Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 08:17 PM EDT

PDB ID	:	6TVR
Title	:	Crystal structure of the haemagglutinin mutant (Gln226Leu) from an H10N7 seal influenza virus isolated in Germany
Authors	:	Zhang, J.; Xiong, X.; Purkiss, A.; Walker, P.; Gamblin, S.; Skehel, J.J.
Deposited on	:	2020-01-10
Resolution	:	2.63 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 (i) 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 (i)) were used in the production of this report:

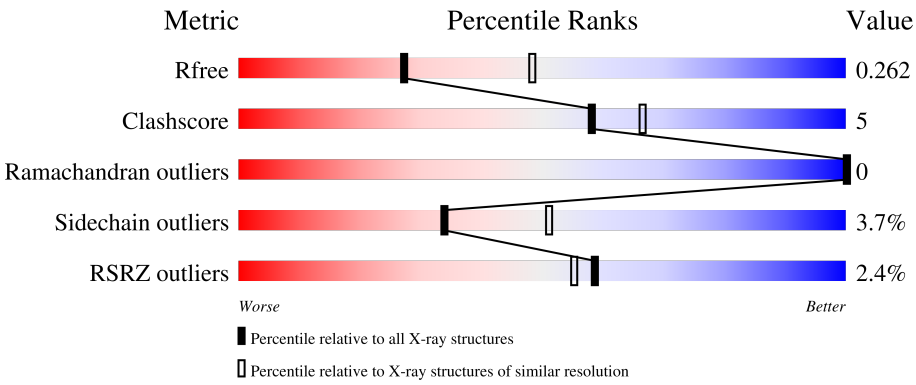
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.63 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	325	90% 9% •
1	C	325	% 89% 9% • •
1	E	325	3% 83% 14% • •
1	G	325	8% 82% 15% • •
1	I	325	8% 82% 16% •

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Mol	Chain	Length	Quality of chain
1	K	325	%, 90%, 8%
2	B	177	88%, 10%
2	D	177	88%, 9%
2	F	177	%, 84%, 14%
2	H	177	88%, 8%
2	J	177	%, 89%, 8%
2	L	177	%, 91%, 6%
3	M	2	50%, 50%
3	N	2	100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 23416 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 HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	321	2450	1521	443	470	16	0	0	0
1	C	320	2442	1515	442	469	16	0	0	0
1	E	320	2442	1515	442	469	16	0	0	0
1	G	319	2434	1511	441	466	16	0	0	0
1	I	319	2435	1512	440	467	16	0	0	0
1	K	320	2442	1515	442	469	16	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ASP	-	expression tag	UNP A0A0A7HR51
A	2	PRO	-	expression tag	UNP A0A0A7HR51
C	1	ASP	-	expression tag	UNP A0A0A7HR51
C	2	PRO	-	expression tag	UNP A0A0A7HR51
E	1	ASP	-	expression tag	UNP A0A0A7HR51
E	2	PRO	-	expression tag	UNP A0A0A7HR51
G	0	ASP	-	expression tag	UNP A0A0A7HR51
G	1	PRO	-	expression tag	UNP A0A0A7HR51
I	1	ASP	-	expression tag	UNP A0A0A7HR51
I	2	PRO	-	expression tag	UNP A0A0A7HR51
K	1	ASP	-	expression tag	UNP A0A0A7HR51
K	2	PRO	-	expression tag	UNP A0A0A7HR51

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	172	1383	855	240	280	8	0	0	0
2	D	172	1383	855	240	280	8	0	0	0
2	F	172	1383	855	240	280	8	0	0	0
2	H	172	1383	855	240	280	8	0	0	0
2	J	172	1383	855	240	280	8	0	0	0
2	L	172	1383	855	240	280	8	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	LYS	-	expression tag	UNP A0A0A7HR51
D	177	LYS	-	expression tag	UNP A0A0A7HR51
F	177	LYS	-	expression tag	UNP A0A0A7HR51
H	177	LYS	-	expression tag	UNP A0A0A7HR51
J	177	LYS	-	expression tag	UNP A0A0A7HR51
L	177	LYS	-	expression tag	UNP A0A0A7HR51

- 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
			Total	C	N	O			
3	M	2	28	16	2	10	0	0	0
3	N	2	28	16	2	10	0	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	1	1	1	0	0
4	D	2	2	2	0	0

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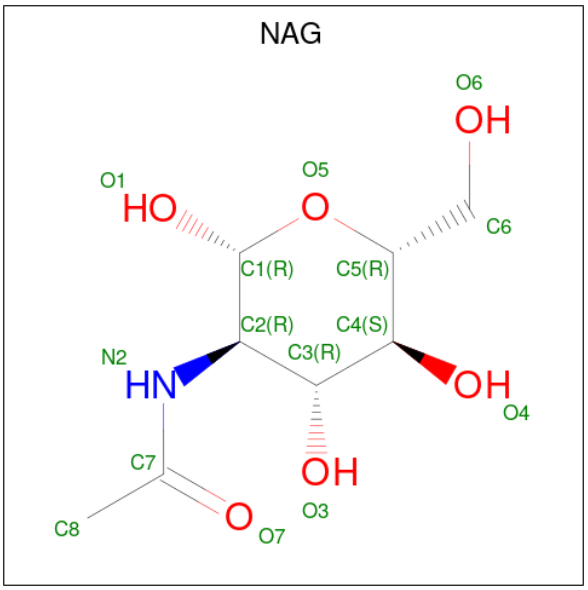
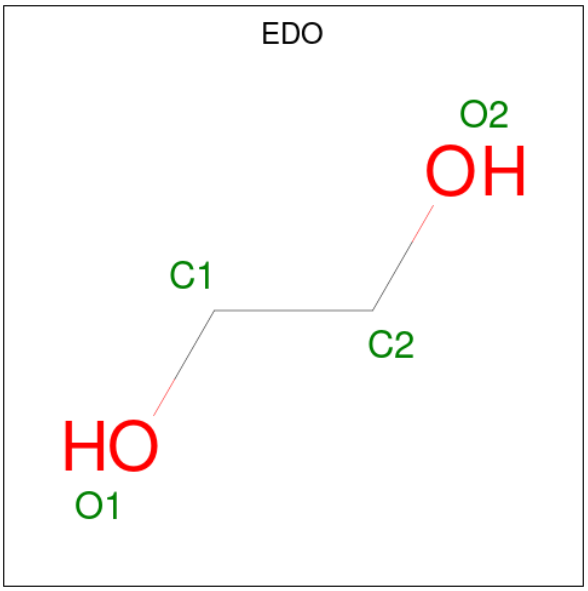
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	G	1	1	1	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	14	8	1	5	0	0
5	F	1	14	8	1	5	0	0
5	H	1	14	8	1	5	0	0
5	I	1	14	8	1	5	0	0
5	J	1	14	8	1	5	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	K	1	4	2	2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	42	42	42	0	0
7	B	37	37	37	0	0
7	C	26	26	26	0	0
7	D	34	34	34	0	0
7	E	16	16	16	0	0
7	F	17	17	17	0	0
7	G	22	22	22	0	0
7	H	30	30	30	0	0
7	I	17	17	17	0	0
7	J	18	18	18	0	0
7	K	51	51	51	0	0

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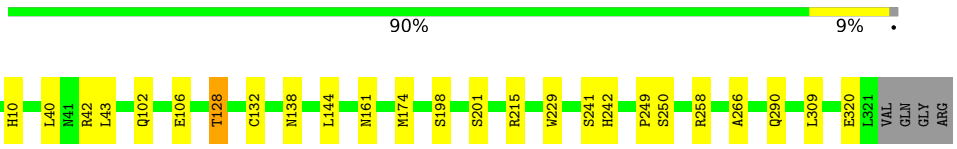
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	L	29	29	29	0	0

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.

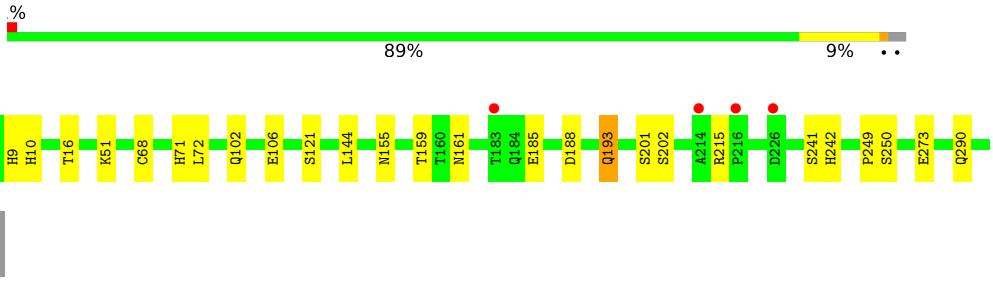
• Molecule 1: Hemagglutinin HA1

Chain A:



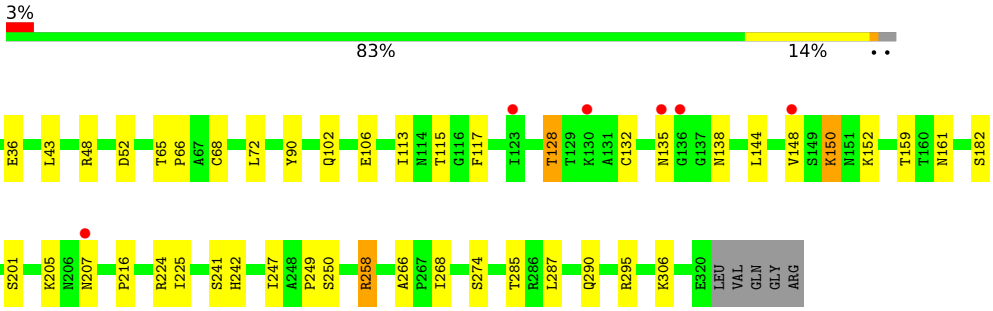
• Molecule 1: Hemagglutinin HA1

Chain C:



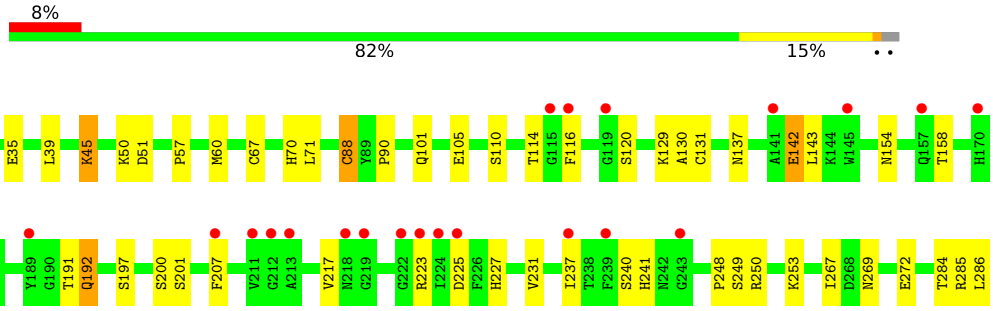
• Molecule 1: Hemagglutinin HA1

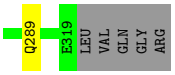
Chain E:



• Molecule 1: Hemagglutinin HA1

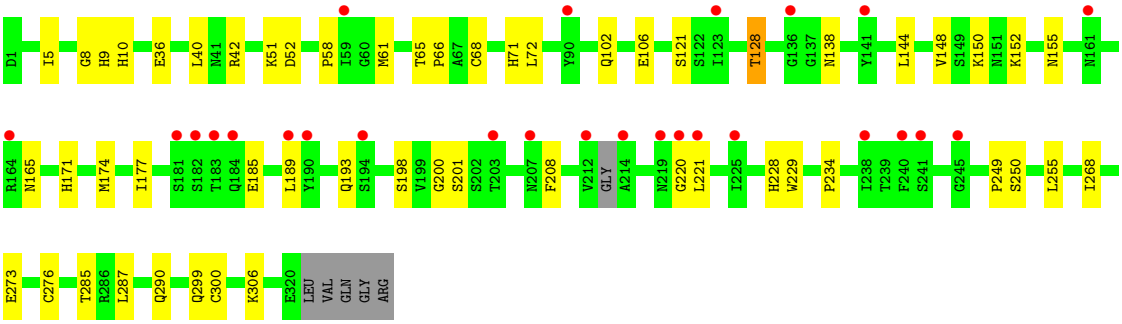
Chain G:





• Molecule 1: Hemagglutinin HA1

Chain I:

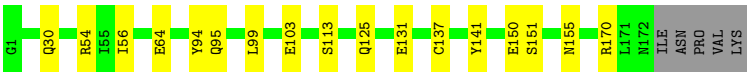


• Molecule 1: Hemagglutinin HA1

Chain K:

• Molecule 2: Hemagglutinin HA2

Chain B:

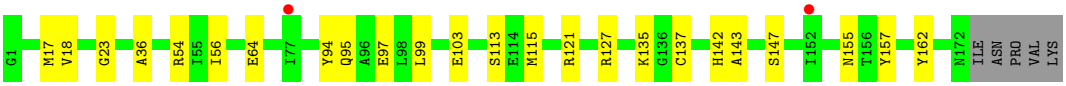


• Molecule 2: Hemagglutinin HA2

Chain D:

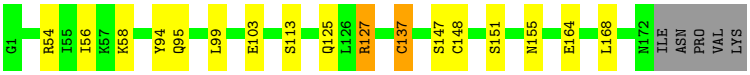
• Molecule 2: Hemagglutinin HA2

Chain F:



• Molecule 2: Hemagglutinin HA2

Chain H:

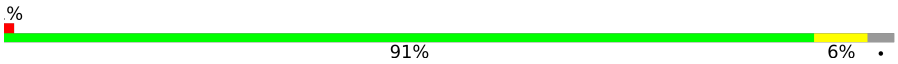


• Molecule 2: Hemagglutinin HA2

Chain J:

• Molecule 2: Hemagglutinin HA2

Chain L:

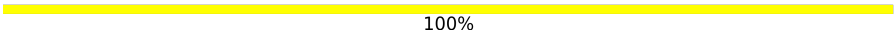


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

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

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.35Å 214.10Å 157.16Å 90.00° 102.06° 90.00°	Depositor
Resolution (Å)	72.33 – 2.63 72.33 – 2.63	Depositor EDS
% Data completeness (in resolution range)	100.0 (72.33-2.63) 100.0 (72.33-2.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.241 , 0.264 0.239 , 0.262	Depositor DCC
R_{free} test set	6486 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	48.8	Xtriage
Anisotropy	0.775	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 32.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	23416	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6327e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, EDO

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	0.65	0/2500	0.76	0/3388
1	C	0.66	0/2492	0.78	0/3377
1	E	0.66	0/2492	0.77	0/3377
1	G	0.66	0/2484	0.79	0/3365
1	I	0.67	0/2484	0.78	0/3365
1	K	0.65	0/2492	0.76	0/3377
2	B	0.65	0/1408	0.72	0/1900
2	D	0.64	0/1408	0.72	0/1900
2	F	0.65	0/1408	0.72	0/1900
2	H	0.64	0/1408	0.74	0/1900
2	J	0.65	0/1408	0.72	0/1900
2	L	0.65	0/1408	0.72	0/1900
All	All	0.65	0/23392	0.76	0/31649

There are no bond length outliers.

There are no bond angle outliers.

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	2450	0	2410	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2442	0	2399	18	0
1	E	2442	0	2399	44	0
1	G	2434	0	2395	38	0
1	I	2435	0	2390	46	0
1	K	2442	0	2399	15	0
2	B	1383	0	1282	10	0
2	D	1383	0	1282	14	0
2	F	1383	0	1282	24	0
2	H	1383	0	1282	9	0
2	J	1383	0	1282	15	0
2	L	1383	0	1282	8	0
3	M	28	0	25	1	0
3	N	28	0	25	0	0
4	A	1	0	0	0	0
4	D	2	0	0	0	0
4	G	1	0	0	0	0
5	B	14	0	13	0	0
5	F	14	0	13	0	0
5	H	14	0	13	0	0
5	I	14	0	13	0	0
5	J	14	0	13	0	0
6	K	4	0	6	0	0
7	A	42	0	0	0	0
7	B	37	0	0	0	0
7	C	26	0	0	0	0
7	D	34	0	0	0	0
7	E	16	0	0	0	0
7	F	17	0	0	1	0
7	G	22	0	0	1	0
7	H	30	0	0	1	0
7	I	17	0	0	0	0
7	J	18	0	0	0	0
7	K	51	0	0	1	0
7	L	29	0	0	0	0
All	All	23416	0	22205	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 5.

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)
1:E:90:TYR:CE1	1:E:225:ILE:HD13	1.81	1.16
1:E:90:TYR:CD1	1:E:225:ILE:HD13	2.01	0.96
1:I:276:CYS:SG	1:I:299:GLN:O	2.31	0.89
1:E:90:TYR:CE1	1:E:225:ILE:CD1	2.58	0.85
1:E:207:ASN:HB2	1:K:211:VAL:HG21	1.59	0.82
1:I:285:THR:HG22	1:I:287:LEU:H	1.45	0.82
1:G:88:CYS:SG	1:G:131:CYS:N	2.54	0.81
1:G:176:ILE:HD13	1:G:207:PHE:HB3	1.62	0.81
1:E:285:THR:HG22	1:E:287:LEU:H	1.44	0.81
1:I:177:ILE:HD13	1:I:208:PHE:HB3	1.63	0.80
1:G:284:THR:HG22	1:G:286:LEU:H	1.46	0.79
1:C:155:ASN:HD21	1:C:193:GLN:HB3	1.51	0.75
2:F:17:MET:CE	2:F:36:ALA:HA	2.18	0.73
1:I:276:CYS:SG	1:I:299:GLN:C	2.66	0.73
1:A:128:THR:CG2	1:A:138:ASN:HB3	2.20	0.71
2:F:17:MET:HE1	2:F:36:ALA:HA	1.71	0.71
1:I:9:HIS:HB3	2:J:115:MET:CE	2.21	0.71
1:I:128:THR:CG2	1:I:138:ASN:HB3	2.19	0.70
1:I:148:VAL:HG23	1:I:189:LEU:HG	1.73	0.70
1:E:9:HIS:HB3	2:F:115:MET:CE	2.22	0.70
1:G:231:VAL:HG22	1:G:237:ILE:CD1	2.22	0.69
1:C:9:HIS:HB3	2:D:115:MET:CE	2.22	0.69
1:E:225:ILE:HG23	1:E:247:ILE:HD12	1.75	0.69
1:E:128:THR:CG2	1:E:138:ASN:HB3	2.23	0.69
1:G:176:ILE:HD12	1:G:227:HIS:CE1	2.28	0.68
1:G:88:CYS:SG	1:G:130:ALA:C	2.72	0.68
1:I:58:PRO:O	1:I:61:MET:HG2	1.93	0.68
1:E:43:LEU:HD13	1:E:266:ALA:O	1.94	0.68
1:K:115:THR:HG21	1:K:249:PRO:O	1.94	0.67
1:G:57:PRO:O	1:G:60:MET:HG2	1.94	0.67
1:E:115:THR:HG21	1:E:249:PRO:O	1.96	0.66
1:G:176:ILE:HD11	1:G:207:PHE:CG	2.31	0.66
1:A:43:LEU:HD23	1:A:266:ALA:O	1.96	0.66
1:I:177:ILE:HD12	1:I:228:HIS:CE1	2.31	0.66
1:G:114:THR:HG21	1:G:248:PRO:O	1.96	0.65
1:I:177:ILE:HD11	1:I:208:PHE:CG	2.32	0.64
2:D:95:GLN:NE2	2:F:95:GLN:OE1	2.31	0.64
1:G:231:VAL:HG22	1:G:237:ILE:HD11	1.78	0.64
2:F:142:HIS:HE1	2:F:157:TYR:OH	1.79	0.63
1:K:115:THR:HG23	1:K:117:PHE:H	1.63	0.63
1:A:258:ARG:NH2	2:B:64:GLU:OE1	2.32	0.63
1:E:115:THR:HG23	1:E:117:PHE:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:GLU:OE2	2:B:170:ARG:HD2	2.00	0.62
1:I:148:VAL:CG2	1:I:189:LEU:HG	2.30	0.61
1:E:43:LEU:CD1	1:E:266:ALA:HB3	2.31	0.61
2:F:56:ILE:O	2:F:56:ILE:HG22	2.02	0.60
1:E:205:LYS:HD3	1:K:224:ARG:HG3	1.84	0.60
2:F:127:ARG:NH2	2:L:139:GLU:OE1	2.24	0.60
1:G:114:THR:HG23	1:G:116:PHE:H	1.64	0.60
2:L:56:ILE:HG22	2:L:56:ILE:O	2.02	0.60
1:C:9:HIS:HB3	2:D:115:MET:HE1	1.83	0.59
2:F:18:VAL:HG12	2:F:18:VAL:O	2.01	0.59
1:G:50:LYS:HE2	1:G:70:HIS:CE1	2.37	0.59
1:I:9:HIS:HB3	2:J:115:MET:HE1	1.84	0.59
2:F:143:ALA:N	7:F:301:HOH:O	2.33	0.59
1:I:52:ASP:OD2	1:I:268:ILE:HD11	2.03	0.59
1:K:258:ARG:NH2	2:L:64:GLU:OE1	2.36	0.59
2:H:56:ILE:HG22	2:H:56:ILE:O	2.03	0.58
1:K:96:ASN:ND2	7:K:501:HOH:O	2.37	0.58
1:G:154:ASN:CG	1:G:192:GLN:HG3	2.23	0.58
1:E:225:ILE:HG13	1:E:247:ILE:HD11	1.85	0.57
1:E:207:ASN:HB2	1:K:211:VAL:CG2	2.31	0.57
1:E:161:ASN:HD22	1:E:242:HIS:HE1	1.52	0.57
2:L:51:LYS:HE3	2:L:103:GLU:OE1	2.04	0.57
2:D:56:ILE:O	2:D:56:ILE:HG22	2.04	0.57
2:F:99:LEU:HD22	2:L:94:TYR:OH	2.04	0.57
2:B:94:TYR:OH	2:J:99:LEU:HD22	2.05	0.57
1:E:225:ILE:CG2	1:E:247:ILE:HD12	2.35	0.56
2:B:56:ILE:HG22	2:B:56:ILE:O	2.04	0.56
1:G:35:GLU:HG2	1:G:284:THR:OG1	2.06	0.56
1:G:200:SER:HB2	1:G:237:ILE:HG12	1.87	0.56
1:G:284:THR:CG2	1:G:286:LEU:HG	2.35	0.56
2:J:56:ILE:HG22	2:J:56:ILE:O	2.06	0.56
1:A:43:LEU:CD2	1:A:266:ALA:HB3	2.35	0.56
1:E:9:HIS:HB3	2:F:115:MET:HE1	1.88	0.56
2:H:125:GLN:CD	2:H:155:ASN:HD22	2.09	0.56
1:I:36:GLU:HG2	1:I:285:THR:OG1	2.06	0.55
1:C:161:ASN:HD22	1:C:242:HIS:HE1	1.53	0.55
1:E:306:LYS:HE3	2:F:97:GLU:OE1	2.07	0.55
1:G:176:ILE:HD13	1:G:207:PHE:CB	2.36	0.55
1:G:176:ILE:CD1	1:G:207:PHE:CG	2.90	0.55
1:A:161:ASN:HD22	1:A:242:HIS:HE1	1.52	0.55
1:I:5:ILE:HD12	2:J:149:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:155:ASN:ND2	1:I:193:GLN:HB3	2.22	0.54
1:E:36:GLU:HG2	1:E:285:THR:OG1	2.06	0.54
2:H:99:LEU:HD22	2:J:94:TYR:OH	2.08	0.54
1:I:177:ILE:CD1	1:I:208:PHE:CG	2.91	0.54
1:I:285:THR:CG2	1:I:287:LEU:HG	2.38	0.54
2:F:17:MET:CE	2:F:23:GLY:HA3	2.37	0.54
2:H:127:ARG:HG3	7:H:308:HOH:O	2.09	0.53
1:G:101:GLN:O	1:G:105:GLU:HG3	2.09	0.53
1:E:258:ARG:NH2	2:F:64:GLU:OE2	2.42	0.53
1:G:50:LYS:HE2	1:G:70:HIS:ND1	2.24	0.53
1:A:102:GLN:O	1:A:106:GLU:HG3	2.09	0.53
1:I:177:ILE:HD13	1:I:208:PHE:CB	2.37	0.53
1:G:110:SER:OG	1:G:253:LYS:HB3	2.09	0.52
1:E:285:THR:CG2	1:E:287:LEU:HG	2.40	0.52
1:G:154:ASN:OD1	1:G:192:GLN:HG3	2.10	0.52
1:I:306:LYS:HE3	2:J:97:GLU:OE2	2.09	0.52
1:C:51:LYS:HE3	1:C:71:HIS:ND1	2.25	0.51
1:A:43:LEU:HD22	1:A:266:ALA:HB3	1.92	0.51
1:K:102:GLN:O	1:K:106:GLU:HG3	2.11	0.51
1:I:51:LYS:HE3	1:I:71:HIS:ND1	2.25	0.51
1:I:220:GLY:C	1:I:221:LEU:HD22	2.31	0.51
1:C:319:PRO:O	1:C:320:GLU:HB2	2.11	0.50
2:D:99:LEU:HD22	2:F:94:TYR:OH	2.11	0.50
2:F:142:HIS:CE1	2:F:157:TYR:OH	2.63	0.50
1:G:142:GLU:HG3	1:G:250:ARG:HB2	1.94	0.49
1:E:148:VAL:HG21	1:E:189:LEU:HD22	1.93	0.49
1:I:155:ASN:HD21	1:I:193:GLN:HB3	1.78	0.49
1:A:161:ASN:ND2	1:A:242:HIS:HE1	2.11	0.49
2:B:54:ARG:NH2	2:B:103:GLU:OE2	2.43	0.49
1:I:9:HIS:HB3	2:J:115:MET:HE2	1.94	0.49
1:E:9:HIS:HB3	2:F:115:MET:HE2	1.95	0.49
1:I:220:GLY:O	1:I:221:LEU:HD22	2.12	0.49
2:L:54:ARG:NH2	2:L:103:GLU:OE2	2.42	0.49
1:G:158:THR:HG23	1:G:241:HIS:NE2	2.27	0.49
1:K:152:LYS:HE3	1:K:188:ASP:OD1	2.12	0.49
2:B:125:GLN:HE22	2:B:155:ASN:HA	1.78	0.48
1:K:148:VAL:HG12	1:K:149:SER:O	2.13	0.48
1:E:102:GLN:O	1:E:106:GLU:HG3	2.13	0.48
2:J:125:GLN:HE22	2:J:155:ASN:HA	1.78	0.48
2:F:17:MET:HE3	2:F:23:GLY:HA3	1.94	0.48
2:L:51:LYS:HE2	2:L:107:THR:OG1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:GLU:O	2:D:168:LEU:HD23	2.13	0.47
1:I:5:ILE:HD13	2:J:152:ILE:HG21	1.96	0.47
2:B:95:GLN:HG2	2:J:95:GLN:HE21	1.78	0.47
1:C:201:SER:C	1:E:216:PRO:HD2	2.35	0.47
1:I:121:SER:O	1:I:150:LYS:HE2	2.15	0.47
2:D:54:ARG:NH2	2:D:103:GLU:OE2	2.42	0.47
1:G:129:LYS:HD3	1:G:137:ASN:HD21	1.80	0.47
1:I:68:CYS:O	1:I:72:LEU:CD1	2.63	0.47
1:E:43:LEU:HD12	1:E:266:ALA:HB3	1.97	0.46
1:E:48:ARG:NH1	1:E:274:SER:O	2.48	0.46
1:G:67:CYS:O	1:G:71:LEU:CD1	2.63	0.46
1:C:68:CYS:O	1:C:72:LEU:CD1	2.64	0.46
1:A:1:ASP:N	1:A:2:PRO:CD	2.78	0.46
2:D:94:TYR:OH	2:L:99:LEU:HD22	2.16	0.46
1:G:39:LEU:HD12	1:G:39:LEU:N	2.31	0.46
2:H:54:ARG:NH2	2:H:103:GLU:OE1	2.44	0.46
1:E:68:CYS:O	1:E:72:LEU:HD13	2.16	0.46
1:E:224:ARG:C	1:E:225:ILE:HD12	2.36	0.46
2:H:164:GLU:O	2:H:168:LEU:HD23	2.15	0.46
1:I:177:ILE:HD11	1:I:208:PHE:CD1	2.51	0.46
1:C:9:HIS:HB3	2:D:115:MET:HE2	1.97	0.46
1:G:45:LYS:HG3	1:G:269:ASN:O	2.15	0.46
1:I:5:ILE:HB	2:J:149:MET:HE1	1.98	0.46
1:C:201:SER:OG	1:C:202:SER:N	2.48	0.46
1:I:102:GLN:O	1:I:106:GLU:HG3	2.16	0.46
1:I:68:CYS:O	1:I:72:LEU:HD13	2.16	0.46
1:E:150:LYS:O	1:E:150:LYS:HD3	2.16	0.45
1:I:144:LEU:HD23	1:I:249:PRO:HA	1.99	0.45
1:C:144:LEU:HD23	1:C:249:PRO:HA	1.98	0.45
1:E:43:LEU:HD11	1:E:266:ALA:HB3	1.99	0.45
3:M:2:NAG:H3	3:M:2:NAG:H83	1.99	0.45
2:B:99:LEU:HD22	2:H:94:TYR:OH	2.16	0.45
1:E:68:CYS:O	1:E:72:LEU:CD1	2.65	0.45
1:K:1:ASP:N	1:K:2:PRO:CD	2.78	0.45
1:C:161:ASN:ND2	1:C:242:HIS:HE1	2.14	0.45
1:E:52:ASP:HB2	1:E:268:ILE:HD11	1.97	0.45
1:G:200:SER:OG	1:G:201:SER:N	2.49	0.45
1:K:52:ASP:HB2	1:K:268:ILE:HD11	1.99	0.45
2:F:18:VAL:O	2:F:18:VAL:CG1	2.65	0.45
1:C:1:ASP:N	1:C:2:PRO:CD	2.80	0.45
1:E:6:CYS:HA	2:F:137:CYS:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:HD23	1:A:249:PRO:HA	1.98	0.44
1:C:9:HIS:HA	2:D:21:TRP:O	2.17	0.44
1:C:102:GLN:O	1:C:106:GLU:HG3	2.17	0.44
1:E:144:LEU:HD23	1:E:249:PRO:HA	1.98	0.44
1:G:143:LEU:HD23	1:G:248:PRO:HA	1.98	0.44
1:G:3:LYS:HG2	2:H:137:CYS:SG	2.58	0.44
1:I:165:ASN:OD1	1:I:171:HIS:CG	2.71	0.44
2:F:17:MET:CE	2:F:36:ALA:CA	2.93	0.44
1:K:144:LEU:HD23	1:K:249:PRO:HA	1.98	0.44
1:I:165:ASN:HD22	1:I:234:PRO:HA	1.81	0.44
2:D:148:CYS:O	2:D:151:SER:OG	2.27	0.43
1:E:65:THR:HG22	1:E:66:PRO:HD2	1.99	0.43
1:E:207:ASN:CB	1:K:211:VAL:HG21	2.38	0.43
2:J:54:ARG:NH2	2:J:103:GLU:OE2	2.43	0.43
1:E:161:ASN:ND2	1:E:242:HIS:HE1	2.14	0.43
1:K:121:SER:O	1:K:150:LYS:HE2	2.18	0.43
1:A:309:LEU:HD12	1:A:309:LEU:HA	1.87	0.43
2:B:141:TYR:CG	2:B:170:ARG:HG2	2.53	0.43
2:F:121:ARG:NH1	2:F:155:ASN:OD1	2.52	0.43
2:F:54:ARG:NH2	2:F:103:GLU:OE2	2.43	0.43
2:F:142:HIS:ND1	2:F:162:TYR:HB3	2.34	0.43
1:G:176:ILE:HD11	1:G:207:PHE:CD1	2.54	0.43
1:C:4:LYS:HG2	2:D:137:CYS:SG	2.59	0.42
1:C:68:CYS:O	1:C:72:LEU:HD13	2.19	0.42
1:I:36:GLU:HB2	1:I:285:THR:HG21	2.01	0.42
1:G:51:ASP:HB2	1:G:267:ILE:HD11	2.01	0.42
1:I:276:CYS:SG	1:I:300:CYS:N	2.84	0.42
1:E:36:GLU:HB2	1:E:285:THR:HG21	2.02	0.42
1:C:7:LEU:CD2	2:D:118:LEU:HG	2.50	0.42
1:I:177:ILE:CD1	1:I:208:PHE:CD1	3.03	0.42
1:I:40:LEU:N	1:I:40:LEU:HD12	2.35	0.42
1:A:6:CYS:HA	2:B:137:CYS:HA	2.02	0.41
1:E:225:ILE:CG1	1:E:247:ILE:HD11	2.48	0.41
1:I:36:GLU:OE1	1:I:285:THR:CG2	2.68	0.41
1:A:215:ARG:HB3	1:I:200:GLY:HA3	2.01	0.41
1:E:36:GLU:OE1	1:E:285:THR:CG2	2.69	0.41
1:E:182:SER:HB2	1:E:184:GLN:HG2	2.02	0.41
1:I:5:ILE:HD12	2:J:149:MET:CE	2.48	0.41
1:G:35:GLU:HB2	1:G:284:THR:HG21	2.01	0.41
1:G:67:CYS:O	1:G:71:LEU:HD13	2.21	0.41
2:H:148:CYS:O	2:H:151:SER:OG	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HD12	1:A:40:LEU:N	2.36	0.41
1:G:90:PRO:HB3	1:G:217:VAL:HB	2.02	0.41
2:D:2:LEU:HD23	2:D:2:LEU:HA	1.93	0.41
1:E:128:THR:CG2	1:E:138:ASN:CB	2.98	0.41
1:G:35:GLU:OE1	1:G:284:THR:CG2	2.69	0.41
1:A:128:THR:HG23	1:A:138:ASN:HB3	2.01	0.40
1:I:65:THR:HG22	1:I:66:PRO:HD2	2.03	0.40
1:A:174:MET:HG2	1:A:229:TRP:HB3	2.03	0.40
1:I:177:ILE:HD12	1:I:228:HIS:HE1	1.84	0.40
1:G:101:GLN:HB2	7:G:514:HOH:O	2.20	0.40
1:I:8:GLY:C	2:J:115:MET:HE3	2.42	0.40
1:I:174:MET:HG2	1:I:229:TRP:HB3	2.03	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	319/325 (98%)	310 (97%)	9 (3%)	0	100	100
1	C	318/325 (98%)	309 (97%)	9 (3%)	0	100	100
1	E	318/325 (98%)	309 (97%)	9 (3%)	0	100	100
1	G	317/325 (98%)	309 (98%)	8 (2%)	0	100	100
1	I	315/325 (97%)	306 (97%)	9 (3%)	0	100	100
1	K	318/325 (98%)	310 (98%)	8 (2%)	0	100	100
2	B	170/177 (96%)	165 (97%)	5 (3%)	0	100	100
2	D	170/177 (96%)	165 (97%)	5 (3%)	0	100	100
2	F	170/177 (96%)	165 (97%)	5 (3%)	0	100	100
2	H	170/177 (96%)	165 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	170/177 (96%)	165 (97%)	5 (3%)	0	100	100
2	L	170/177 (96%)	165 (97%)	5 (3%)	0	100	100
All	All	2925/3012 (97%)	2843 (97%)	82 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	271/275 (98%)	260 (96%)	11 (4%)	30	47
1	C	270/275 (98%)	256 (95%)	14 (5%)	23	36
1	E	270/275 (98%)	256 (95%)	14 (5%)	23	36
1	G	269/275 (98%)	254 (94%)	15 (6%)	21	32
1	I	269/275 (98%)	258 (96%)	11 (4%)	30	47
1	K	270/275 (98%)	262 (97%)	8 (3%)	41	59
2	B	145/151 (96%)	141 (97%)	4 (3%)	43	61
2	D	145/151 (96%)	142 (98%)	3 (2%)	53	71
2	F	145/151 (96%)	142 (98%)	3 (2%)	53	71
2	H	145/151 (96%)	139 (96%)	6 (4%)	30	47
2	J	145/151 (96%)	143 (99%)	2 (1%)	67	80
2	L	145/151 (96%)	143 (99%)	2 (1%)	67	80
All	All	2489/2556 (97%)	2396 (96%)	93 (4%)	34	51

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	10	HIS
1	A	42	ARG
1	A	128	THR

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Mol	Chain	Res	Type
1	A	132	CYS
1	A	198	SER
1	A	201	SER
1	A	241	SER
1	A	250	SER
1	A	290	GLN
1	A	320	GLU
2	B	30	GLN
2	B	113	SER
2	B	150	GLU
2	B	151	SER
1	C	1	ASP
1	C	10	HIS
1	C	16	THR
1	C	121	SER
1	C	159	THR
1	C	185	GLU
1	C	188	ASP
1	C	193	GLN
1	C	215	ARG
1	C	241	SER
1	C	250	SER
1	C	273	GLU
1	C	290	GLN
1	C	320	GLU
2	D	113	SER
2	D	137	CYS
2	D	147	SER
1	E	10	HIS
1	E	113	ILE
1	E	128	THR
1	E	132	CYS
1	E	135	ASN
1	E	150	LYS
1	E	152	LYS
1	E	159	THR
1	E	201	SER
1	E	241	SER
1	E	250	SER
1	E	258	ARG
1	E	290	GLN
1	E	295	ARG

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Mol	Chain	Res	Type
2	F	113	SER
2	F	135	LYS
2	F	147	SER
1	G	9	HIS
1	G	45	LYS
1	G	88	CYS
1	G	120	SER
1	G	142	GLU
1	G	191	THR
1	G	192	GLN
1	G	197	SER
1	G	223	ARG
1	G	225	ASP
1	G	240	SER
1	G	249	SER
1	G	272	GLU
1	G	285	ARG
1	G	289	GLN
2	H	58	LYS
2	H	95	GLN
2	H	113	SER
2	H	127	ARG
2	H	137	CYS
2	H	147	SER
1	I	10	HIS
1	I	42	ARG
1	I	128	THR
1	I	152	LYS
1	I	185	GLU
1	I	198	SER
1	I	201	SER
1	I	250	SER
1	I	255	LEU
1	I	273	GLU
1	I	290	GLN
2	J	30	GLN
2	J	113	SER
1	K	5	ILE
1	K	10	HIS
1	K	42	ARG
1	K	188	ASP
1	K	198	SER

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Mol	Chain	Res	Type
1	K	201	SER
1	K	250	SER
1	K	290	GLN
2	L	30	GLN
2	L	113	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	161	ASN
1	A	193	GLN
1	A	207	ASN
1	A	242	HIS
1	A	270	ASN
2	B	27	GLN
2	B	30	GLN
2	B	95	GLN
2	B	155	ASN
1	C	10	HIS
1	C	161	ASN
1	C	178	HIS
1	C	242	HIS
1	C	270	ASN
2	D	161	GLN
1	E	102	GLN
1	E	161	ASN
1	E	207	ASN
1	E	217	GLN
1	E	242	HIS
1	E	270	ASN
2	F	27	GLN
2	F	142	HIS
1	G	137	ASN
1	G	177	HIS
1	G	206	ASN
1	G	227	HIS
1	G	283	ASN
2	H	27	GLN
2	H	95	GLN
2	H	155	ASN
1	I	10	HIS

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Mol	Chain	Res	Type
1	I	102	GLN
1	I	155	ASN
1	I	193	GLN
1	I	207	ASN
1	I	228	HIS
2	J	75	HIS
2	J	95	GLN
2	J	125	GLN
1	K	10	HIS
1	K	193	GLN
1	K	270	ASN
2	L	30	GLN
2	L	95	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	NAG	M	1	3,2,4	14,14,15	0.33	0	17,19,21	0.93	1 (5%)
3	NAG	M	2	3	14,14,15	0.39	0	17,19,21	1.81	2 (11%)
3	NAG	N	1	3,2	14,14,15	0.36	0	17,19,21	1.09	1 (5%)
3	NAG	N	2	3	14,14,15	0.47	0	17,19,21	1.07	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
3	NAG	M	1	3,2,4	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	3/6/23/26	0/1/1/1
3	NAG	N	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	2	NAG	C2-N2-C7	4.66	129.53	122.90
3	M	2	NAG	C8-C7-N2	3.35	121.78	116.10
3	M	1	NAG	C1-O5-C5	2.45	115.51	112.19
3	N	1	NAG	C4-C3-C2	2.22	114.28	111.02
3	N	2	NAG	C1-O5-C5	2.15	115.11	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	2	NAG	C8-C7-N2-C2
3	M	2	NAG	O7-C7-N2-C2
3	N	1	NAG	O5-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	M	2	NAG	C3-C2-N2-C7
3	N	2	NAG	C4-C5-C6-O6

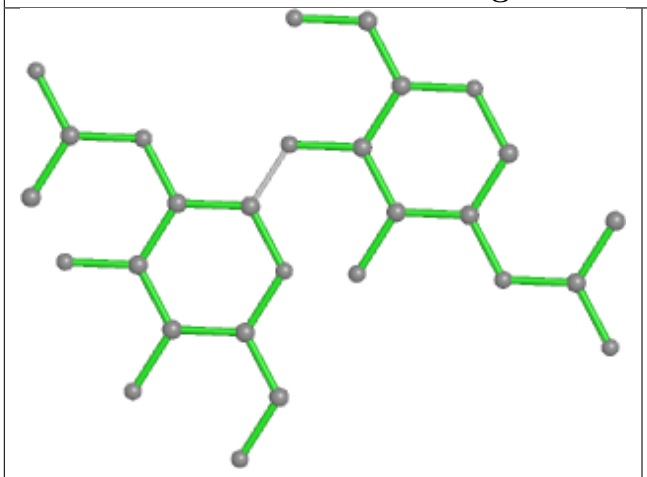
There are no ring outliers.

1 monomer is involved in 1 short contact:

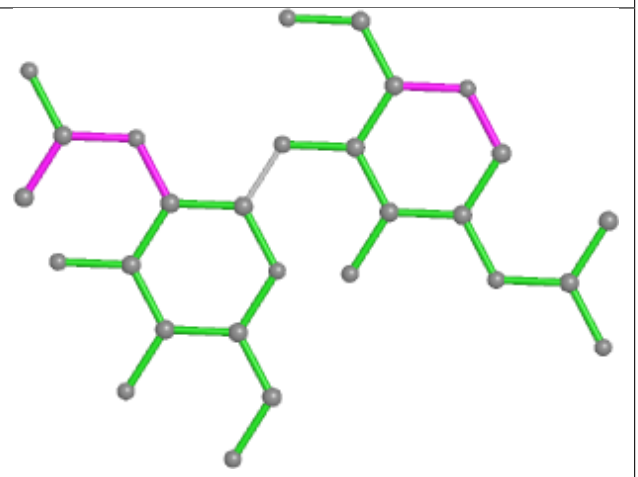
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	2	NAG	1	0

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

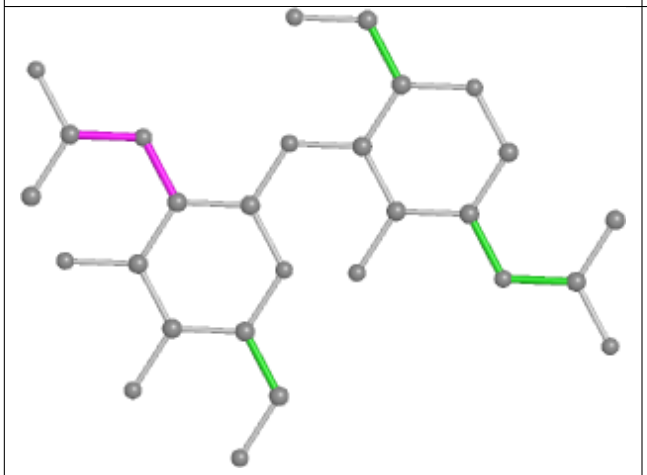
Oligosaccharide Chain M



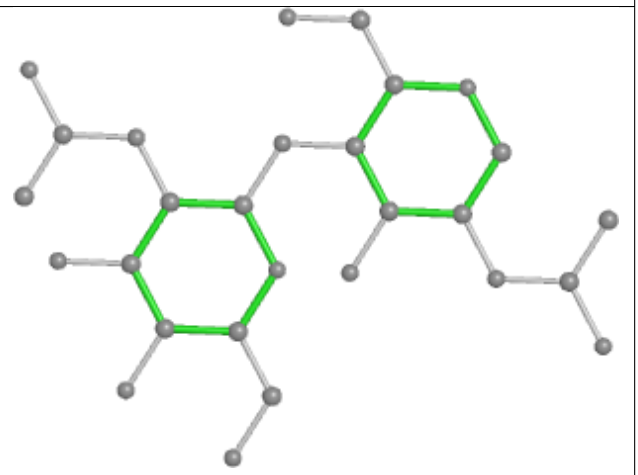
Bond lengths



Bond angles

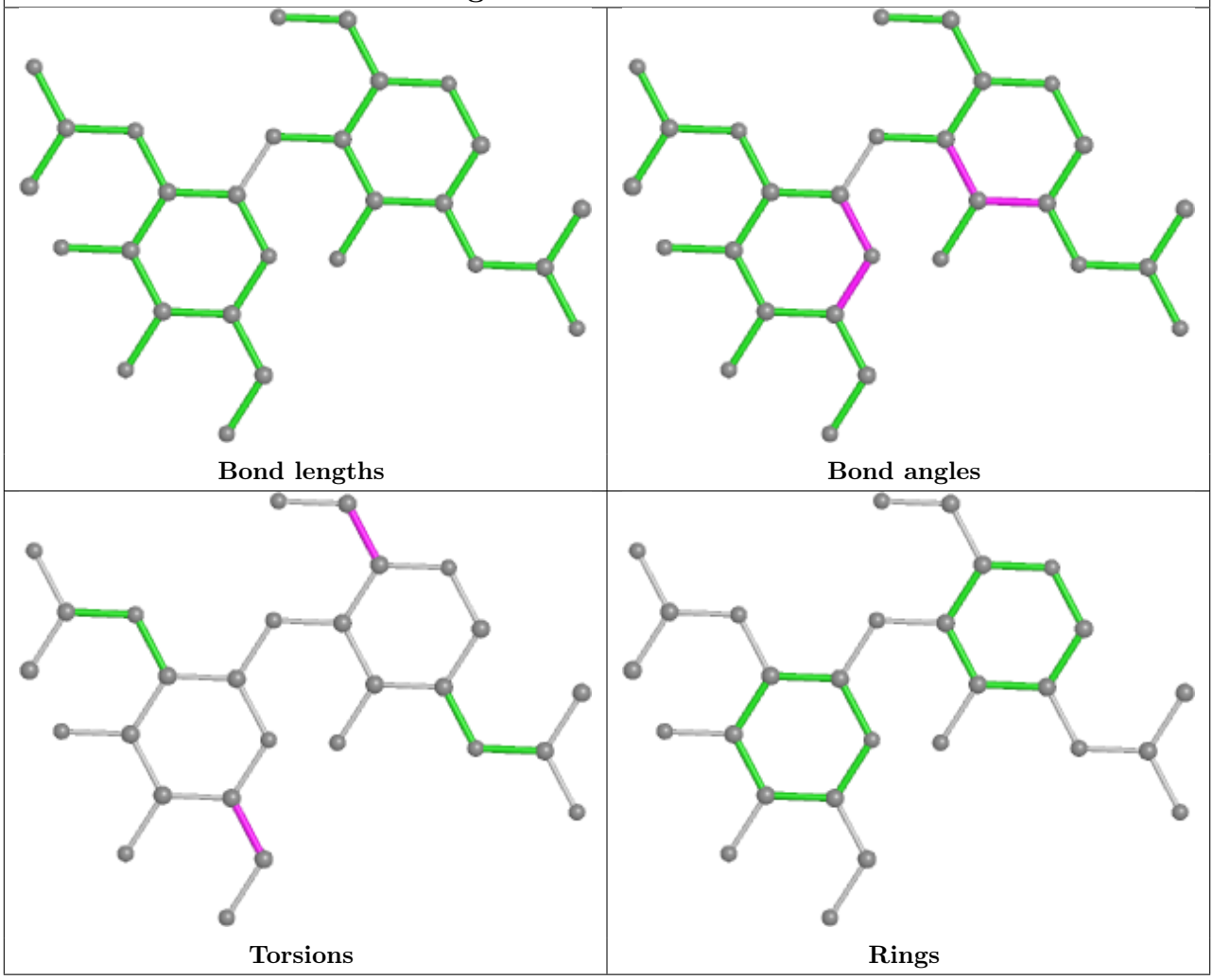


Torsions



Rings

Oligosaccharide Chain N



5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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	$\#\|Z\| > 2$
5	NAG	B	201	2	14,14,15	0.48	0	17,19,21	1.76	2 (11%)
5	NAG	H	201	2,4	14,14,15	0.76	0	17,19,21	1.41	1 (5%)
5	NAG	I	401	1	14,14,15	0.66	0	17,19,21	2.02	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	J	201	2,4	14,14,15	0.41	0	17,19,21	1.60	1 (5%)
5	NAG	F	201	2,4	14,14,15	0.51	0	17,19,21	1.74	1 (5%)
6	EDO	K	401	-	3,3,3	0.09	0	2,2,2	0.18	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
5	NAG	B	201	2	-	1/6/23/26	0/1/1/1
5	NAG	H	201	2,4	-	2/6/23/26	0/1/1/1
5	NAG	I	401	1	-	3/6/23/26	0/1/1/1
5	NAG	J	201	2,4	-	1/6/23/26	0/1/1/1
5	NAG	F	201	2,4	-	0/6/23/26	0/1/1/1
6	EDO	K	401	-	-	1/1/1/1	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	201	NAG	C1-O5-C5	6.51	121.02	112.19
5	J	201	NAG	C1-O5-C5	6.11	120.47	112.19
5	B	201	NAG	C1-O5-C5	6.08	120.43	112.19
5	H	201	NAG	C1-O5-C5	4.05	117.68	112.19
5	I	401	NAG	C3-C4-C5	3.75	116.93	110.24
5	I	401	NAG	O5-C1-C2	-3.64	105.53	111.29
5	I	401	NAG	C2-N2-C7	3.55	127.97	122.90
5	I	401	NAG	C1-O5-C5	2.80	115.98	112.19
5	B	201	NAG	O5-C1-C2	-2.70	107.02	111.29
5	I	401	NAG	C1-C2-N2	2.31	114.44	110.49
5	I	401	NAG	O5-C5-C4	2.16	116.07	110.83
5	I	401	NAG	C4-C3-C2	-2.03	108.05	111.02

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	401	NAG	C3-C2-N2-C7
5	I	401	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	H	201	NAG	O5-C5-C6-O6
5	I	401	NAG	O5-C5-C6-O6
5	H	201	NAG	C4-C5-C6-O6
6	K	401	EDO	O1-C1-C2-O2
5	B	201	NAG	O5-C5-C6-O6
5	J	201	NAG	C4-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	321/325 (98%)	0.24	0	100	100	44, 64, 98, 119	0
1	C	320/325 (98%)	0.29	4 (1%)	77	75	39, 73, 119, 142	0
1	E	320/325 (98%)	0.31	9 (2%)	53	49	56, 90, 143, 159	0
1	G	319/325 (98%)	0.68	25 (7%)	13	10	45, 92, 153, 185	0
1	I	319/325 (98%)	0.55	26 (8%)	11	9	52, 91, 160, 200	0
1	K	320/325 (98%)	0.25	2 (0%)	89	88	43, 60, 90, 115	0
2	B	172/177 (97%)	0.20	0	100	100	41, 64, 94, 104	0
2	D	172/177 (97%)	0.22	0	100	100	37, 58, 75, 92	0
2	F	172/177 (97%)	0.31	2 (1%)	79	77	44, 73, 101, 118	0
2	H	172/177 (97%)	0.27	0	100	100	39, 61, 81, 101	0
2	J	172/177 (97%)	0.18	2 (1%)	79	77	46, 69, 90, 108	0
2	L	172/177 (97%)	0.23	1 (0%)	89	88	44, 62, 85, 104	0
All	All	2951/3012 (97%)	0.33	71 (2%)	59	55	37, 71, 134, 200	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	212	GLY	10.1
1	I	214	ALA	7.2
1	G	213	ALA	6.4
1	I	182	SER	6.3
1	G	219	GLY	5.6
1	G	237	ILE	5.3
1	I	221	LEU	5.1
1	G	189	TYR	5.0
1	I	219	ASN	4.8
1	G	145	TRP	4.4
1	E	130	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	225	ASP	3.8
1	I	90	TYR	3.7
1	I	220	GLY	3.7
1	E	184	GLN	3.6
1	G	218	ASN	3.6
1	I	190	TYR	3.5
1	G	182	THR	3.4
1	I	183	THR	3.4
1	G	211	VAL	3.3
1	G	243	GLY	3.0
1	I	164	ARG	2.9
1	I	184	GLN	2.8
1	C	226	ASP	2.8
1	I	194	SER	2.8
1	I	123	ILE	2.8
1	I	241	SER	2.7
1	G	119	GLY	2.7
1	G	170	HIS	2.7
1	I	240	PHE	2.7
1	G	239	PHE	2.6
1	E	123	ILE	2.6
1	G	177	HIS	2.6
1	I	245	GLY	2.6
1	I	189	LEU	2.6
1	C	216	PRO	2.5
1	I	59	ILE	2.5
1	I	225	ILE	2.5
1	E	136	GLY	2.5
1	C	214	ALA	2.5
1	C	183	THR	2.4
1	E	135	ASN	2.4
1	I	141	TYR	2.4
1	G	141	ALA	2.3
1	I	207	ASN	2.3
1	G	223	ARG	2.3
2	L	66	ILE	2.3
1	E	188	ASP	2.3
2	F	152	ILE	2.3
1	G	157	GLN	2.2
1	E	148	VAL	2.2
1	K	286	ARG	2.2
1	G	207	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	115	GLY	2.2
1	G	222	GLY	2.2
1	I	212	VAL	2.1
1	K	35	VAL	2.1
1	E	207	ASN	2.1
1	E	190	TYR	2.1
1	I	238	ILE	2.1
1	G	181	SER	2.1
1	I	203	THR	2.1
1	I	161	ASN	2.1
1	I	181	SER	2.1
2	F	77	ILE	2.1
1	I	136	GLY	2.1
2	J	98	LEU	2.1
1	G	224	ILE	2.0
2	J	102	MET	2.0
1	G	116	PHE	2.0
1	G	171	LEU	2.0

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

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

6.3 Carbohydrates (i)

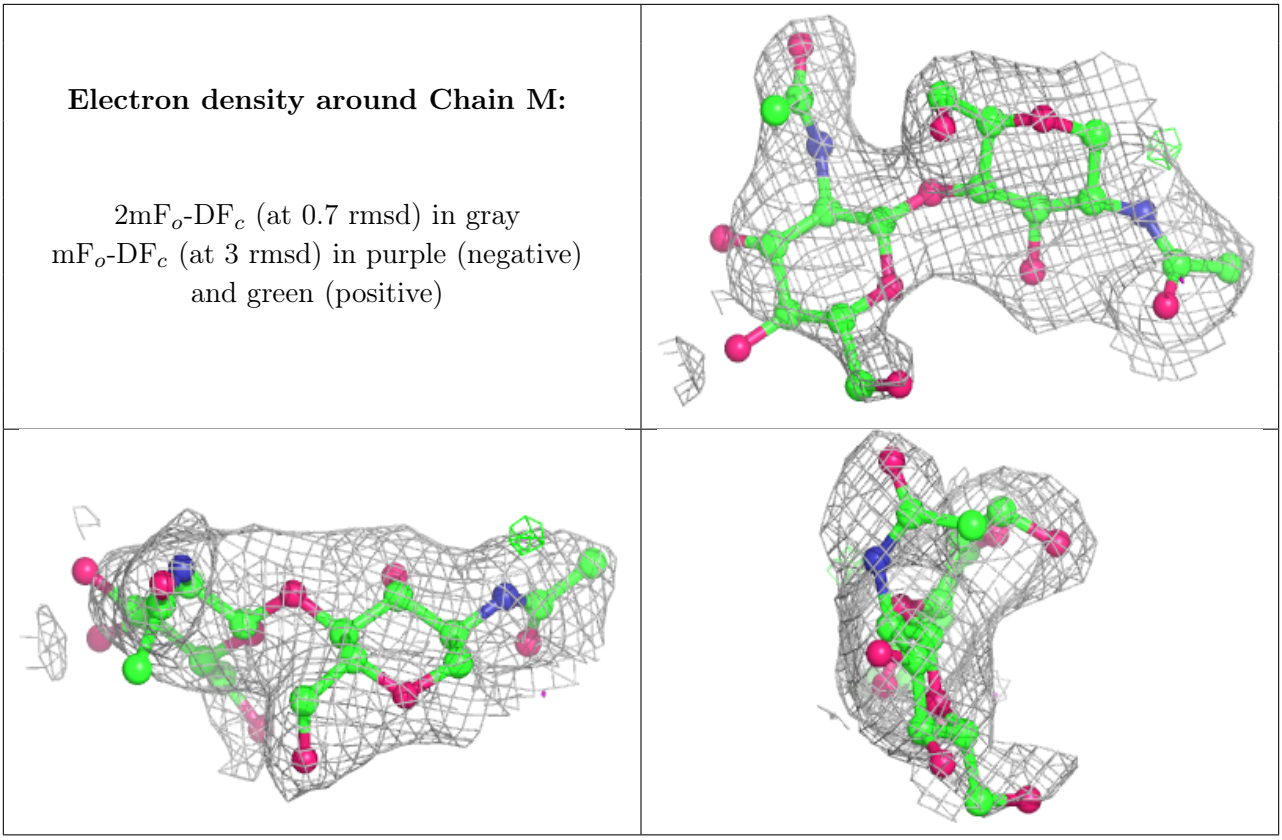
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	M	2	14/15	0.84	0.32	94,102,112,114	0
3	NAG	N	2	14/15	0.85	0.40	114,119,128,129	0
3	NAG	N	1	14/15	0.89	0.14	84,90,97,108	0
3	NAG	M	1	14/15	0.96	0.11	60,64,70,82	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.

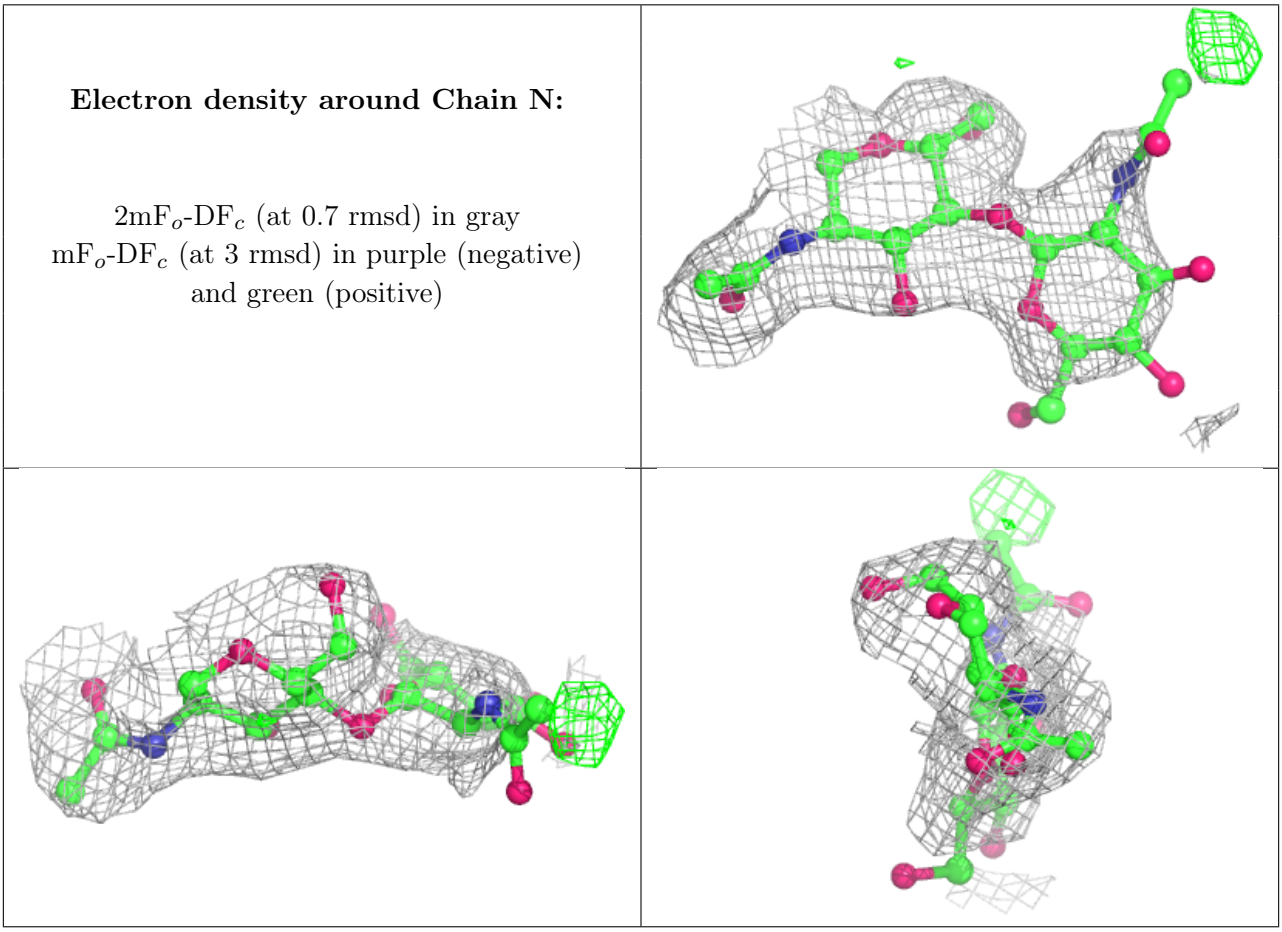
Electron density around Chain M:

$2mF_o$-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 N:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	D	401	1/1	0.70	0.07	114,114,114,114	0
5	NAG	I	401	14/15	0.72	0.15	110,127,132,133	0
4	CA	G	401	1/1	0.78	0.08	105,105,105,105	0
5	NAG	J	201	14/15	0.83	0.19	96,103,107,107	0
5	NAG	F	201	14/15	0.89	0.13	91,98,101,105	0
5	NAG	B	201	14/15	0.90	0.14	76,85,91,100	0
5	NAG	H	201	14/15	0.90	0.14	53,59,61,62	0
6	EDO	K	401	4/4	0.94	0.25	62,65,66,70	0
4	CA	D	404	1/1	0.96	0.11	55,55,55,55	0
4	CA	A	401	1/1	0.97	0.11	53,53,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.