



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:57 AM UTC

PDB ID : 7UJK / pdb_00007ujk
Title : Integrin alpha IIB beta3 complex with lamifiban
Authors : Lin, F.-Y.; Zhu, J.; Zhu, J.; Springer, T.A.
Deposited on : 2022-03-30
Resolution : 2.43 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

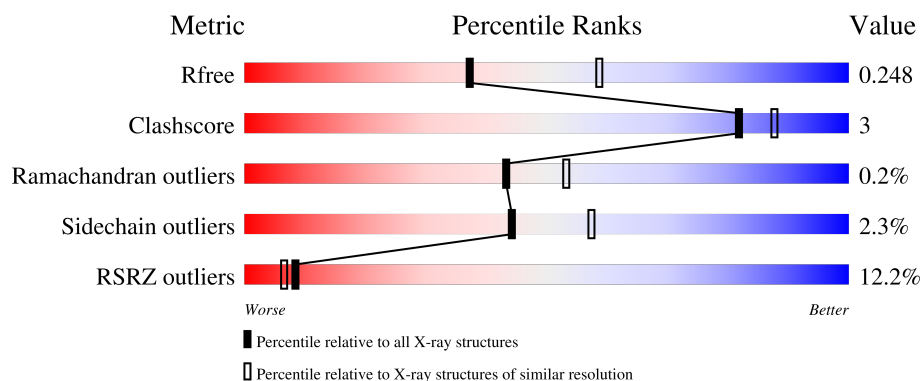
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	457	3% 90% 9%
1	C	457	3% 94% 5%
2	B	472	11% 91% 7%
2	D	472	11% 92% 7%
3	E	221	38% 89% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	221	
4	F	214	
4	L	214	
5	G	5	
6	I	2	
6	K	2	
7	J	4	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 22145 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 Integrin alpha-IIb heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	8	0
			3532	2245	611	668	8			
1	C	453	Total	C	N	O	S	0	4	0
			3502	2224	604	666	8			

- Molecule 2 is a protein called Isoform Beta-3C of Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	466	Total	C	N	O	S	4	8	0
			3649	2273	622	720	34			
2	D	471	Total	C	N	O	S	3	2	0
			3642	2270	621	716	35			

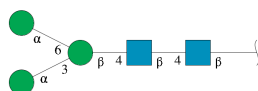
- Molecule 3 is a protein called 10E5 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	214	Total	C	N	O	S	0	0	0
			1631	1035	264	326	6			
3	H	216	Total	C	N	O	S	0	0	0
			1642	1041	266	329	6			

- Molecule 4 is a protein called 10E5 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			
4	L	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



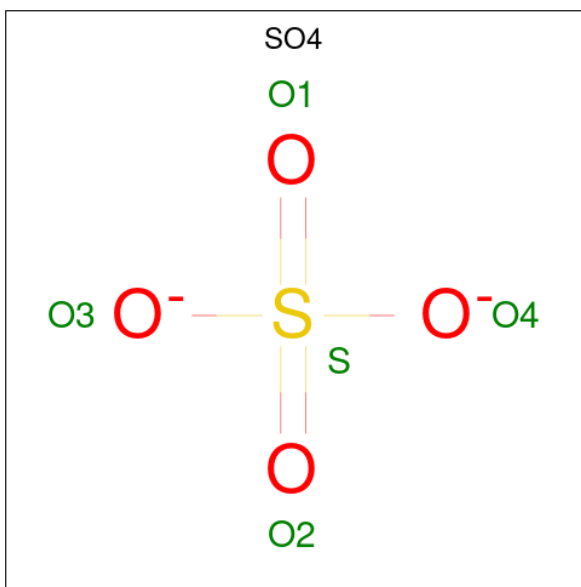
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



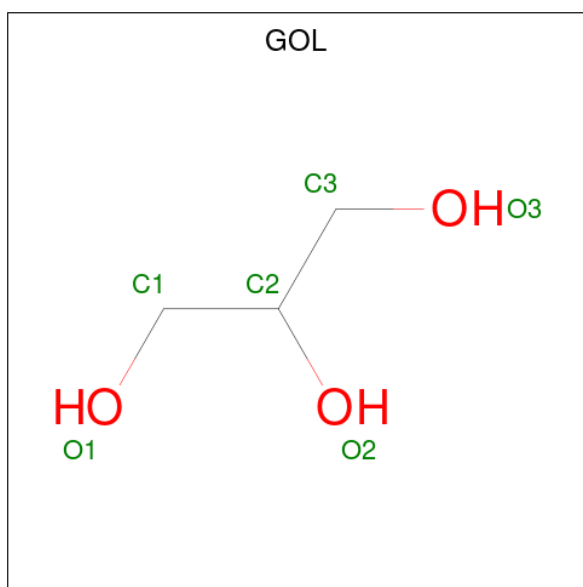
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	J	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	4	Total	Ca	0	0
			4	4		
10	B	2	Total	Ca	0	0
			2	2		
10	C	4	Total	Ca	0	0
			4	4		
10	D	2	Total	Ca	0	0
			2	2		

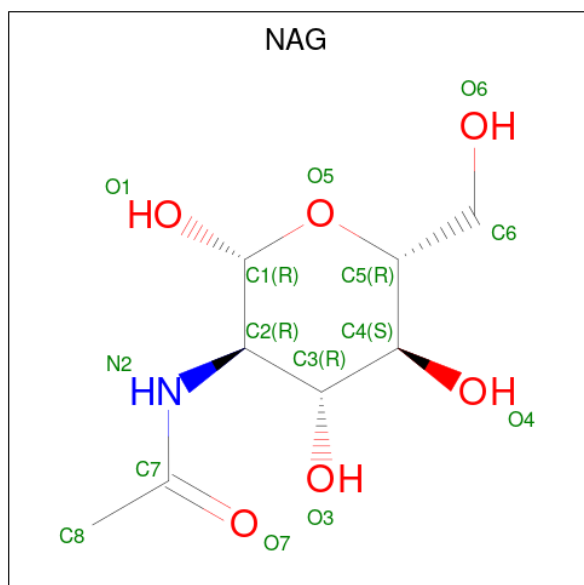
- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	Cl	0	0
			1	1		
11	C	2	Total	Cl	0	0
			2	2		

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

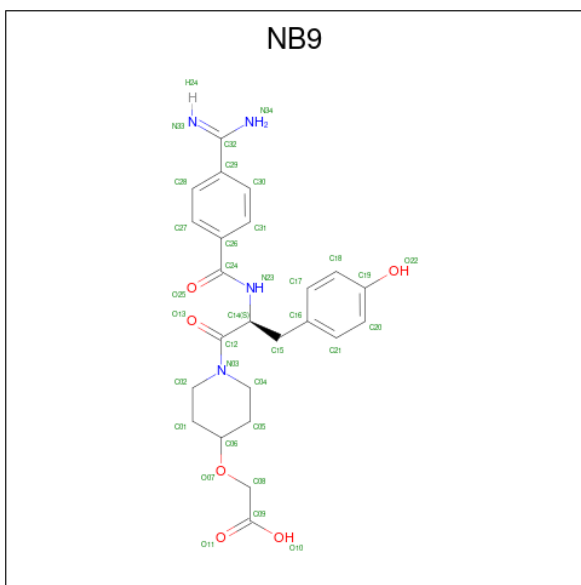
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	1	Total	Mg	0	0
			1	1		
12	D	1	Total	Mg	0	0
			1	1		

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	N	O	0	0
			14	8	1	5		
13	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 14 is Lamifiban (CCD ID: NB9) (formula: $C_{24}H_{28}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	B	1	Total	C	N	O	0	0
			34	24	4	6		
14	D	1	Total	C	N	O	0	0
			34	24	4	6		

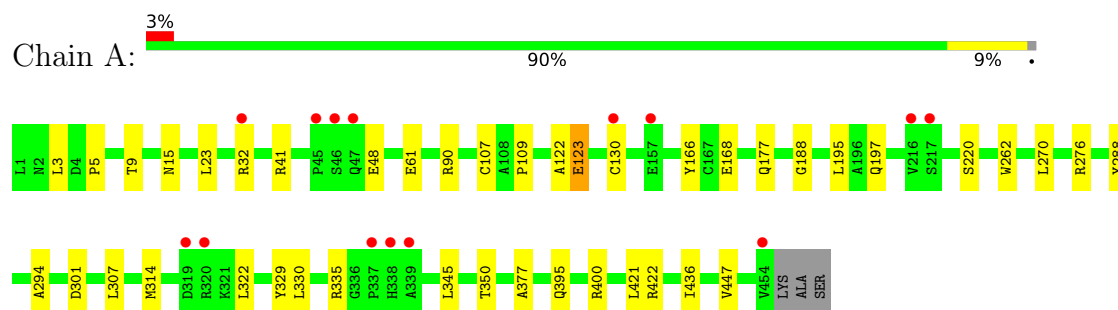
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	323	Total	O	0	0
			323	323		
15	B	214	Total	O	0	0
			214	214		
15	C	125	Total	O	0	0
			125	125		
15	D	118	Total	O	0	0
			118	118		
15	E	35	Total	O	0	0
			35	35		
15	F	35	Total	O	0	0
			35	35		
15	H	46	Total	O	0	0
			46	46		
15	L	56	Total	O	0	0
			56	56		

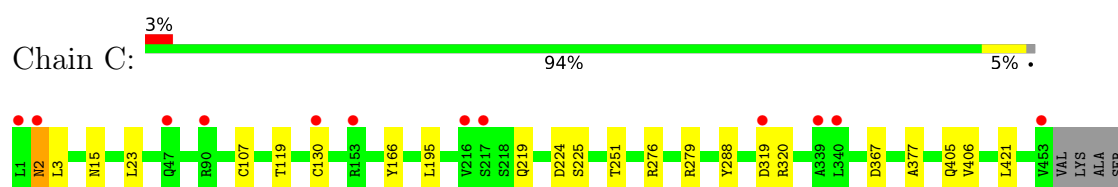
3 Residue-property plots [i](#)

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.

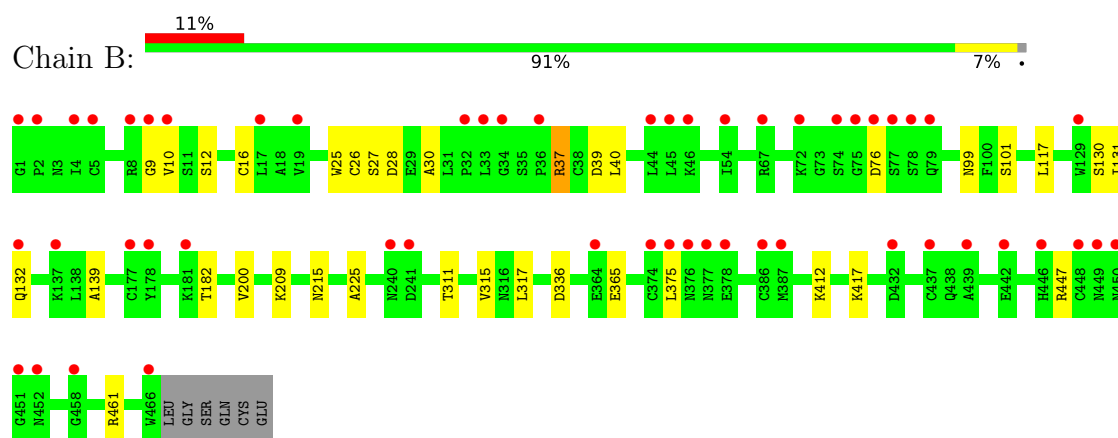
- Molecule 1: Integrin alpha-IIb heavy chain



- Molecule 1: Integrin alpha-IIb heavy chain

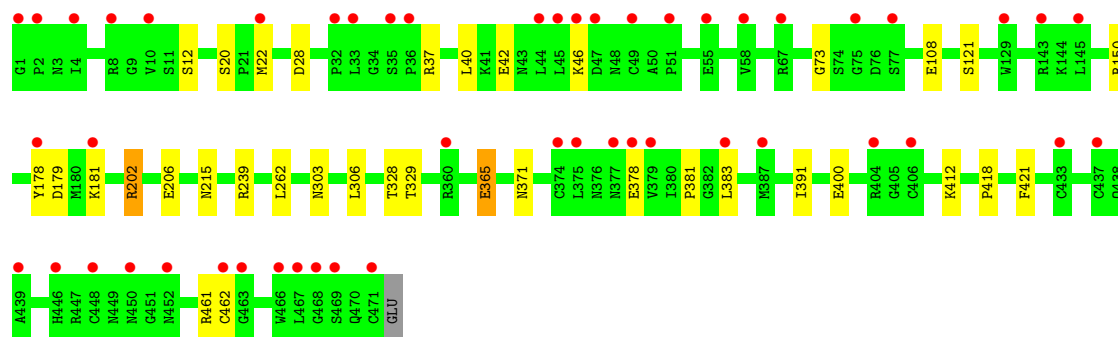


- Molecule 2: Isoform Beta-3C of Integrin beta-3

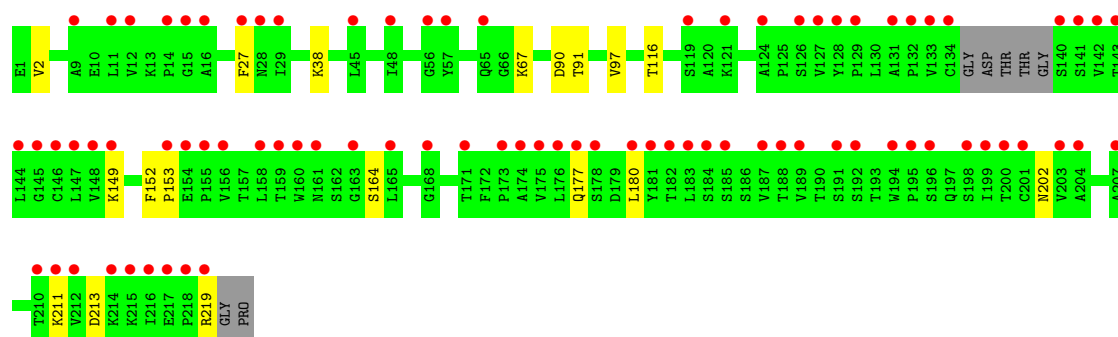
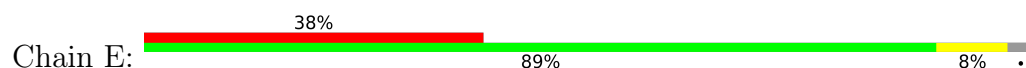


- Molecule 2: Isoform Beta-3C of Integrin beta-3

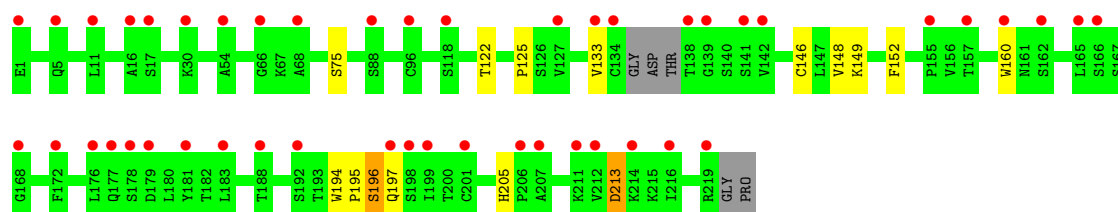




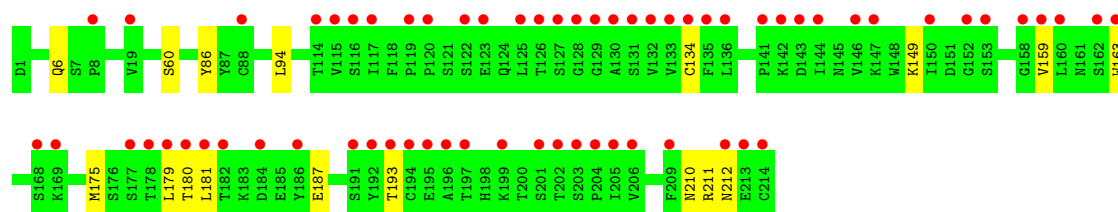
• Molecule 3: 10E5 Fab heavy chain



• Molecule 3: 10E5 Fab heavy chain

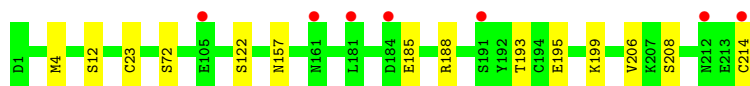


• Molecule 4: 10E5 Fab light chain



• Molecule 4: 10E5 Fab light chain





- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 60% 40%



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

Chain I: 100%



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

Chain K: 50% 50%



- Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	259.38Å 145.25Å 105.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.78 – 2.43 48.78 – 2.43	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.78-2.43) 86.6 (48.78-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.221 , 0.247 0.222 , 0.248	Depositor DCC
R_{free} test set	1981 reflections (1.32%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22145	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, NB9, CA, SO4, GOL, BMA, MG, MAN, CL

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	0.11	0/3647	0.34	0/4969
1	C	0.11	0/3605	0.34	0/4912
2	B	0.12	0/3725	0.32	0/5049
2	D	0.12	0/3714	0.33	0/5036
3	E	0.12	0/1673	0.31	0/2290
3	H	0.10	0/1684	0.31	0/2305
4	F	0.13	0/1673	0.33	0/2269
4	L	0.12	0/1673	0.32	0/2269
All	All	0.12	0/21394	0.33	0/29099

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3532	0	3383	29	0
1	C	3502	0	3334	8	0
2	B	3649	0	3571	17	0
2	D	3642	0	3558	18	0
3	E	1631	0	1590	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	0	1600	9	0
4	F	1637	0	1553	8	0
4	L	1637	0	1553	6	0
5	G	61	0	52	0	0
6	I	28	0	25	0	0
6	K	28	0	25	2	0
7	J	50	0	43	0	0
8	A	15	0	0	1	0
8	C	15	0	0	0	0
8	L	5	0	0	0	0
9	A	6	0	8	0	0
10	A	4	0	0	0	0
10	B	2	0	0	0	0
10	C	4	0	0	0	0
10	D	2	0	0	0	0
11	A	1	0	0	0	0
11	C	2	0	0	0	0
12	B	1	0	0	0	0
12	D	1	0	0	0	0
13	B	14	0	13	1	0
13	D	14	0	13	0	0
14	B	34	0	0	0	0
14	D	34	0	0	2	0
15	A	323	0	0	18	0
15	B	214	0	0	3	0
15	C	125	0	0	1	0
15	D	118	0	0	3	0
15	E	35	0	0	2	0
15	F	35	0	0	2	0
15	H	46	0	0	6	0
15	L	56	0	0	1	0
All	All	22145	0	20321	104	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 3.

All (104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLU:OE2	1:A:90[B]:ARG:NH1	2.20	0.74
15:H:333:HOH:O	4:L:214:CYS:SG	2.45	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:365:GLU:OE2	2:B:412:LYS:NZ	2.22	0.72
2:D:181:LYS:NZ	15:D:2101:HOH:O	2.20	0.68
1:A:436:ILE:O	15:A:601:HOH:O	2.13	0.66
3:H:152:PHE:O	15:H:301:HOH:O	2.15	0.65
4:F:6:GLN:NE2	15:F:303:HOH:O	2.28	0.65
3:E:149:LYS:NZ	4:F:180:THR:HG21	2.12	0.64
2:D:202:ARG:NH2	2:D:206:GLU:OE2	2.30	0.64
1:A:422:ARG:O	15:A:601:HOH:O	2.15	0.64
2:B:28:ASP:OD1	2:B:30:ALA:N	2.31	0.64
1:A:330:LEU:O	15:A:603:HOH:O	2.15	0.64
1:A:90[A]:ARG:NH2	15:A:608:HOH:O	2.31	0.63
3:E:67:LYS:NZ	3:E:90:ASP:OD2	2.26	0.61
1:A:177[A]:GLN:NE2	15:A:611:HOH:O	2.33	0.61
2:B:131:ILE:O	15:B:2101:HOH:O	2.16	0.60
1:A:15[B]:ASN:ND2	15:A:612:HOH:O	2.34	0.59
2:D:365:GLU:OE2	2:D:412:LYS:NZ	2.35	0.59
2:D:73:GLY:N	2:D:108:GLU:O	2.36	0.58
2:D:121:SER:HB2	14:D:2005:NB9:O10	2.03	0.58
1:C:2:ASN:N	1:C:2:ASN:OD1	2.37	0.58
1:C:3:LEU:O	1:C:405:GLN:NE2	2.28	0.57
1:A:32[B]:ARG:NH2	15:A:613:HOH:O	2.36	0.57
3:H:213:ASP:OD1	3:H:213:ASP:N	2.37	0.57
1:A:188:GLY:HA2	15:A:772:HOH:O	2.03	0.57
4:F:210:ASN:ND2	15:F:307:HOH:O	2.38	0.56
2:D:306:LEU:HB3	2:D:328:THR:HG22	1.88	0.56
2:B:130:SER:OG	2:B:336:ASP:O	2.21	0.56
2:B:26:CYS:O	2:B:37:ARG:NH1	2.42	0.52
2:B:132[A]:GLN:NE2	15:B:2108:HOH:O	2.37	0.52
3:E:219:ARG:NH2	15:E:303:HOH:O	2.42	0.52
1:A:301:ASP:OD2	15:A:604:HOH:O	2.19	0.51
1:A:307:LEU:O	15:A:605:HOH:O	2.19	0.51
2:D:12:SER:HB3	2:D:461:ARG:HD3	1.92	0.51
2:B:25:TRP:CD1	2:B:27:SER:HG	2.28	0.50
4:L:185:GLU:OE1	15:L:401:HOH:O	2.18	0.50
4:L:193:THR:HG23	4:L:208:SER:HB3	1.93	0.50
1:A:307:LEU:HA	1:A:329:TYR:O	2.11	0.50
1:A:377:ALA:HB2	1:A:421:LEU:HD11	1.93	0.50
2:D:418:PRO:HB2	2:D:421:PHE:CD1	2.47	0.50
2:B:39:ASP:OD1	2:B:40:LEU:N	2.45	0.49
4:F:187:GLU:HG2	4:F:211:ARG:NH1	2.28	0.48
1:C:107:CYS:HA	1:C:130:CYS:HA	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:SER:HB3	2:B:461:ARG:HD3	1.94	0.48
3:H:125:PRO:HB2	15:H:330:HOH:O	2.13	0.48
2:B:311:THR:O	2:B:315[B]:VAL:HG23	2.14	0.47
1:A:345:LEU:O	15:A:603:HOH:O	2.20	0.47
1:A:9:THR:HB	1:A:447:VAL:HB	1.96	0.47
1:A:197:GLN:OE1	15:A:606:HOH:O	2.21	0.47
1:A:276:ARG:NH1	15:A:630:HOH:O	2.45	0.47
1:C:377:ALA:HB2	1:C:421:LEU:HD11	1.96	0.47
2:D:150:ARG:HE	2:D:239:ARG:HD3	1.79	0.47
1:A:262:TRP:HB3	2:B:317:LEU:HD13	1.97	0.47
2:B:99:ASN:O	13:B:2004:NAG:H82	2.15	0.47
3:E:202:ASN:HA	3:E:213:ASP:HB3	1.98	0.46
6:K:1:NAG:O3	6:K:2:NAG:O5	2.30	0.46
1:A:294:ALA:N	15:A:605:HOH:O	2.40	0.46
3:H:196:SER:OG	3:H:197:GLN:N	2.48	0.46
1:A:107:CYS:HA	1:A:130:CYS:HA	1.97	0.45
1:A:400:ARG:HD2	8:A:502:SO4:O2	2.17	0.45
3:H:205:HIS:HE1	15:H:301:HOH:O	1.99	0.45
2:D:22:MET:HG2	2:D:40:LEU:HD22	1.99	0.45
1:A:436:ILE:N	15:A:601:HOH:O	2.49	0.44
3:H:149:LYS:NZ	15:H:302:HOH:O	2.23	0.44
1:A:15[A]:ASN:ND2	15:A:627:HOH:O	2.44	0.44
3:H:148:VAL:HG13	15:H:330:HOH:O	2.18	0.44
2:D:28:ASP:O	2:D:37:ARG:NH2	2.51	0.44
1:C:224:ASP:OD1	1:C:225:SER:N	2.47	0.44
3:E:38:LYS:N	15:E:307:HOH:O	2.51	0.44
3:E:91:THR:HG23	3:E:116:THR:HA	2.00	0.44
2:B:10:VAL:HG11	2:B:16:CYS:HA	1.99	0.43
3:E:177:GLN:N	3:E:180:LEU:O	2.42	0.43
2:D:178:TYR:CG	2:D:179:ASP:N	2.86	0.43
1:A:122:ALA:O	1:A:123:GLU:HB2	2.19	0.43
2:D:400:GLU:HB2	6:K:1:NAG:H83	2.00	0.43
1:A:41:ARG:NH2	15:A:641:HOH:O	2.51	0.42
3:E:2:VAL:HG13	3:E:27:PHE:CE1	2.54	0.42
4:F:149:LYS:HB2	4:F:193:THR:HB	2.01	0.42
3:H:194:TRP:CG	3:H:195:PRO:HA	2.54	0.42
1:A:3:LEU:O	1:A:5:PRO:HD3	2.19	0.42
1:A:314:MET:HB3	1:A:322:LEU:HB3	2.02	0.42
3:H:146:CYS:HB2	3:H:160:TRP:CH2	2.54	0.42
2:D:329:THR:HB	15:D:2169:HOH:O	2.19	0.42
3:E:213:ASP:OD1	3:E:213:ASP:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:365:GLU:H	2:B:365:GLU:CD	2.28	0.41
4:L:195:GLU:HG2	4:L:206:VAL:HG22	2.02	0.41
2:D:42:GLU:O	2:D:46:LYS:HG3	2.20	0.41
1:C:276:ARG:HD2	1:C:279:ARG:HB2	2.03	0.41
4:L:185:GLU:HG3	4:L:188:ARG:NH1	2.35	0.41
4:F:163:TRP:CZ2	4:F:175:MET:HE3	2.56	0.41
1:C:367:ASP:OD1	1:C:367:ASP:N	2.49	0.41
2:D:391:ILE:HG22	15:D:2137:HOH:O	2.20	0.41
4:F:6:GLN:NE2	4:F:86:TYR:O	2.49	0.41
4:F:159:VAL:HG22	4:F:179:LEU:HD13	2.03	0.41
1:A:109:PRO:O	1:A:168:GLU:HA	2.20	0.41
2:B:139:ALA:HB2	2:B:200:VAL:HG11	2.02	0.41
1:C:320:ARG:NH1	15:C:612:HOH:O	2.49	0.41
2:D:121:SER:HB2	14:D:2005:NB9:C09	2.51	0.41
2:B:117:LEU:HD11	2:B:225:ALA:HB1	2.02	0.40
2:B:209:LYS:NZ	15:B:2121:HOH:O	2.54	0.40
2:D:371:ASN:OD1	2:D:381:PRO:HA	2.20	0.40
3:E:152:PHE:HA	3:E:153:PRO:HA	1.90	0.40
4:L:4:MET:HE3	4:L:23:CYS:SG	2.61	0.40
1:A:15[A]:ASN:ND2	15:A:648:HOH:O	2.55	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	460/457 (101%)	444 (96%)	15 (3%)	1 (0%)	43	53
1	C	455/457 (100%)	437 (96%)	18 (4%)	0	100	100
2	B	472/472 (100%)	451 (96%)	18 (4%)	3 (1%)	21	25
2	D	471/472 (100%)	445 (94%)	26 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	210/221 (95%)	191 (91%)	18 (9%)	1 (0%)	24	29
3	H	212/221 (96%)	195 (92%)	17 (8%)	0	100	100
4	F	212/214 (99%)	193 (91%)	18 (8%)	1 (0%)	24	29
4	L	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
All	All	2704/2728 (99%)	2560 (95%)	138 (5%)	6 (0%)	43	53

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	164	SER
1	A	123	GLU
2	B	9	GLY
2	B	76	ASP
2	B	375	LEU
4	F	212	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/364 (102%)	359 (97%)	11 (3%)	36	48
1	C	365/364 (100%)	354 (97%)	11 (3%)	36	48
2	B	420/417 (101%)	414 (99%)	6 (1%)	59	70
2	D	418/417 (100%)	409 (98%)	9 (2%)	45	59
3	E	186/190 (98%)	184 (99%)	2 (1%)	65	75
3	H	187/190 (98%)	182 (97%)	5 (3%)	39	52
4	F	188/188 (100%)	184 (98%)	4 (2%)	47	60
4	L	188/188 (100%)	183 (97%)	5 (3%)	39	52
All	All	2322/2318 (100%)	2269 (98%)	53 (2%)	44	57

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

Mol	Chain	Res	Type
1	A	23	LEU
1	A	61	GLU
1	A	166	TYR
1	A	195	LEU
1	A	220	SER
1	A	270	LEU
1	A	288	TYR
1	A	335	ARG
1	A	350[A]	THR
1	A	350[B]	THR
1	A	395	GLN
2	B	37	ARG
2	B	101	SER
2	B	182	THR
2	B	215	ASN
2	B	417	LYS
2	B	447	ARG
1	C	2	ASN
1	C	15	ASN
1	C	23	LEU
1	C	119	THR
1	C	166	TYR
1	C	195	LEU
1	C	219	GLN
1	C	251	THR
1	C	288	TYR
1	C	319	ASP
1	C	406	VAL
2	D	20	SER
2	D	202	ARG
2	D	215	ASN
2	D	262	LEU
2	D	303	ASN
2	D	365	GLU
2	D	378	GLU
2	D	383	LEU
2	D	462	CYS
3	E	97	VAL
3	E	211	LYS
4	F	60	SER
4	F	94	LEU
4	F	134	CYS
4	F	181	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	75	SER
3	H	122	THR
3	H	133	VAL
3	H	196	SER
3	H	213	ASP
4	L	12	SER
4	L	72	SER
4	L	122	SER
4	L	157	ASN
4	L	199	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	372	ASN
2	B	15	GLN
2	B	106	GLN
2	B	305	ASN
1	C	85	GLN
2	D	204	ASN
2	D	280	HIS
2	D	376	ASN
3	E	82	GLN
4	F	137	ASN
4	L	27	GLN
4	L	161	ASN

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](#)

13 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	$\# Z > 2$
5	NAG	G	1	5,2	14,14,15	0.31	0	17,19,21	0.62	0
5	NAG	G	2	5	14,14,15	0.32	0	17,19,21	0.42	0
5	BMA	G	3	5	11,11,12	0.61	0	15,15,17	0.77	0
5	MAN	G	4	5	11,11,12	0.61	0	15,15,17	0.98	2 (13%)
5	MAN	G	5	5	11,11,12	0.63	0	15,15,17	0.92	2 (13%)
6	NAG	I	1	2,6	14,14,15	0.33	0	17,19,21	0.45	0
6	NAG	I	2	6	14,14,15	0.27	0	17,19,21	0.40	0
7	NAG	J	1	2,7	14,14,15	0.34	0	17,19,21	0.63	1 (5%)
7	NAG	J	2	7	14,14,15	0.26	0	17,19,21	0.48	0
7	BMA	J	3	7	11,11,12	0.57	0	15,15,17	0.87	0
7	MAN	J	4	7	11,11,12	0.68	0	15,15,17	0.99	2 (13%)
6	NAG	K	1	2,6	14,14,15	0.30	0	17,19,21	0.55	0
6	NAG	K	2	6	14,14,15	0.36	0	17,19,21	0.77	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
5	NAG	G	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	1/2/19/22	0/1/1/1
6	NAG	I	1	2,6	-	1/6/23/26	0/1/1/1
6	NAG	I	2	6	-	3/6/23/26	0/1/1/1
7	NAG	J	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
7	BMA	J	3	7	-	2/2/19/22	0/1/1/1
7	MAN	J	4	7	-	2/2/19/22	0/1/1/1
6	NAG	K	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	4	MAN	C1-O5-C5	2.68	115.78	112.19
7	J	4	MAN	C1-O5-C5	2.37	115.36	112.19
6	K	2	NAG	C1-O5-C5	2.25	115.20	112.19
5	G	5	MAN	C1-O5-C5	2.15	115.07	112.19
5	G	4	MAN	O2-C2-C3	-2.12	105.77	110.15
7	J	4	MAN	O2-C2-C3	-2.11	105.79	110.15
5	G	5	MAN	O2-C2-C3	-2.08	105.83	110.15
7	J	1	NAG	C1-O5-C5	2.08	114.97	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

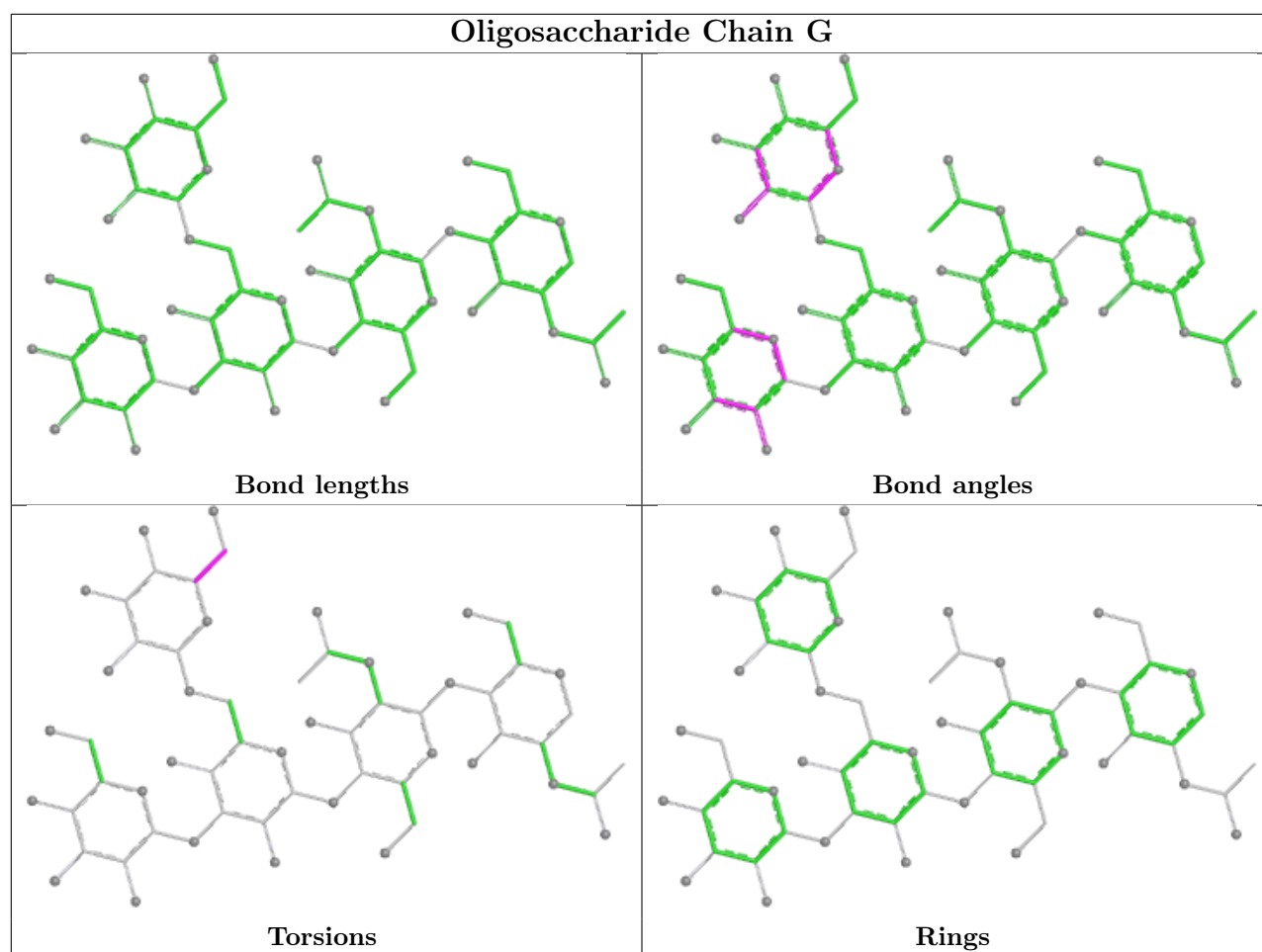
Mol	Chain	Res	Type	Atoms
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
7	J	4	MAN	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
5	G	5	MAN	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
7	J	3	BMA	C4-C5-C6-O6
7	J	3	BMA	O5-C5-C6-O6
7	J	4	MAN	C4-C5-C6-O6

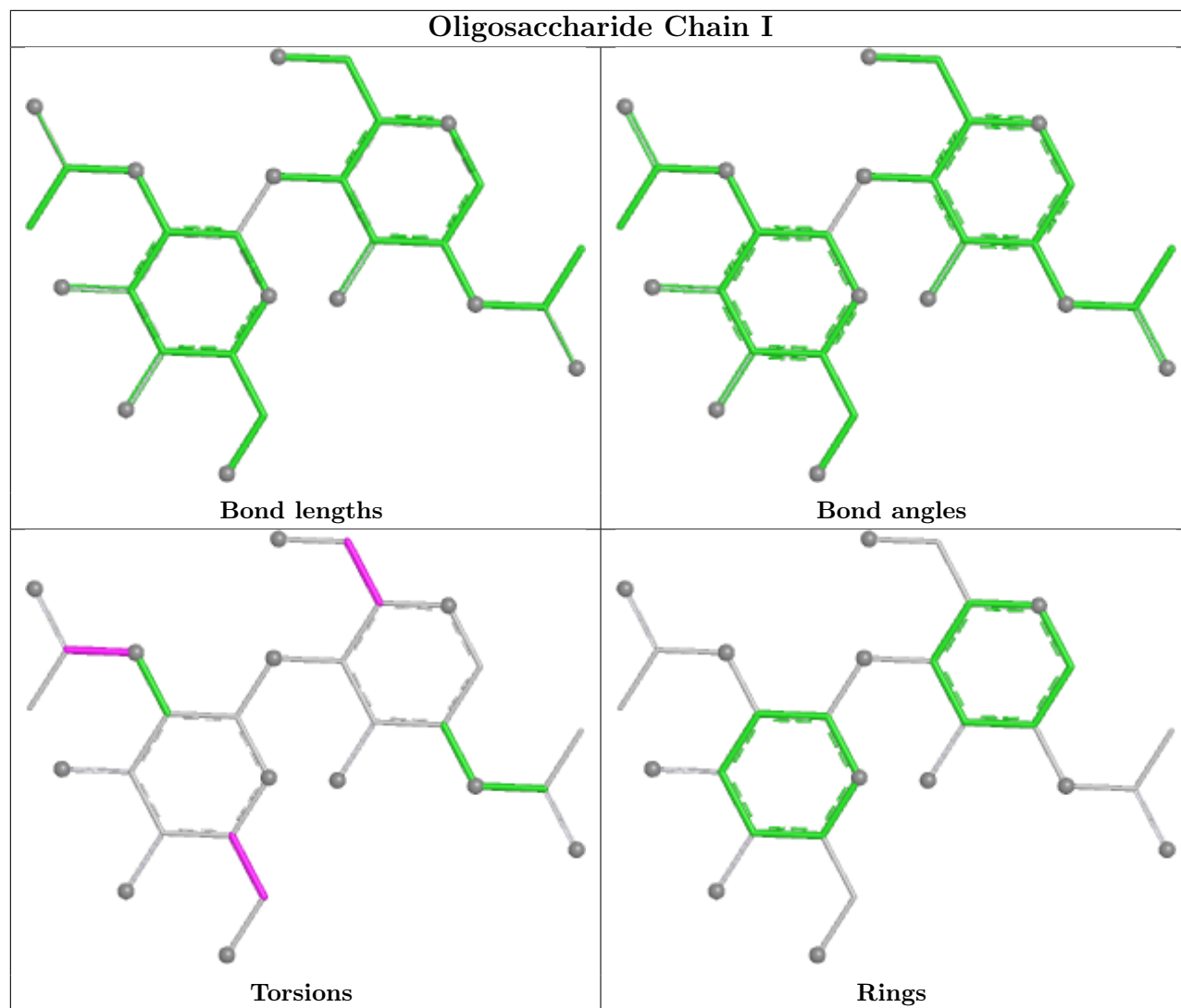
There are no ring outliers.

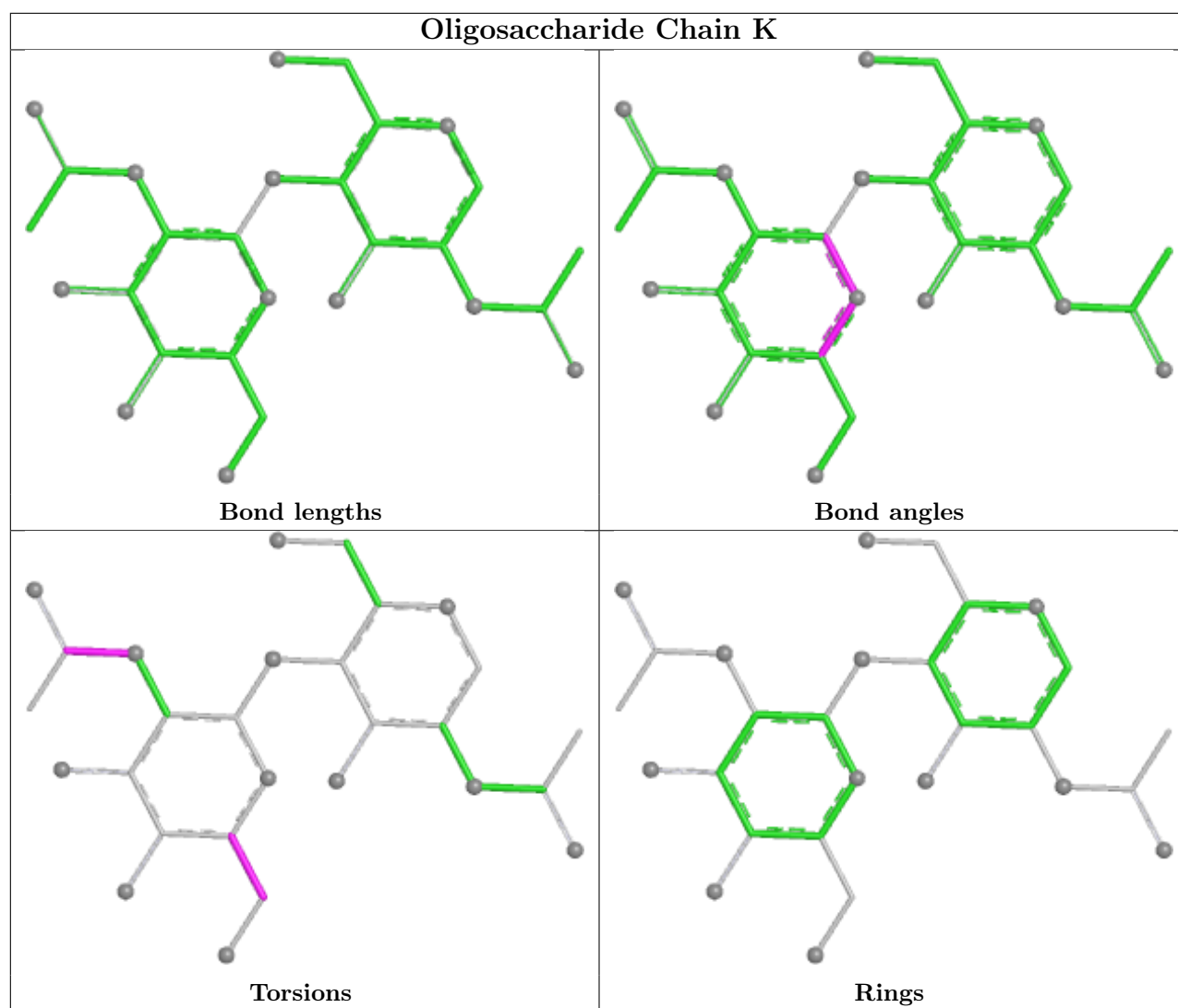
2 monomers are involved in 2 short contacts:

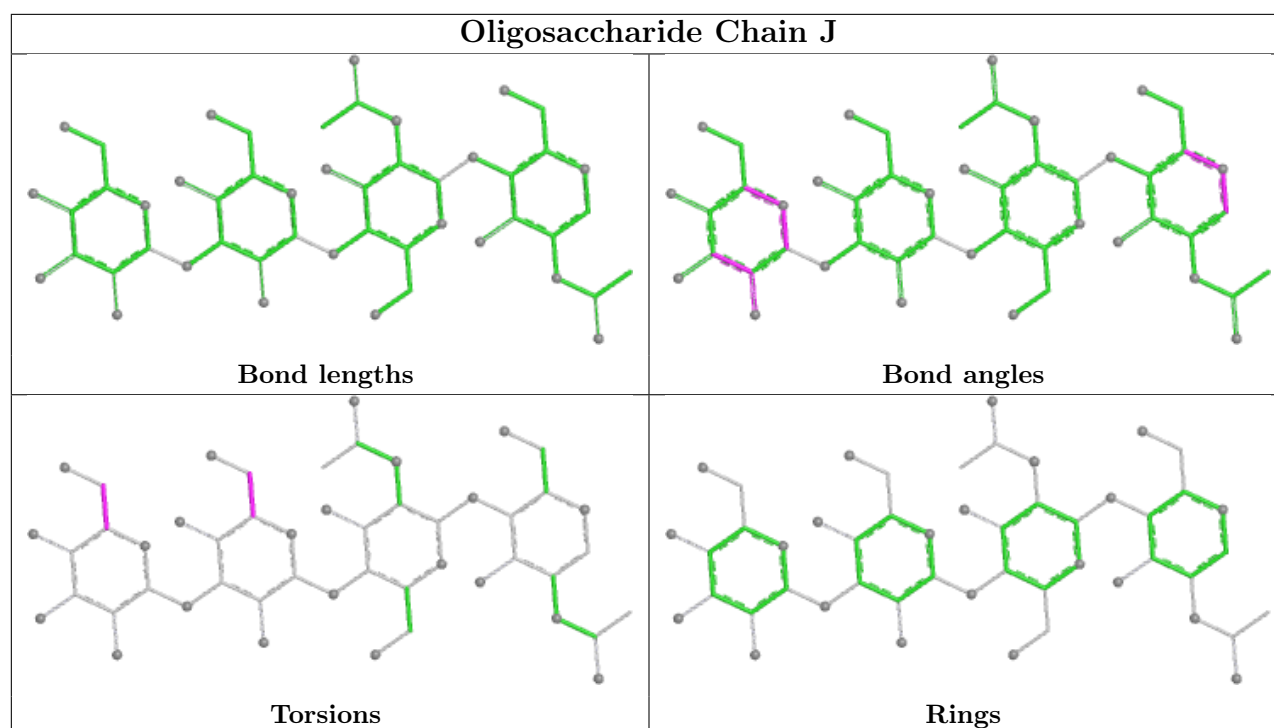
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	2	NAG	1	0
6	K	1	NAG	2	0

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









5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 17 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	SO4	C	501	-	4,4,4	0.24	0	6,6,6	0.07	0
8	SO4	C	502	-	4,4,4	0.24	0	6,6,6	0.07	0
13	NAG	B	2004	2	14,14,15	0.41	0	17,19,21	0.49	0
14	NB9	B	2005	12	36,36,36	2.55	9 (25%)	44,49,49	1.52	3 (6%)
14	NB9	D	2005	12	36,36,36	2.57	9 (25%)	44,49,49	1.28	3 (6%)
8	SO4	A	501	-	4,4,4	0.24	0	6,6,6	0.07	0
8	SO4	A	502	-	4,4,4	0.24	0	6,6,6	0.07	0
9	GOL	A	503	-	5,5,5	0.36	0	5,5,5	0.42	0
13	NAG	D	2004	2	14,14,15	0.55	0	17,19,21	0.39	0
8	SO4	C	503	-	4,4,4	0.24	0	6,6,6	0.07	0
8	SO4	L	301	-	4,4,4	0.24	0	6,6,6	0.07	0
8	SO4	A	508	-	4,4,4	0.25	0	6,6,6	0.21	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	B	2004	2	-	1/6/23/26	0/1/1/1
14	NB9	B	2005	12	-	2/29/39/39	0/3/3/3
14	NB9	D	2005	12	-	2/29/39/39	0/3/3/3
9	GOL	A	503	-	-	2/4/4/4	-
13	NAG	D	2004	2	-	2/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	D	2005	NB9	C12-N03	10.39	1.50	1.35
14	B	2005	NB9	C12-N03	10.30	1.49	1.35
14	B	2005	NB9	C24-N23	6.64	1.49	1.34
14	D	2005	NB9	C24-N23	6.63	1.49	1.34
14	B	2005	NB9	O13-C12	-4.52	1.14	1.22
14	D	2005	NB9	O13-C12	-4.47	1.14	1.22
14	D	2005	NB9	C32-N34	4.15	1.44	1.33
14	B	2005	NB9	C32-N34	4.15	1.44	1.33
14	D	2005	NB9	C04-N03	2.80	1.52	1.47
14	B	2005	NB9	C04-N03	2.70	1.51	1.47
14	B	2005	NB9	C15-C16	2.60	1.57	1.51
14	D	2005	NB9	C15-C16	2.56	1.57	1.51
14	D	2005	NB9	C02-N03	2.54	1.51	1.47
14	B	2005	NB9	C14-N23	2.50	1.51	1.45
14	D	2005	NB9	C14-N23	2.50	1.51	1.45
14	B	2005	NB9	C02-N03	2.37	1.51	1.47
14	B	2005	NB9	C26-C24	2.35	1.55	1.50
14	D	2005	NB9	C26-C24	2.35	1.55	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	2005	NB9	C02-C01-C06	5.95	116.77	110.32
14	B	2005	NB9	C04-C05-C06	5.09	115.83	110.32
14	D	2005	NB9	C02-C01-C06	4.58	115.28	110.32
14	D	2005	NB9	C04-C05-C06	3.85	114.50	110.32
14	B	2005	NB9	C05-C06-C01	3.11	118.02	111.67
14	D	2005	NB9	C05-C06-C01	2.11	115.97	111.67

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	D	2004	NAG	C4-C5-C6-O6
13	D	2004	NAG	O5-C5-C6-O6
9	A	503	GOL	O1-C1-C2-C3
9	A	503	GOL	O1-C1-C2-O2
13	B	2004	NAG	O5-C5-C6-O6
14	B	2005	NB9	C28-C29-C32-N33
14	D	2005	NB9	C30-C29-C32-N33
14	B	2005	NB9	C30-C29-C32-N34
14	D	2005	NB9	C28-C29-C32-N33

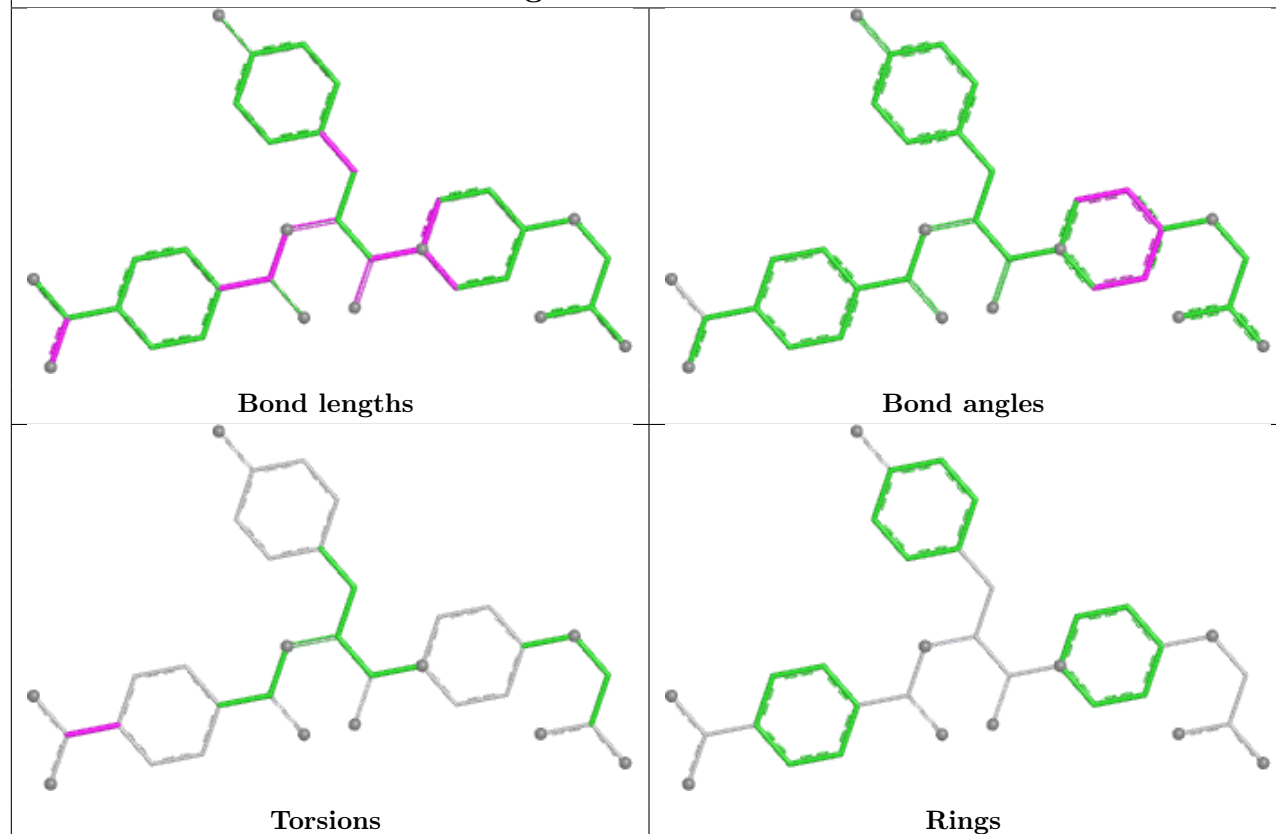
There are no ring outliers.

3 monomers are involved in 4 short contacts:

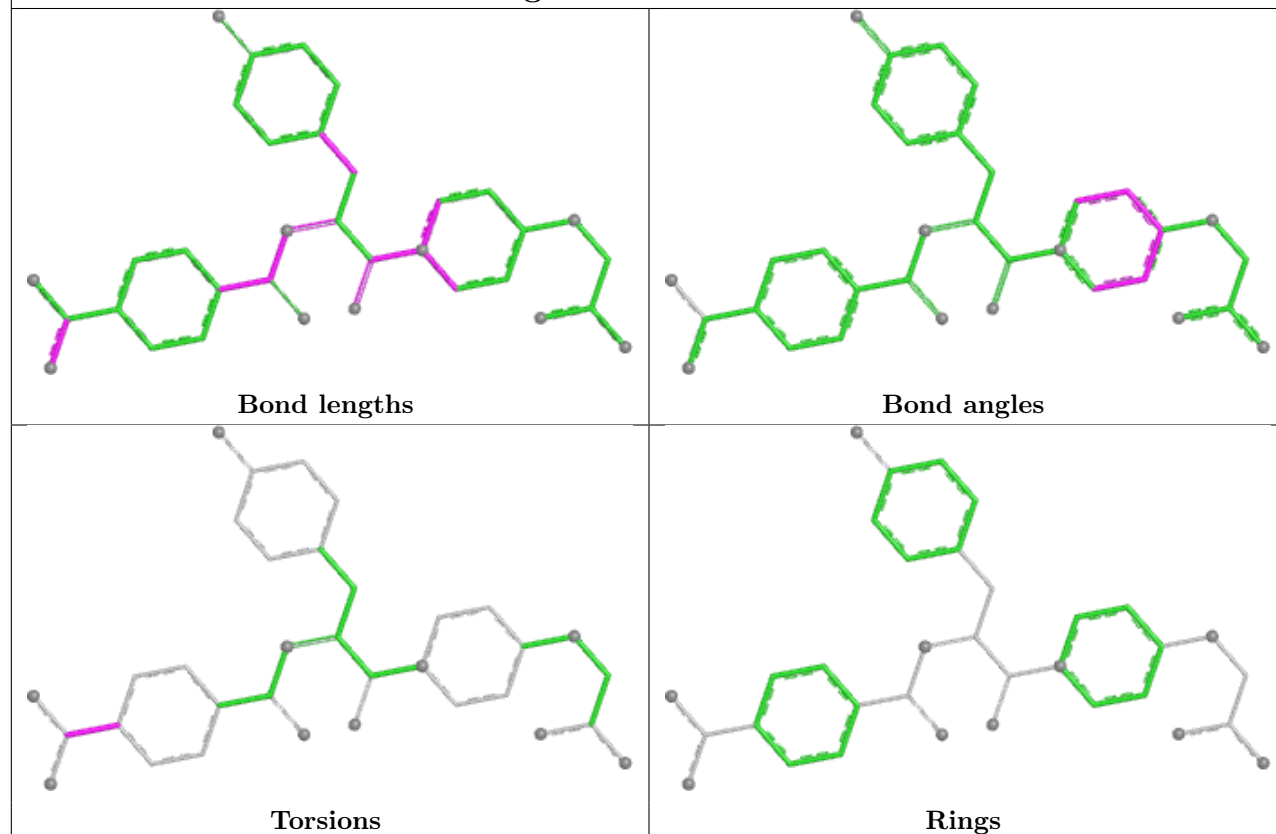
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	2004	NAG	1	0
14	D	2005	NB9	2	0
8	A	502	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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 than 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 NB9 B 2005



Ligand NB9 D 2005



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	454/457 (99%)	0.11	14 (3%)	51	50	22, 39, 55, 71	8 (1%)
1	C	453/457 (99%)	0.30	12 (2%)	57	57	22, 50, 68, 86	4 (0%)
2	B	466/472 (98%)	0.76	53 (11%)	10	8	19, 59, 114, 132	9 (1%)
2	D	471/472 (99%)	0.87	50 (10%)	11	8	24, 67, 106, 119	3 (0%)
3	E	214/221 (96%)	1.97	83 (38%)	1	0	67, 107, 157, 163	0
3	H	216/221 (97%)	1.33	46 (21%)	2	2	50, 86, 115, 120	0
4	F	214/214 (100%)	1.65	65 (30%)	1	1	69, 112, 150, 158	0
4	L	214/214 (100%)	0.90	7 (3%)	49	48	53, 77, 91, 109	0
All	All	2702/2728 (99%)	0.82	330 (12%)	8	6	19, 63, 135, 163	24 (0%)

All (330) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	454	VAL	8.9
3	E	212	VAL	7.9
2	D	129[A]	TRP	7.7
1	C	1	LEU	6.8
2	B	33	LEU	6.3
3	E	147	LEU	6.1
2	B	77	SER	6.1
3	E	216	ILE	5.8
3	E	165	LEU	5.7
2	D	471	CYS	5.7
3	E	203	VAL	5.5
3	E	144	LEU	5.4
3	E	214	LYS	5.1
4	F	125	LEU	5.1
4	F	130	ALA	5.1
2	D	375	LEU	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	201	CYS	4.8
3	E	127	VAL	4.8
2	D	469	SER	4.4
3	E	133	VAL	4.4
4	F	115	VAL	4.4
1	A	217	SER	4.3
3	E	128	TYR	4.3
4	F	135	PHE	4.3
2	B	132[A]	GLN	4.2
3	E	149	LYS	4.2
2	B	76	ASP	4.2
2	D	468	GLY	4.2
4	F	180	THR	4.2
3	E	183	LEU	4.1
2	B	466	TRP	4.0
4	L	214	CYS	4.0
3	E	192	SER	4.0
3	E	134	CYS	4.0
2	B	375	LEU	4.0
4	F	181	LEU	4.0
2	B	74	SER	4.0
2	D	33	LEU	4.0
4	F	126	THR	3.9
4	F	182	THR	3.9
2	B	129	TRP	3.9
3	E	160	TRP	3.9
1	C	2	ASN	3.9
3	E	196	SER	3.8
4	L	212	ASN	3.8
4	F	179	LEU	3.8
4	F	131	SER	3.7
1	A	130	CYS	3.7
4	F	160	LEU	3.7
3	E	148	VAL	3.7
3	E	176	LEU	3.7
4	F	134	CYS	3.7
2	D	466	TRP	3.6
2	D	446	HIS	3.6
3	E	145	GLY	3.6
3	E	204	ALA	3.6
3	E	174	ALA	3.6
3	E	199	ILE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	171	THR	3.6
2	D	1	GLY	3.6
3	E	168	GLY	3.6
2	B	4	ILE	3.6
3	E	215	LYS	3.5
3	E	210	THR	3.5
4	F	117	ILE	3.5
3	H	198	SER	3.4
3	E	194	TRP	3.4
4	F	214	CYS	3.4
4	F	209	PHE	3.4
4	F	169	LYS	3.4
4	F	119	PRO	3.4
4	F	196	ALA	3.4
2	D	387	MET	3.4
2	D	2	PRO	3.4
4	F	202	THR	3.4
1	C	130	CYS	3.3
2	D	374	CYS	3.3
2	D	437	CYS	3.3
3	E	146	CYS	3.3
3	E	132	PRO	3.3
2	D	406	CYS	3.3
3	E	129	PRO	3.3
3	E	188	THR	3.3
3	E	189	VAL	3.3
4	F	152	GLY	3.3
4	F	114	THR	3.3
2	D	4	ILE	3.3
3	E	9	ALA	3.3
2	B	452	ASN	3.2
3	H	212	VAL	3.2
2	D	77	SER	3.2
3	H	134	CYS	3.2
2	B	78	SER	3.2
2	D	378	GLU	3.2
2	D	467	LEU	3.2
4	F	213	GLU	3.2
4	F	194	CYS	3.2
2	D	462	CYS	3.2
4	F	150	ILE	3.2
4	F	178	THR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	319	ASP	3.1
3	E	181	TYR	3.1
3	H	219	ARG	3.1
2	B	378	GLU	3.1
4	L	191	SER	3.1
2	B	75	GLY	3.1
2	D	178	TYR	3.1
1	A	339	ALA	3.1
2	B	36	PRO	3.1
2	B	2	PRO	3.1
3	E	126	SER	3.1
1	C	453	VAL	3.1
4	F	205	ILE	3.1
4	F	163	TRP	3.0
3	E	121	LYS	3.0
4	F	204	PRO	3.0
4	F	116	SER	3.0
2	B	10	VAL	3.0
2	D	143	ARG	3.0
4	F	147	LYS	3.0
3	H	139	GLY	3.0
3	E	180	LEU	3.0
4	F	143	ASP	3.0
3	H	168	GLY	2.9
3	E	217	GLU	2.9
2	D	49	CYS	2.9
4	F	193	THR	2.9
4	F	133	VAL	2.9
4	F	206	VAL	2.9
2	B	137[A]	LYS	2.9
3	H	214	LYS	2.9
2	D	32	PRO	2.9
4	L	181	LEU	2.9
2	B	79	GLN	2.9
2	B	364	GLU	2.9
4	F	122	SER	2.8
3	E	175	VAL	2.8
3	E	218	PRO	2.8
3	E	131	ALA	2.8
3	E	11	LEU	2.8
4	F	195	GLU	2.8
2	B	178	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	H	138	THR	2.8
2	B	450	ASN	2.8
4	F	132	VAL	2.8
2	B	446	HIS	2.8
3	E	142	VAL	2.8
4	F	142	LYS	2.8
3	H	5	GLN	2.8
2	B	376	ASN	2.7
3	E	184	SER	2.7
3	H	192	SER	2.7
4	F	146	VAL	2.7
3	H	177	GLN	2.7
2	D	44	LEU	2.7
2	B	432	ASP	2.7
2	D	181	LYS	2.7
1	C	216	VAL	2.7
1	C	339	ALA	2.7
1	A	45	PRO	2.6
2	B	32	PRO	2.6
2	D	8	ARG	2.6
1	C	47	GLN	2.6
2	B	241	ASP	2.6
2	B	458	GLY	2.6
4	F	129	GLY	2.6
4	F	199	LYS	2.6
3	H	216	ILE	2.6
3	H	176	LEU	2.6
1	A	46	SER	2.6
1	A	47	GLN	2.6
3	E	200	THR	2.6
4	F	186	TYR	2.6
2	D	67	ARG	2.6
3	E	195	PRO	2.6
4	F	120	PRO	2.6
3	E	187	VAL	2.6
3	E	141	SER	2.6
2	D	47	ASP	2.6
2	D	51	PRO	2.6
3	E	219	ARG	2.6
1	A	32[A]	ARG	2.5
4	L	184	ASP	2.5
4	F	136	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	212	ASN	2.5
3	E	140	SER	2.5
3	E	143	THR	2.5
2	B	67	ARG	2.5
2	B	9	GLY	2.5
2	D	45	LEU	2.5
2	D	452	ASN	2.5
3	E	119	SER	2.5
3	E	182	THR	2.5
3	H	206	PRO	2.5
2	D	377	ASN	2.5
3	E	28	ASN	2.5
3	E	124	ALA	2.5
3	E	198	SER	2.5
2	D	433	CYS	2.5
2	D	55	GLU	2.5
2	D	75	GLY	2.5
2	B	46	LYS	2.5
3	E	158	LEU	2.5
3	H	165	LEU	2.5
2	D	10	VAL	2.5
2	B	177	CYS	2.4
2	B	374	CYS	2.4
2	B	34	GLY	2.4
3	E	56	GLY	2.4
3	E	45	LEU	2.4
3	E	156	VAL	2.4
3	H	127	VAL	2.4
3	H	68	ALA	2.4
4	F	123	GLU	2.4
2	B	72	LYS	2.4
2	B	181	LYS	2.4
1	C	319	ASP	2.4
3	E	57	TYR	2.4
3	E	177	GLN	2.4
3	E	16	ALA	2.4
4	F	197	THR	2.4
3	E	29	ILE	2.4
3	H	183	LEU	2.4
2	B	449	ASN	2.4
3	H	16	ALA	2.4
4	F	141	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	L	105	GLU	2.4
2	D	35	SER	2.4
3	E	178	SER	2.4
2	D	463	GLY	2.4
1	C	90	ARG	2.4
3	E	12	VAL	2.4
3	H	142	VAL	2.4
3	E	207	ALA	2.4
3	E	173	PRO	2.3
1	A	338	HIS	2.3
3	H	133	VAL	2.3
3	H	207	ALA	2.3
3	E	159	THR	2.3
4	F	153	SER	2.3
3	H	172	PHE	2.3
1	C	217	SER	2.3
3	H	118	SER	2.3
3	H	162	SER	2.3
3	H	197	GLN	2.3
2	B	386	CYS	2.3
2	B	448	CYS	2.3
4	F	88	CYS	2.3
3	E	153	PRO	2.3
2	D	404	ARG	2.3
4	F	158	GLY	2.3
3	E	48	ILE	2.3
2	D	36	PRO	2.3
3	E	65	GLN	2.2
2	B	17	LEU	2.2
2	B	44	LEU	2.2
3	H	17	SER	2.2
3	H	30	LYS	2.2
3	H	141	SER	2.2
4	F	201	SER	2.2
4	F	184	ASP	2.2
1	A	157	GLU	2.2
1	A	320	ARG	2.2
2	D	360	ARG	2.2
2	B	5	CYS	2.2
3	H	201	CYS	2.2
2	B	451	GLY	2.2
3	H	211	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	145	LEU	2.2
3	H	166	SER	2.2
4	F	144	ILE	2.2
3	H	1	GLU	2.2
1	A	337	PRO	2.2
3	E	211	LYS	2.2
3	H	96	CYS	2.2
4	F	177	SER	2.2
3	H	179	ASP	2.2
2	D	58	VAL	2.2
2	D	439	ALA	2.2
4	F	168	SER	2.2
2	B	8	ARG	2.2
2	D	46	LYS	2.2
2	D	22	MET	2.1
2	B	54	ILE	2.1
1	C	153	ARG	2.1
3	E	27	PHE	2.1
2	B	442	GLU	2.1
3	H	181	TYR	2.1
4	F	192	TYR	2.1
3	H	88	SER	2.1
4	F	191	SER	2.1
3	E	14	PRO	2.1
4	F	8	PRO	2.1
4	F	19	VAL	2.1
3	H	54	ALA	2.1
3	E	15	GLY	2.1
3	E	163	GLY	2.1
4	F	162	SER	2.1
4	F	159	VAL	2.1
2	B	45	LEU	2.1
3	E	154	GLU	2.1
3	E	185	SER	2.1
4	F	127	SER	2.1
4	F	203	SER	2.1
2	B	437	CYS	2.1
2	D	448	CYS	2.1
3	E	155	PRO	2.1
1	A	216	VAL	2.0
2	D	450	ASN	2.0
3	H	11	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	L	161	ASN	2.0
3	H	157	THR	2.0
3	H	160	TRP	2.0
2	B	387	MET	2.0
3	E	191	SER	2.0
3	H	178	SER	2.0
2	B	19	VAL	2.0
2	D	379	VAL	2.0
1	C	340	LEU	2.0
2	B	439	ALA	2.0
2	D	383	LEU	2.0
2	B	1	GLY	2.0
2	B	240	ASN	2.0
2	B	377	ASN	2.0
3	E	161	ASN	2.0
3	H	66	GLY	2.0
4	F	128	GLY	2.0
3	H	188	THR	2.0
3	H	199	ILE	2.0
3	H	155	PRO	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.

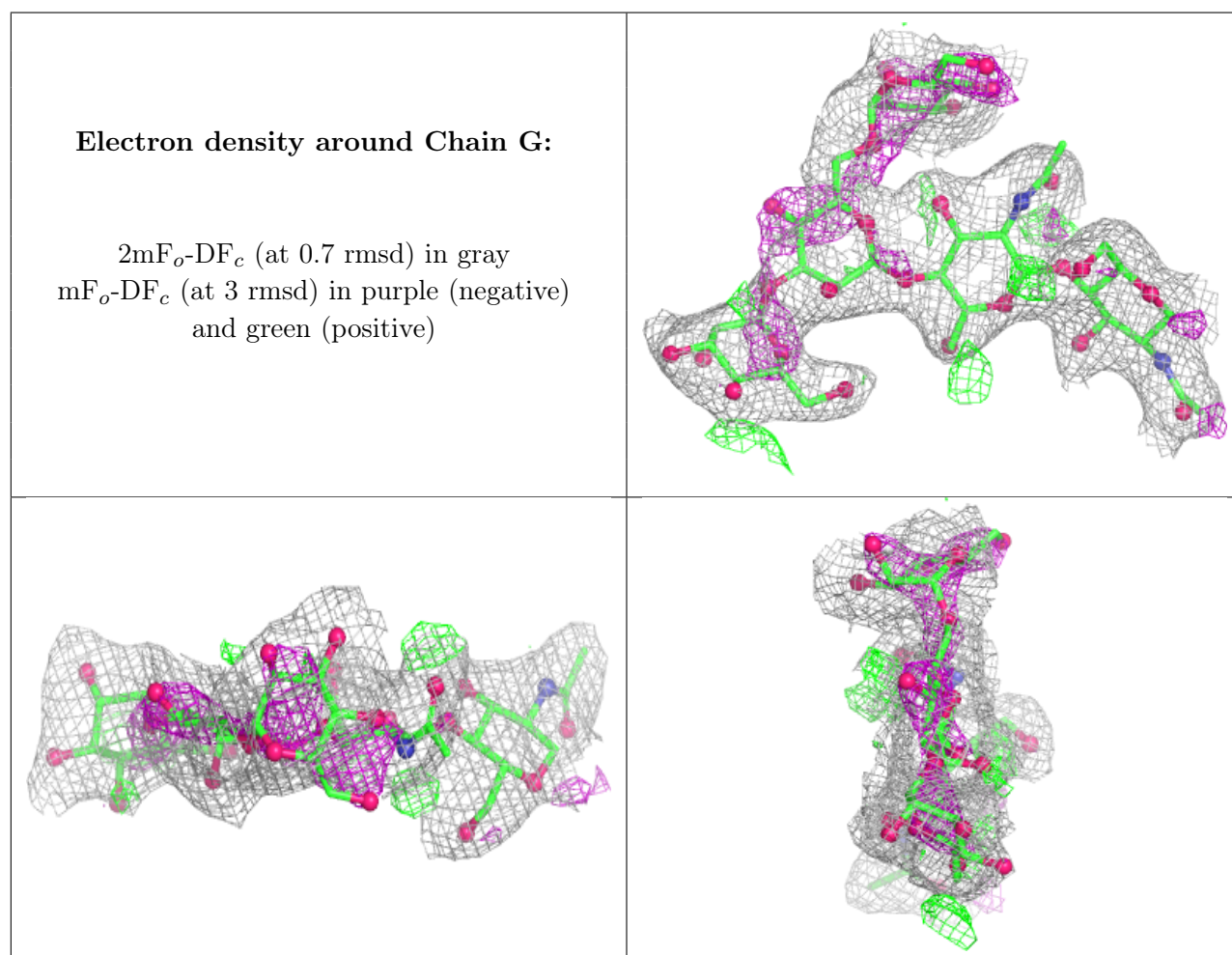
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	G	1	14/15	-	-	48,48,48,48	0
5	NAG	G	2	14/15	-	-	61,61,61,61	0
5	BMA	G	3	11/12	-	-	70,70,70,70	0
5	MAN	G	4	11/12	-	-	68,68,68,68	0
5	MAN	G	5	11/12	-	-	75,75,75,75	0
7	NAG	J	2	14/15	0.63	0.15	69,69,69,69	0
6	NAG	I	2	14/15	0.76	0.15	85,85,85,85	0
7	NAG	J	1	14/15	0.78	0.14	58,58,58,58	0

Continued on next page...

Continued from previous page...

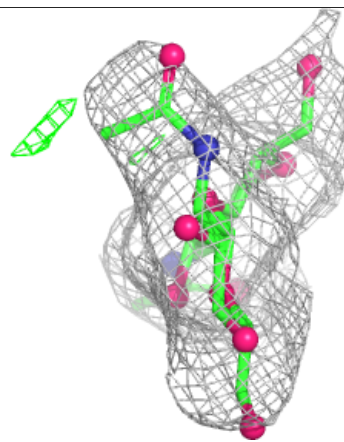
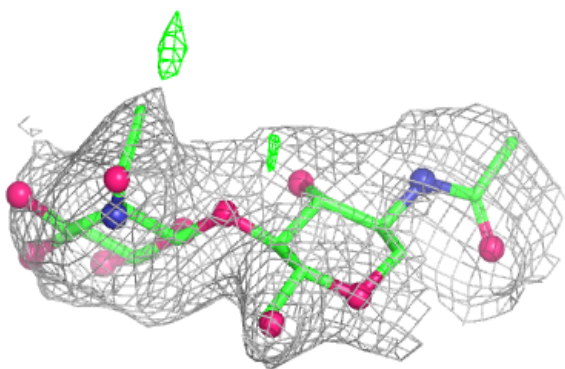
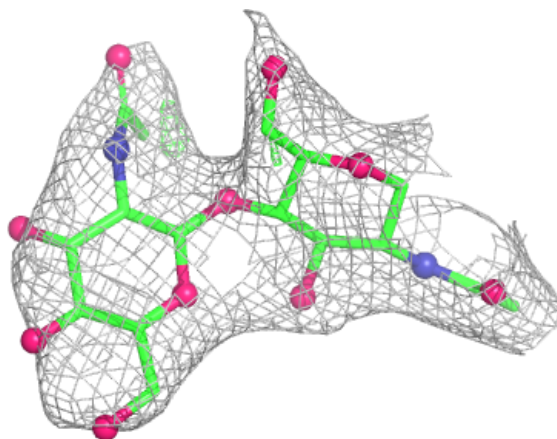
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	K	2	14/15	0.80	0.14	94,94,94,94	0
6	NAG	I	1	14/15	0.87	0.12	83,83,83,83	0
6	NAG	K	1	14/15	0.89	0.10	89,89,89,89	0
7	BMA	J	3	11/12	-	-	76,76,76,76	0
7	MAN	J	4	11/12	-	-	76,76,76,76	0

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.



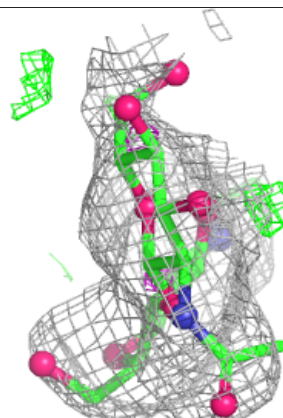
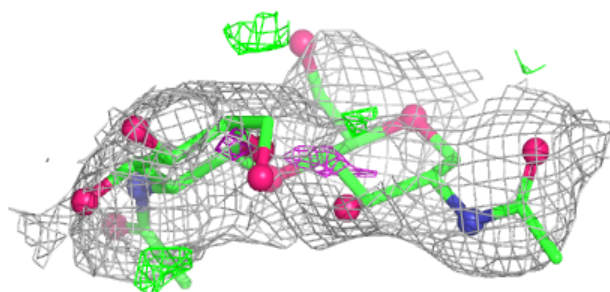
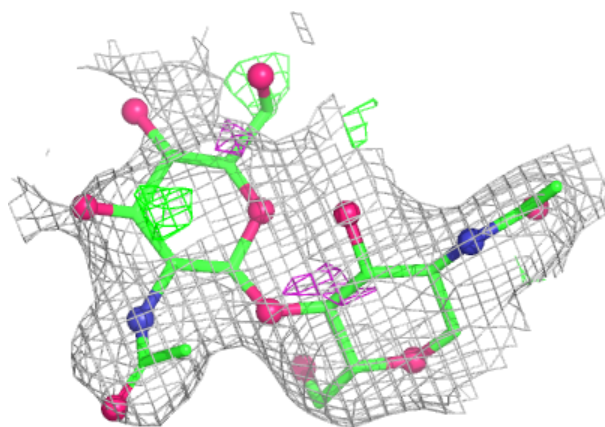
Electron density around Chain I:

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

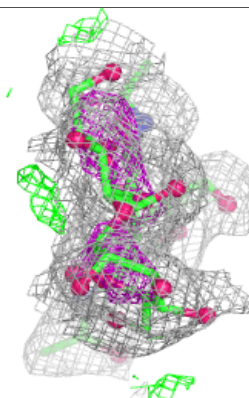
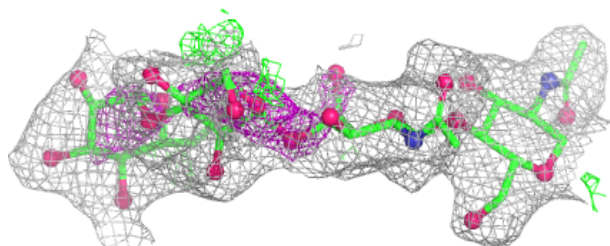
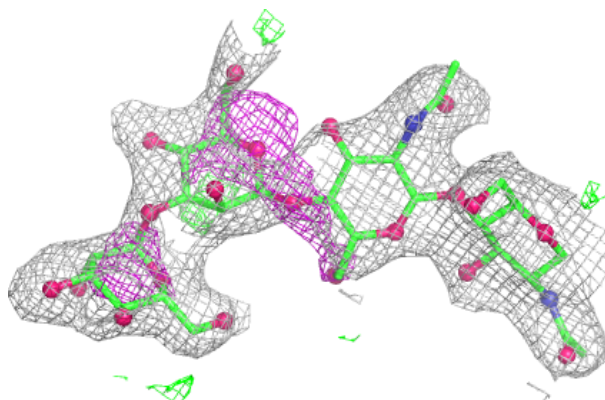


Electron density around Chain K:

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

**Electron density around Chain J:**

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



6.4 Ligands ⓘ

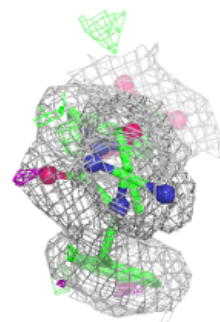
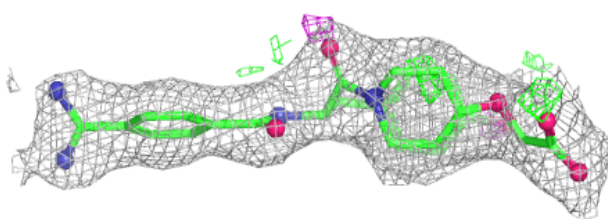
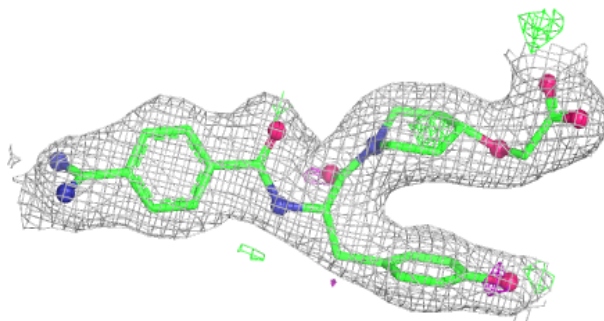
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
13	NAG	B	2004	14/15	0.66	0.15	86,86,86,86	0
13	NAG	D	2004	14/15	0.66	0.17	85,85,85,85	0
8	SO4	A	508	5/5	0.73	0.20	52,52,52,52	0
8	SO4	C	501	5/5	0.78	0.25	65,65,65,65	0
8	SO4	C	502	5/5	0.78	0.22	70,70,70,70	0
9	GOL	A	503	6/6	0.84	0.14	48,48,48,48	0
8	SO4	A	501	5/5	0.85	0.32	61,61,61,61	0
8	SO4	L	301	5/5	0.87	0.21	71,71,71,71	0
11	CL	C	505	1/1	0.91	0.18	67,67,67,67	0
10	CA	B	2002	1/1	0.93	0.13	52,52,52,52	0
8	SO4	C	503	5/5	0.93	0.12	61,61,61,61	5
14	NB9	B	2005	34/34	0.93	0.10	38,38,38,38	0
14	NB9	D	2005	34/34	0.93	0.10	48,48,48,48	0
11	CL	C	504	1/1	0.94	0.09	56,56,56,56	0
11	CL	A	509	1/1	0.96	0.09	53,53,53,53	0
10	CA	C	508	1/1	0.97	0.04	51,51,51,51	0
10	CA	A	507	1/1	0.97	0.04	36,36,36,36	0
8	SO4	A	502	5/5	0.97	0.08	50,50,50,50	0
10	CA	C	506	1/1	0.97	0.05	64,64,64,64	0
10	CA	A	506	1/1	0.98	0.04	36,36,36,36	0
12	MG	D	2001	1/1	0.98	0.07	40,40,40,40	0
10	CA	D	2002	1/1	0.98	0.05	53,53,53,53	0
10	CA	D	2003	1/1	0.98	0.03	42,42,42,42	0
10	CA	A	504	1/1	0.98	0.03	48,48,48,48	0
10	CA	C	507	1/1	0.98	0.03	56,56,56,56	0
10	CA	A	505	1/1	0.99	0.03	38,38,38,38	0
10	CA	C	509	1/1	0.99	0.02	49,49,49,49	0
10	CA	B	2003	1/1	0.99	0.02	33,33,33,33	0
12	MG	B	2001	1/1	1.00	0.09	28,28,28,28	0

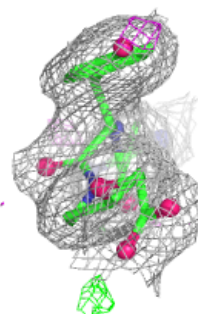
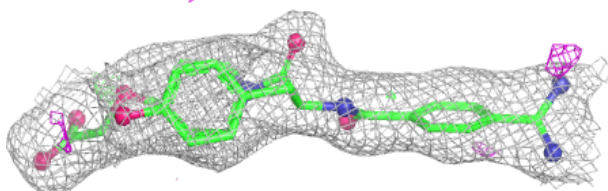
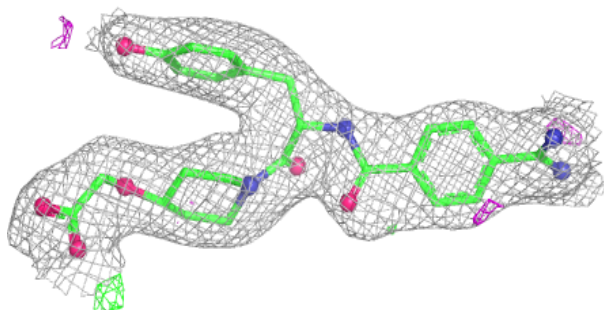
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NB9 B 2005:

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

**Electron density around NB9 D 2005:**

$2mF_o-DF_c$ (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.