Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 12:33 PM EDT

PDB ID	:	2I9B
Title	:	Crystal structure of ATF-urokinase receptor complex
Authors	:	Lubkowski, J.; Barinka, C.
Deposited on	:	2006-09-05
Resolution	:	2.80 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:

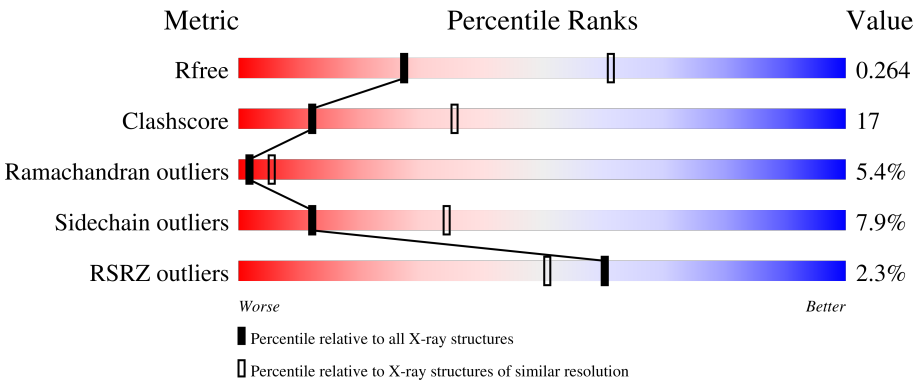
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	145	59% 21% • 16%
1	B	145	60% 21% • 16%
1	C	145	55% 25% • • 16%
1	D	145	.% 52% 26% 6% • 16%
2	E	279	3% 57% 32% 5% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	279	%, 59%, 29%, 6%, 5%
2	G	279	5%, 54%, 28%, 6%, 11%
2	H	279	3%, 51%, 30%, 6%, 11%
3	I	3	33%, 67%
3	J	3	33%, 67%
4	K	2	100%
4	L	2	50%, 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	E	318	-	-	X	-
5	SO4	F	328	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11892 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 Urokinase-type plasminogen activator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	122	966	596	183	173	14	0	0	0
1	B	122	966	596	183	173	14	0	0	0
1	C	122	966	596	183	173	14	0	0	0
1	D	122	966	596	183	173	14	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	cloning artifact	UNP P00749
A	0	SER	-	cloning artifact	UNP P00749
B	-1	ARG	-	cloning artifact	UNP P00749
B	0	SER	-	cloning artifact	UNP P00749
C	-1	ARG	-	cloning artifact	UNP P00749
C	0	SER	-	cloning artifact	UNP P00749
D	-1	ARG	-	cloning artifact	UNP P00749
D	0	SER	-	cloning artifact	UNP P00749

- Molecule 2 is a protein called Urokinase plasminogen activator surface receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	265	2034	1222	374	406	32	0	0	0
2	F	265	2034	1222	374	406	32	0	0	0
2	G	248	1882	1127	344	379	32	0	0	0
2	H	248	1882	1127	344	379	32	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ARG	-	cloning artifact	UNP Q03405
E	0	SER	-	cloning artifact	UNP Q03405
E	162	GLN	ASN	engineered mutation	UNP Q03405
E	172	GLN	ASN	engineered mutation	UNP Q03405
E	200	GLN	ASN	engineered mutation	UNP Q03405
E	233	GLN	ASN	engineered mutation	UNP Q03405
F	-1	ARG	-	cloning artifact	UNP Q03405
F	0	SER	-	cloning artifact	UNP Q03405
F	162	GLN	ASN	engineered mutation	UNP Q03405
F	172	GLN	ASN	engineered mutation	UNP Q03405
F	200	GLN	ASN	engineered mutation	UNP Q03405
F	233	GLN	ASN	engineered mutation	UNP Q03405
G	-1	ARG	-	cloning artifact	UNP Q03405
G	0	SER	-	cloning artifact	UNP Q03405
G	162	GLN	ASN	engineered mutation	UNP Q03405
G	172	GLN	ASN	engineered mutation	UNP Q03405
G	200	GLN	ASN	engineered mutation	UNP Q03405
G	233	GLN	ASN	engineered mutation	UNP Q03405
H	-1	ARG	-	cloning artifact	UNP Q03405
H	0	SER	-	cloning artifact	UNP Q03405
H	162	GLN	ASN	engineered mutation	UNP Q03405
H	172	GLN	ASN	engineered mutation	UNP Q03405
H	200	GLN	ASN	engineered mutation	UNP Q03405
H	233	GLN	ASN	engineered mutation	UNP Q03405

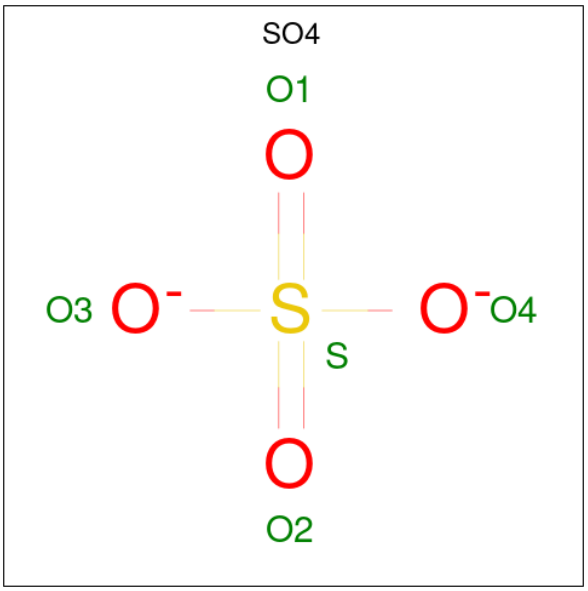
- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	I	3	39	22	2	15	0	0	0
			Total	C	N	O			
3	J	3	39	22	2	15	0	0	0

- Molecule 4 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			
4	K	2	28	16	2	10	0	0	0
			Total	C	N	O			
4	L	2	28	16	2	10	0	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	E	1	5	4	1	0	0
			Total	O	S		
5	F	1	5	4	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	14	14	14	0	0
			Total	O		
6	B	13	13	13	0	0
			Total	O		
6	C	3	3	3	0	0

Continued on next page...

Continued from previous page...

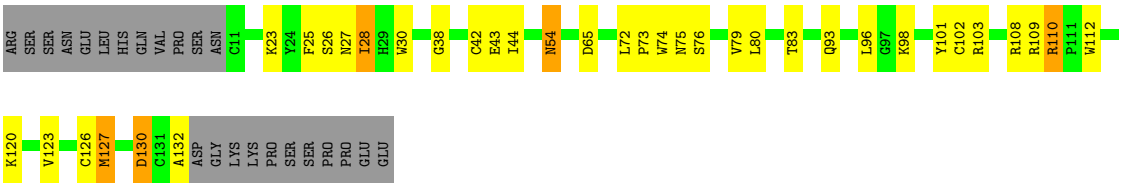
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	D	2	2	2	0	0
			Total	O		
6	E	11	11	11	0	0
			Total	O		
6	F	7	7	7	0	0
			Total	O		
6	G	2	2	2	0	0

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.

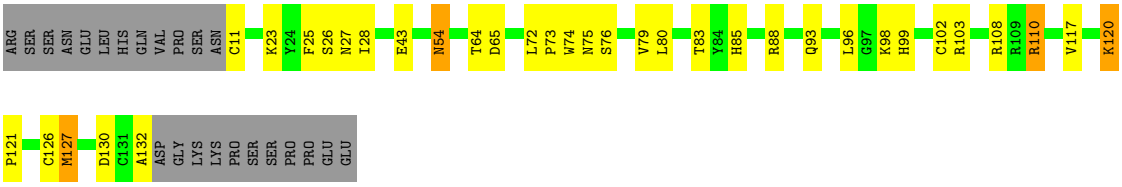
• Molecule 1: Urokinase-type plasminogen activator

Chain A:



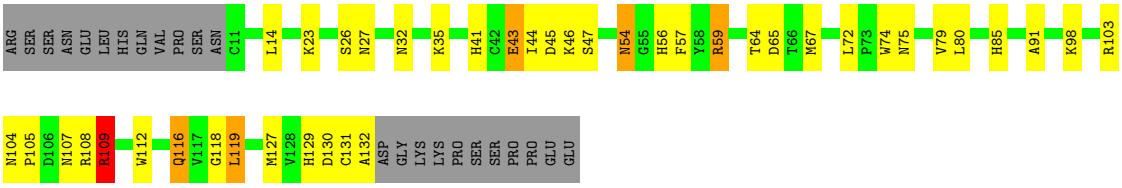
• Molecule 1: Urokinase-type plasminogen activator

Chain B:



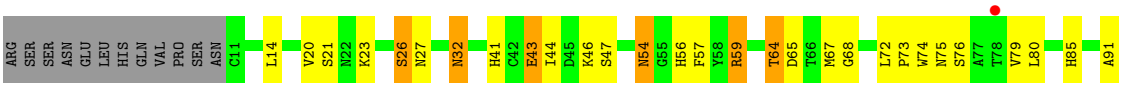
• Molecule 1: Urokinase-type plasminogen activator

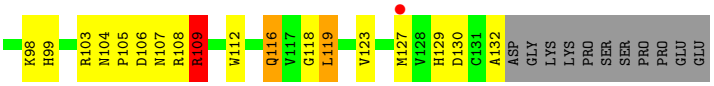
Chain C:



• Molecule 1: Urokinase-type plasminogen activator

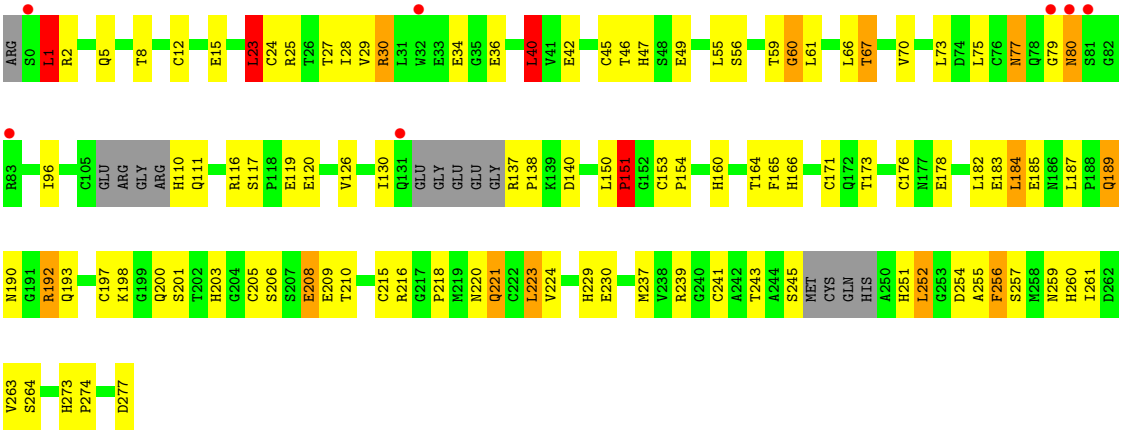
Chain D:





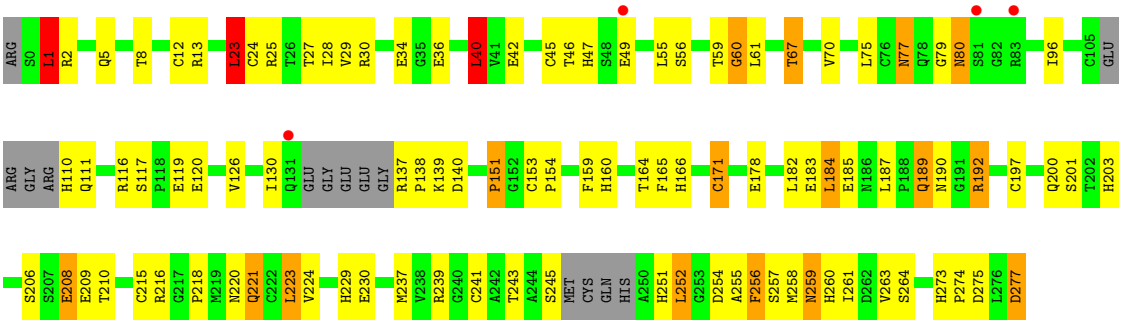
• Molecule 2: Urokinase plasminogen activator surface receptor

Chain E:



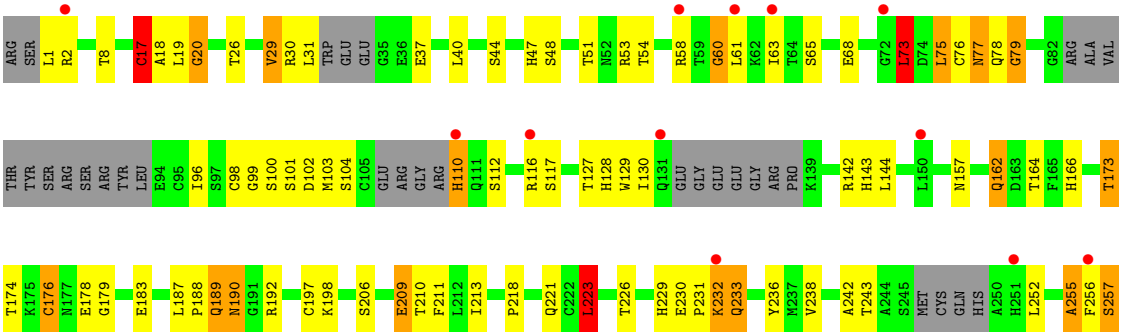
• Molecule 2: Urokinase plasminogen activator surface receptor

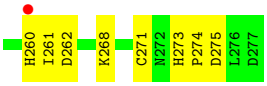
Chain F:



• Molecule 2: Urokinase plasminogen activator surface receptor

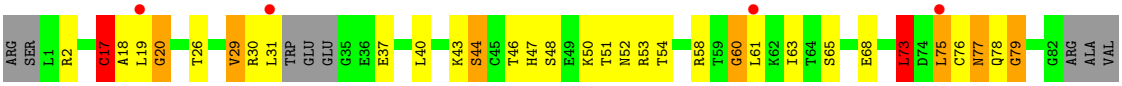
Chain G:

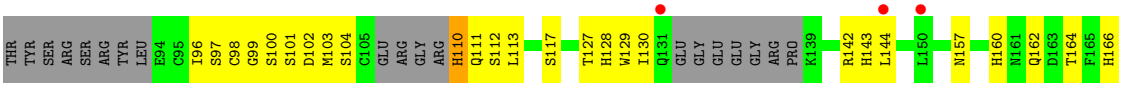


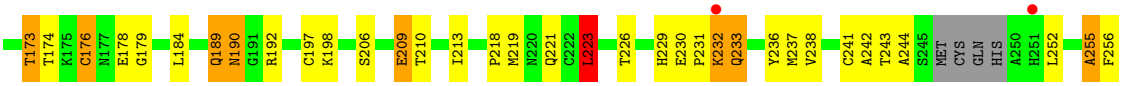


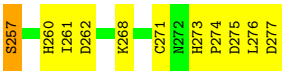
• Molecule 2: Urokinase plasminogen activator surface receptor

Chain H:









• Molecule 3: beta-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

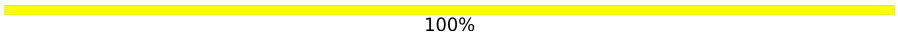
Chain I:

• Molecule 3: beta-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

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

Chain K:



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

Chain L:

NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.91Å 281.92Å 62.81Å 90.00° 105.41° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 14.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.2 (15.00-2.80) 90.8 (14.98-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.222 , 0.265 0.221 , 0.264	Depositor DCC
R_{free} test set	1911 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å^2)	79.5	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 63.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.468 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11892	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, SO4

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	0.60	0/993	0.85	0/1342
1	B	0.62	0/993	0.86	0/1342
1	C	0.48	0/993	0.77	1/1342 (0.1%)
1	D	0.59	0/993	0.81	1/1342 (0.1%)
2	E	0.66	1/2065 (0.0%)	1.00	6/2780 (0.2%)
2	F	0.66	2/2065 (0.1%)	0.98	5/2780 (0.2%)
2	G	0.56	1/1906 (0.1%)	0.89	2/2561 (0.1%)
2	H	0.56	1/1906 (0.1%)	0.88	2/2561 (0.1%)
All	All	0.60	5/11914 (0.0%)	0.90	17/16050 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	176	CYS	CB-SG	-6.75	1.70	1.82
2	H	176	CYS	CB-SG	-6.33	1.71	1.82
2	E	49	GLU	CG-CD	5.25	1.59	1.51
2	F	49	GLU	CG-CD	5.19	1.59	1.51
2	F	171	CYS	CB-SG	-5.19	1.73	1.81

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	223	LEU	CA-CB-CG	6.49	130.22	115.30
2	G	223	LEU	CA-CB-CG	5.86	128.78	115.30
2	F	61	LEU	CA-CB-CG	5.77	128.56	115.30
2	H	223	LEU	CA-CB-CG	5.73	128.48	115.30
2	F	1	LEU	CA-CB-CG	5.72	128.47	115.30
2	F	223	LEU	CA-CB-CG	5.69	128.39	115.30
2	E	40	LEU	CA-CB-CG	5.60	128.17	115.30
1	D	109	ARG	NE-CZ-NH2	5.57	123.09	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	LEU	CA-CB-CG	5.54	128.05	115.30
2	E	23	LEU	CA-CB-CG	5.48	127.91	115.30
1	C	109	ARG	NE-CZ-NH2	5.45	123.03	120.30
2	E	61	LEU	CA-CB-CG	5.40	127.72	115.30
2	F	23	LEU	CA-CB-CG	5.38	127.68	115.30
2	E	73	LEU	CA-CB-CG	5.35	127.60	115.30
2	G	144	LEU	CA-CB-CG	5.06	126.94	115.30
2	H	144	LEU	CA-CB-CG	5.05	126.91	115.30
2	F	40	LEU	CA-CB-CG	5.03	126.86	115.30

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	966	0	900	31	0
1	B	966	0	900	30	0
1	C	966	0	900	27	0
1	D	966	0	900	34	0
2	E	2034	0	1908	69	0
2	F	2034	0	1908	69	0
2	G	1882	0	1760	73	0
2	H	1882	0	1761	75	0
3	I	39	0	34	1	0
3	J	39	0	34	1	0
4	K	28	0	25	0	0
4	L	28	0	25	1	0
5	E	5	0	0	4	0
5	F	5	0	0	3	0
6	A	14	0	0	0	0
6	B	13	0	0	1	0
6	C	3	0	0	0	0
6	D	2	0	0	0	0
6	E	11	0	0	0	0
6	F	7	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	2	0	0	0	0
All	All	11892	0	11055	391	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 17.

All (391) 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:H:47:HIS:NE2	2:H:260:HIS:CE1	2.24	1.06
2:G:47:HIS:NE2	2:G:260:HIS:CE1	2.25	1.03
2:E:137:ARG:HG2	2:E:138:PRO:HD3	1.37	1.01
2:F:137:ARG:HG2	2:F:138:PRO:HD3	1.44	0.99
2:G:47:HIS:NE2	2:G:260:HIS:HE1	1.71	0.88
2:H:47:HIS:CD2	2:H:260:HIS:CE1	2.62	0.86
2:E:263:VAL:HG12	2:E:264:SER:H	1.40	0.86
2:G:47:HIS:CD2	2:G:260:HIS:CE1	2.63	0.85
2:F:130:ILE:HG21	2:F:166:HIS:HE2	1.41	0.84
2:H:47:HIS:NE2	2:H:260:HIS:HE1	1.73	0.84
2:G:103:MET:HG3	2:H:103:MET:HG3	1.61	0.83
2:F:263:VAL:HG12	2:F:264:SER:H	1.42	0.82
2:F:263:VAL:HG12	2:F:264:SER:N	1.93	0.82
2:E:130:ILE:HG21	2:E:166:HIS:HE2	1.46	0.81
2:E:263:VAL:HG12	2:E:264:SER:N	1.98	0.79
1:B:108:ARG:NH2	1:D:105:PRO:O	2.12	0.78
2:H:173:THR:O	2:H:176:CYS:HB2	1.82	0.78
2:H:47:HIS:HE1	2:H:233:GLN:NE2	1.82	0.78
1:D:54:ASN:H	1:D:54:ASN:HD22	1.30	0.78
2:G:162:GLN:HG2	2:G:211:PHE:HE1	1.49	0.77
1:C:54:ASN:HD22	1:C:54:ASN:H	1.33	0.77
2:G:47:HIS:HE1	2:G:233:GLN:NE2	1.81	0.77
2:G:162:GLN:HG2	2:G:211:PHE:CE1	2.20	0.77
2:F:229:HIS:CD2	2:F:230:GLU:HG2	2.18	0.77
2:E:229:HIS:CD2	2:E:230:GLU:HG2	2.20	0.76
2:F:197:CYS:HB3	2:F:210:THR:HG22	1.68	0.76
2:G:96:ILE:HD13	2:G:110:HIS:HD2	1.51	0.76
2:E:197:CYS:HB3	2:E:210:THR:HG22	1.67	0.75
2:F:59:THR:HG22	2:F:59:THR:O	1.84	0.75
2:H:96:ILE:HD13	2:H:110:HIS:HD2	1.52	0.75
1:D:104:ASN:HD21	1:D:108:ARG:H	1.34	0.74
1:A:102:CYS:O	1:A:103:ARG:NH1	2.22	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:47:HIS:ND1	5:E:318:SO4:O4	2.15	0.73
1:B:102:CYS:O	1:B:103:ARG:NH1	2.21	0.72
2:E:130:ILE:HG23	2:E:130:ILE:O	1.89	0.72
2:F:60:GLY:H	2:F:111:GLN:HE22	1.36	0.72
3:I:1:NAG:H61	3:I:2:NAG:HN2	1.54	0.72
1:B:25:PHE:HB2	1:B:28:ILE:HD11	1.71	0.71
2:E:59:THR:O	2:E:59:THR:HG22	1.91	0.70
2:G:173:THR:O	2:G:176:CYS:HB2	1.92	0.70
1:A:108:ARG:NH2	1:C:105:PRO:O	2.21	0.70
2:F:28:ILE:HG21	2:F:30:ARG:HH11	1.56	0.70
2:E:200:GLN:HB2	2:E:203:HIS:HB2	1.72	0.69
2:G:99:GLY:H	2:G:104:SER:HB2	1.57	0.69
2:F:117:SER:HB2	2:F:120:GLU:HG3	1.73	0.69
1:C:104:ASN:HD21	1:C:108:ARG:H	1.38	0.69
2:F:200:GLN:HB2	2:F:203:HIS:HB2	1.75	0.69
2:E:60:GLY:H	2:E:111:GLN:HE22	1.41	0.69
2:F:206:SER:OG	2:F:209:GLU:HG3	1.94	0.68
2:G:29:VAL:HG13	2:G:40:LEU:HB2	1.75	0.68
2:G:47:HIS:CE1	2:G:233:GLN:NE2	2.61	0.68
2:E:130:ILE:HG21	2:E:166:HIS:NE2	2.08	0.68
2:H:47:HIS:CE1	2:H:233:GLN:NE2	2.61	0.68
2:E:137:ARG:HG2	2:E:138:PRO:CD	2.21	0.68
2:F:130:ILE:HG21	2:F:166:HIS:NE2	2.07	0.68
2:F:263:VAL:CG1	2:F:264:SER:H	2.07	0.68
2:F:237:MET:SD	2:F:239:ARG:NH1	2.67	0.67
2:F:189:GLN:HA	2:F:189:GLN:HE21	1.58	0.67
2:H:29:VAL:HG13	2:H:40:LEU:HB2	1.77	0.67
2:F:229:HIS:HD2	2:F:230:GLU:HG2	1.58	0.67
2:G:162:GLN:HE21	2:G:213:ILE:HD11	1.58	0.67
2:E:229:HIS:HD2	2:E:230:GLU:HG2	1.59	0.66
1:A:25:PHE:HB2	1:A:28:ILE:HD11	1.78	0.66
1:A:54:ASN:H	1:A:54:ASN:HD22	1.40	0.66
1:C:109:ARG:HH21	1:C:109:ARG:HG3	1.58	0.66
2:F:130:ILE:HG23	2:F:130:ILE:O	1.94	0.66
2:G:130:ILE:HG21	2:G:166:HIS:HE1	1.60	0.66
2:E:206:SER:OG	2:E:209:GLU:HG3	1.96	0.66
2:E:208:GLU:N	2:E:208:GLU:OE1	2.27	0.66
2:E:189:GLN:HA	2:E:189:GLN:HE21	1.60	0.65
2:H:130:ILE:HG21	2:H:166:HIS:HE1	1.61	0.65
2:E:237:MET:SD	2:E:239:ARG:NH1	2.69	0.65
2:H:99:GLY:H	2:H:104:SER:HB2	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:117:SER:HB2	2:E:120:GLU:HG3	1.78	0.65
1:A:75:ASN:ND2	1:A:98:LYS:HG2	2.12	0.64
2:F:47:HIS:ND1	5:F:328:SO4:O2	2.26	0.64
2:E:263:VAL:CG1	2:E:264:SER:H	2.09	0.64
2:H:268:LYS:O	2:H:271:CYS:SG	2.56	0.64
2:G:47:HIS:HE1	2:G:233:GLN:CD	2.01	0.64
1:D:64:THR:OG1	1:D:68:GLY:HA2	1.97	0.64
1:B:54:ASN:HD22	1:B:54:ASN:H	1.45	0.63
1:D:109:ARG:HH21	1:D:109:ARG:HG3	1.62	0.63
2:F:218:PRO:O	2:F:243:THR:HG22	1.98	0.63
3:J:1:NAG:H61	3:J:2:NAG:HN2	1.63	0.63
1:A:27:ASN:HB2	2:E:42:GLU:OE2	1.98	0.63
2:H:51:THR:H	2:H:53:ARG:HH11	1.45	0.63
1:C:109:ARG:HH21	1:C:109:ARG:CG	2.12	0.63
2:H:52:ASN:HD21	4:L:1:NAG:HN2	1.47	0.63
2:E:260:HIS:CE1	5:E:318:SO4:O3	2.52	0.63
2:G:31:LEU:O	2:G:37:GLU:HA	1.99	0.62
2:F:263:VAL:CG1	2:F:264:SER:N	2.62	0.62
2:G:268:LYS:O	2:G:271:CYS:SG	2.58	0.62
2:H:31:LEU:O	2:H:37:GLU:HA	2.00	0.62
1:B:75:ASN:ND2	1:B:98:LYS:HG2	2.14	0.62
1:D:72:LEU:HD21	1:D:116:GLN:HB2	1.82	0.61
1:A:76:SER:O	1:A:80:LEU:HG	2.01	0.61
2:H:47:HIS:HE1	2:H:233:GLN:CD	2.05	0.60
1:D:14:LEU:HD12	1:D:43:GLU:HB3	1.83	0.60
1:D:109:ARG:HH21	1:D:109:ARG:CG	2.13	0.60
1:B:76:SER:O	1:B:80:LEU:HG	2.01	0.60
2:E:218:PRO:O	2:E:243:THR:HG22	2.02	0.60
1:B:117:VAL:O	1:B:120:LYS:HG2	2.01	0.59
2:F:190:ASN:ND2	2:F:192:ARG:HB3	2.16	0.59
2:G:103:MET:CG	2:H:103:MET:HG3	2.30	0.59
2:H:223:LEU:HD23	2:H:242:ALA:CB	2.33	0.59
2:E:28:ILE:HG21	2:E:30:ARG:HH11	1.66	0.59
2:G:103:MET:HG3	2:H:103:MET:CG	2.31	0.58
2:F:137:ARG:HG2	2:F:138:PRO:CD	2.27	0.58
2:G:51:THR:H	2:G:53:ARG:HH11	1.51	0.58
1:C:14:LEU:HD12	1:C:43:GLU:HB3	1.83	0.58
2:E:130:ILE:O	2:E:130:ILE:CG2	2.51	0.58
2:F:29:VAL:HG12	2:F:40:LEU:HB2	1.86	0.58
2:F:25:ARG:HB3	2:F:70:VAL:HG12	1.86	0.58
2:G:130:ILE:HG21	2:G:166:HIS:CE1	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:TRP:HA	1:D:79:VAL:HG11	1.85	0.58
2:H:273:HIS:HD2	2:H:275:ASP:H	1.49	0.58
2:G:47:HIS:CE1	2:G:233:GLN:CD	2.77	0.58
2:F:208:GLU:OE1	2:F:208:GLU:N	2.29	0.57
2:F:273:HIS:ND1	2:F:274:PRO:HD2	2.19	0.57
2:E:190:ASN:ND2	2:E:192:ARG:HB3	2.19	0.57
1:C:72:LEU:HD21	1:C:116:GLN:HB2	1.87	0.56
1:C:74:TRP:HA	1:C:79:VAL:HG11	1.87	0.56
1:D:41:HIS:HB2	1:D:43:GLU:HG3	1.87	0.56
2:G:96:ILE:HD13	2:G:110:HIS:CD2	2.37	0.56
2:H:47:HIS:CE1	2:H:233:GLN:CD	2.79	0.56
2:H:130:ILE:HG21	2:H:166:HIS:CE1	2.38	0.56
2:F:184:LEU:HD22	2:F:216:ARG:HD2	1.88	0.56
2:G:273:HIS:HD2	2:G:275:ASP:H	1.53	0.56
2:E:29:VAL:HG12	2:E:40:LEU:HB2	1.88	0.56
1:D:54:ASN:HD21	1:D:56:HIS:HD2	1.52	0.55
2:F:59:THR:O	2:F:59:THR:CG2	2.54	0.55
2:E:206:SER:HG	2:E:209:GLU:HG3	1.71	0.55
1:D:118:GLY:O	1:D:119:LEU:HB2	2.07	0.55
1:A:93:GLN:HG2	2:H:273:HIS:CD2	2.42	0.55
2:F:260:HIS:ND1	5:F:328:SO4:O4	2.40	0.55
2:F:130:ILE:O	2:F:130:ILE:CG2	2.56	0.54
2:H:128:HIS:HB2	2:H:142:ARG:NH2	2.22	0.54
2:E:273:HIS:ND1	2:E:274:PRO:HD2	2.23	0.54
1:A:75:ASN:HD22	1:A:98:LYS:HG2	1.72	0.54
2:H:128:HIS:HD2	2:H:142:ARG:CZ	2.21	0.54
1:D:112:TRP:CE3	1:D:123:VAL:HG23	2.43	0.54
2:G:2:ARG:HA	2:G:17:CYS:HB2	1.89	0.53
2:E:96:ILE:HG13	2:E:178:GLU:HB3	1.89	0.53
2:E:184:LEU:HD22	2:E:216:ARG:HD2	1.91	0.53
2:G:273:HIS:CD2	2:G:274:PRO:HD2	2.44	0.53
1:B:93:GLN:HG2	2:G:273:HIS:CD2	2.44	0.53
2:G:223:LEU:HD23	2:G:242:ALA:CB	2.39	0.53
1:B:27:ASN:HB2	2:F:42:GLU:OE2	2.09	0.52
2:E:183:GLU:OE2	2:E:183:GLU:HA	2.09	0.52
2:E:220:ASN:OD1	2:E:221:GLN:NE2	2.42	0.52
2:F:183:GLU:OE2	2:F:183:GLU:HA	2.10	0.52
2:F:55:LEU:HD23	2:F:56:SER:N	2.24	0.52
1:B:25:PHE:CB	1:B:28:ILE:HD11	2.39	0.52
2:E:29:VAL:HG23	2:E:66:LEU:HG	1.92	0.52
2:G:58:ARG:NH2	2:G:112:SER:O	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ARG:HH11	1:B:110:ARG:CG	2.22	0.52
1:D:65:ASP:C	1:D:67:MET:H	2.14	0.52
2:H:96:ILE:HD13	2:H:110:HIS:CD2	2.39	0.52
1:A:25:PHE:CB	1:A:28:ILE:HD11	2.40	0.52
2:G:77:ASN:O	2:G:79:GLY:N	2.42	0.51
2:H:2:ARG:HA	2:H:17:CYS:HB2	1.91	0.51
2:H:77:ASN:O	2:H:79:GLY:N	2.43	0.51
1:C:41:HIS:HB2	1:C:43:GLU:HG3	1.92	0.51
1:C:54:ASN:HD21	1:C:56:HIS:HD2	1.59	0.51
2:F:96:ILE:HG13	2:F:178:GLU:HB3	1.91	0.51
2:G:197:CYS:HB3	2:G:210:THR:HG22	1.92	0.51
1:A:74:TRP:CE3	1:A:96:LEU:HD22	2.45	0.51
2:F:254:ASP:C	2:F:256:PHE:H	2.14	0.51
2:F:260:HIS:CE1	5:F:328:SO4:S	3.04	0.51
2:H:198:LYS:HG2	2:H:236:TYR:OH	2.11	0.51
1:A:44:ILE:HD13	1:A:101:TYR:HE2	1.76	0.51
2:E:137:ARG:CG	2:E:138:PRO:HD3	2.26	0.51
2:G:198:LYS:HG3	2:G:238:VAL:HG22	1.92	0.50
2:H:198:LYS:HG3	2:H:238:VAL:HG22	1.92	0.50
2:H:75:LEU:C	2:H:77:ASN:H	2.15	0.50
2:E:190:ASN:HD22	2:E:215:CYS:HB2	1.76	0.50
2:H:102:ASP:OD1	2:H:104:SER:OG	2.30	0.50
2:F:220:ASN:OD1	2:F:221:GLN:NE2	2.45	0.50
1:C:118:GLY:O	1:C:119:LEU:HB2	2.11	0.50
2:G:75:LEU:C	2:G:77:ASN:H	2.14	0.50
1:A:110:ARG:CG	1:A:110:ARG:HH11	2.24	0.50
2:E:260:HIS:CE1	5:E:318:SO4:S	3.04	0.50
1:B:23:LYS:HD2	2:F:255:ALA:HA	1.94	0.50
2:G:26:THR:O	2:G:68:GLU:HA	2.12	0.49
1:C:129:HIS:CG	1:C:130:ASP:H	2.31	0.49
1:B:74:TRP:CE3	1:B:96:LEU:HD22	2.47	0.49
1:B:127:MET:HA	1:B:127:MET:CE	2.43	0.49
1:A:65:ASP:HA	1:A:126:CYS:HA	1.95	0.49
2:E:197:CYS:CB	2:E:210:THR:HG22	2.40	0.49
2:H:73:LEU:H	2:H:73:LEU:HD23	1.76	0.49
2:H:218:PRO:O	2:H:243:THR:HG22	2.13	0.49
1:B:110:ARG:HH11	1:B:110:ARG:HG2	1.76	0.49
1:D:23:LYS:HE3	2:H:127:THR:OG1	2.12	0.49
1:D:76:SER:O	1:D:80:LEU:HG	2.13	0.49
2:G:142:ARG:HG3	2:G:143:HIS:HD2	1.78	0.49
2:G:174:THR:C	2:G:176:CYS:N	2.66	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ARG:HD2	1:C:112:TRP:CD1	2.48	0.49
2:E:24:CYS:HA	2:E:45:CYS:HA	1.95	0.49
1:A:28:ILE:HD12	1:A:28:ILE:O	2.13	0.48
1:C:54:ASN:HD22	1:C:54:ASN:N	2.05	0.48
2:F:75:LEU:C	2:F:77:ASN:H	2.17	0.48
2:H:98:CYS:HB3	2:H:110:HIS:HB3	1.95	0.48
2:F:160:HIS:HA	2:F:164:THR:O	2.13	0.48
2:G:255:ALA:C	2:G:257:SER:H	2.16	0.48
2:H:58:ARG:NH2	2:H:112:SER:O	2.44	0.48
1:A:112:TRP:CE3	1:A:123:VAL:HG13	2.48	0.48
1:B:75:ASN:HD22	1:B:98:LYS:HG2	1.74	0.48
2:H:197:CYS:HB3	2:H:210:THR:HG22	1.95	0.48
1:B:76:SER:HB2	1:B:79:VAL:H	1.79	0.48
2:E:25:ARG:HB3	2:E:70:VAL:HG12	1.95	0.48
2:G:128:HIS:HD2	2:G:142:ARG:CZ	2.26	0.48
1:B:28:ILE:HD12	1:B:28:ILE:O	2.13	0.48
1:D:108:ARG:HD2	1:D:112:TRP:CD1	2.49	0.48
1:D:129:HIS:CG	1:D:130:ASP:H	2.31	0.48
1:B:11:CYS:SG	2:F:138:PRO:HG3	2.54	0.48
2:E:224:VAL:HG13	2:E:264:SER:HB3	1.96	0.48
2:F:251:HIS:H	2:F:252:LEU:HG	1.78	0.48
2:G:142:ARG:HG3	2:G:143:HIS:CD2	2.49	0.48
1:B:64:THR:HG22	6:B:154:HOH:O	2.14	0.48
2:E:160:HIS:CD2	2:E:241:CYS:HB2	2.48	0.48
1:C:65:ASP:C	1:C:67:MET:H	2.17	0.47
2:G:98:CYS:HB3	2:G:110:HIS:HB3	1.96	0.47
2:H:18:ALA:O	2:H:20:GLY:N	2.46	0.47
2:H:26:THR:O	2:H:68:GLU:HA	2.13	0.47
2:F:160:HIS:CE1	2:F:241:CYS:HB2	2.49	0.47
1:A:73:PRO:HD2	1:A:76:SER:OG	2.14	0.47
1:C:104:ASN:HD22	1:C:112:TRP:HE1	1.62	0.47
2:F:1:LEU:HD23	2:F:2:ARG:N	2.29	0.47
2:G:157:ASN:ND2	2:G:252:LEU:HD23	2.28	0.47
2:H:229:HIS:CD2	2:H:230:GLU:H	2.32	0.47
1:D:80:LEU:HD23	1:D:85:HIS:HB2	1.97	0.47
2:E:75:LEU:C	2:E:77:ASN:H	2.18	0.47
2:G:73:LEU:HD23	2:G:73:LEU:H	1.79	0.47
2:G:198:LYS:HG2	2:G:236:TYR:OH	2.15	0.47
1:B:65:ASP:HA	1:B:126:CYS:HA	1.97	0.47
1:C:59:ARG:HA	1:C:103:ARG:CZ	2.44	0.47
1:D:54:ASN:HD22	1:D:54:ASN:N	2.02	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:PHE:CD2	2:G:189:GLN:HG3	2.50	0.47
2:E:160:HIS:HA	2:E:164:THR:O	2.15	0.47
2:E:254:ASP:C	2:E:256:PHE:H	2.18	0.47
2:F:5:GLN:O	2:F:12:CYS:HA	2.15	0.47
2:F:197:CYS:CB	2:F:210:THR:HG22	2.41	0.47
2:H:162:GLN:NE2	2:H:213:ILE:HD11	2.30	0.47
2:H:255:ALA:C	2:H:257:SER:H	2.18	0.47
2:G:30:ARG:HB3	2:G:65:SER:HB2	1.97	0.47
1:C:44:ILE:O	1:C:46:LYS:N	2.48	0.46
2:H:174:THR:C	2:H:176:CYS:N	2.69	0.46
2:H:276:LEU:O	2:H:277:ASP:HB2	2.16	0.46
1:A:110:ARG:HH11	1:A:110:ARG:HG2	1.80	0.46
2:E:5:GLN:O	2:E:12:CYS:HA	2.15	0.46
2:E:251:HIS:H	2:E:252:LEU:HG	1.80	0.46
2:G:18:ALA:O	2:G:20:GLY:N	2.48	0.46
1:C:57:PHE:CD2	2:H:189:GLN:HG3	2.50	0.46
2:F:184:LEU:HD23	2:F:187:LEU:HD12	1.98	0.46
1:B:74:TRP:CD2	1:B:96:LEU:HD22	2.50	0.46
1:A:72:LEU:HD23	1:A:72:LEU:HA	1.63	0.46
1:C:23:LYS:HE3	2:G:127:THR:OG1	2.15	0.46
2:E:23:LEU:O	2:E:46:THR:N	2.49	0.46
2:G:130:ILE:HD12	2:G:130:ILE:HA	1.87	0.46
2:E:130:ILE:HG21	2:E:166:HIS:CE1	2.51	0.46
2:E:153:CYS:HA	2:E:154:PRO:HA	1.68	0.46
2:G:128:HIS:HB2	2:G:142:ARG:NH2	2.31	0.46
1:D:26:SER:O	1:D:27:ASN:HB3	2.16	0.45
1:D:26:SER:O	1:D:27:ASN:CB	2.64	0.45
2:G:130:ILE:CG2	2:G:166:HIS:HE1	2.29	0.45
2:E:1:LEU:HD23	2:E:2:ARG:N	2.32	0.45
2:H:30:ARG:HB3	2:H:65:SER:HB2	1.97	0.45
1:A:127:MET:HA	1:A:127:MET:CE	2.45	0.45
1:B:120:LYS:HA	1:B:121:PRO:HD3	1.76	0.45
1:C:130:ASP:O	1:C:132:ALA:N	2.48	0.45
2:E:55:LEU:HD23	2:E:56:SER:N	2.31	0.45
2:G:206:SER:OG	2:G:209:GLU:OE2	2.34	0.45
2:H:43:LYS:O	2:H:44:SER:HB3	2.17	0.45
2:H:273:HIS:CD2	2:H:274:PRO:HD2	2.51	0.45
1:A:38:GLY:O	1:A:42:CYS:HA	2.16	0.45
1:A:74:TRP:CD2	1:A:96:LEU:HD22	2.51	0.45
1:A:130:ASP:C	1:A:132:ALA:N	2.70	0.45
2:H:157:ASN:HB3	2:H:244:ALA:HB3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:28:ILE:HB	2:E:67:THR:HG23	1.99	0.45
2:G:99:GLY:N	2:G:104:SER:HB2	2.26	0.45
2:H:46:THR:OG1	2:H:50:LYS:HG3	2.17	0.45
1:B:72:LEU:HA	1:B:72:LEU:HD23	1.59	0.44
2:F:28:ILE:HB	2:F:67:THR:HG23	1.99	0.44
2:F:190:ASN:HD22	2:F:215:CYS:HB2	1.81	0.44
2:G:190:ASN:HD22	2:G:192:ARG:H	1.66	0.44
2:H:142:ARG:HG3	2:H:143:HIS:CD2	2.52	0.44
2:H:157:ASN:ND2	2:H:252:LEU:HD23	2.32	0.44
2:H:219:MET:HG3	2:H:243:THR:HG23	1.99	0.44
1:A:76:SER:HB2	1:A:79:VAL:H	1.82	0.44
2:E:5:GLN:HG3	2:E:15:GLU:HB2	1.99	0.44
1:D:130:ASP:O	1:D:132:ALA:N	2.50	0.44
2:E:150:LEU:HB3	2:E:151:PRO:HD2	2.00	0.44
2:F:190:ASN:HD22	2:F:192:ARG:HB3	1.81	0.44
1:A:23:LYS:N	2:E:140:ASP:OD1	2.49	0.44
1:A:30:TRP:CH2	2:E:66:LEU:HD21	2.52	0.44
1:C:109:ARG:HG3	1:C:109:ARG:NH2	2.31	0.44
2:E:184:LEU:HD23	2:E:187:LEU:HD12	2.00	0.44
1:D:44:ILE:O	1:D:46:LYS:N	2.51	0.44
2:G:102:ASP:OD1	2:G:104:SER:OG	2.35	0.44
1:B:73:PRO:HA	1:B:99:HIS:O	2.18	0.44
2:E:263:VAL:CG1	2:E:264:SER:N	2.67	0.44
2:E:260:HIS:HE1	5:E:318:SO4:O3	1.98	0.44
2:H:190:ASN:HD22	2:H:192:ARG:H	1.65	0.44
2:H:206:SER:OG	2:H:209:GLU:OE2	2.36	0.44
2:H:142:ARG:HG3	2:H:143:HIS:HD2	1.83	0.43
2:H:99:GLY:N	2:H:104:SER:HB2	2.31	0.43
2:H:190:ASN:ND2	2:H:192:ARG:HB3	2.33	0.43
2:G:178:GLU:HG2	2:G:179:GLY:N	2.34	0.43
2:G:261:ILE:HG12	2:G:262:ASP:N	2.34	0.43
1:D:73:PRO:HA	1:D:99:HIS:O	2.19	0.43
1:B:130:ASP:C	1:B:132:ALA:N	2.71	0.43
2:E:25:ARG:NH1	2:E:27:THR:OG1	2.46	0.43
2:E:189:GLN:HE21	2:E:189:GLN:CA	2.29	0.43
2:F:25:ARG:NH1	2:F:27:THR:OG1	2.46	0.43
2:F:126:VAL:HG11	2:F:165:PHE:CE2	2.53	0.43
1:C:80:LEU:HD23	1:C:85:HIS:HB2	2.00	0.43
2:F:206:SER:HG	2:F:209:GLU:HG3	1.83	0.43
2:G:174:THR:C	2:G:176:CYS:H	2.22	0.43
2:H:160:HIS:CE1	2:H:241:CYS:HB2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:60:GLY:O	2:G:61:LEU:HB2	2.18	0.43
2:G:142:ARG:NH1	2:G:183:GLU:OE2	2.52	0.43
2:G:218:PRO:O	2:G:243:THR:HG22	2.18	0.43
2:E:126:VAL:HG11	2:E:165:PHE:CE2	2.54	0.42
2:E:192:ARG:HG3	2:E:193:GLN:N	2.34	0.42
2:H:128:HIS:CD2	2:H:142:ARG:CZ	3.01	0.42
2:H:128:HIS:CE1	2:H:129:TRP:HB2	2.54	0.42
2:H:261:ILE:HG12	2:H:262:ASP:N	2.34	0.42
2:H:130:ILE:CG2	2:H:166:HIS:HE1	2.29	0.42
2:F:159:PHE:CE2	2:F:256:PHE:HZ	2.37	0.42
2:G:187:LEU:HA	2:G:188:PRO:HD2	1.89	0.42
2:F:24:CYS:HA	2:F:45:CYS:HA	2.01	0.42
2:F:224:VAL:HG13	2:F:264:SER:HB3	2.01	0.42
2:H:60:GLY:O	2:H:61:LEU:HB2	2.20	0.42
1:C:75:ASN:HD22	1:C:98:LYS:HG2	1.84	0.42
2:G:100:SER:CB	2:G:142:ARG:HB3	2.49	0.42
2:G:213:ILE:HD12	2:G:213:ILE:HA	1.90	0.42
1:A:54:ASN:HD22	1:A:54:ASN:N	2.08	0.42
2:F:256:PHE:O	2:F:257:SER:C	2.58	0.42
2:H:58:ARG:HG3	2:H:113:LEU:HD13	2.01	0.42
1:C:26:SER:O	1:C:27:ASN:CB	2.67	0.42
1:C:26:SER:O	1:C:27:ASN:HB3	2.20	0.42
1:C:109:ARG:CG	1:C:109:ARG:NH2	2.80	0.42
2:H:178:GLU:HG2	2:H:179:GLY:N	2.35	0.42
1:B:127:MET:HA	1:B:127:MET:HE3	2.02	0.42
1:D:20:VAL:HG12	1:D:21:SER:N	2.35	0.42
1:D:54:ASN:H	1:D:54:ASN:ND2	2.08	0.42
1:D:75:ASN:HD22	1:D:98:LYS:HG2	1.85	0.42
1:D:106:ASP:OD2	1:D:106:ASP:N	2.53	0.42
1:A:23:LYS:HD2	2:E:255:ALA:HA	2.02	0.42
2:F:139:LYS:HB3	2:F:139:LYS:HE2	1.83	0.42
2:H:276:LEU:O	2:H:277:ASP:CB	2.68	0.42
2:G:197:CYS:CB	2:G:210:THR:HG22	2.50	0.41
2:H:100:SER:CB	2:H:142:ARG:HB3	2.50	0.41
2:H:213:ILE:HD12	2:H:213:ILE:HA	1.89	0.41
2:F:239:ARG:NH2	2:F:274:PRO:HA	2.35	0.41
1:B:73:PRO:HD2	1:B:76:SER:OG	2.19	0.41
2:F:153:CYS:HA	2:F:154:PRO:HA	1.65	0.41
2:G:190:ASN:HD22	2:G:190:ASN:C	2.22	0.41
2:E:256:PHE:O	2:E:257:SER:C	2.58	0.41
2:G:190:ASN:HD21	2:G:192:ARG:HB3	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:190:ASN:ND2	2:G:192:ARG:HB3	2.35	0.41
2:G:229:HIS:CD2	2:G:230:GLU:H	2.38	0.41
2:G:1:LEU:HD23	2:G:2:ARG:N	2.35	0.41
2:G:75:LEU:O	2:G:77:ASN:N	2.54	0.41
2:H:198:LYS:HA	2:H:237:MET:O	2.21	0.41
1:A:109:ARG:HG3	1:A:110:ARG:HG2	2.03	0.41
1:A:130:ASP:C	1:A:132:ALA:H	2.24	0.41
2:F:259:ASN:O	2:F:260:HIS:C	2.58	0.41
2:G:47:HIS:CE1	2:G:233:GLN:OE1	2.74	0.41
1:A:73:PRO:O	1:A:76:SER:OG	2.29	0.41
1:D:32:ASN:HD22	1:D:32:ASN:HA	1.55	0.41
1:D:59:ARG:HA	1:D:103:ARG:CZ	2.51	0.41
2:G:128:HIS:CE1	2:G:129:TRP:HB2	2.54	0.41
2:H:31:LEU:HA	2:H:63:ILE:O	2.21	0.41
2:H:58:ARG:HG2	2:H:63:ILE:HG13	2.03	0.41
2:H:97:SER:N	2:H:111:GLN:O	2.51	0.41
1:D:65:ASP:OD2	1:D:67:MET:HB2	2.21	0.40
1:D:109:ARG:HG3	1:D:109:ARG:NH2	2.34	0.40
2:F:137:ARG:CG	2:F:138:PRO:HD3	2.32	0.40
2:F:275:ASP:C	2:F:277:ASP:H	2.23	0.40
2:H:160:HIS:CD2	2:H:184:LEU:HD11	2.56	0.40
2:E:173:THR:HB	2:E:176:CYS:HB3	2.03	0.40
2:F:23:LEU:O	2:F:46:THR:N	2.53	0.40
2:F:273:HIS:ND1	2:F:274:PRO:CD	2.84	0.40
1:B:23:LYS:N	2:F:140:ASP:OD1	2.51	0.40
2:E:198:LYS:O	2:E:205:CYS:SG	2.80	0.40
1:B:85:HIS:CE1	1:B:88:ARG:HG3	2.57	0.40
2:F:256:PHE:HB3	2:F:258:MET:HG3	2.04	0.40
2:G:31:LEU:HA	2:G:63:ILE:O	2.21	0.40
2:E:206:SER:O	2:E:210:THR:HG23	2.21	0.40
2:F:229:HIS:CD2	2:F:230:GLU:N	2.89	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	120/145 (83%)	109 (91%)	9 (8%)	2 (2%)	9	29
1	B	120/145 (83%)	108 (90%)	11 (9%)	1 (1%)	19	49
1	C	120/145 (83%)	94 (78%)	18 (15%)	8 (7%)	1	3
1	D	120/145 (83%)	98 (82%)	16 (13%)	6 (5%)	2	6
2	E	257/279 (92%)	209 (81%)	37 (14%)	11 (4%)	2	8
2	F	257/279 (92%)	208 (81%)	37 (14%)	12 (5%)	2	7
2	G	236/279 (85%)	194 (82%)	22 (9%)	20 (8%)	1	1
2	H	236/279 (85%)	196 (83%)	21 (9%)	19 (8%)	1	2
All	All	1466/1696 (86%)	1216 (83%)	171 (12%)	79 (5%)	2	5

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	119	LEU
1	D	119	LEU
2	E	36	GLU
2	E	201	SER
2	F	36	GLU
2	F	201	SER
2	G	78	GLN
2	G	79	GLY
2	G	209	GLU
2	H	19	LEU
2	H	78	GLN
2	H	209	GLU
2	H	233	GLN
1	D	107	ASN
2	E	8	THR
2	E	60	GLY
2	E	79	GLY
2	E	185	GLU
2	F	60	GLY
2	F	79	GLY
2	F	185	GLU
2	G	19	LEU
2	G	73	LEU
2	G	76	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	232	LYS
2	G	233	GLN
2	G	257	SER
2	H	73	LEU
2	H	75	LEU
2	H	76	CYS
2	H	79	GLY
2	H	173	THR
2	H	232	LYS
2	H	257	SER
1	C	91	ALA
1	C	107	ASN
1	C	131	CYS
2	E	1	LEU
2	E	34	GLU
2	E	80	ASN
2	E	256	PHE
2	F	8	THR
2	F	80	ASN
2	F	151	PRO
2	F	256	PHE
2	G	17	CYS
2	G	75	LEU
2	G	101	SER
2	G	173	THR
2	G	255	ALA
2	H	17	CYS
2	H	44	SER
2	H	101	SER
2	H	255	ALA
1	A	26	SER
1	C	116	GLN
1	D	26	SER
1	D	91	ALA
1	D	116	GLN
2	E	151	PRO
2	F	1	LEU
2	F	34	GLU
2	G	8	THR
2	G	20	GLY
2	G	44	SER
2	G	231	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	20	GLY
2	H	231	PRO
1	B	26	SER
1	C	35	LYS
1	C	45	ASP
1	D	47	SER
2	F	13	ARG
2	G	60	GLY
2	H	60	GLY
1	C	47	SER
2	G	48	SER
2	H	48	SER
1	A	28	ILE

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	106/128 (83%)	99 (93%)	7 (7%)	16	44
1	B	106/128 (83%)	100 (94%)	6 (6%)	20	50
1	C	106/128 (83%)	99 (93%)	7 (7%)	16	44
1	D	106/128 (83%)	99 (93%)	7 (7%)	16	44
2	E	236/247 (96%)	212 (90%)	24 (10%)	7	22
2	F	236/247 (96%)	213 (90%)	23 (10%)	8	24
2	G	220/247 (89%)	203 (92%)	17 (8%)	13	35
2	H	220/247 (89%)	205 (93%)	15 (7%)	16	42
All	All	1336/1500 (89%)	1230 (92%)	106 (8%)	12	34

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	54	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	83	THR
1	A	110	ARG
1	A	120	LYS
1	A	127	MET
1	A	130	ASP
1	B	43	GLU
1	B	54	ASN
1	B	83	THR
1	B	110	ARG
1	B	120	LYS
1	B	127	MET
1	C	32	ASN
1	C	43	GLU
1	C	54	ASN
1	C	59	ARG
1	C	64	THR
1	C	109	ARG
1	C	127	MET
1	D	32	ASN
1	D	43	GLU
1	D	54	ASN
1	D	59	ARG
1	D	64	THR
1	D	109	ARG
1	D	127	MET
2	E	1	LEU
2	E	23	LEU
2	E	30	ARG
2	E	40	LEU
2	E	67	THR
2	E	77	ASN
2	E	80	ASN
2	E	110	HIS
2	E	116	ARG
2	E	119	GLU
2	E	151	PRO
2	E	171	CYS
2	E	182	LEU
2	E	184	LEU
2	E	189	GLN
2	E	192	ARG
2	E	208	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	221	GLN
2	E	223	LEU
2	E	245	SER
2	E	252	LEU
2	E	259	ASN
2	E	261	ILE
2	E	277	ASP
2	F	1	LEU
2	F	23	LEU
2	F	40	LEU
2	F	67	THR
2	F	77	ASN
2	F	80	ASN
2	F	110	HIS
2	F	116	ARG
2	F	119	GLU
2	F	151	PRO
2	F	171	CYS
2	F	182	LEU
2	F	184	LEU
2	F	189	GLN
2	F	192	ARG
2	F	208	GLU
2	F	221	GLN
2	F	223	LEU
2	F	245	SER
2	F	252	LEU
2	F	259	ASN
2	F	261	ILE
2	F	277	ASP
2	G	17	CYS
2	G	29	VAL
2	G	54	THR
2	G	73	LEU
2	G	77	ASN
2	G	110	HIS
2	G	116	ARG
2	G	117	SER
2	G	162	GLN
2	G	164	THR
2	G	189	GLN
2	G	190	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	221	GLN
2	G	223	LEU
2	G	226	THR
2	G	232	LYS
2	G	256	PHE
2	H	17	CYS
2	H	29	VAL
2	H	54	THR
2	H	73	LEU
2	H	77	ASN
2	H	110	HIS
2	H	117	SER
2	H	164	THR
2	H	189	GLN
2	H	190	ASN
2	H	221	GLN
2	H	223	LEU
2	H	226	THR
2	H	232	LYS
2	H	256	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	41	HIS
1	A	54	ASN
1	A	93	GLN
1	A	107	ASN
1	A	116	GLN
1	B	40	GLN
1	B	41	HIS
1	B	54	ASN
1	B	93	GLN
1	B	107	ASN
1	B	116	GLN
1	C	15	ASN
1	C	32	ASN
1	C	54	ASN
1	C	56	HIS
1	C	82	GLN
1	C	93	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	104	ASN
1	D	15	ASN
1	D	54	ASN
1	D	56	HIS
1	D	82	GLN
1	D	93	GLN
1	D	104	ASN
2	E	77	ASN
2	E	78	GLN
2	E	80	ASN
2	E	111	GLN
2	E	121	GLN
2	E	128	HIS
2	E	189	GLN
2	E	190	ASN
2	E	193	GLN
2	E	221	GLN
2	E	233	GLN
2	E	259	ASN
2	F	77	ASN
2	F	78	GLN
2	F	80	ASN
2	F	111	GLN
2	F	121	GLN
2	F	128	HIS
2	F	160	HIS
2	F	189	GLN
2	F	190	ASN
2	F	193	GLN
2	F	221	GLN
2	F	233	GLN
2	F	259	ASN
2	G	21	GLN
2	G	78	GLN
2	G	80	ASN
2	G	110	HIS
2	G	111	GLN
2	G	114	GLN
2	G	128	HIS
2	G	131	GLN
2	G	160	HIS
2	G	162	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	166	HIS
2	G	172	GLN
2	G	190	ASN
2	G	193	GLN
2	G	221	GLN
2	G	229	HIS
2	G	233	GLN
2	G	234	GLN
2	G	260	HIS
2	G	273	HIS
2	H	21	GLN
2	H	78	GLN
2	H	80	ASN
2	H	110	HIS
2	H	111	GLN
2	H	114	GLN
2	H	128	HIS
2	H	131	GLN
2	H	160	HIS
2	H	162	GLN
2	H	166	HIS
2	H	172	GLN
2	H	190	ASN
2	H	193	GLN
2	H	221	GLN
2	H	229	HIS
2	H	234	GLN
2	H	260	HIS
2	H	273	HIS

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)

10 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	I	1	2,3	14,14,15	0.48	0	17,19,21	1.30	1 (5%)
3	NAG	I	2	3	14,14,15	0.44	0	17,19,21	1.95	2 (11%)
3	BMA	I	3	3	11,11,12	0.69	0	15,15,17	0.97	0
3	NAG	J	1	2,3	14,14,15	0.60	0	17,19,21	1.28	1 (5%)
3	NAG	J	2	3	14,14,15	0.52	0	17,19,21	1.89	3 (17%)
3	BMA	J	3	3	11,11,12	0.68	0	15,15,17	0.73	0
4	NAG	K	1	2,4	14,14,15	0.49	0	17,19,21	1.52	1 (5%)
4	NAG	K	2	4	14,14,15	0.50	0	17,19,21	1.80	4 (23%)
4	NAG	L	1	4	14,14,15	0.49	0	17,19,21	1.28	2 (11%)
4	NAG	L	2	4	14,14,15	0.55	0	17,19,21	1.71	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	I	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1
3	BMA	I	3	3	-	2/2/19/22	0/1/1/1
3	NAG	J	1	2,3	-	4/6/23/26	0/1/1/1
3	NAG	J	2	3	-	4/6/23/26	0/1/1/1
3	BMA	J	3	3	-	2/2/19/22	0/1/1/1
4	NAG	K	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	K	2	4	-	6/6/23/26	0/1/1/1
4	NAG	L	1	4	-	3/6/23/26	0/1/1/1
4	NAG	L	2	4	-	6/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	2	NAG	C1-O5-C5	6.00	120.32	112.19
3	I	2	NAG	C1-O5-C5	5.57	119.73	112.19
4	K	2	NAG	C1-O5-C5	5.56	119.73	112.19
3	J	2	NAG	C4-C3-C2	-4.95	103.77	111.02
4	K	1	NAG	O5-C5-C6	4.48	114.23	107.20
3	J	2	NAG	C1-O5-C5	4.21	117.90	112.19
3	I	2	NAG	C4-C3-C2	-4.13	104.97	111.02
3	I	1	NAG	O5-C1-C2	-3.65	105.52	111.29
4	L	1	NAG	C1-O5-C5	3.01	116.27	112.19
4	K	2	NAG	O5-C5-C6	2.87	111.70	107.20
4	L	1	NAG	O5-C5-C6	2.56	111.22	107.20
3	J	1	NAG	O4-C4-C3	-2.52	104.53	110.35
3	J	2	NAG	O5-C5-C6	-2.46	103.35	107.20
4	K	2	NAG	C3-C4-C5	2.33	114.40	110.24
4	K	2	NAG	C2-N2-C7	2.09	125.88	122.90

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	1	NAG	C3-C2-N2-C7
3	J	1	NAG	C8-C7-N2-C2
3	J	1	NAG	O7-C7-N2-C2
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
4	K	2	NAG	C8-C7-N2-C2
4	K	2	NAG	O7-C7-N2-C2
4	L	1	NAG	C8-C7-N2-C2
4	L	1	NAG	O7-C7-N2-C2
4	L	2	NAG	C1-C2-N2-C7
4	L	2	NAG	C8-C7-N2-C2
4	L	2	NAG	O7-C7-N2-C2
4	L	2	NAG	C4-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
3	J	3	BMA	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
4	L	2	NAG	O5-C5-C6-O6
3	I	3	BMA	C4-C5-C6-O6
3	J	3	BMA	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	K	1	NAG	C4-C5-C6-O6
3	J	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
3	J	2	NAG	O5-C5-C6-O6
4	K	2	NAG	C1-C2-N2-C7
4	K	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
4	K	2	NAG	C3-C2-N2-C7
3	J	1	NAG	C4-C5-C6-O6
4	L	2	NAG	C3-C2-N2-C7
3	J	2	NAG	C4-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6

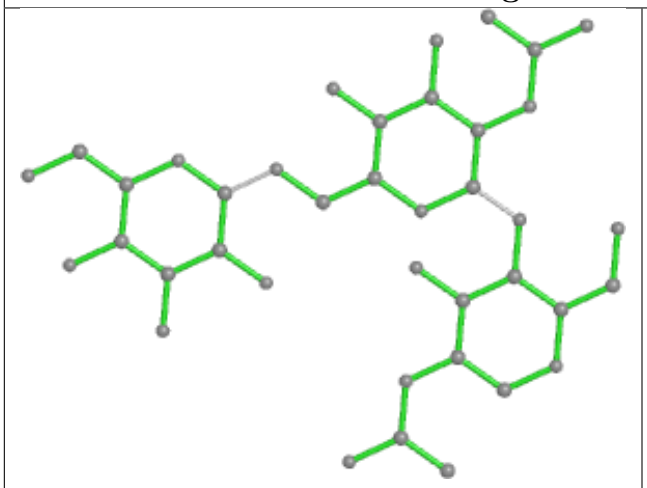
There are no ring outliers.

5 monomers are involved in 3 short contacts:

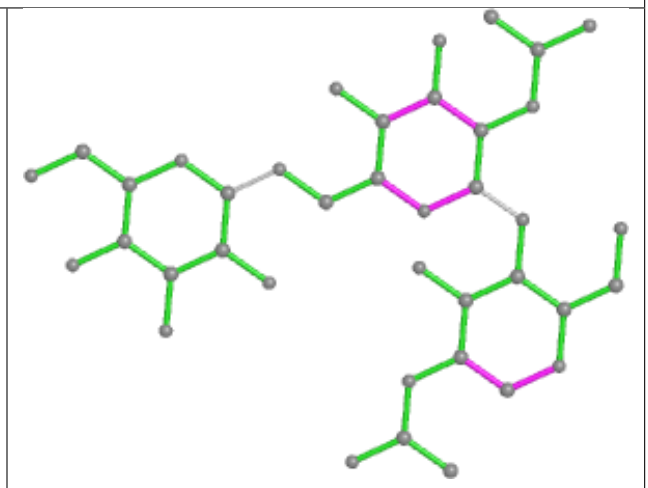
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	2	NAG	1	0
4	L	1	NAG	1	0
3	J	1	NAG	1	0
3	I	2	NAG	1	0
3	I	1	NAG	1	0

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

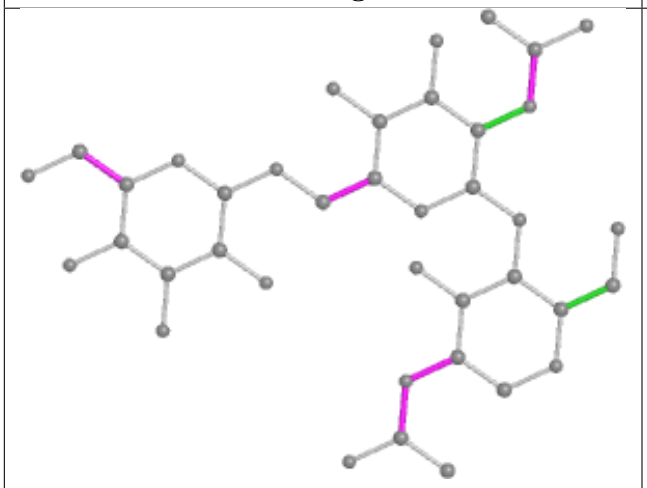
Oligosaccharide Chain I



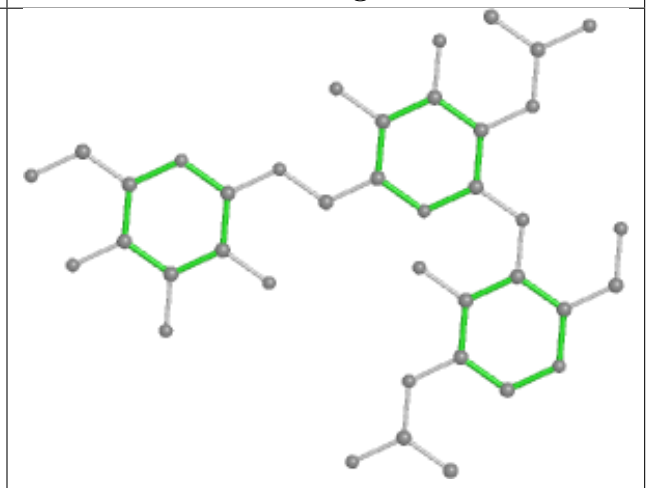
Bond lengths



Bond angles

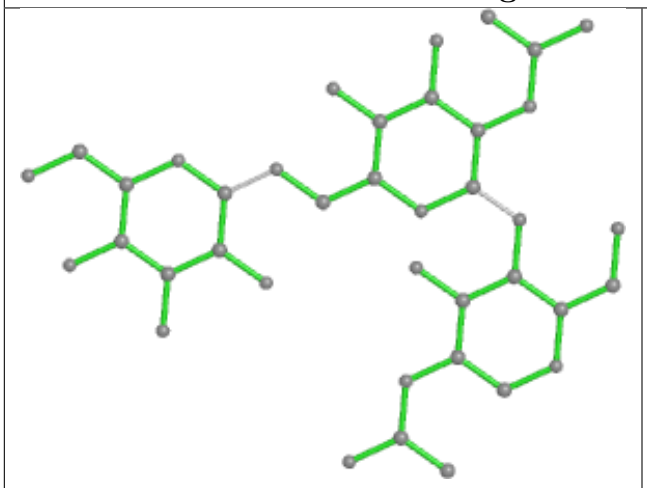


Torsions

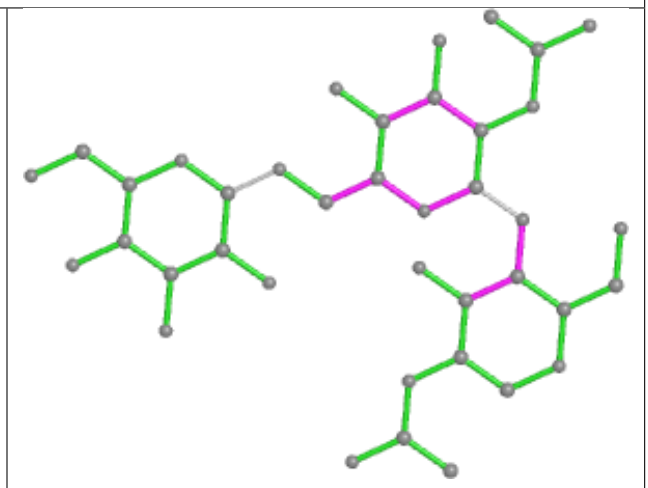


Rings

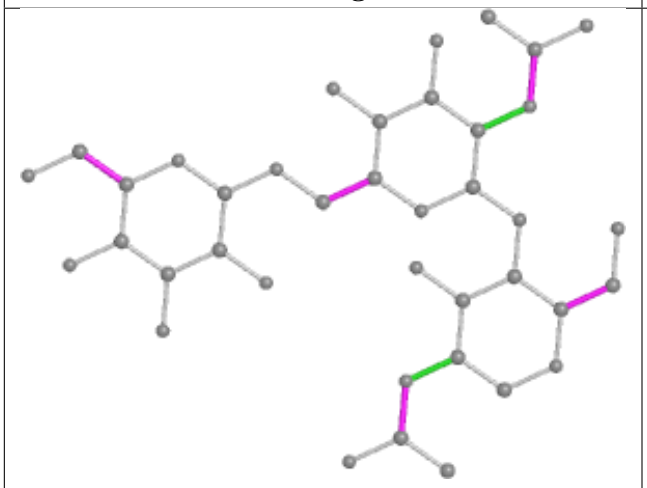
Oligosaccharide Chain J



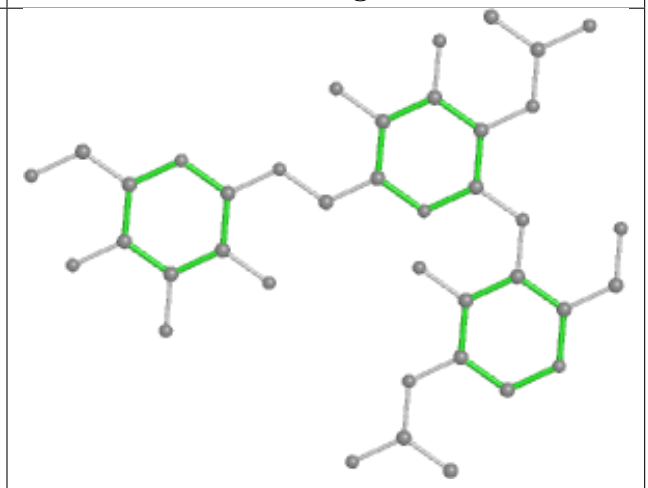
Bond lengths



Bond angles

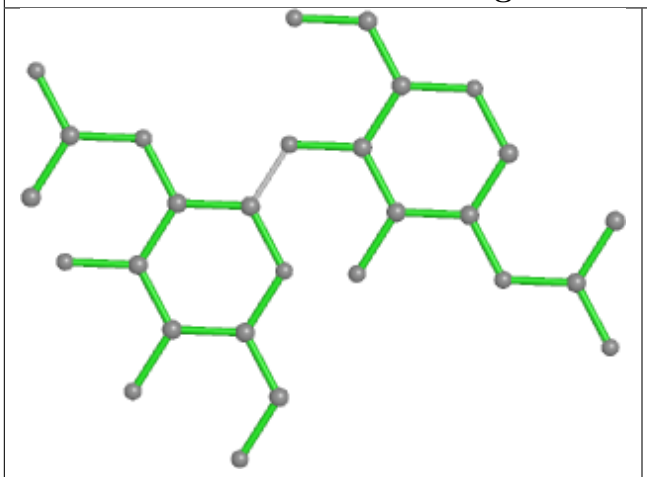


Torsions

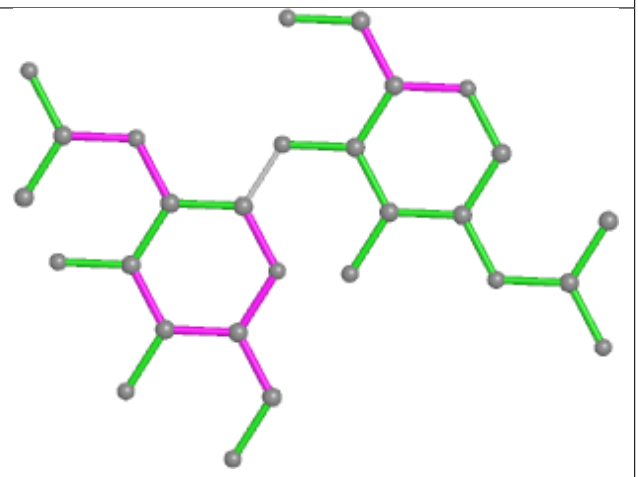


Rings

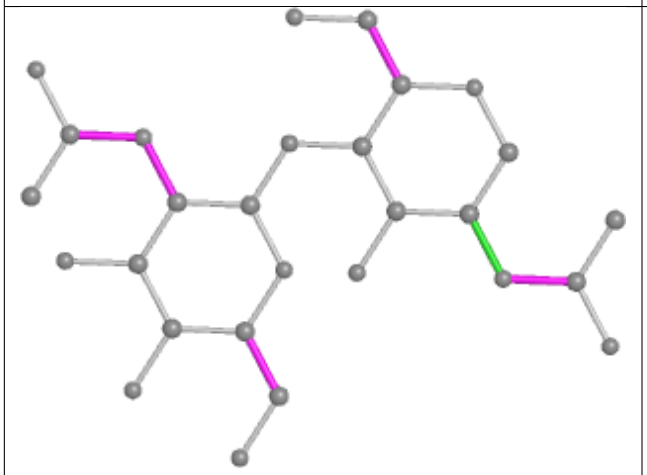
Oligosaccharide Chain K



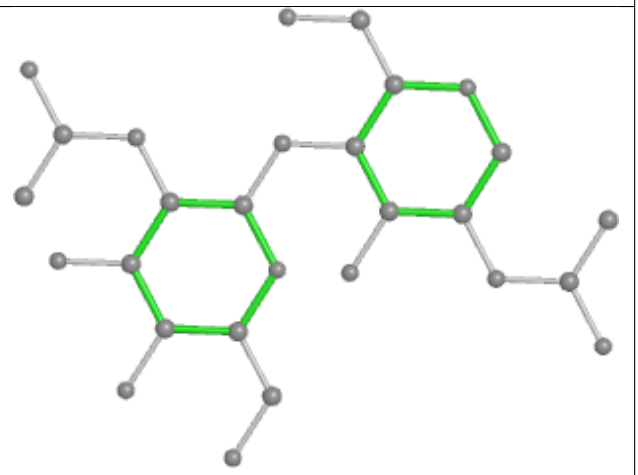
Bond lengths



Bond angles

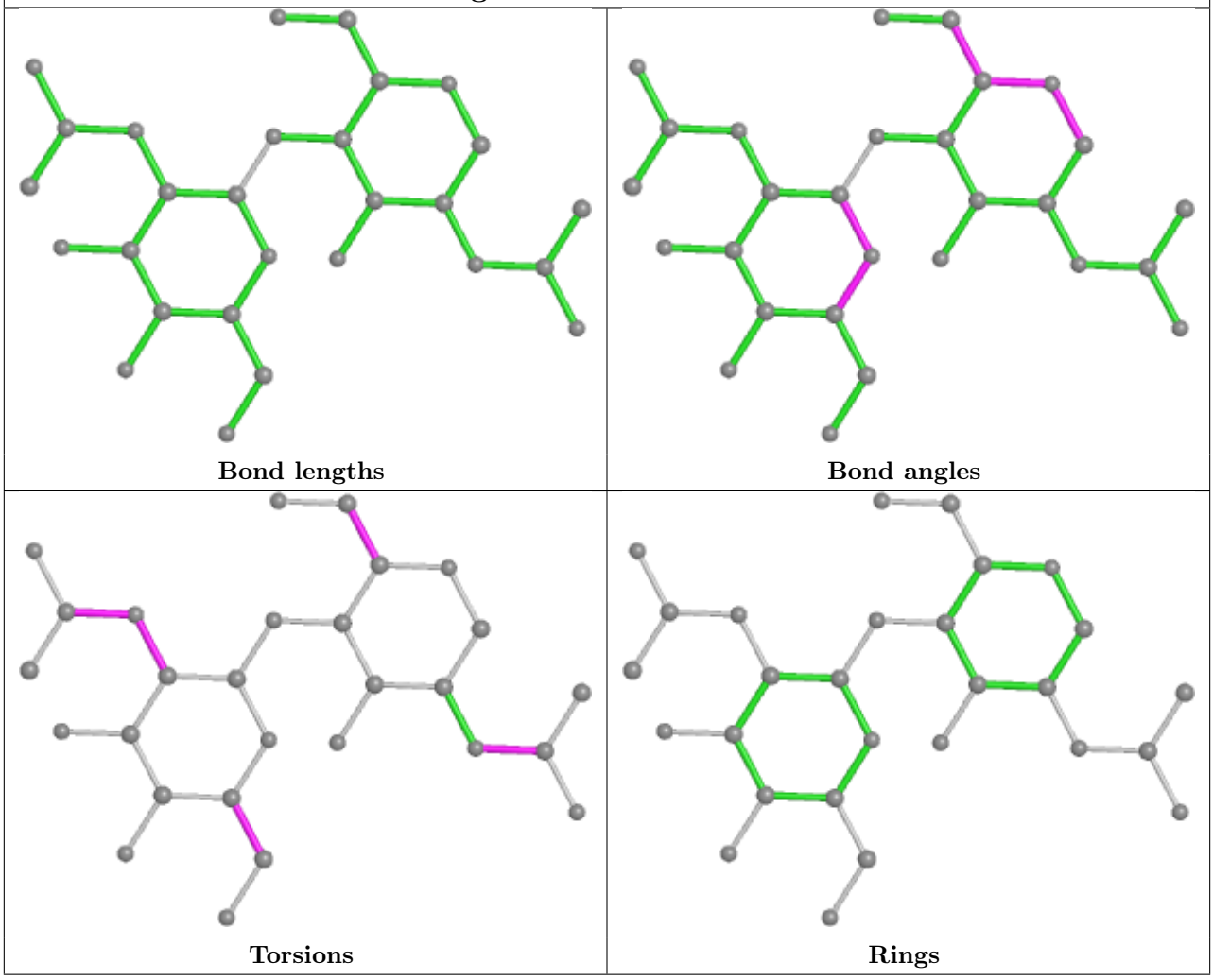


Torsions



Rings

Oligosaccharide Chain L



5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	F	328	-	4,4,4	0.24	0	6,6,6	1.05	0
5	SO4	E	318	-	4,4,4	0.15	0	6,6,6	0.96	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	328	SO4	3	0
5	E	318	SO4	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	122/145 (84%)	-0.15	0	100	100	50, 65, 80, 92	0
1	B	122/145 (84%)	-0.14	0	100	100	50, 65, 80, 92	0
1	C	122/145 (84%)	-0.07	0	100	100	49, 67, 77, 80	0
1	D	122/145 (84%)	0.06	2 (1%)	72	66	49, 67, 76, 80	0
2	E	265/279 (94%)	-0.11	7 (2%)	56	46	48, 70, 91, 104	0
2	F	265/279 (94%)	-0.05	4 (1%)	73	68	48, 70, 91, 104	0
2	G	248/279 (88%)	0.14	13 (5%)	27	18	48, 68, 80, 92	0
2	H	248/279 (88%)	0.14	9 (3%)	42	32	48, 68, 80, 92	0
All	All	1514/1696 (89%)	-0.01	35 (2%)	60	51	48, 68, 85, 104	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	131	GLN	6.6
2	H	19	LEU	6.0
2	F	131	GLN	5.4
2	H	131	GLN	4.4
2	E	131	GLN	4.2
2	G	251	HIS	4.0
2	H	251	HIS	3.5
2	G	61	LEU	3.4
2	E	81	SER	3.3
2	F	49	GLU	3.2
2	G	63	ILE	3.2
2	G	232	LYS	3.1
2	F	83	ARG	3.1
2	G	256	PHE	3.0
2	G	110	HIS	3.0
2	G	116	ARG	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	80	ASN	2.9
2	H	150	LEU	2.8
2	G	150	LEU	2.7
2	G	72	GLY	2.7
2	E	79	GLY	2.7
2	H	61	LEU	2.7
2	H	144	LEU	2.6
2	H	31	LEU	2.5
2	E	0	SER	2.5
1	D	127	MET	2.5
2	E	32	TRP	2.4
2	G	260	HIS	2.3
2	H	232	LYS	2.3
2	G	2	ARG	2.3
2	H	75	LEU	2.3
2	F	81	SER	2.2
2	G	58	ARG	2.1
2	E	83	ARG	2.0
1	D	78	THR	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
4	NAG	L	1	14/15	0.51	0.25	80,164,186,192	0
3	BMA	J	3	11/12	0.69	0.23	97,155,174,194	0
3	BMA	I	3	11/12	0.73	0.20	107,159,168,181	0
4	NAG	L	2	14/15	0.82	0.17	85,138,149,150	0
3	NAG	J	2	14/15	0.84	0.19	55,99,125,152	0
4	NAG	K	2	14/15	0.85	0.16	94,129,153,156	0
3	NAG	I	2	14/15	0.87	0.16	73,96,142,161	0
4	NAG	K	1	14/15	0.88	0.10	80,138,160,163	0
3	NAG	I	1	14/15	0.95	0.12	66,91,107,116	0

Continued on next page...

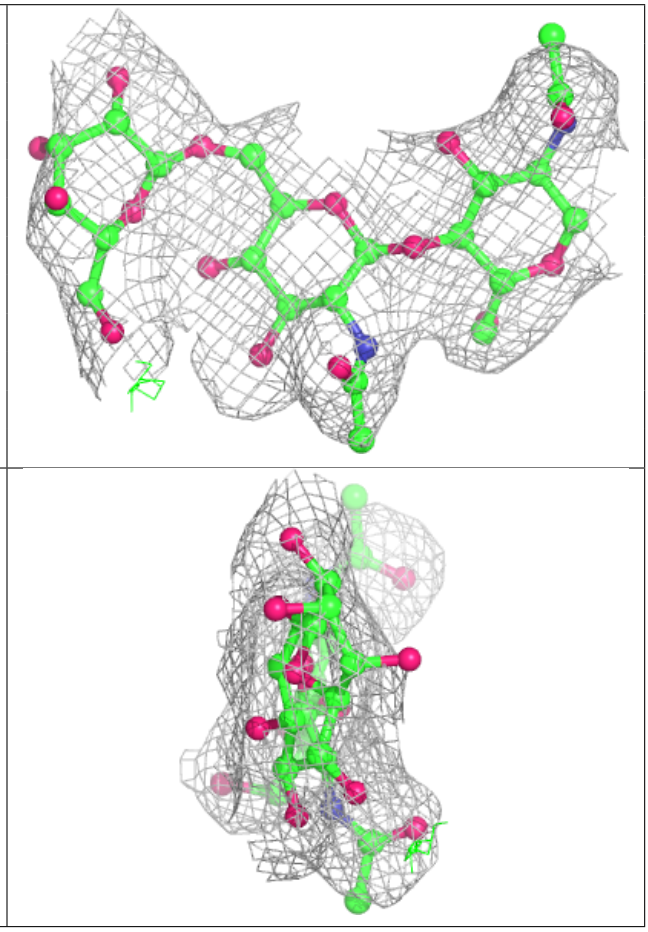
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	J	1	14/15	0.95	0.13	58,83,112,116	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.

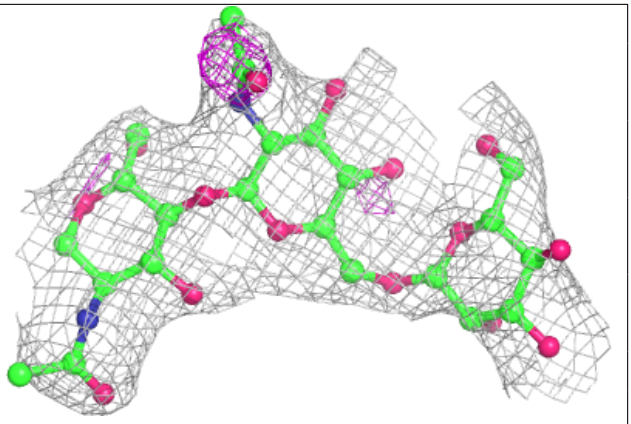
Electron density around Chain I:

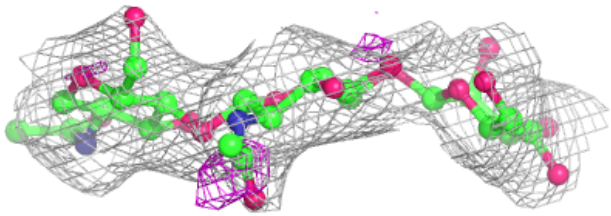
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

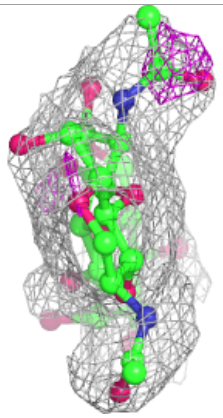


Electron density around Chain J:

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

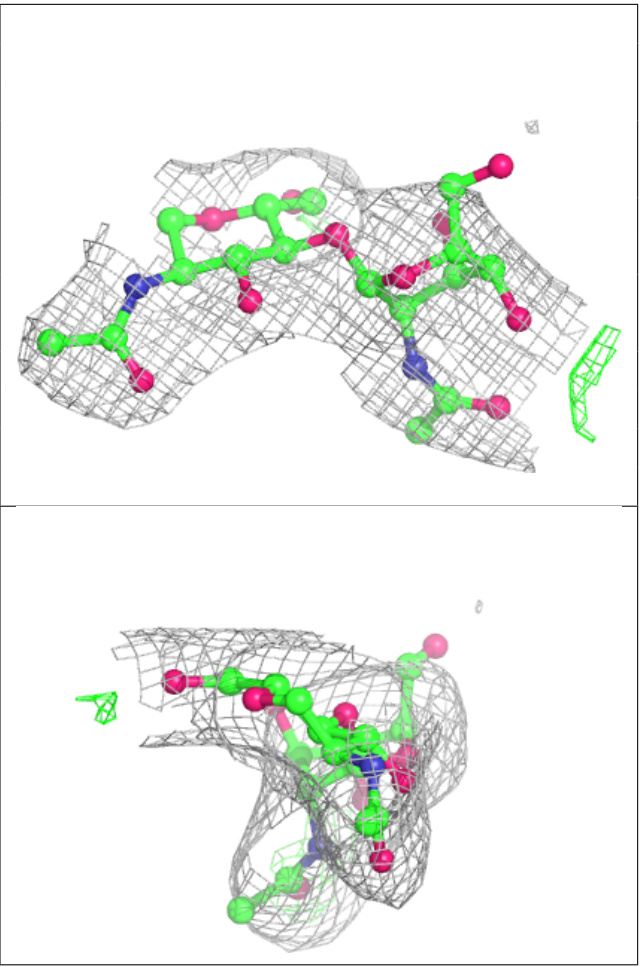






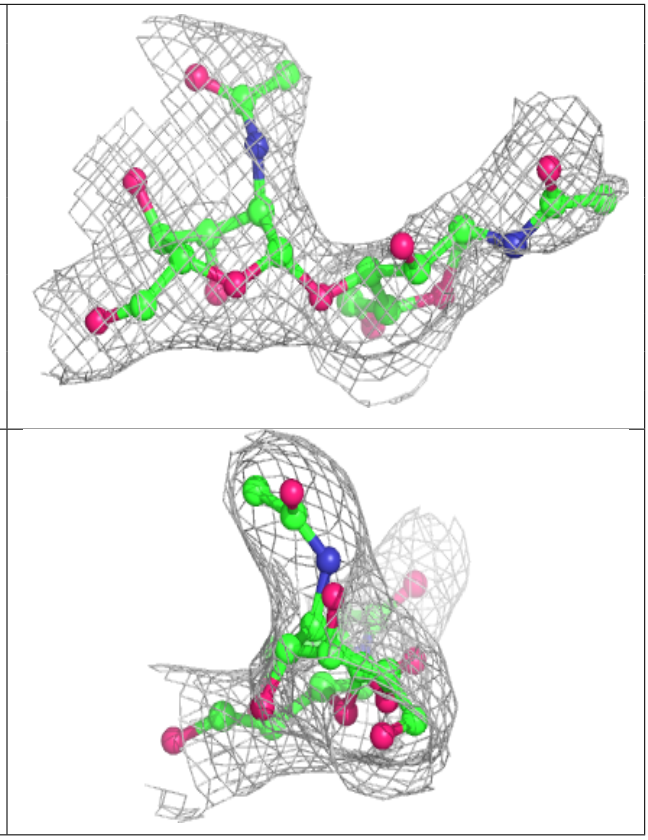
Electron density around Chain K:

$2mF_o$-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 L:

$2mF_o$-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
5	SO4	F	328	5/5	0.97	0.16	54,56,74,88	0
5	SO4	E	318	5/5	0.98	0.16	52,57,75,81	0

6.5 Other polymers (i)

There are no such residues in this entry.