Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 04:08 AM JST

PDB ID	:	6KN9
Title	:	Crystal structure of human interleukin 18 receptor beta extracellular domain in complex with an antagonistic scFv
Authors	:	Wu, D.H.; Liu, C.C.
Deposited on	:	2019-08-05
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

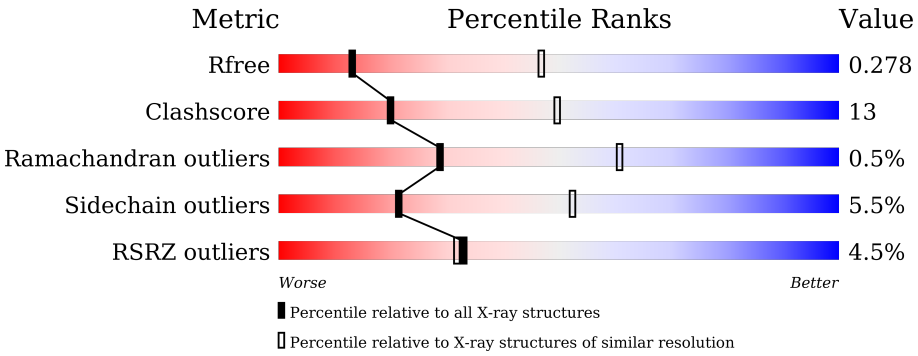
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	337	53% 23% 23%
1	B	337	5% 48% 17% 34%
1	C	337	55% 20% 23%
2	D	257	2% 61% 23% 14%
2	E	257	8% 40% 12% 48%
2	F	257	4% 59% 25% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	2	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9768 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 Interleukin-18 receptor accessory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1939	1236	327	368	8			
1	B	224	Total	C	N	O	S	0	0	0
			1609	1024	270	307	8			
1	C	261	Total	C	N	O	S	0	0	0
			1957	1251	333	366	7			

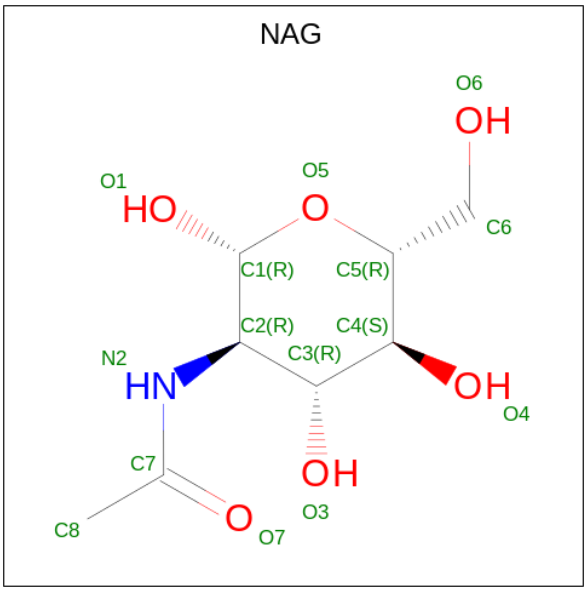
- Molecule 2 is a protein called scFv.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	220	Total	C	N	O	S	0	0	0
			1622	1035	262	320	5			
2	E	134	Total	C	N	O	S	0	0	0
			939	593	153	189	4			
2	F	221	Total	C	N	O	S	0	0	0
			1646	1052	270	318	6			

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

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



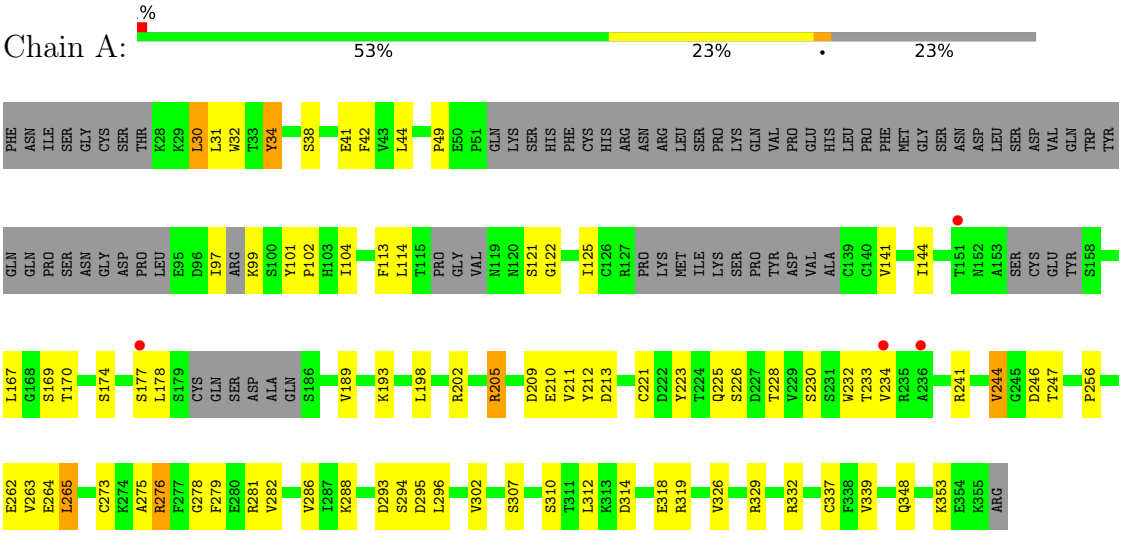
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0

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.

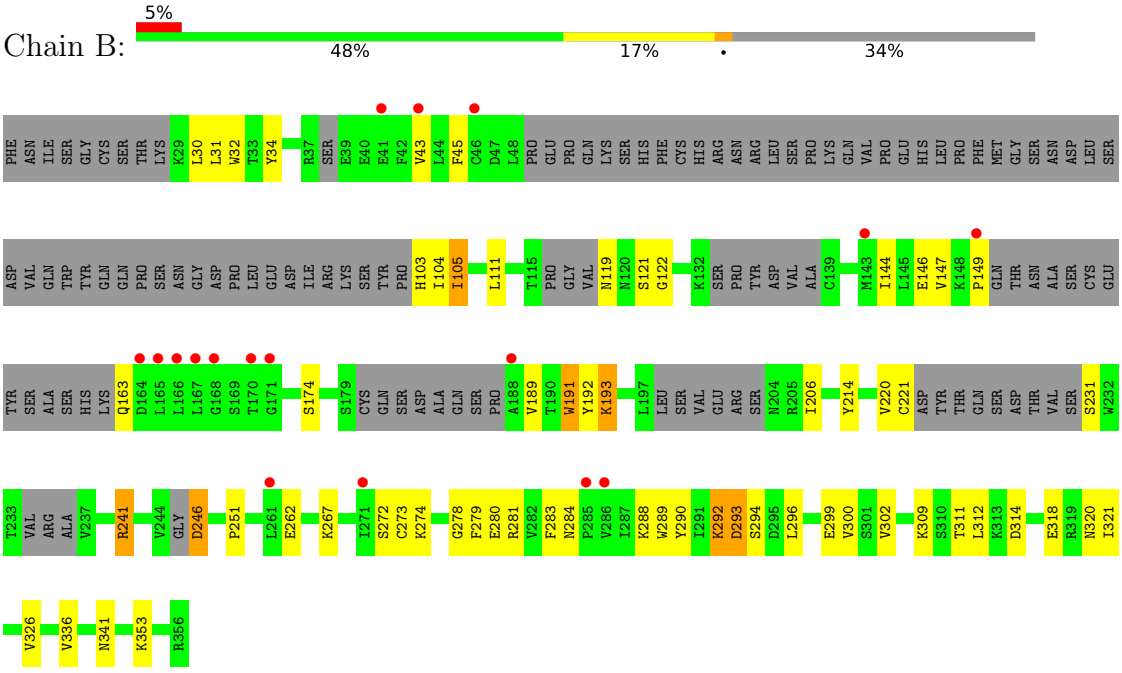
• Molecule 1: Interleukin-18 receptor accessory protein

Chain A:



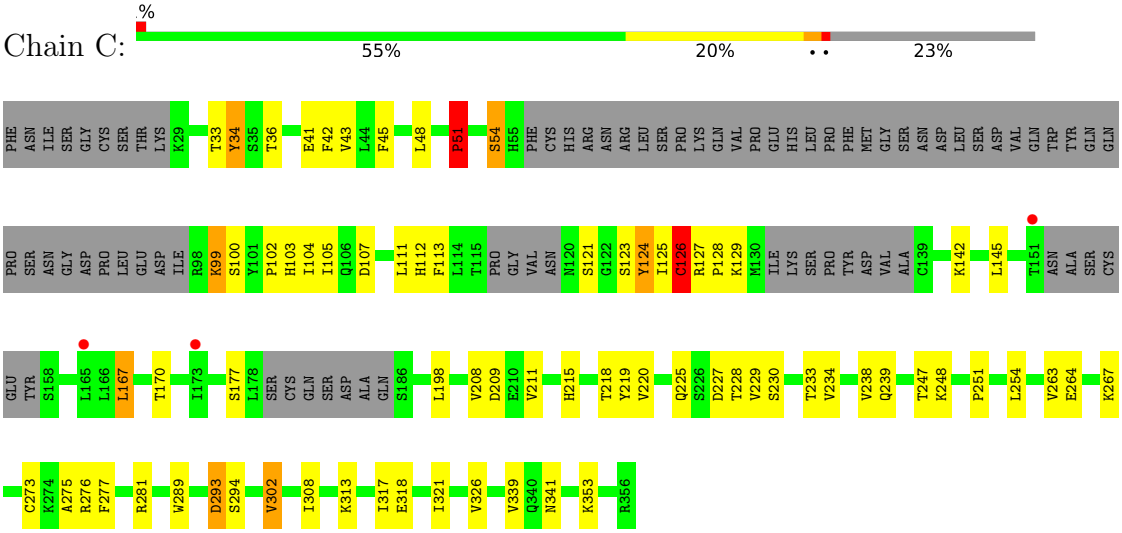
• Molecule 1: Interleukin-18 receptor accessory protein

Chain B:



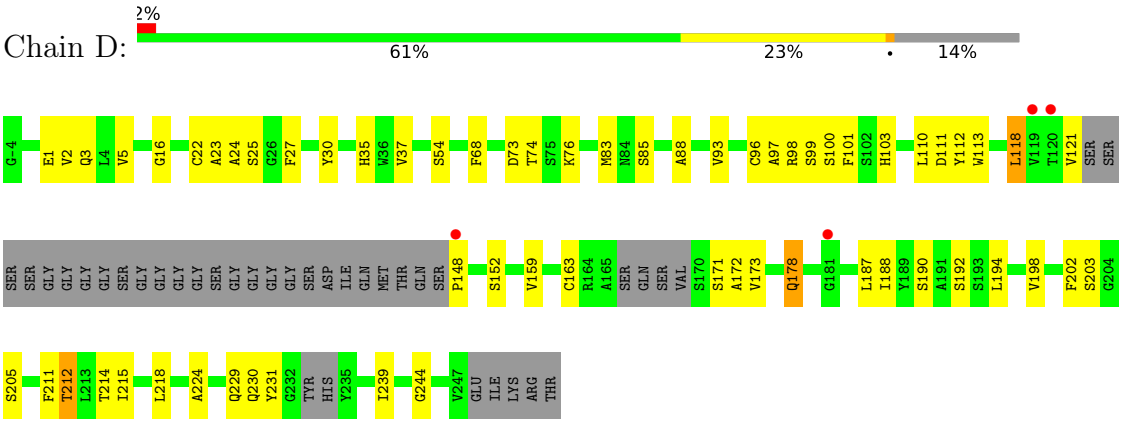
• Molecule 1: Interleukin-18 receptor accessory protein

Chain C:



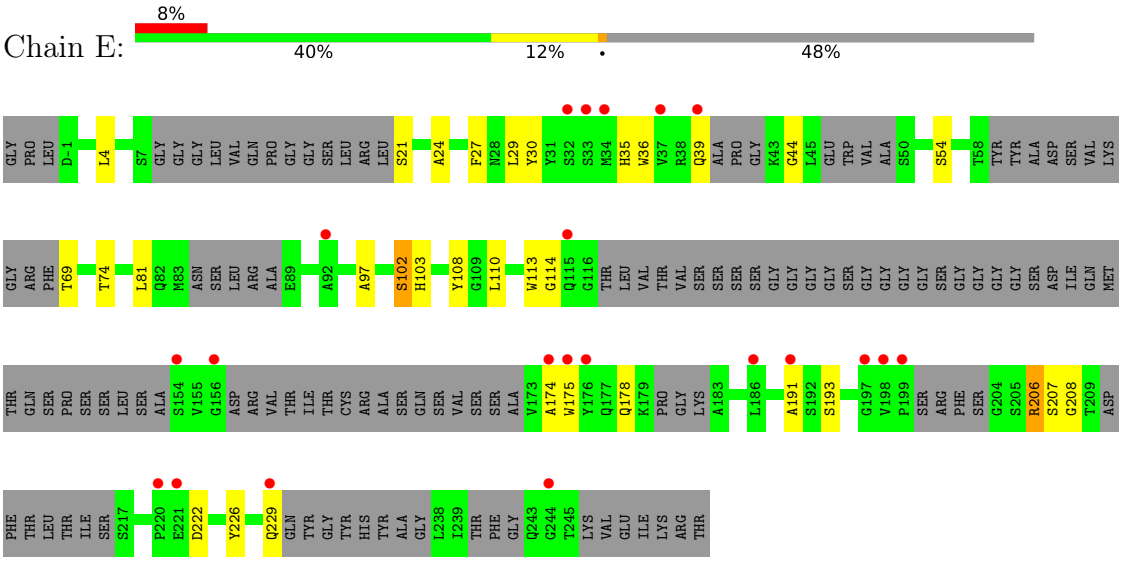
• Molecule 2: scFv

Chain D:



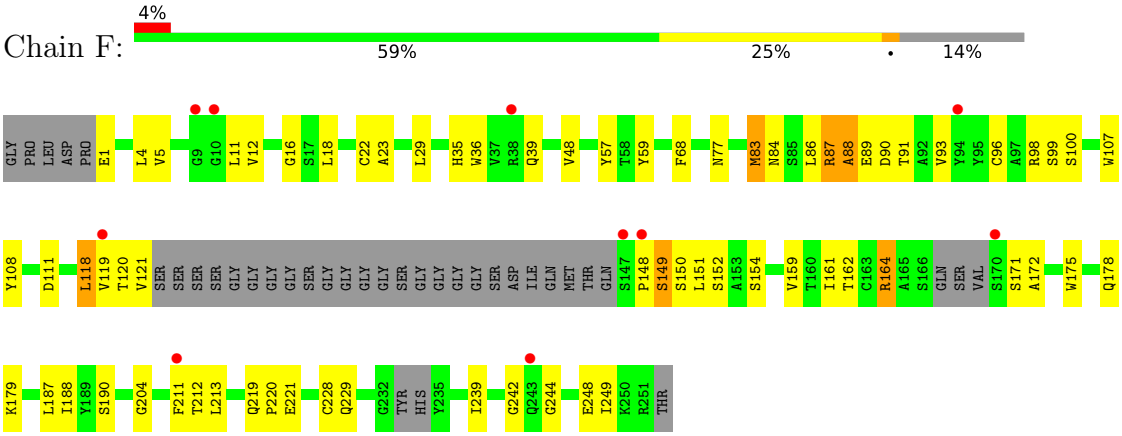
• Molecule 2: scFv

Chain E:



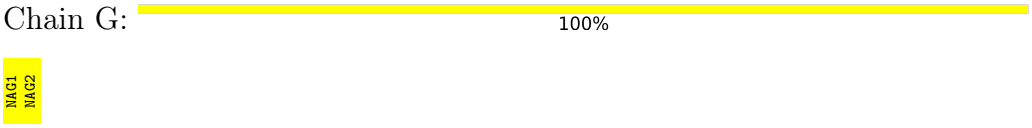
• Molecule 2: scFv

Chain F:



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

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	163.16Å 163.16Å 64.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.19 – 3.30 47.49 – 3.30	Depositor EDS
% Data completeness (in resolution range)	87.0 (39.19-3.30) 87.0 (47.49-3.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.247 , 0.277 0.251 , 0.278	Depositor DCC
R_{free} test set	1257 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 23.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l 0.029 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	9768	wwPDB-VP
Average B, all atoms (Å^2)	50.0	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 23.08 % 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 5.0027e-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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.61	1/1969 (0.1%)	0.84	5/2678 (0.2%)
1	B	0.46	0/1626	0.62	0/2206
1	C	0.57	1/1990 (0.1%)	0.78	2/2707 (0.1%)
2	D	0.63	1/1663 (0.1%)	0.73	0/2264
2	E	0.40	0/954	0.59	0/1291
2	F	0.52	0/1686	0.72	0/2292
All	All	0.55	3/9888 (0.0%)	0.73	7/13438 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	6
1	C	0	3
2	D	0	1
2	F	0	2
All	All	0	15

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	178	GLN	C-N	-5.57	1.21	1.34
1	C	126	CYS	CB-SG	5.18	1.91	1.82
1	A	273	CYS	CB-SG	-5.16	1.73	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	30	LEU	CA-CB-CG	7.41	132.35	115.30
1	A	337	CYS	CA-CB-SG	-6.47	102.36	114.00
1	A	205	ARG	NE-CZ-NH1	-6.03	117.29	120.30
1	A	49	PRO	C-N-CA	5.61	135.73	121.70
1	C	167	LEU	CA-CB-CG	5.44	127.81	115.30
1	C	254	LEU	CB-CG-CD2	-5.22	102.12	111.00
1	A	312	LEU	CB-CG-CD2	-5.19	102.18	111.00

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	THR	Peptide
1	A	293	ASP	Peptide
1	A	302	VAL	Peptide
1	B	103	HIS	Peptide
1	B	104	ILE	Peptide
1	B	189	VAL	Peptide
1	B	231	SER	Peptide
1	B	293	ASP	Peptide
1	B	45	PHE	Peptide
1	C	124	TYR	Peptide
1	C	293	ASP	Peptide
1	C	51	PRO	Peptide
2	D	1	GLU	Peptide
2	F	1	GLU	Peptide
2	F	249	ILE	Peptide

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	1939	0	1830	49	0
1	B	1609	0	1445	40	0
1	C	1957	0	1871	46	0
2	D	1622	0	1491	45	0
2	E	939	0	769	23	0
2	F	1646	0	1535	49	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	28	0	25	0	0
4	A	14	0	13	0	0
4	C	14	0	13	0	0
All	All	9768	0	8992	237	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 13.

All (237) 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:F:16:GLY:O	2:F:84:ASN:O	1.75	1.03
1:A:276:ARG:NH2	1:A:314:ASP:OD1	1.97	0.98
1:B:191:TRP:HE1	1:B:206:ILE:HB	1.30	0.96
1:C:251:PRO:HD3	1:C:341:ASN:HB2	1.45	0.96
2:E:102:SER:HG	2:E:103:HIS:HD1	1.20	0.89
1:C:218:THR:HG22	1:C:239:GLN:HG3	1.60	0.82
1:A:193:LYS:HB2	1:A:198:LEU:HD11	1.62	0.82
2:F:83:MET:HE1	2:F:119:VAL:HG21	1.62	0.81
2:F:91:THR:HG23	2:F:120:THR:HA	1.63	0.79
2:F:87:ARG:O	2:F:89:GLU:N	2.17	0.77
2:E:222:ASP:O	2:E:226:TYR:OH	2.03	0.76
2:F:68:PHE:CD1	2:F:83:MET:HA	2.23	0.74
1:A:31:LEU:HD22	1:A:144:ILE:HB	1.69	0.73
2:F:68:PHE:CE1	2:F:83:MET:HB3	2.24	0.73
2:F:171:SER:OG	2:F:172:ALA:N	2.22	0.73
1:A:247:THR:HG21	1:A:278:GLY:HA3	1.69	0.72
2:D:171:SER:HB2	2:D:231:TYR:O	1.89	0.72
1:A:281:ARG:NH1	2:D:111:ASP:OD1	2.23	0.72
1:A:232:TRP:HE1	1:A:234:VAL:HG22	1.55	0.71
1:A:169:SER:OG	1:A:170:THR:N	2.23	0.71
2:D:148:PRO:HB3	2:D:244:GLY:HA3	1.74	0.68
1:C:167:LEU:HA	1:C:211:VAL:HB	1.75	0.68
1:A:210:GLU:HG2	1:A:212:TYR:CZ	2.29	0.67
1:A:167:LEU:HD21	1:A:244:VAL:HG23	1.75	0.67
1:B:121:SER:HB2	1:B:147:VAL:HB	1.78	0.66
1:C:100:SER:O	1:C:102:PRO:HD3	1.97	0.65
1:C:227:ASP:HB3	1:C:229:VAL:H	1.62	0.64
2:D:187:LEU:HA	2:D:198:VAL:HG21	1.80	0.63
1:A:310:SER:OG	2:D:103:HIS:O	2.14	0.63
1:C:51:PRO:HG2	1:C:54:SER:N	2.13	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:SER:HA	1:C:145:LEU:H	1.63	0.63
1:A:294:SER:OG	1:A:295:ASP:N	2.29	0.63
2:D:93:VAL:HG22	2:D:118:LEU:HG	1.81	0.62
1:C:41:GLU:HG2	1:C:42:PHE:H	1.63	0.62
2:D:187:LEU:HD22	2:D:198:VAL:HG13	1.80	0.62
1:B:191:TRP:CZ3	1:B:221:CYS:HA	2.34	0.62
1:C:103:HIS:O	1:C:103:HIS:ND1	2.33	0.62
2:D:159:VAL:HB	2:D:218:LEU:HD11	1.82	0.62
2:D:205:SER:HB3	2:D:212:THR:HG23	1.82	0.62
2:F:164:ARG:HH21	2:F:244:GLY:H	1.45	0.61
1:B:300:VAL:HG11	1:B:321:ILE:HD12	1.83	0.61
1:C:276:ARG:NH2	1:C:313:LYS:O	2.33	0.61
2:F:87:ARG:C	2:F:89:GLU:H	2.03	0.61
2:D:229:GLN:HE21	2:D:239:ILE:HG23	1.65	0.60
1:B:251:PRO:HD3	1:B:341:ASN:OD1	2.01	0.60
1:A:318:GLU:O	1:A:318:GLU:HG3	2.02	0.59
1:C:263:VAL:HG22	1:C:353:LYS:O	2.04	0.58
2:F:179:LYS:NZ	2:F:221:GLU:O	2.34	0.58
1:C:302:VAL:HG22	1:C:321:ILE:HA	1.85	0.57
2:D:5:VAL:O	2:D:22:CYS:HA	2.04	0.57
2:F:68:PHE:CZ	2:F:83:MET:HB3	2.40	0.57
2:D:35:HIS:O	2:D:96:CYS:HA	2.05	0.57
2:F:148:PRO:HB3	2:F:244:GLY:HA3	1.86	0.57
1:A:279:PHE:HA	2:D:103:HIS:CE1	2.39	0.56
2:D:203:SER:HB3	2:D:214:THR:HB	1.86	0.56
2:F:88:ALA:HA	2:F:121:VAL:HG11	1.87	0.56
2:F:152:SER:OG	2:F:152:SER:O	2.21	0.56
2:F:164:ARG:H	2:F:164:ARG:HD3	1.70	0.56
1:A:167:LEU:HA	1:A:211:VAL:HB	1.87	0.56
1:A:41:GLU:HG2	1:A:42:PHE:H	1.71	0.55
2:F:187:LEU:HB3	2:F:188:ILE:HD12	1.89	0.55
2:F:12:VAL:O	2:F:121:VAL:HA	2.06	0.55
2:F:228:CYS:O	2:F:242:GLY:N	2.41	0.54
1:B:281:ARG:HH12	2:E:108:TYR:HB3	1.73	0.54
1:C:275:ALA:HB2	1:C:339:VAL:HG11	1.88	0.54
2:F:98:ARG:HG2	2:F:99:SER:N	2.22	0.54
2:E:30:TYR:O	2:E:54:SER:HB3	2.07	0.54
1:A:232:TRP:HE1	1:A:234:VAL:CG2	2.20	0.54
1:A:263:VAL:HG21	1:A:326:VAL:HG11	1.90	0.54
1:C:126:CYS:O	1:C:128:PRO:HD3	2.08	0.54
2:F:5:VAL:HB	2:F:23:ALA:HB3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LYS:HA	1:A:319:ARG:HH11	1.73	0.53
2:F:93:VAL:HG22	2:F:118:LEU:HD13	1.90	0.53
2:F:175:TRP:CD2	2:F:213:LEU:HB2	2.43	0.53
2:D:171:SER:OG	2:D:172:ALA:N	2.42	0.53
2:D:172:ALA:HB1	2:D:190:SER:HA	1.90	0.53
1:A:170:THR:HG22	1:A:209:ASP:O	2.09	0.52
1:B:191:TRP:CE3	1:B:221:CYS:HA	2.44	0.52
1:A:42:PHE:HB3	1:A:113:PHE:HB2	1.90	0.52
2:D:98:ARG:HG2	2:D:99:SER:N	2.24	0.52
2:D:88:ALA:HA	2:D:121:VAL:HB	1.91	0.52
1:B:241:ARG:NH1	2:E:193:SER:HA	2.25	0.52
2:D:202:PHE:HA	2:D:214:THR:O	2.10	0.52
1:C:281:ARG:NH2	2:F:108:TYR:O	2.44	0.51
2:F:57:TYR:HB3	2:F:59:TYR:HE1	1.76	0.51
1:A:256:PRO:O	1:A:348:GLN:HG2	2.10	0.51
1:B:262:GLU:HA	1:B:353:LYS:O	2.10	0.51
1:B:273:CYS:HB2	1:B:289:TRP:CZ2	2.44	0.51
1:C:227:ASP:HB3	1:C:230:SER:H	1.73	0.51
2:D:171:SER:CB	2:D:231:TYR:H	2.23	0.51
2:F:149:SER:OG	2:F:150:SER:N	2.43	0.51
1:B:32:TRP:O	1:B:146:GLU:N	2.39	0.51
2:F:39:GLN:OE1	2:F:178:GLN:NE2	2.20	0.51
1:B:246:ASP:OD2	1:B:281:ARG:N	2.42	0.50
1:C:208:VAL:HG21	1:C:215:HIS:CE1	2.46	0.50
1:B:293:ASP:OD1	1:B:294:SER:N	2.44	0.50
1:C:105:ILE:O	1:C:112:HIS:N	2.41	0.50
2:F:88:ALA:HA	2:F:121:VAL:CG1	2.42	0.50
2:F:35:HIS:O	2:F:96:CYS:HA	2.12	0.50
2:D:5:VAL:HB	2:D:23:ALA:HB3	1.94	0.50
2:E:24:ALA:HB1	2:E:27:PHE:CE2	2.46	0.50
2:E:35:HIS:CD2	2:E:110:LEU:HD21	2.47	0.50
1:B:290:TYR:HB2	1:B:336:VAL:HB	1.94	0.49
1:C:41:GLU:HG2	1:C:42:PHE:N	2.26	0.49
2:F:87:ARG:C	2:F:89:GLU:N	2.64	0.49
2:D:68:PHE:CD1	2:D:83:MET:HA	2.48	0.49
1:B:121:SER:OG	1:B:122:GLY:N	2.46	0.49
1:C:275:ALA:CB	1:C:339:VAL:HG11	2.42	0.49
2:E:174:ALA:N	2:E:229:GLN:O	2.45	0.49
2:F:18:LEU:O	2:F:83:MET:HG3	2.12	0.49
1:B:312:LEU:HA	2:E:103:HIS:O	2.13	0.49
1:C:293:ASP:OD1	1:C:294:SER:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:VAL:HA	1:C:111:LEU:O	2.13	0.48
2:E:29:LEU:HB2	2:E:74:THR:HG22	1.93	0.48
1:A:34:TYR:HB2	1:A:42:PHE:CE1	2.48	0.48
1:A:241:ARG:HG2	2:D:192:SER:HB2	1.95	0.48
2:F:164:ARG:NH2	2:F:244:GLY:H	2.10	0.48
1:A:213:ASP:OD2	2:D:172:ALA:HB2	2.13	0.48
1:A:125:ILE:HG13	1:A:141:VAL:O	2.13	0.48
1:B:119:ASN:N	1:B:149:PRO:HG3	2.29	0.48
2:D:111:ASP:HB2	2:D:112:TYR:CD2	2.48	0.48
1:A:210:GLU:HG2	1:A:212:TYR:OH	2.13	0.47
2:F:107:TRP:CH2	2:F:229:GLN:OE1	2.67	0.47
1:B:281:ARG:NH2	2:E:108:TYR:O	2.47	0.47
2:F:151:LEU:HA	2:F:151:LEU:HD23	1.52	0.47
1:B:32:TRP:N	1:B:144:ILE:O	2.42	0.47
1:C:263:VAL:HG21	1:C:326:VAL:HG11	1.95	0.47
2:D:202:PHE:CE2	2:D:215:ILE:HG12	2.49	0.47
1:B:278:GLY:O	2:E:103:HIS:NE2	2.48	0.47
1:C:264:GLU:O	1:C:267:LYS:HB2	2.13	0.47
1:C:273:CYS:HB2	1:C:289:TRP:CZ2	2.49	0.47
2:F:219:GLN:HB3	2:F:220:PRO:HD2	1.95	0.47
2:F:229:GLN:NE2	2:F:239:ILE:HG23	2.30	0.47
1:A:282:VAL:HA	2:D:98:ARG:NH2	2.30	0.47
2:F:188:ILE:HD13	2:F:213:LEU:HD13	1.96	0.47
1:B:163:GLN:NE2	1:B:174:SER:O	2.42	0.46
1:B:274:LYS:HE3	1:B:318:GLU:OE1	2.14	0.46
2:D:2:VAL:HG13	2:D:27:PHE:HD1	1.79	0.46
2:F:4:LEU:HD22	2:F:22:CYS:SG	2.55	0.46
2:D:98:ARG:O	2:D:110:LEU:HA	2.14	0.46
1:C:103:HIS:O	1:C:103:HIS:CG	2.69	0.46
2:E:39:GLN:NE2	2:E:178:GLN:OE1	2.45	0.46
2:D:178:GLN:O	2:D:224:ALA:HB1	2.15	0.46
1:A:246:ASP:HA	1:A:279:PHE:O	2.15	0.46
1:B:292:LYS:HG2	1:B:296:LEU:O	2.15	0.46
2:F:204:GLY:HA2	2:F:212:THR:O	2.16	0.46
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.66	0.45
1:C:281:ARG:O	2:F:100:SER:OG	2.34	0.45
1:A:113:PHE:CD1	1:A:113:PHE:N	2.85	0.45
1:A:225:GLN:HG2	1:A:232:TRP:CH2	2.51	0.45
1:B:267:LYS:O	1:B:326:VAL:HG23	2.16	0.45
1:A:281:ARG:O	2:D:98:ARG:NH2	2.45	0.45
1:C:45:PHE:HZ	1:C:220:VAL:HG21	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:229:GLN:HE21	2:F:239:ILE:HG23	1.82	0.45
2:E:39:GLN:HA	2:E:44:GLY:O	2.16	0.45
2:D:24:ALA:HB1	2:D:27:PHE:CZ	2.51	0.45
2:D:101:PHE:O	2:D:101:PHE:CD2	2.70	0.45
2:E:97:ALA:HB3	2:E:110:LEU:HD13	1.98	0.45
1:B:191:TRP:NE1	1:B:206:ILE:HB	2.13	0.45
1:C:228:THR:HG23	1:C:229:VAL:HG23	1.99	0.45
1:A:353:LYS:HD3	1:A:353:LYS:HA	1.82	0.45
2:D:37:VAL:HB	2:D:113:TRP:HZ3	1.80	0.45
2:F:86:LEU:HA	2:F:90:ASP:OD2	2.17	0.45
1:B:272:SER:HA	1:B:320:ASN:OD1	2.17	0.45
1:A:99:LYS:O	1:A:101:TYR:N	2.49	0.44
1:A:178:LEU:HD21	1:A:223:TYR:CZ	2.53	0.44
1:C:124:TYR:CD1	1:C:145:LEU:HD23	2.51	0.44
1:B:191:TRP:HZ3	1:B:221:CYS:HA	1.80	0.44
2:D:2:VAL:HA	2:D:25:SER:O	2.18	0.44
1:B:300:VAL:HG22	1:B:302:VAL:HG13	1.99	0.44
2:F:29:LEU:HD13	2:F:77:ASN:OD1	2.17	0.44
1:B:311:THR:O	1:B:312:LEU:C	2.54	0.44
2:D:97:ALA:HA	2:D:112:TYR:O	2.18	0.44
2:D:229:GLN:HG2	2:D:230:GLN:N	2.33	0.44
2:E:97:ALA:HB2	2:E:113:TRP:CD2	2.52	0.44
2:D:3:GLN:HB2	2:D:25:SER:HB3	2.00	0.44
1:B:280:GLU:HB2	1:B:283:PHE:HD1	1.83	0.43
1:C:34:TYR:CE2	1:C:42:PHE:HB2	2.53	0.43
1:C:113:PHE:N	1:C:113:PHE:CD1	2.84	0.43
2:F:162:THR:HA	2:F:211:PHE:O	2.18	0.43
1:B:43:VAL:HA	1:B:111:LEU:O	2.17	0.43
1:B:309:LYS:NZ	1:B:314:ASP:OD2	2.51	0.43
1:C:170:THR:HG22	1:C:209:ASP:O	2.18	0.43
1:A:189:VAL:CG1	1:A:221:CYS:HB2	2.48	0.43
2:D:163:CYS:N	2:D:211:PHE:O	2.51	0.43
1:A:275:ALA:CB	1:A:339:VAL:HG11	2.48	0.43
2:E:21:SER:O	2:E:36:TRP:HH2	2.01	0.43
1:A:265:LEU:H	1:A:265:LEU:HG	1.45	0.43
1:C:308:ILE:CG2	1:C:318:GLU:HG2	2.49	0.43
2:F:68:PHE:CE1	2:F:83:MET:CB	2.98	0.43
1:B:246:ASP:N	1:B:246:ASP:OD1	2.52	0.42
1:C:104:ILE:HG23	1:C:113:PHE:HA	2.00	0.42
2:E:35:HIS:HD2	2:E:110:LEU:HD21	1.84	0.42
1:A:41:GLU:HG2	1:A:42:PHE:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:PRO:HG2	1:A:104:ILE:HD12	2.01	0.42
1:A:121:SER:OG	1:A:122:GLY:N	2.52	0.42
1:B:288:LYS:HD3	1:B:299:GLU:OE1	2.20	0.42
1:C:99:LYS:HD3	1:C:100:SER:N	2.34	0.42
1:C:277:PHE:CD1	1:C:317:ILE:HD12	2.54	0.42
1:B:34:TYR:HB3	1:B:147:VAL:HA	2.02	0.42
1:B:192:TYR:HB2	1:B:220:VAL:HB	2.01	0.42
1:B:246:ASP:HB2	1:B:279:PHE:O	2.19	0.42
1:A:232:TRP:CD1	1:A:233:THR:N	2.88	0.42
1:B:284:ASN:HD21	2:E:27:PHE:HA	1.85	0.42
2:D:188:ILE:HG12	2:D:194:LEU:HD12	2.02	0.42
1:A:226:SER:HA	1:A:230:SER:O	2.19	0.42
1:C:219:TYR:HB2	1:C:238:VAL:HG13	2.02	0.42
2:D:30:TYR:CZ	2:D:74:THR:HG21	2.55	0.42
2:E:175:TRP:HZ3	2:E:191:ALA:HA	1.85	0.42
1:C:198:LEU:HD11	1:C:219:TYR:CE2	2.54	0.41
1:A:329:ARG:O	1:A:332:ARG:N	2.27	0.41
2:E:69:THR:O	2:E:81:LEU:HD12	2.20	0.41
1:C:121:SER:HB3	1:C:124:TYR:OH	2.20	0.41
2:F:151:LEU:HD12	2:F:159:VAL:HG13	2.02	0.41
2:F:36:TRP:O	2:F:48:VAL:HB	2.20	0.41
1:C:129:LYS:HD2	1:C:129:LYS:O	2.20	0.41
2:E:206:ARG:C	2:E:208:GLY:H	2.24	0.41
2:E:4:LEU:O	2:E:114:GLY:HA3	2.21	0.41
2:F:162:THR:HG22	2:F:212:THR:HG23	2.03	0.41
2:F:172:ALA:HA	2:F:190:SER:HA	2.03	0.41
1:C:126:CYS:HA	1:C:142:LYS:HA	2.02	0.41
2:D:24:ALA:HB1	2:D:27:PHE:CE1	2.56	0.41
1:B:119:ASN:HA	1:B:149:PRO:HG3	2.03	0.41
1:B:193:LYS:HE2	1:B:214:TYR:O	2.21	0.41
1:C:104:ILE:HG23	1:C:112:HIS:O	2.20	0.41
1:A:32:TRP:HA	1:A:233:THR:O	2.21	0.40
1:A:286:VAL:O	1:A:339:VAL:HA	2.22	0.40
1:C:225:GLN:HG3	1:C:234:VAL:HG23	2.02	0.40
2:D:194:LEU:HD11	2:D:202:PHE:HB2	2.02	0.40
1:A:167:LEU:HD21	1:A:244:VAL:CG2	2.49	0.40
1:A:296:LEU:HA	1:A:296:LEU:HD23	1.78	0.40
1:C:321:ILE:HD13	1:C:321:ILE:HG21	1.83	0.40
2:D:16:GLY:O	2:D:85:SER:N	2.54	0.40
2:D:73:ASP:OD2	2:D:76:LYS:HG3	2.20	0.40
2:F:161:ILE:O	2:F:213:LEU:N	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:THR:CG2	1:A:278:GLY:HA3	2.45	0.40
1:C:126:CYS:HB2	1:C:142:LYS:CB	2.52	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	246/337 (73%)	215 (87%)	31 (13%)	0	100	100
1	B	202/337 (60%)	178 (88%)	23 (11%)	1 (0%)	29	61
1	C	249/337 (74%)	219 (88%)	28 (11%)	2 (1%)	19	51
2	D	212/257 (82%)	189 (89%)	23 (11%)	0	100	100
2	E	108/257 (42%)	93 (86%)	14 (13%)	1 (1%)	17	48
2	F	213/257 (83%)	190 (89%)	21 (10%)	2 (1%)	17	48
All	All	1230/1782 (69%)	1084 (88%)	140 (11%)	6 (0%)	29	61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	105	ILE
2	F	88	ALA
1	C	51	PRO
2	F	87	ARG
2	E	207	SER
1	C	125	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	202/316 (64%)	187 (93%)	15 (7%)	13	40
1	B	155/316 (49%)	147 (95%)	8 (5%)	23	54
1	C	205/316 (65%)	191 (93%)	14 (7%)	16	44
2	D	161/202 (80%)	155 (96%)	6 (4%)	34	63
2	E	84/202 (42%)	82 (98%)	2 (2%)	49	73
2	F	165/202 (82%)	157 (95%)	8 (5%)	25	56
All	All	972/1554 (62%)	919 (94%)	53 (6%)	21	52

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	34	TYR
1	A	38	SER
1	A	97	ILE
1	A	114	LEU
1	A	174	SER
1	A	177	SER
1	A	202	ARG
1	A	205	ARG
1	A	244	VAL
1	A	262	GLU
1	A	264	GLU
1	A	265	LEU
1	A	276	ARG
1	A	307	SER
1	B	30	LEU
1	B	31	LEU
1	B	105	ILE
1	B	191	TRP
1	B	193	LYS
1	B	241	ARG
1	B	246	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	292	LYS
1	C	33	THR
1	C	34	TYR
1	C	36	THR
1	C	48	LEU
1	C	54	SER
1	C	99	LYS
1	C	107	ASP
1	C	126	CYS
1	C	127	ARG
1	C	177	SER
1	C	233	THR
1	C	247	THR
1	C	248	LYS
1	C	302	VAL
2	D	54	SER
2	D	100	SER
2	D	118	LEU
2	D	152	SER
2	D	173	VAL
2	D	212	THR
2	E	102	SER
2	E	206	ARG
2	F	11	LEU
2	F	83	MET
2	F	111	ASP
2	F	118	LEU
2	F	149	SER
2	F	154	SER
2	F	164	ARG
2	F	248	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	HIS
1	C	225	GLN
2	D	103	HIS
2	E	35	HIS
2	F	243	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	G	1	3,1	14,14,15	1.53	2 (14%)	17,19,21	1.22	2 (11%)
3	NAG	G	2	3	14,14,15	1.63	3 (21%)	17,19,21	1.04	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	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2	NAG	O5-C1	4.17	1.50	1.43
3	G	1	NAG	O5-C1	3.89	1.49	1.43
3	G	1	NAG	C7-N2	2.72	1.43	1.34
3	G	2	NAG	C7-N2	2.71	1.43	1.34
3	G	2	NAG	C3-C2	-2.38	1.47	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	2	NAG	C4-C3-C2	2.19	114.22	111.02
3	G	1	NAG	C8-C7-N2	2.11	119.66	116.10
3	G	1	NAG	O3-C3-C4	2.09	115.19	110.35

There are no chirality outliers.

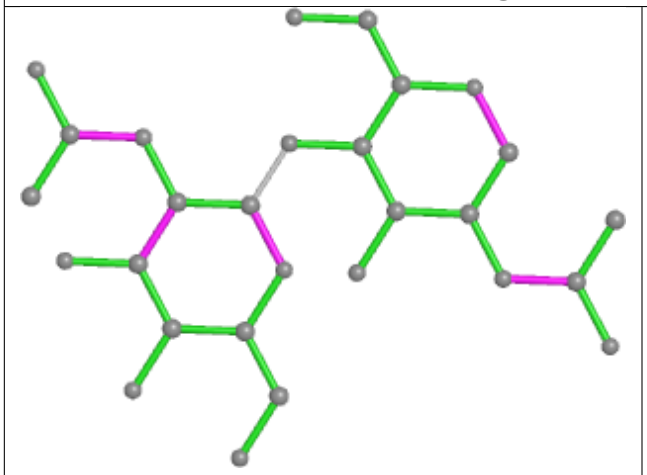
There are no torsion outliers.

There are no ring outliers.

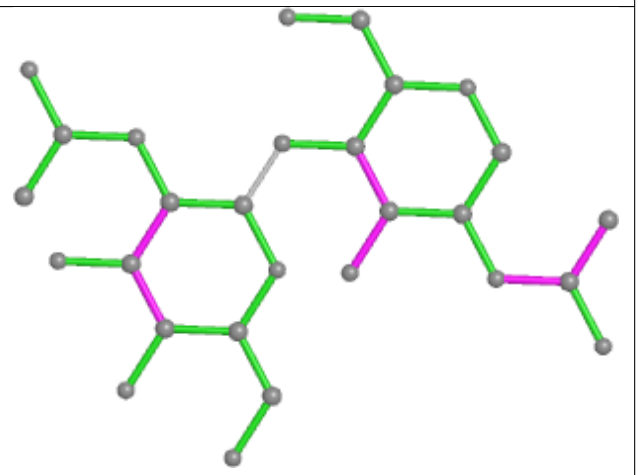
No monomer is involved in short contacts.

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

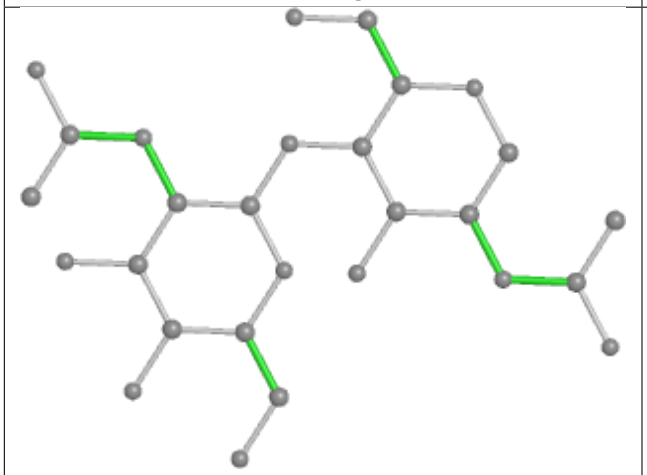
Oligosaccharide Chain G



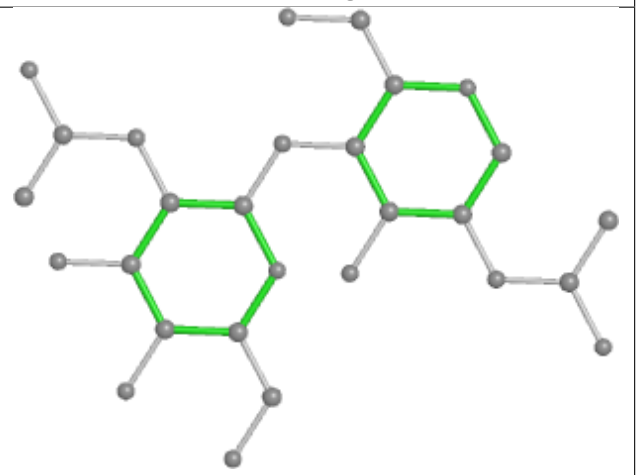
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	C	401	1	14,14,15	1.63	3 (21%)	17,19,21	2.68	7 (41%)
4	NAG	A	401	1	14,14,15	1.71	4 (28%)	17,19,21	3.50	8 (47%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	401	1	-	2/6/23/26	0/1/1/1
4	NAG	A	401	1	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	NAG	O5-C1	4.27	1.50	1.43
4	A	401	NAG	O5-C1	4.00	1.50	1.43
4	A	401	NAG	O3-C3	2.77	1.49	1.43
4	A	401	NAG	C7-N2	2.47	1.42	1.34
4	C	401	NAG	C7-N2	2.36	1.42	1.34
4	C	401	NAG	O5-C5	2.34	1.48	1.43
4	A	401	NAG	O5-C5	2.24	1.48	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	401	NAG	C2-N2-C7	-10.61	107.79	122.90
4	C	401	NAG	C2-N2-C7	-8.48	110.83	122.90
4	A	401	NAG	O5-C5-C6	4.25	113.86	107.20
4	A	401	NAG	C4-C3-C2	-4.17	104.90	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	401	NAG	O4-C4-C3	3.73	118.98	110.35
4	A	401	NAG	C6-C5-C4	-3.61	104.56	113.00
4	C	401	NAG	O5-C5-C6	3.02	111.94	107.20
4	C	401	NAG	C3-C4-C5	2.90	115.41	110.24
4	A	401	NAG	O3-C3-C4	2.76	116.73	110.35
4	A	401	NAG	O7-C7-N2	-2.65	117.08	121.95
4	A	401	NAG	C8-C7-N2	2.52	120.37	116.10
4	C	401	NAG	C4-C3-C2	2.41	114.56	111.02
4	C	401	NAG	C1-O5-C5	2.32	115.34	112.19
4	C	401	NAG	C8-C7-N2	2.19	119.81	116.10
4	C	401	NAG	O7-C7-N2	-2.15	118.01	121.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

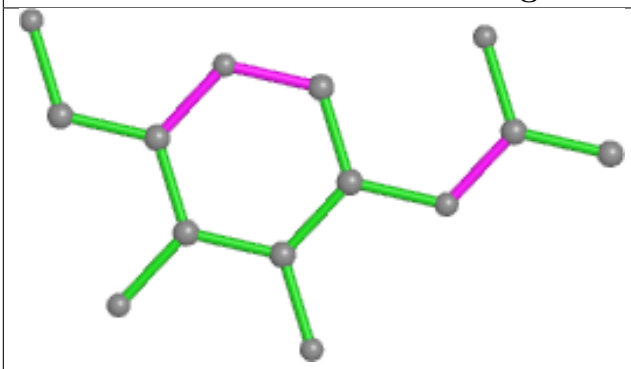
Mol	Chain	Res	Type	Atoms
4	C	401	NAG	O5-C5-C6-O6
4	C	401	NAG	C4-C5-C6-O6

There are no ring outliers.

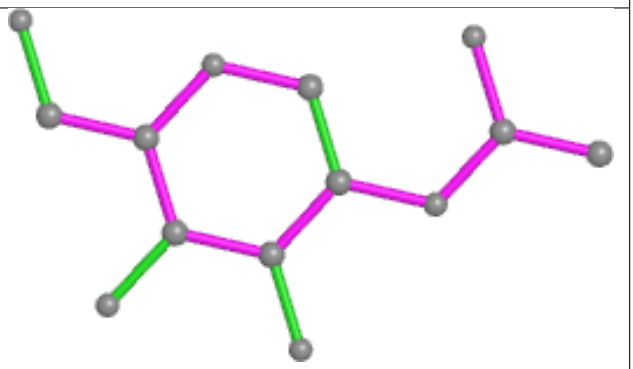
No monomer is involved in short contacts.

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

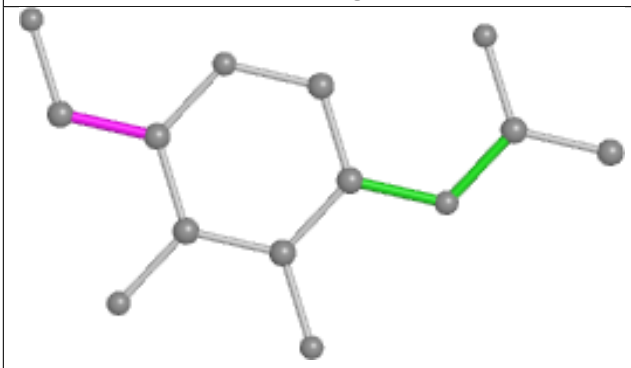
Ligand NAG C 401



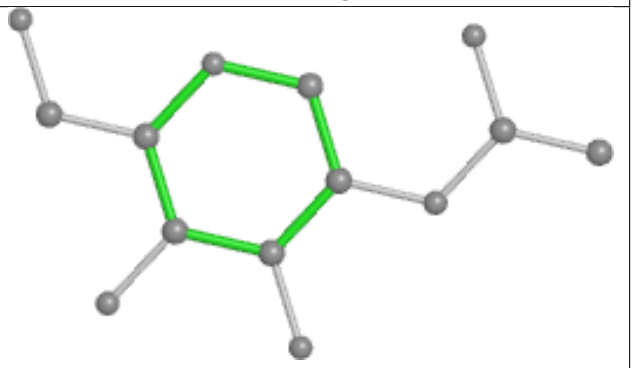
Bond lengths



Bond angles

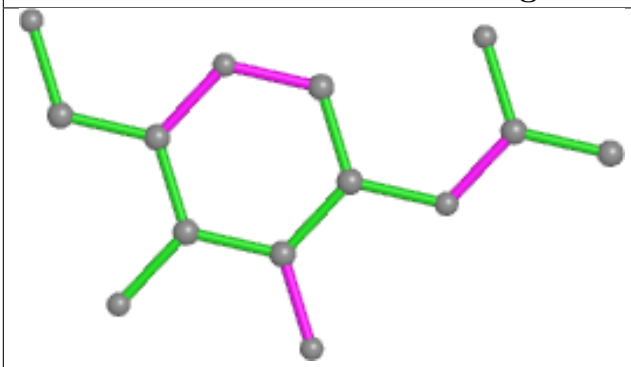


Torsions

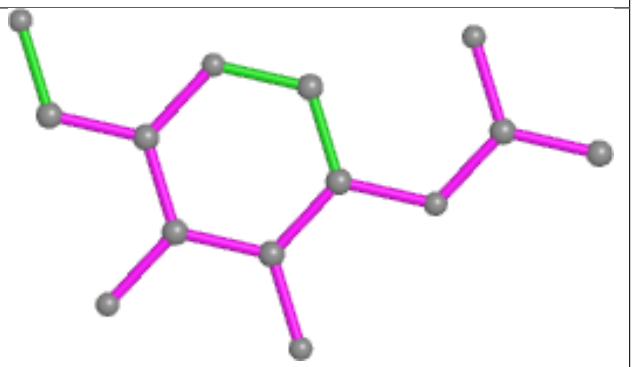


Rings

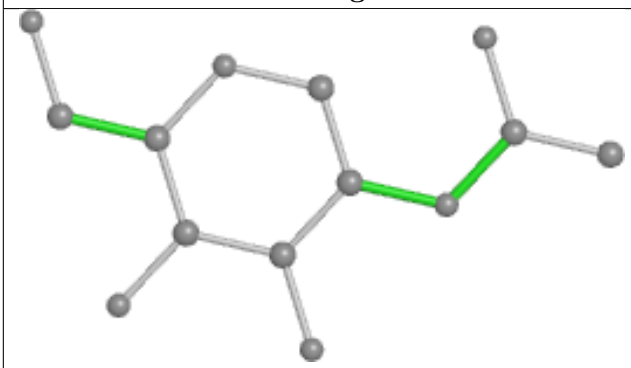
Ligand NAG A 401



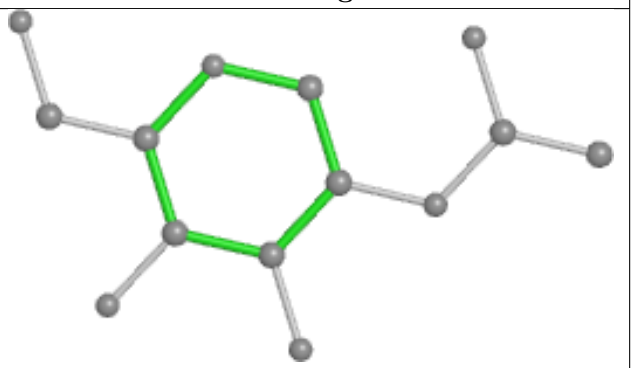
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	260/337 (77%)	0.05	4 (1%) 73 72	9, 40, 84, 117	0
1	B	224/337 (66%)	0.25	17 (7%) 13 13	30, 69, 96, 109	0
1	C	261/337 (77%)	0.04	3 (1%) 80 81	18, 45, 69, 104	0
2	D	220/257 (85%)	0.12	4 (1%) 68 67	12, 41, 68, 77	0
2	E	134/257 (52%)	0.70	21 (15%) 2 2	50, 81, 100, 119	0
2	F	221/257 (85%)	0.10	10 (4%) 33 32	17, 42, 70, 89	0
All	All	1320/1782 (74%)	0.17	59 (4%) 33 32	9, 51, 90, 119	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	176	TYR	5.9
2	E	92	ALA	5.1
2	E	199	PRO	4.7
1	B	171	GLY	4.1
2	E	244	GLY	3.7
2	E	175	TRP	3.7
1	B	41	GLU	3.6
1	B	165	LEU	3.6
1	C	165	LEU	3.5
1	B	261	LEU	3.5
1	A	236	ALA	3.4
2	E	34	MET	3.1
2	E	197	GLY	3.1
1	B	46	CYS	3.1
1	B	286	VAL	3.1
2	E	39	GLN	3.0
1	B	167	LEU	3.0
2	D	148	PRO	2.9
1	C	151	THR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	220	PRO	2.9
2	F	243	GLN	2.9
1	B	43	VAL	2.7
1	B	143	MET	2.7
1	B	164	ASP	2.7
2	D	181	GLY	2.7
2	D	119	VAL	2.6
2	E	33	SER	2.6
1	B	170	THR	2.5
2	F	119	VAL	2.5
2	F	147	SER	2.5
1	A	177	SER	2.5
2	E	32	SER	2.5
2	E	174	ALA	2.4
2	E	154	SER	2.4
2	E	198	VAL	2.4
1	B	188	ALA	2.3
1	A	151	THR	2.3
2	F	9	GLY	2.3
2	E	221	GLU	2.3
1	B	168	GLY	2.2
2	F	148	PRO	2.2
2	E	115	GLN	2.2
2	F	10	GLY	2.2
2	E	186	LEU	2.2
1	B	285	PRO	2.1
1	B	166	LEU	2.1
1	B	149	PRO	2.1
1	B	271	ILE	2.1
2	D	120	THR	2.1
2	E	37	VAL	2.1
2	E	156	GLY	2.1
2	E	191	ALA	2.1
2	E	229	GLN	2.1
1	C	173	ILE	2.1
2	F	94	TYR	2.0
2	F	170	SER	2.0
2	F	211	PHE	2.0
1	A	234	VAL	2.0
2	F	38	ARG	2.0

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

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

6.3 Carbohydrates (i)

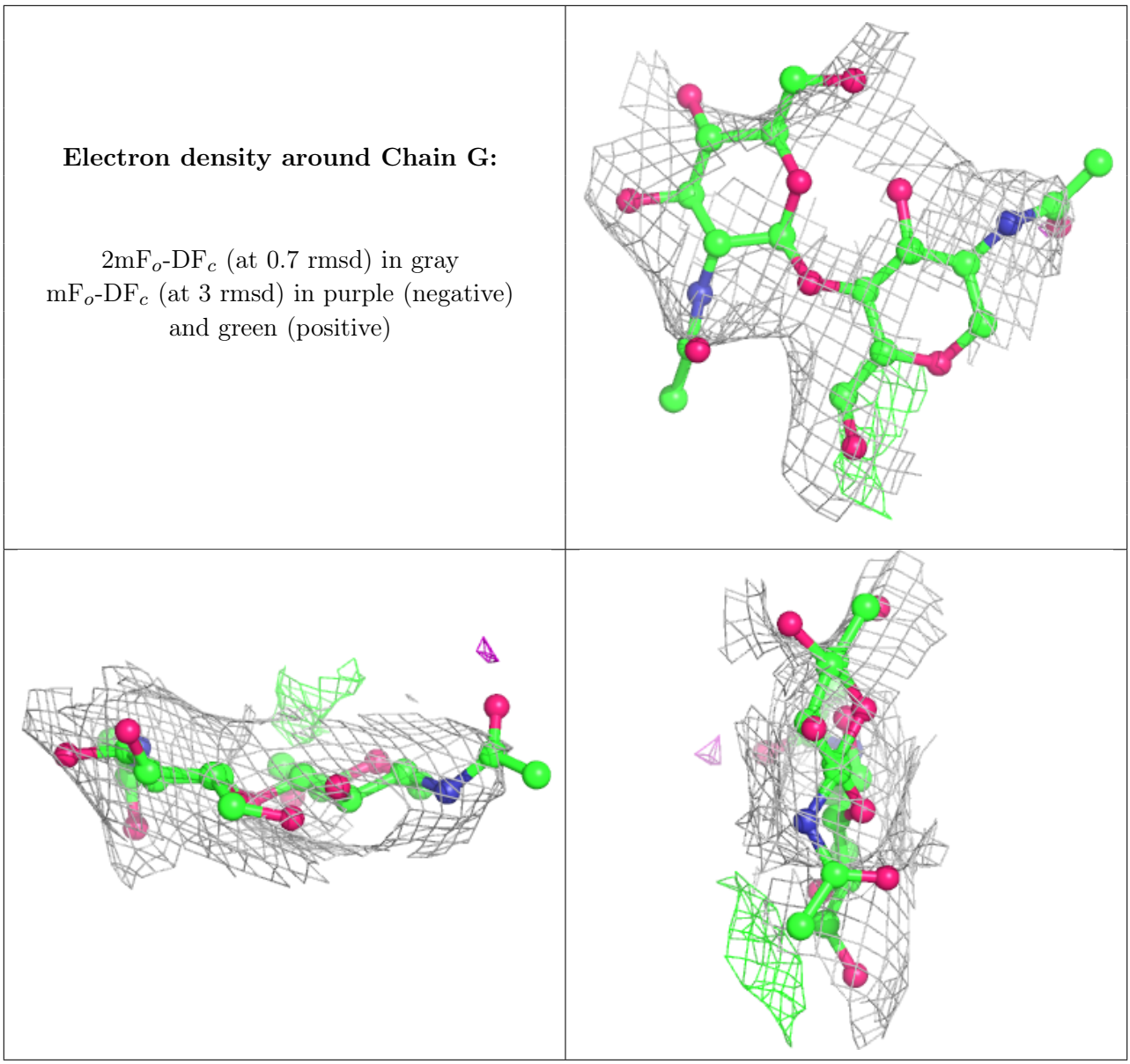
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	G	2	14/15	0.78	0.27	91,107,127,137	0
3	NAG	G	1	14/15	0.81	0.21	73,88,98,103	0

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

Electron density around Chain G:

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



6.4 Ligands

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

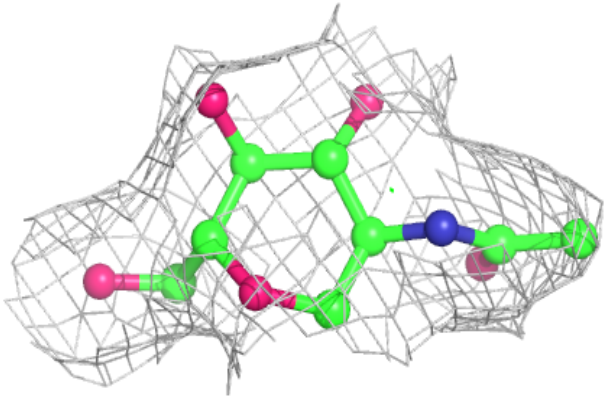
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	C	401	14/15	0.89	0.14	40,46,54,55	0
4	NAG	A	401	14/15	0.94	0.12	10,11,11,11	0

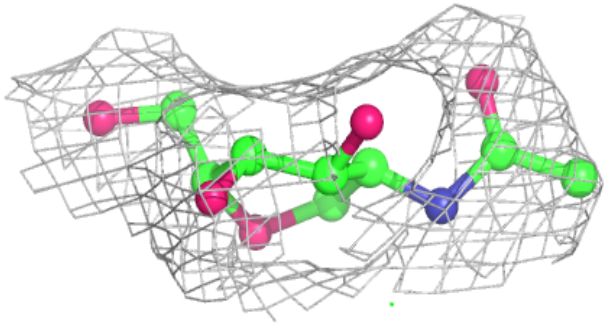
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

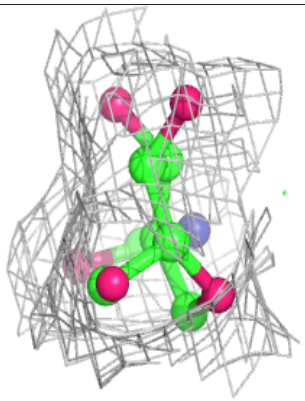
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAG C 401:

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

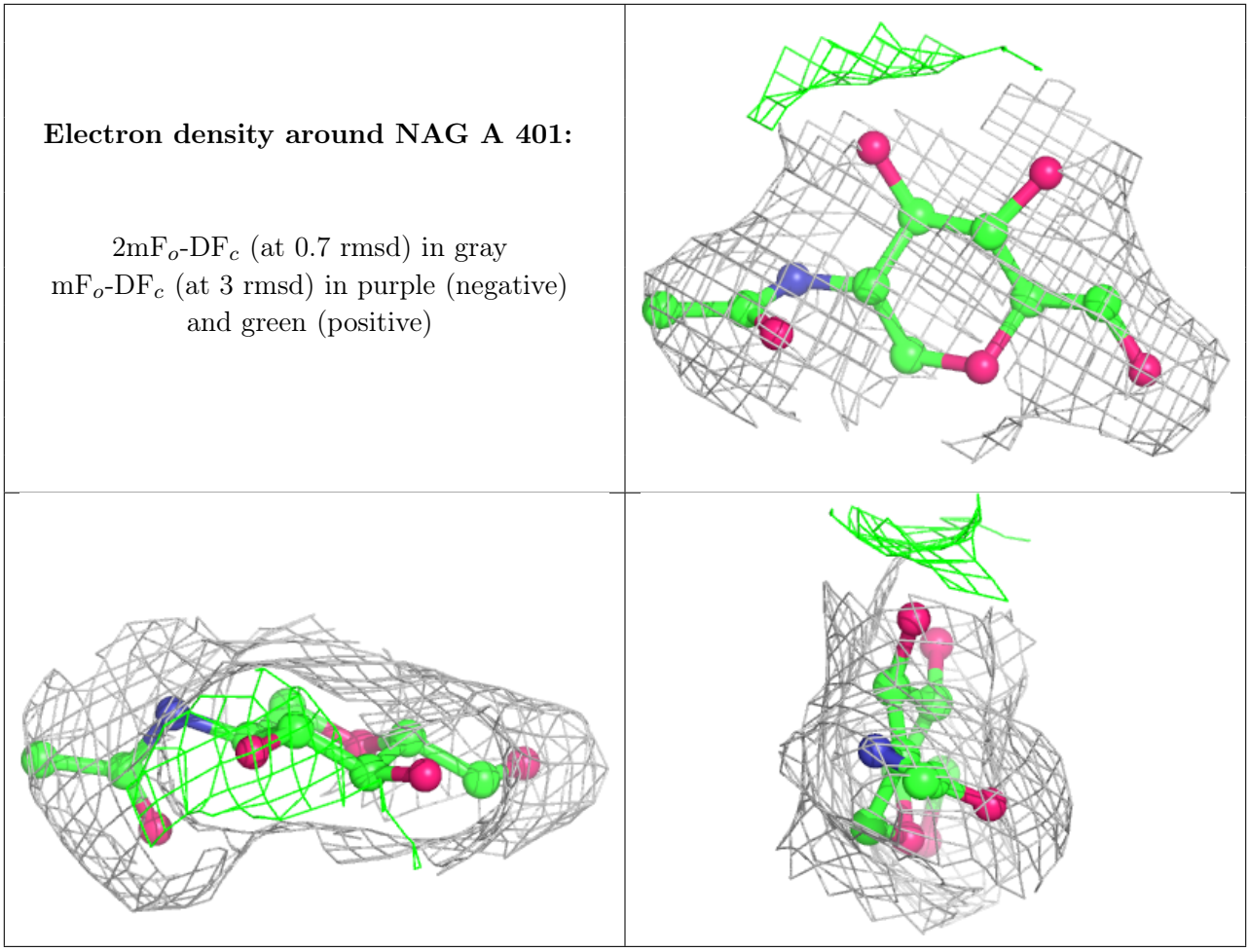






Electron density around NAG A 401:

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



6.5 Other polymers (i)

There are no such residues in this entry.