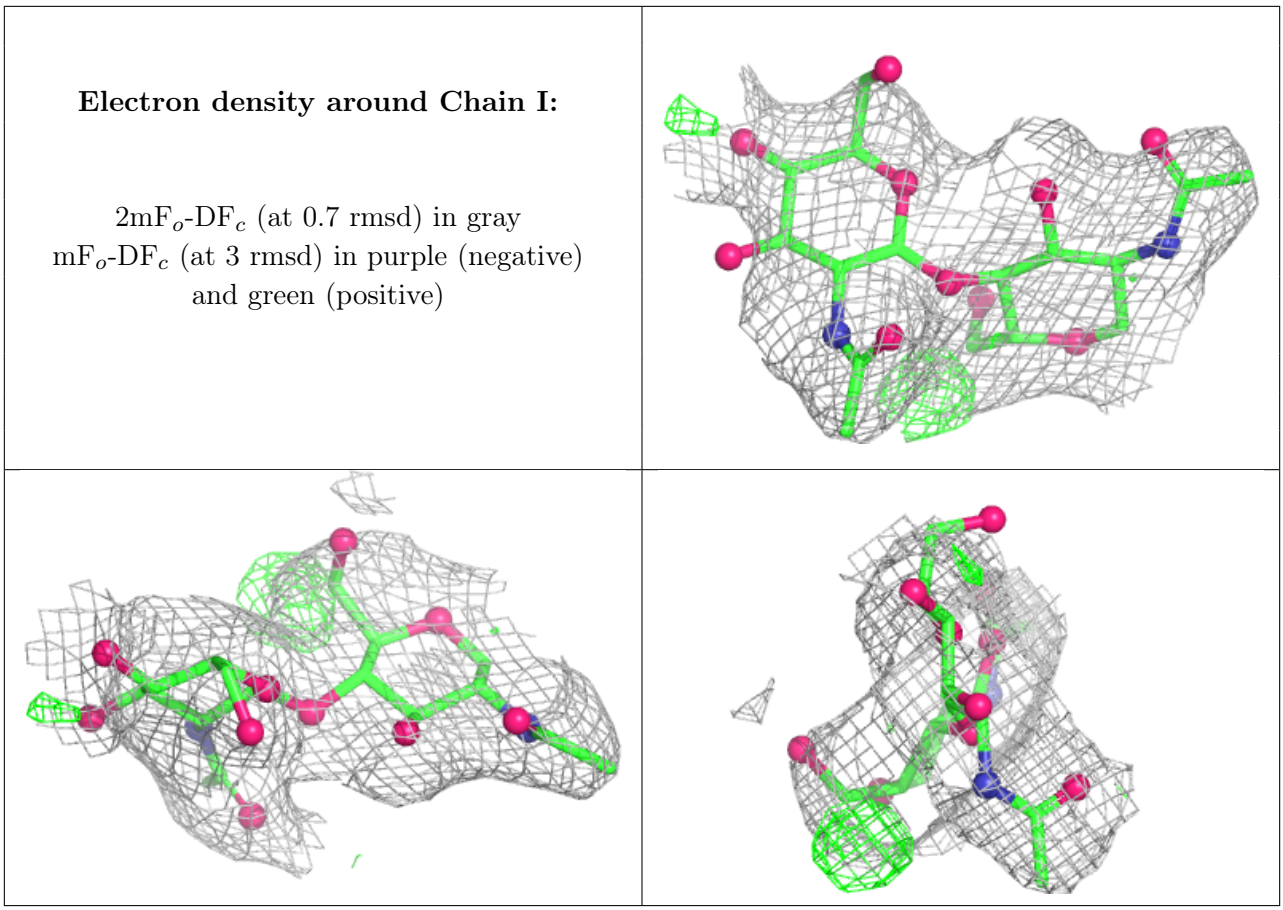






Electron density around Chain I:

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



6.4 Ligands

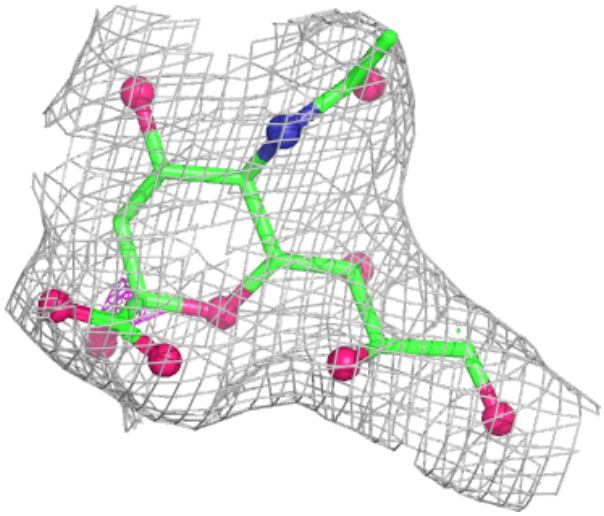
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

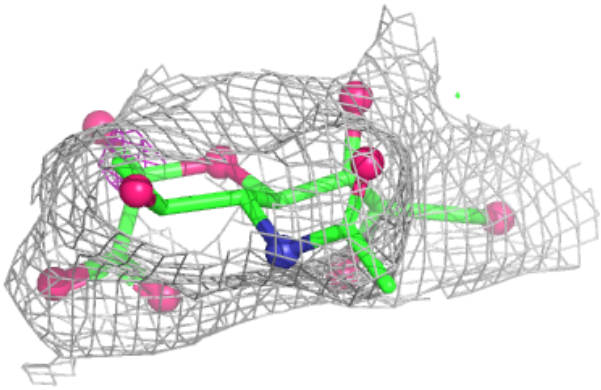
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	E	601	14/15	0.81	0.31	100,107,113,120	0
4	NAG	C	601	14/15	0.87	0.14	110,114,120,120	0
5	SIA	A	604	21/21	0.89	0.13	57,69,80,83	0
5	SIA	C	604	21/21	0.89	0.24	74,84,89,91	0
4	NAG	A	601	14/15	0.90	0.25	78,86,90,92	0

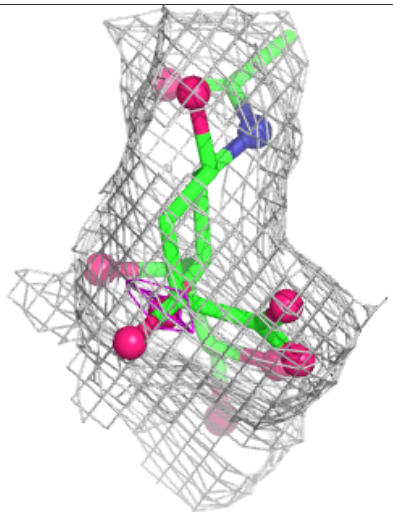
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SIA A 604:

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

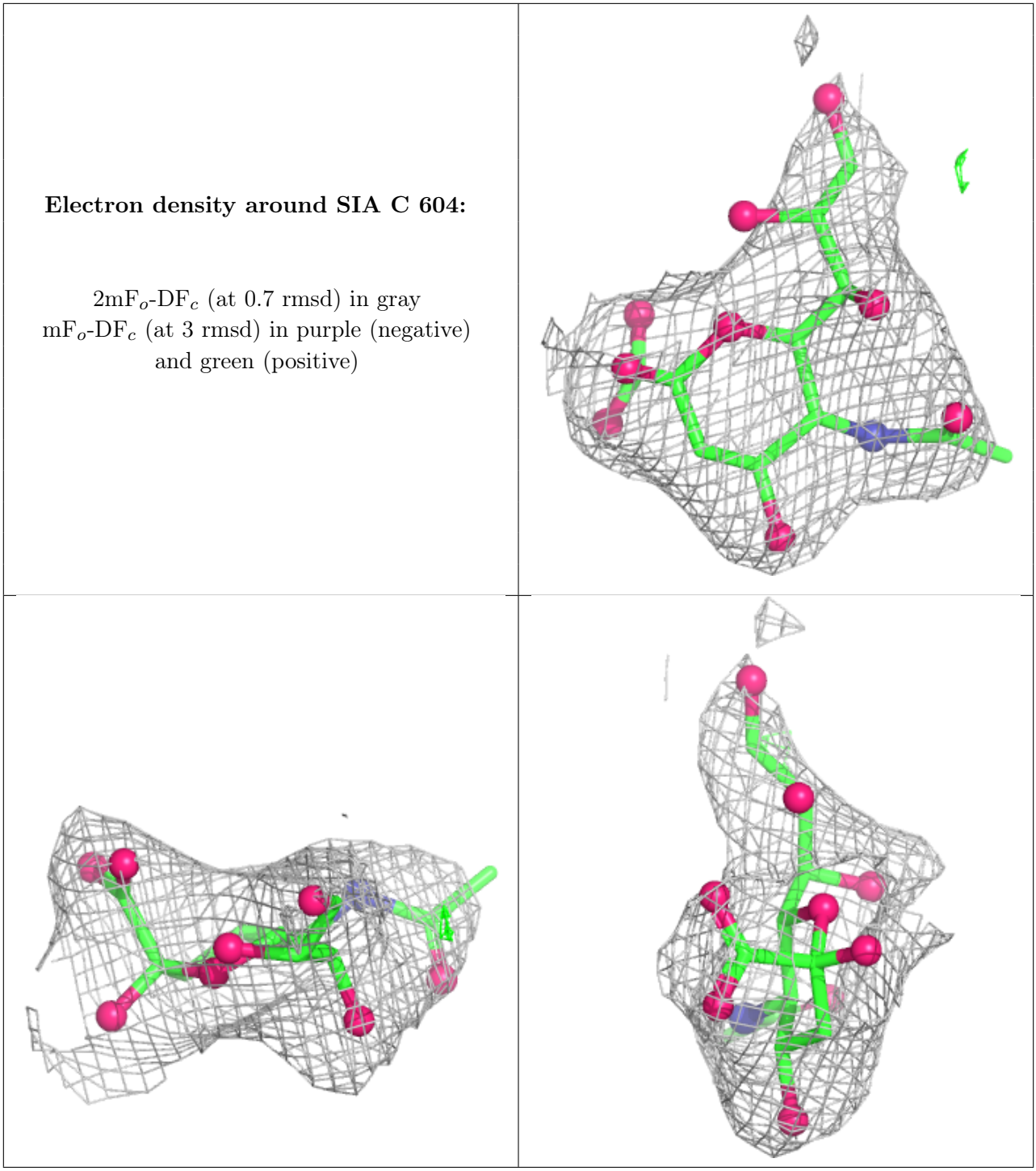






Electron density around SIA C 604:

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



6.5 Other polymers

There are no such residues in this entry.