



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2024 – 12:51 AM EDT

PDB ID : 7UJK
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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.3

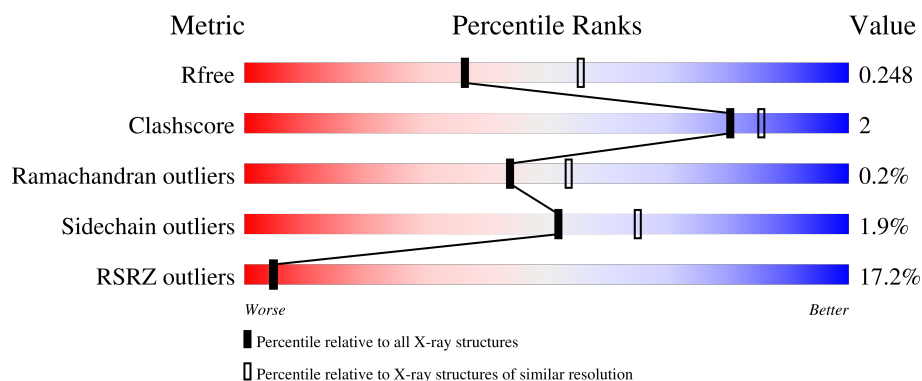
1 Overall quality at a glance

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}	164625	2124 (2.46-2.42)
Clashscore	180529	2259 (2.46-2.42)
Ramachandran outliers	177936	2244 (2.46-2.42)
Sidechain outliers	177891	2244 (2.46-2.42)
RSRZ outliers	164620	2124 (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	<div> <div>3%</div> <div>90%</div> <div>9%</div> </div>
1	C	457	<div> <div>4%</div> <div>94%</div> <div>5%</div> </div>
2	B	472	<div> <div>16%</div> <div>92%</div> <div>7%</div> </div>
2	D	472	<div> <div>15%</div> <div>92%</div> <div>8%</div> </div>
3	E	221	<div> <div>50%</div> <div>89%</div> <div>8%</div> </div>

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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			

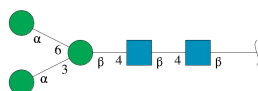
- Molecule 3 is a protein called 10E5 Fab heavy chain.

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 (three-letter code: 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 (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 10 is CALCIUM ION (three-letter code: 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		

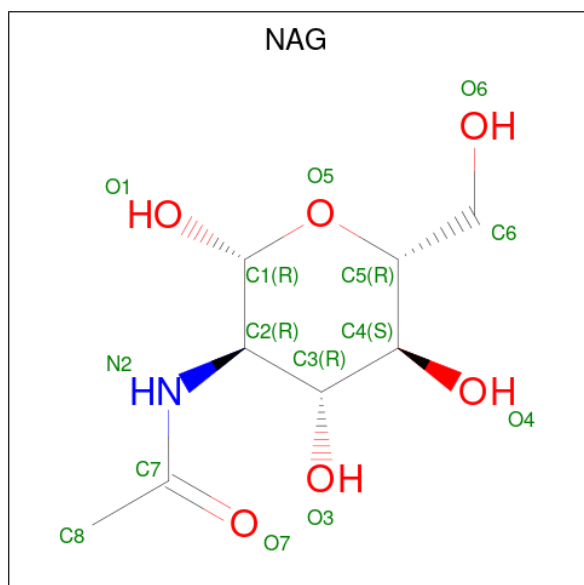
- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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 (three-letter code: MG) (formula: Mg).

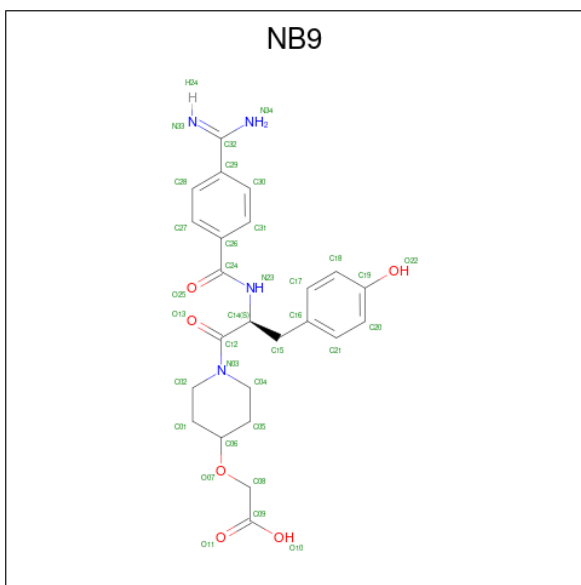
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	1	Total	Mg	0	0
			1	1		
12	D	1	Total	Mg	0	0
			1	1		

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: 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 (three-letter code: 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		

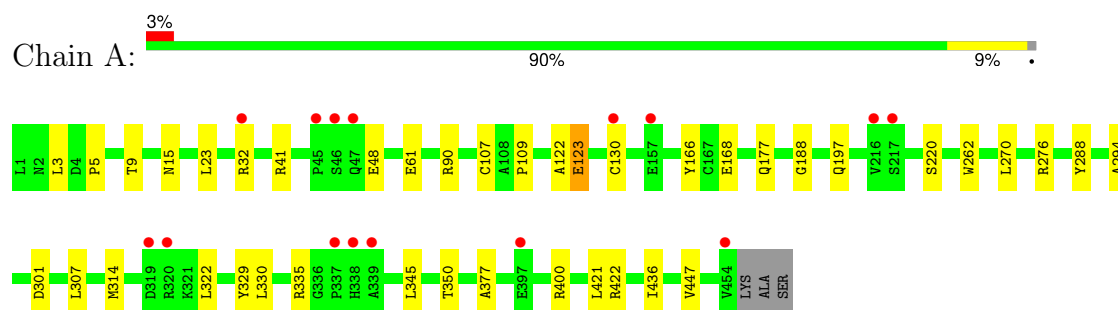
- Molecule 15 is water.

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		

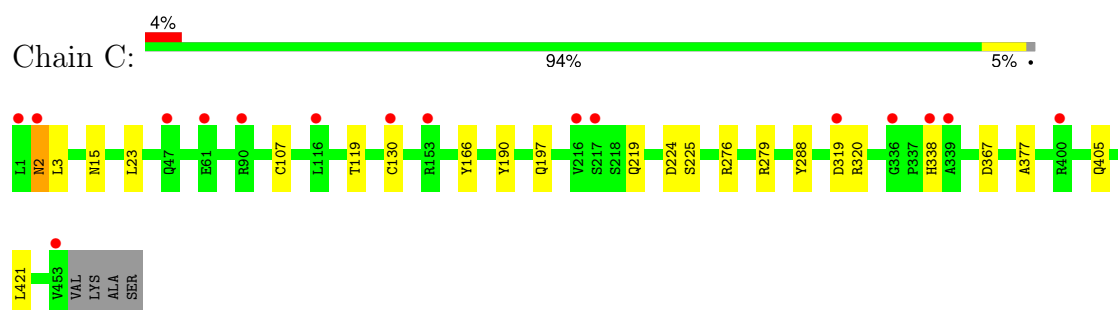
3 Residue-property plots [i](#)

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.

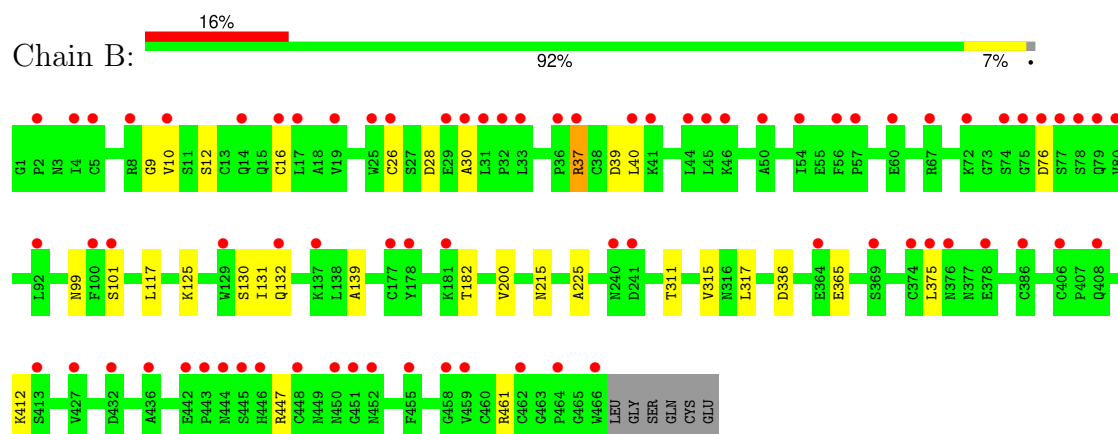
- Molecule 1: Integrin alpha-IIb heavy chain



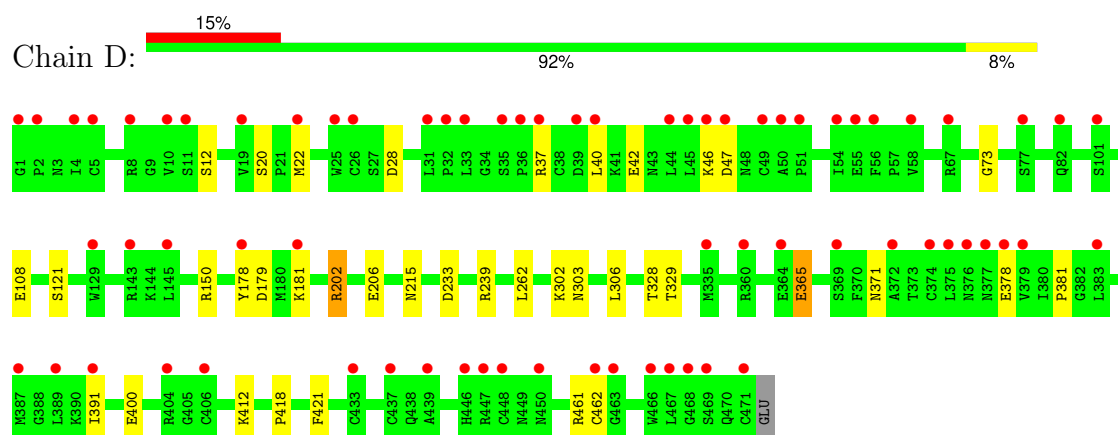
- Molecule 1: Integrin alpha-IIb heavy chain



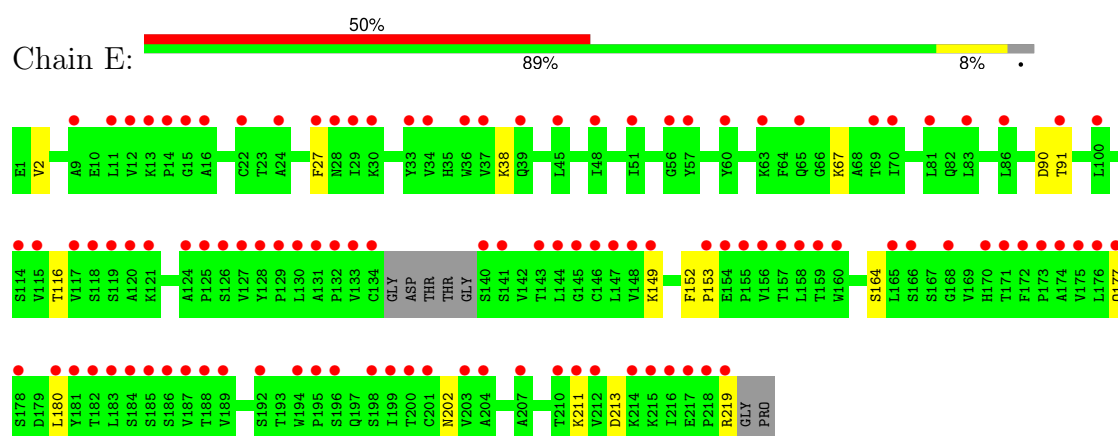
- Molecule 2: Isoform Beta-3C of Integrin beta-3



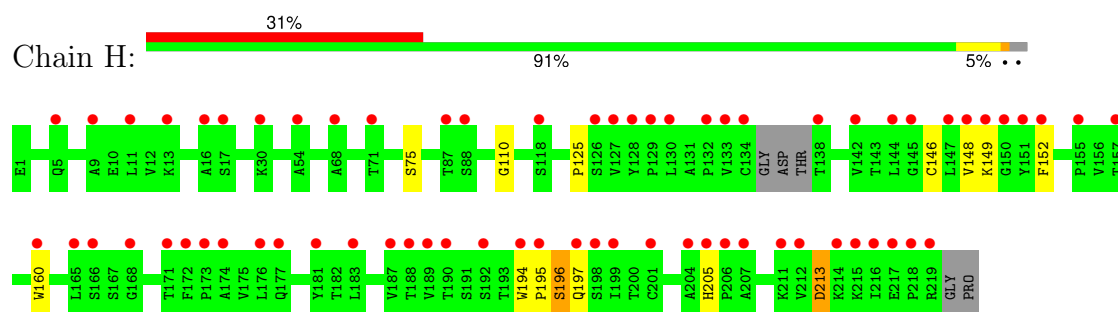
- Molecule 2: Isoform Beta-3C of Integrin beta-3



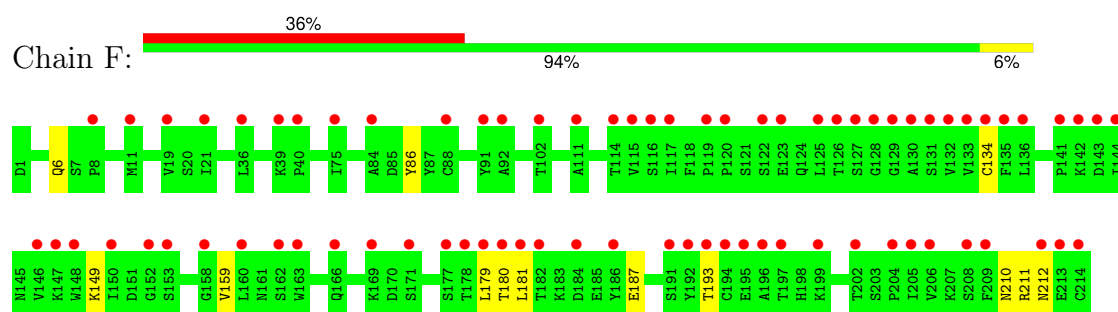
- Molecule 3: 10E5 Fab heavy chain



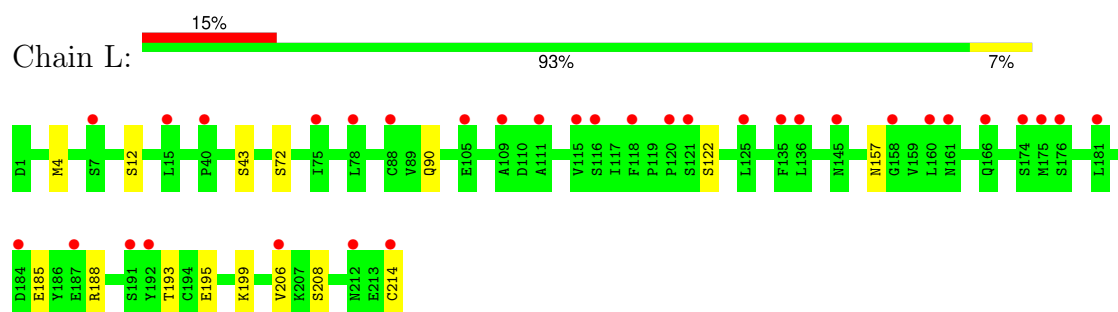
- Molecule 3: 10E5 Fab heavy chain



- Molecule 4: 10E5 Fab light chain



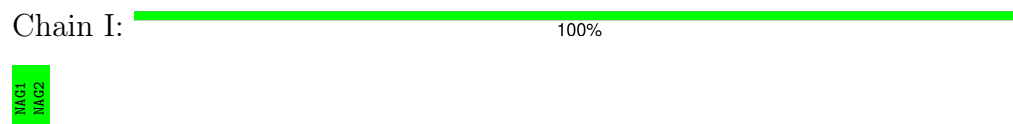
- Molecule 4: 10E5 Fab light chain



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



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



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



- Molecule 7: α -D-mannopyranose-(1-3)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



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	147522 reflections (1.37%)	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 , 42.6	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	0.92	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: CA, MAN, NAG, MG, CL, BMA, SO4, GOL, NB9

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	0.25	0/3647	0.47	0/4969
1	C	0.25	0/3605	0.45	0/4912
2	B	0.25	0/3725	0.44	0/5049
2	D	0.24	0/3714	0.44	0/5036
3	E	0.24	0/1673	0.45	0/2290
3	H	0.24	0/1684	0.46	0/2305
4	F	0.26	0/1673	0.45	0/2269
4	L	0.25	0/1673	0.46	0/2269
All	All	0.25	0/21394	0.45	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	15	0
2	D	3642	0	3558	19	0
3	E	1631	0	1590	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	0	1600	10	0
4	F	1637	0	1553	7	0
4	L	1637	0	1553	7	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	103	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 2.

All (103) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:181:LYS:NZ	15:D:2101:HOH:O	2.20	0.75
1:A:48:GLU:OE2	1:A:90[B]:ARG:NH1	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:333:HOH:O	4:L:214:CYS:SG	2.45	0.73
2:B:365:GLU:OE2	2:B:412:LYS:NZ	2.22	0.72
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
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
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
3:E:67:LYS:NZ	3:E:90:ASP:OD2	2.26	0.49
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
2:B:12:SER:HB3	2:B:461:ARG:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:E:213:ASP:OD1	3:E:213:ASP:N	2.53	0.42
4:L:4:MET:HE2	4:L:90:GLN:HB3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:367:ASP:OD1	1:C:367:ASP:N	2.49	0.41
2:B:125:LYS:NZ	15:B:2119:HOH:O	2.52	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:D:233:ASP:OD2	2:D:302:LYS:NZ	2.46	0.41
2:B:117:LEU:HD11	2:B:225:ALA:HB1	2.02	0.40
3:H:110:GLY:O	4:L:43:SER:OG	2.35	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
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

5.3.1 Protein backbone

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%)	44	53
1	C	455/457 (100%)	437 (96%)	18 (4%)	0	100	100
2	B	472/472 (100%)	451 (96%)	18 (4%)	3 (1%)	22	26
2	D	471/472 (100%)	445 (94%)	26 (6%)	0	100	100
3	E	210/221 (95%)	191 (91%)	18 (9%)	1 (0%)	25	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	212/221 (96%)	195 (92%)	17 (8%)	0	100	100
4	F	212/214 (99%)	193 (91%)	18 (8%)	1 (0%)	25	30
4	L	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
All	All	2704/2728 (99%)	2560 (95%)	138 (5%)	6 (0%)	44	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%)	361 (98%)	9 (2%)	44	57
1	C	365/364 (100%)	354 (97%)	11 (3%)	36	48
2	B	420/417 (101%)	415 (99%)	5 (1%)	67	79
2	D	418/417 (100%)	409 (98%)	9 (2%)	47	60
3	E	186/190 (98%)	185 (100%)	1 (0%)	86	92
3	H	187/190 (98%)	184 (98%)	3 (2%)	58	71
4	F	188/188 (100%)	186 (99%)	2 (1%)	70	80
4	L	188/188 (100%)	183 (97%)	5 (3%)	40	52
All	All	2322/2318 (100%)	2277 (98%)	45 (2%)	52	65

All (45) 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	220	SER
1	A	270	LEU
1	A	288	TYR
1	A	335	ARG
1	A	350[A]	THR
1	A	350[B]	THR
2	B	37	ARG
2	B	101	SER
2	B	182	THR
2	B	215	ASN
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	190	TYR
1	C	197	GLN
1	C	219	GLN
1	C	288	TYR
1	C	319	ASP
1	C	338	HIS
2	D	20	SER
2	D	47	ASP
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	462	CYS
3	E	211	LYS
4	F	134	CYS
4	F	181	LEU
3	H	75	SER
3	H	196	SER
3	H	213	ASP
4	L	12	SER
4	L	72	SER
4	L	122	SER

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Mol	Chain	Res	Type
4	L	157	ASN
4	L	199	LYS

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

Mol	Chain	Res	Type
1	C	372	ASN
2	D	280	HIS
2	D	438	GLN
2	D	452	ASN
4	F	138	ASN
4	L	27	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 ⓘ

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	2,5	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	2,5	-	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	-2.10	105.79	110.15
5	G	5	MAN	O2-C2-C3	-2.08	105.83	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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:

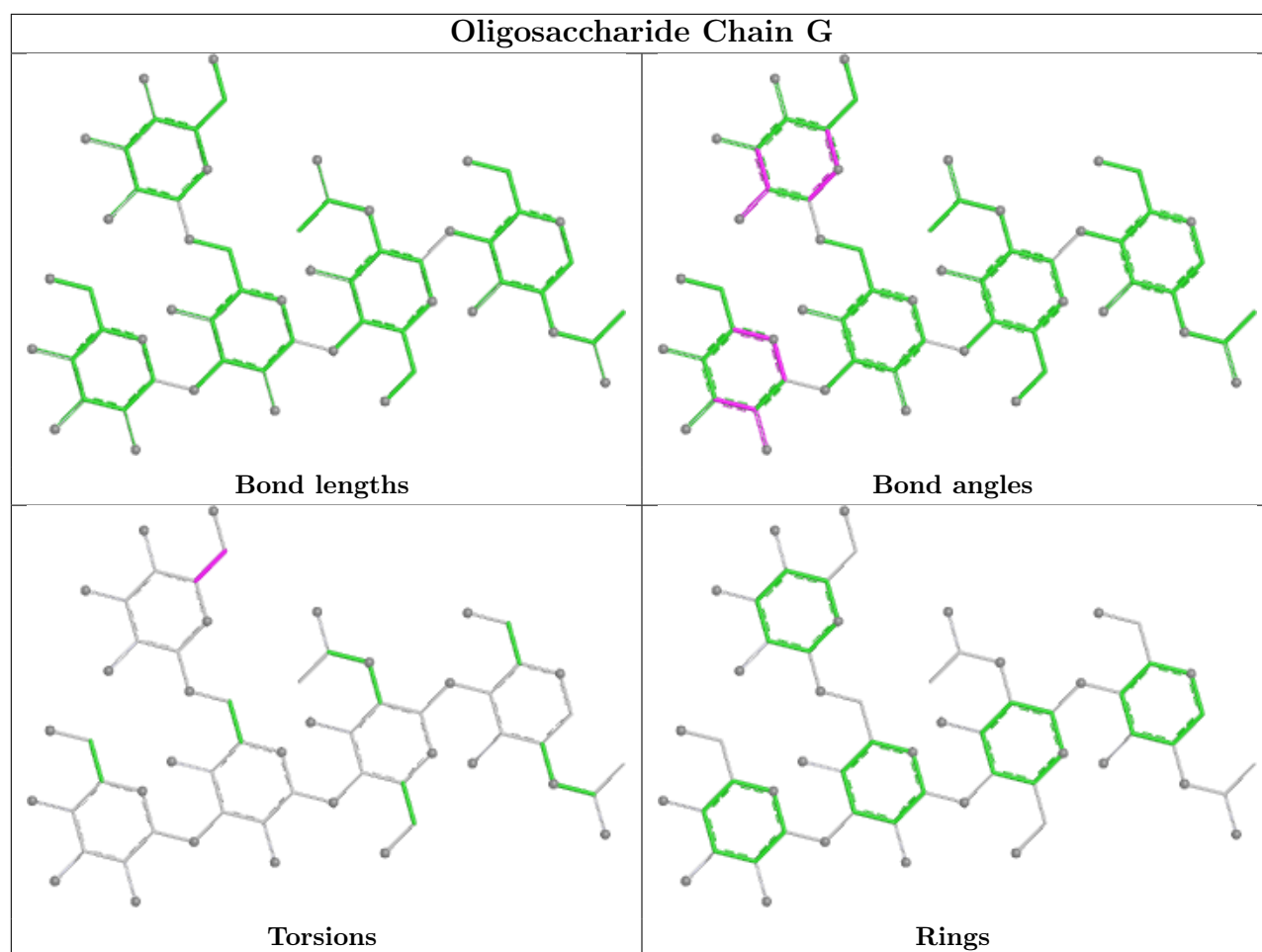
Mol	Chain	Res	Type	Atoms
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
7	J	4	MAN	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
5	G	5	MAN	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
7	J	3	BMA	C4-C5-C6-O6
7	J	3	BMA	O5-C5-C6-O6
7	J	4	MAN	C4-C5-C6-O6

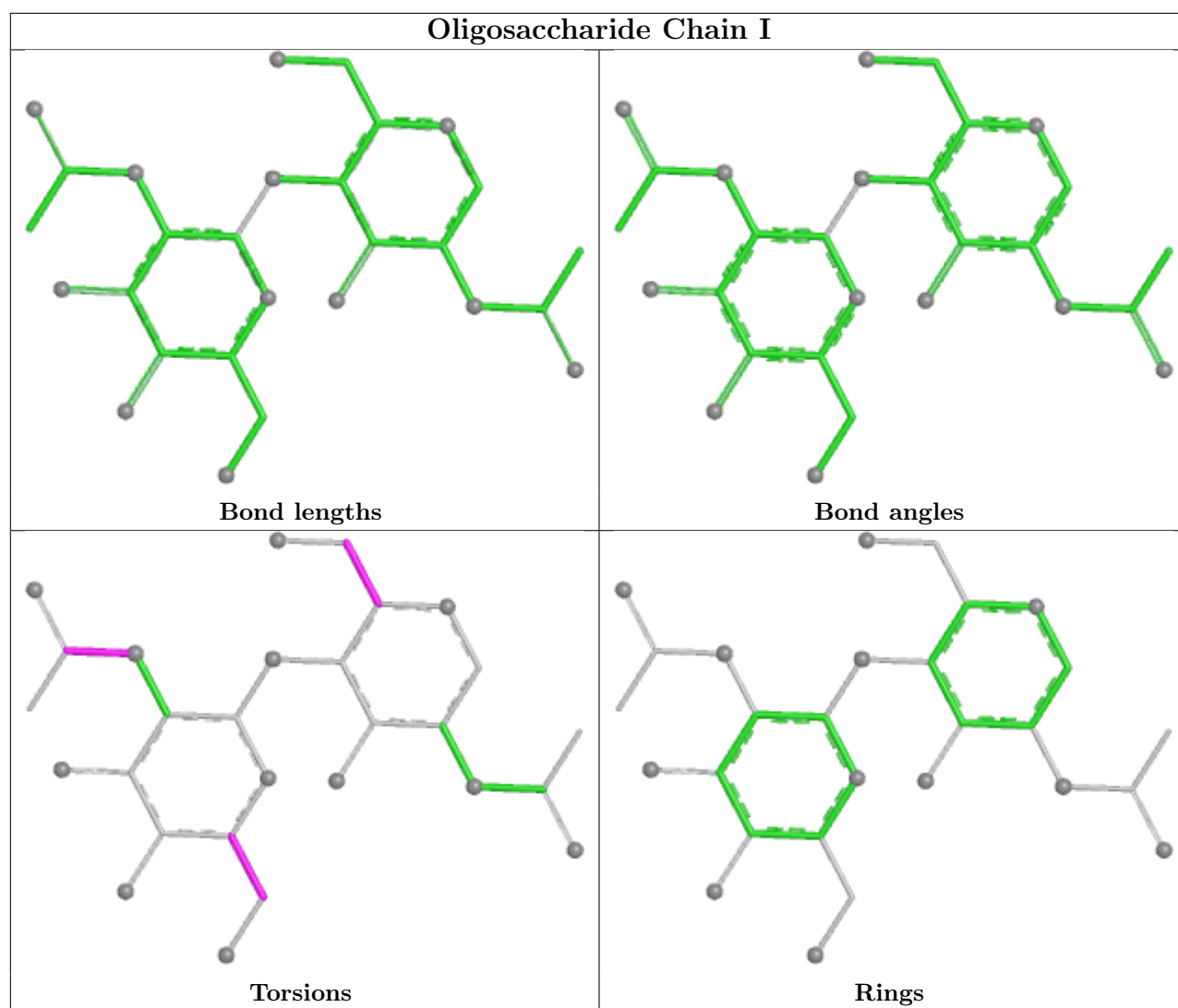
There are no ring outliers.

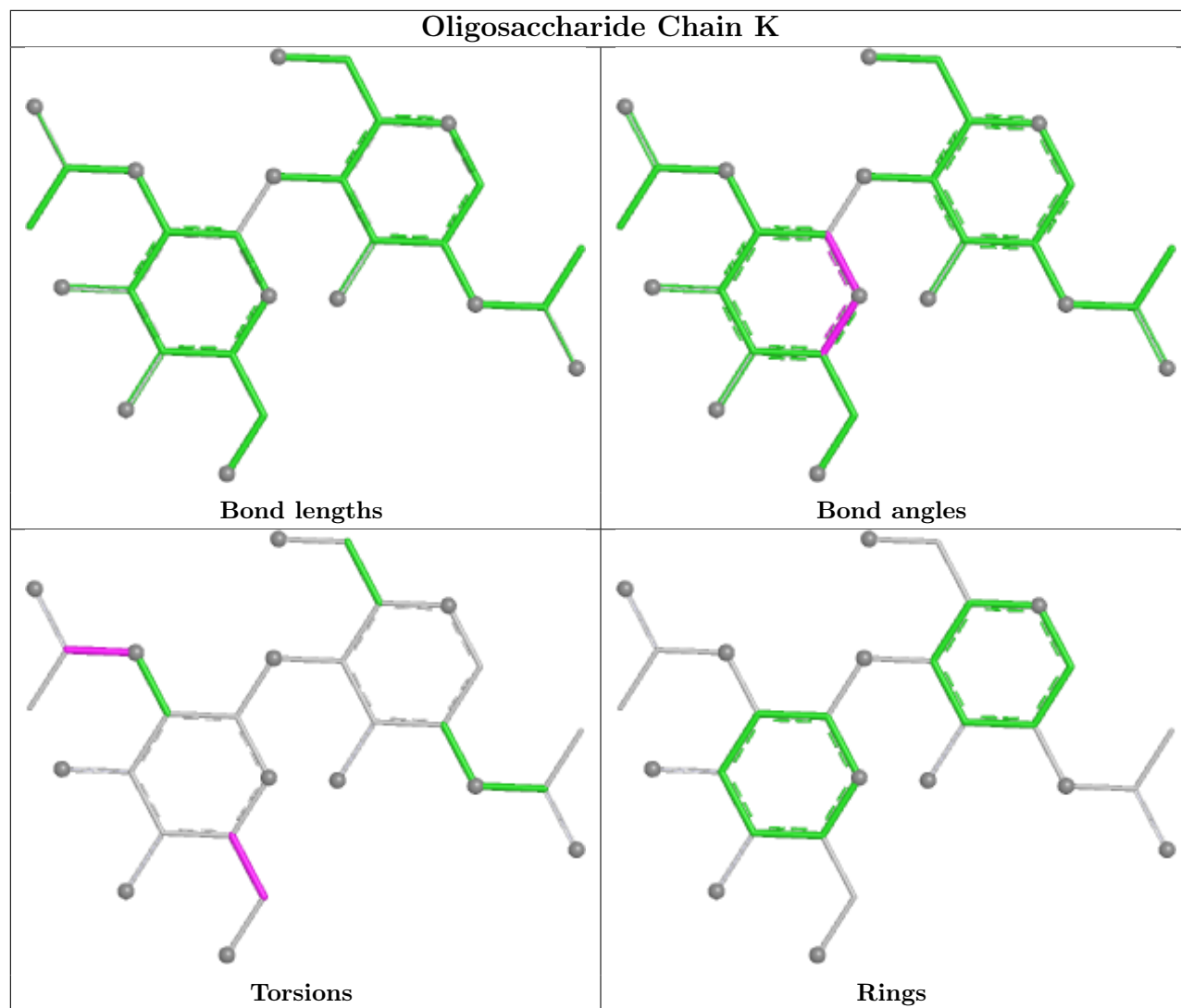
2 monomers are involved in 2 short contacts:

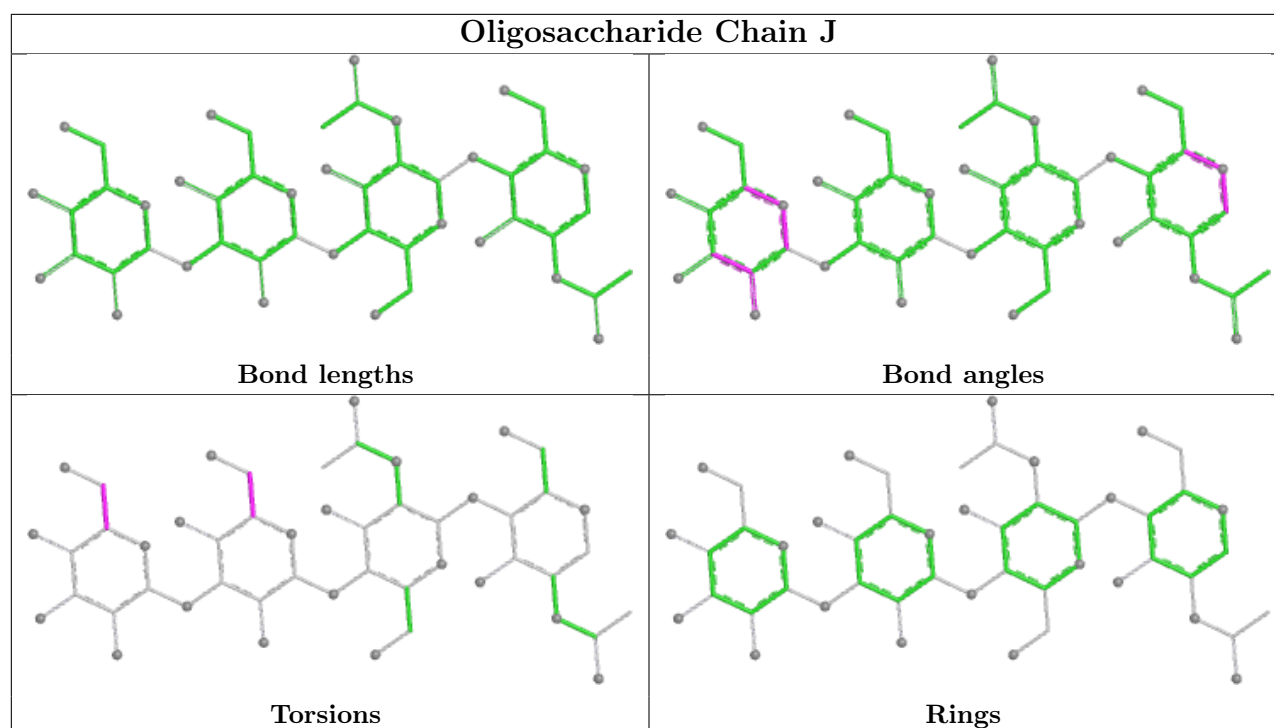
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	2	NAG	1	0
6	K	1	NAG	2	0

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	$\# Z > 2$
14	NB9	B	2005	12	36,36,36	2.55	9 (25%)	44,49,49	1.52	3 (6%)
8	SO4	A	501	-	4,4,4	0.24	0	6,6,6	0.07	0
13	NAG	D	2004	2	14,14,15	0.55	0	17,19,21	0.39	0
8	SO4	C	502	-	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
8	SO4	C	503	-	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
9	GOL	A	503	-	5,5,5	0.36	0	5,5,5	0.42	0
14	NB9	D	2005	12	36,36,36	2.56	9 (25%)	44,49,49	1.28	3 (6%)
8	SO4	C	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
8	SO4	L	301	-	4,4,4	0.24	0	6,6,6	0.07	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
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
13	NAG	D	2004	2	-	2/6/23/26	0/1/1/1
13	NAG	B	2004	2	-	1/6/23/26	0/1/1/1
9	GOL	A	503	-	-	2/4/4/4	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	D	2005	NB9	C12-N03	10.38	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	2.79	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	2.55	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	114.49	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

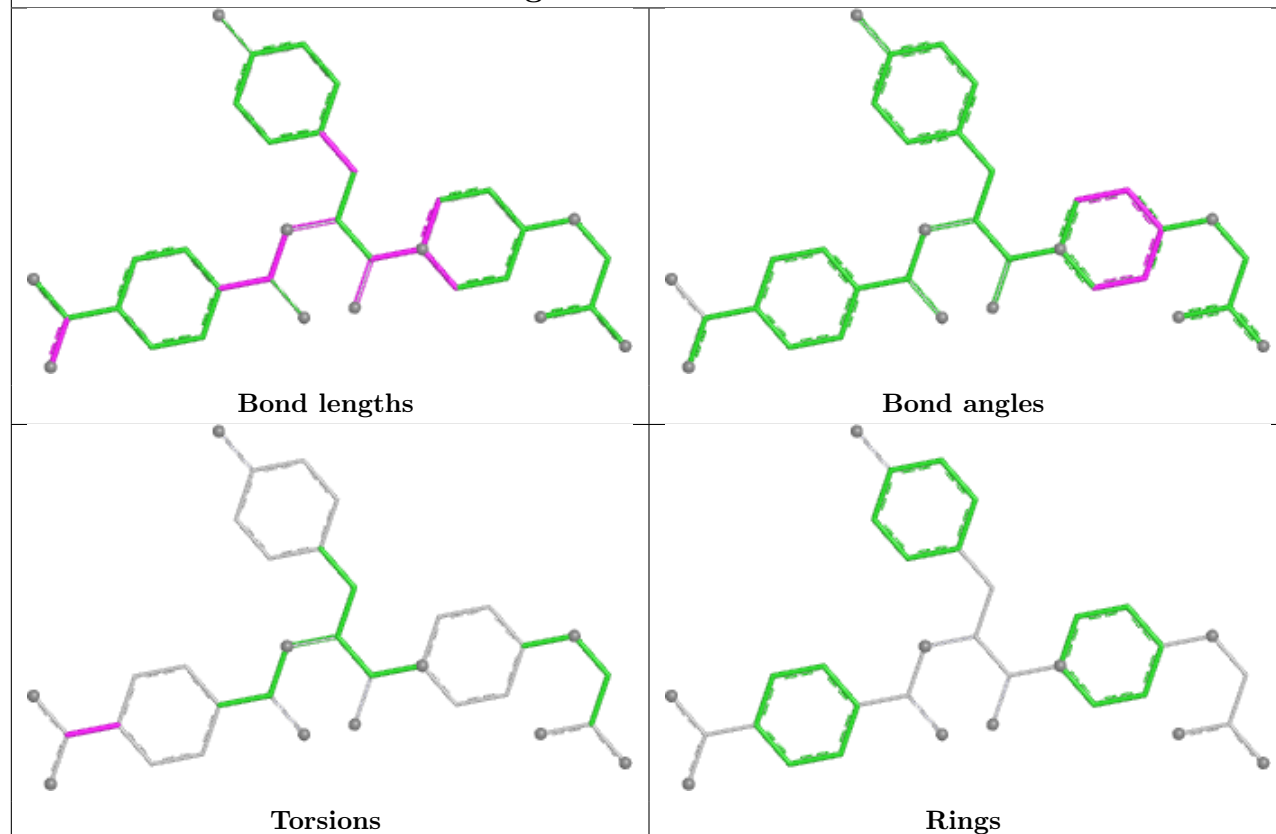
There are no ring outliers.

3 monomers are involved in 4 short contacts:

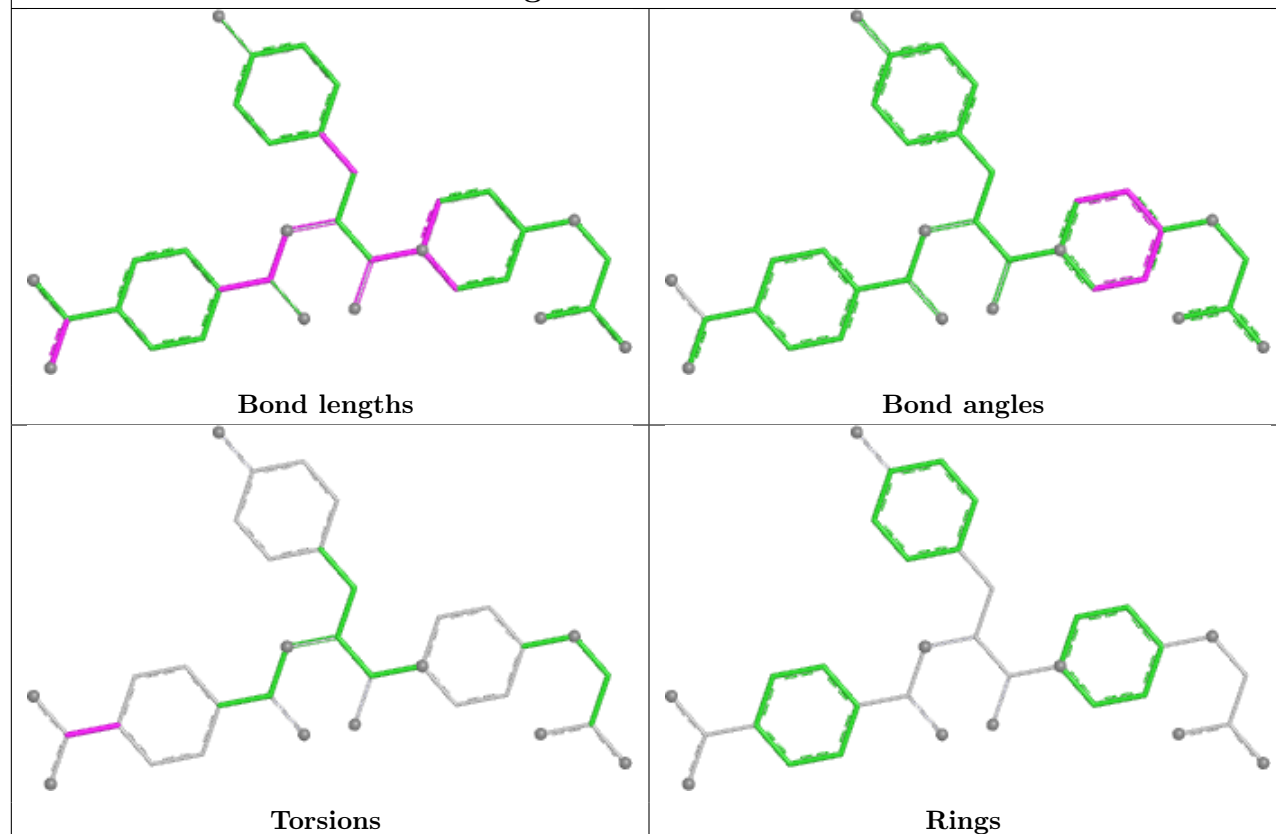
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	2004	NAG	1	0
14	D	2005	NB9	2	0
8	A	502	SO4	1	0

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 [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, 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%)	0.07	15 (3%)	49	50	22, 39, 55, 71	8 (1%)
1	C	453/457 (99%)	0.39	16 (3%)	47	47	22, 50, 68, 86	4 (0%)
2	B	466/472 (98%)	0.85	76 (16%)	5	5	19, 59, 114, 132	9 (1%)
2	D	471/472 (99%)	1.06	70 (14%)	7	6	24, 67, 106, 119	3 (0%)
3	E	214/221 (96%)	2.25	110 (51%)	0	1	67, 107, 157, 163	0
3	H	216/221 (97%)	1.59	68 (31%)	1	1	50, 86, 115, 120	0
4	F	214/214 (100%)	1.95	76 (35%)	1	1	69, 112, 150, 158	0
4	L	214/214 (100%)	1.29	33 (15%)	6	6	53, 77, 91, 109	0
All	All	2702/2728 (99%)	0.97	464 (17%)	5	5	19, 63, 135, 163	24 (0%)

All (464) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	454	VAL	9.2
2	D	129[A]	TRP	8.1
3	E	212	VAL	7.9
1	C	1	LEU	6.9
3	E	147	LEU	6.8
3	E	165	LEU	6.0
2	B	77	SER	5.9
3	E	203	VAL	5.8
2	B	33	LEU	5.8
3	E	216	ILE	5.7
4	F	115	VAL	5.4
4	F	135	PHE	5.4
2	D	471	CYS	5.3
4	F	130	ALA	5.3
3	E	133	VAL	5.3
3	E	174	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
3	E	144	LEU	5.2
3	E	214	LYS	5.0
4	F	125	LEU	4.9
3	E	127	VAL	4.8
4	F	182	THR	4.8
1	A	217	SER	4.7
2	D	375	LEU	4.6
4	F	181	LEU	4.6
3	E	183	LEU	4.5
4	F	179	LEU	4.4
2	D	469	SER	4.4
3	E	199	ILE	4.4
4	F	134	CYS	4.4
3	E	201	CYS	4.3
2	B	4	ILE	4.3
3	E	128	TYR	4.3
4	L	214	CYS	4.2
4	F	204	PRO	4.2
2	B	132[A]	GLN	4.1
3	E	9	ALA	4.1
2	D	44	LEU	4.1
3	H	212	VAL	4.1
4	F	195	GLU	4.0
3	H	216	ILE	4.0
3	E	134	CYS	4.0
3	E	184	SER	4.0
3	E	188	THR	4.0
3	E	132	PRO	3.9
4	F	152	GLY	3.9
3	E	160	TRP	3.9
3	E	171	THR	3.9
4	F	114	THR	3.9
4	F	180	THR	3.9
3	E	204	ALA	3.9
1	C	2	ASN	3.9
4	F	116	SER	3.9
3	E	181	TYR	3.9
4	F	209	PHE	3.8
4	F	132	VAL	3.8
4	F	117	ILE	3.8
2	B	375	LEU	3.8
2	B	74	SER	3.8

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Mol	Chain	Res	Type	RSRZ
3	E	149	LYS	3.8
3	H	142	VAL	3.7
4	F	205	ILE	3.7
3	E	189	VAL	3.7
4	F	206	VAL	3.7
2	D	45	LEU	3.7
2	B	129	TRP	3.7
2	D	468	GLY	3.7
1	A	130	CYS	3.7
2	D	406	CYS	3.6
2	B	458	GLY	3.6
3	E	168	GLY	3.6
2	D	378	GLU	3.6
3	E	148	VAL	3.6
3	E	175	VAL	3.6
4	F	169	LYS	3.6
3	H	134	CYS	3.6
2	B	76	ASP	3.6
3	E	14	PRO	3.5
2	B	378	GLU	3.5
4	F	131	SER	3.5
4	L	191	SER	3.5
4	F	126	THR	3.5
4	F	193	THR	3.5
2	B	466	TRP	3.5
1	C	130	CYS	3.5
2	D	374	CYS	3.5
4	F	136	LEU	3.5
2	D	387	MET	3.5
3	H	201	CYS	3.5
1	A	339	ALA	3.5
2	D	446	HIS	3.5
3	H	198	SER	3.5
3	E	215	LYS	3.5
3	E	210	THR	3.5
4	F	178	THR	3.5
4	F	196	ALA	3.5
4	F	160	LEU	3.4
2	B	178	TYR	3.4
3	E	194	TRP	3.4
2	B	451	GLY	3.4
2	D	4	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
3	E	120	ALA	3.4
2	D	466	TRP	3.4
3	E	187	VAL	3.4
3	H	189	VAL	3.4
3	E	176	LEU	3.3
3	H	165	LEU	3.3
4	F	163	TRP	3.3
3	H	219	ARG	3.3
3	E	121	LYS	3.3
4	F	119	PRO	3.3
2	D	433	CYS	3.3
3	E	145	GLY	3.3
3	H	144	LEU	3.3
2	D	49	CYS	3.3
2	D	58	VAL	3.3
4	F	133	VAL	3.3
4	F	146	VAL	3.3
2	B	44	LEU	3.3
4	F	194	CYS	3.3
2	B	36	PRO	3.2
2	B	10	VAL	3.2
4	L	181	LEU	3.2
4	L	105	GLU	3.2
2	B	432	ASP	3.2
4	F	147	LYS	3.2
3	E	56	GLY	3.2
2	B	452	ASN	3.1
4	F	202	THR	3.1
2	B	67	ARG	3.1
2	D	26	CYS	3.1
2	D	2	PRO	3.1
3	E	195	PRO	3.1
4	F	111	ALA	3.1
4	F	186	TYR	3.1
2	B	137[A]	LYS	3.1
2	D	77	SER	3.1
4	L	135	PHE	3.1
4	L	184	ASP	3.1
2	B	41	LYS	3.1
2	D	463	GLY	3.1
3	E	11	LEU	3.1
3	E	16	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
4	F	142	LYS	3.1
2	B	446	HIS	3.1
2	D	33	LEU	3.0
2	B	2	PRO	3.0
3	H	206	PRO	3.0
3	E	182	THR	3.0
4	F	197	THR	3.0
2	D	467	LEU	3.0
3	H	214	LYS	3.0
1	C	339	ALA	3.0
4	L	212	ASN	3.0
3	H	188	THR	3.0
3	H	118	SER	3.0
3	H	168	GLY	3.0
3	H	127	VAL	3.0
2	B	45	LEU	3.0
3	E	192	SER	3.0
4	L	174	SER	3.0
3	E	153	PRO	3.0
4	F	213	GLU	3.0
3	E	131	ALA	3.0
3	H	207	ALA	3.0
2	B	78	SER	2.9
2	D	1	GLY	2.9
2	D	181	LYS	2.9
1	A	319	ASP	2.9
3	E	12	VAL	2.9
3	E	117	VAL	2.9
4	F	214	CYS	2.9
2	D	178	TYR	2.9
3	E	114	SER	2.9
3	H	128	TYR	2.9
4	F	144	ILE	2.9
3	E	129	PRO	2.9
2	B	181	LYS	2.9
2	D	54	ILE	2.9
1	A	45	PRO	2.9
2	B	56	PHE	2.9
2	B	442	GLU	2.9
3	E	217	GLU	2.9
4	F	148	TRP	2.9
3	E	45	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
3	E	219	ARG	2.8
3	E	146	CYS	2.8
4	F	177	SER	2.8
3	E	158	LEU	2.8
4	F	199	LYS	2.8
3	H	194	TRP	2.8
1	A	47	GLN	2.8
3	E	124	ALA	2.8
3	H	204	ALA	2.8
2	D	55	GLU	2.8
3	E	126	SER	2.8
2	B	5	CYS	2.8
2	D	10	VAL	2.8
4	L	115	VAL	2.8
2	B	450	ASN	2.7
2	D	143	ARG	2.7
3	E	29	ILE	2.7
1	A	337	PRO	2.7
3	E	119	SER	2.7
1	C	453	VAL	2.7
3	E	57	TYR	2.7
2	B	26	CYS	2.7
3	H	183	LEU	2.7
2	D	51	PRO	2.7
3	H	218	PRO	2.7
2	B	79	GLN	2.7
3	H	181	TYR	2.7
2	D	372	ALA	2.7
3	E	28	ASN	2.7
2	D	36	PRO	2.7
3	E	125	PRO	2.7
3	H	129	PRO	2.7
4	F	158	GLY	2.7
3	E	140	SER	2.7
4	F	127	SER	2.7
4	F	162	SER	2.7
4	L	121	SER	2.7
3	E	86	LEU	2.7
3	H	151	TYR	2.7
2	B	57	PRO	2.7
2	B	25	TRP	2.7
3	E	48	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
3	H	132	PRO	2.6
3	H	199	ILE	2.6
4	L	120	PRO	2.6
2	D	25	TRP	2.6
2	D	8	ARG	2.6
3	H	17	SER	2.6
3	H	9	ALA	2.6
3	E	13	LYS	2.6
4	F	91	TYR	2.6
3	H	155	PRO	2.6
4	F	150	ILE	2.6
2	B	364	GLU	2.6
3	H	172	PHE	2.6
2	B	17	LEU	2.6
3	H	166	SER	2.6
3	H	187	VAL	2.6
3	E	159	THR	2.6
3	E	200	THR	2.6
2	B	374	CYS	2.6
2	D	462	CYS	2.6
4	F	212	ASN	2.6
1	C	47	GLN	2.6
2	D	145	LEU	2.6
3	H	215	LYS	2.6
1	A	46	SER	2.6
3	E	156	VAL	2.6
3	E	196	SER	2.6
3	H	126	SER	2.6
4	L	7	SER	2.6
4	L	111	ALA	2.6
2	B	241	ASP	2.6
2	D	391	ILE	2.6
3	H	157	THR	2.6
2	B	75	GLY	2.6
2	D	437	CYS	2.6
2	D	67	ARG	2.6
2	D	383	LEU	2.5
4	L	125	LEU	2.5
3	E	173	PRO	2.5
4	F	21	ILE	2.5
4	F	143	ASP	2.5
3	H	5	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	450	ASN	2.5
2	B	455	PHE	2.5
2	D	37	ARG	2.5
3	E	37	VAL	2.5
4	L	109	ALA	2.5
2	D	22	MET	2.5
3	E	100	LEU	2.5
2	D	379	VAL	2.5
3	E	36	TRP	2.5
3	E	178	SER	2.5
2	D	19	VAL	2.5
3	E	218	PRO	2.5
4	F	8	PRO	2.5
4	F	191	SER	2.5
3	E	177	GLN	2.5
3	H	138	THR	2.5
4	F	192	TYR	2.5
2	B	386	CYS	2.4
3	H	173	PRO	2.4
3	E	118	SER	2.4
4	F	123	GLU	2.4
3	H	177	GLN	2.4
3	H	197	GLN	2.4
2	B	376	ASN	2.4
4	L	145	ASN	2.4
2	B	177	CYS	2.4
4	F	88	CYS	2.4
1	C	216	VAL	2.4
2	B	464	PRO	2.4
3	H	174	ALA	2.4
2	D	360	ARG	2.4
2	D	39	ASP	2.4
4	L	78	LEU	2.4
4	L	136	LEU	2.4
1	A	338	HIS	2.4
3	E	30	LYS	2.4
1	A	32[A]	ARG	2.4
3	E	207	ALA	2.4
2	B	445	SER	2.4
4	F	128	GLY	2.4
2	B	72	LYS	2.4
2	B	448	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	447	ARG	2.4
3	E	154	GLU	2.4
2	B	436	ALA	2.4
2	B	369	SER	2.4
2	D	11	SER	2.4
3	E	157	THR	2.4
2	B	40	LEU	2.3
2	B	92	LEU	2.3
2	D	389	LEU	2.3
3	E	27	PHE	2.3
2	B	19	VAL	2.3
2	B	14	GLN	2.3
3	H	54	ALA	2.3
2	B	413	SER	2.3
3	E	186	SER	2.3
3	H	160	TRP	2.3
4	L	15	LEU	2.3
1	A	320	ARG	2.3
3	E	115	VAL	2.3
3	H	133	VAL	2.3
1	C	336	GLY	2.3
3	H	88	SER	2.3
3	E	180	LEU	2.3
3	H	11	LEU	2.3
3	H	176	LEU	2.3
4	F	102	THR	2.3
2	B	444	ASN	2.3
3	H	30	LYS	2.3
3	E	155	PRO	2.3
4	F	19	VAL	2.3
4	F	92	ALA	2.3
2	D	448	CYS	2.3
1	C	116	LEU	2.3
2	D	31	LEU	2.3
2	D	35	SER	2.3
3	E	166	SER	2.3
3	H	87	THR	2.3
2	D	56	PHE	2.3
3	H	211	LYS	2.3
4	F	184	ASP	2.3
2	B	8	ARG	2.3
3	H	195	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
3	E	34	VAL	2.3
3	E	70	ILE	2.3
2	D	50	ALA	2.3
3	H	16	ALA	2.3
3	H	68	ALA	2.3
2	B	406	CYS	2.3
3	H	145	GLY	2.2
3	H	147	LEU	2.2
4	F	39	LYS	2.2
1	C	90	ARG	2.2
2	D	32	PRO	2.2
4	F	40	PRO	2.2
4	L	75	ILE	2.2
2	D	439	ALA	2.2
2	B	462	CYS	2.2
3	H	130	LEU	2.2
4	L	160	LEU	2.2
2	D	46	LYS	2.2
3	E	22	CYS	2.2
4	F	122	SER	2.2
4	F	153	SER	2.2
3	H	152	PHE	2.2
2	B	240	ASN	2.2
2	D	377	ASN	2.2
4	F	120	PRO	2.2
2	B	29	GLU	2.2
4	L	187	GLU	2.2
2	D	82	GLN	2.2
4	L	166	GLN	2.2
3	E	24	ALA	2.2
4	L	192	TYR	2.2
4	L	158	GLY	2.2
2	B	101	SER	2.2
3	E	185	SER	2.2
3	H	71	THR	2.2
4	L	40	PRO	2.2
3	E	65	GLN	2.2
4	F	75	ILE	2.2
3	E	60	TYR	2.2
3	H	205	HIS	2.2
2	D	40	LEU	2.2
3	E	81	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	83	LEU	2.2
4	L	175	MET	2.2
2	D	5	CYS	2.2
3	E	143	THR	2.2
3	H	192	SER	2.2
2	B	60	GLU	2.2
2	B	80	VAL	2.2
1	C	338	HIS	2.2
2	B	50	ALA	2.2
3	E	170	HIS	2.2
2	B	31	LEU	2.1
3	E	15	GLY	2.1
4	F	129	GLY	2.1
1	C	153	ARG	2.1
3	E	91	THR	2.1
3	H	171	THR	2.1
3	H	190	THR	2.1
2	B	16	CYS	2.1
3	E	141	SER	2.1
3	E	198	SER	2.1
4	F	171	SER	2.1
1	C	319	ASP	2.1
2	B	46	LYS	2.1
3	E	211	LYS	2.1
2	B	459	VAL	2.1
3	H	148	VAL	2.1
4	L	206	VAL	2.1
2	B	30	ALA	2.1
4	F	84	ALA	2.1
3	E	33	TYR	2.1
2	B	100	PHE	2.1
4	F	208	SER	2.1
4	L	88	CYS	2.1
1	C	61	GLU	2.1
3	H	217	GLU	2.1
2	D	47	ASP	2.1
3	H	149	LYS	2.1
1	A	216	VAL	2.1
4	F	11	MET	2.1
4	F	36	LEU	2.1
4	L	118	PHE	2.1
1	A	157	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	217	SER	2.1
4	L	161	ASN	2.1
2	B	427	VAL	2.1
3	E	130	LEU	2.1
1	C	400	ARG	2.1
2	D	404	ARG	2.1
3	E	69	THR	2.1
4	F	141	PRO	2.1
4	L	116	SER	2.1
4	L	176	SER	2.1
2	B	54	ILE	2.1
2	D	335	MET	2.1
2	B	32	PRO	2.0
3	E	63	LYS	2.0
3	E	172	PHE	2.0
3	H	13	LYS	2.0
1	A	397	GLU	2.0
2	B	408	GLN	2.0
4	F	166	GLN	2.0
2	D	101	SER	2.0
2	D	369	SER	2.0
3	E	51	ILE	2.0
2	D	376	ASN	2.0
2	B	37	ARG	2.0
3	H	150	GLY	2.0
2	B	443	PRO	2.0
2	D	364	GLU	2.0
3	E	39	GLN	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](#)

SUGAR-RSR INFOmissingINFO

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,

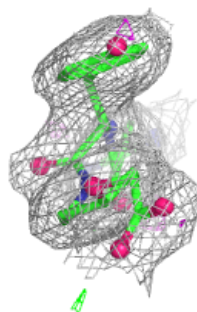
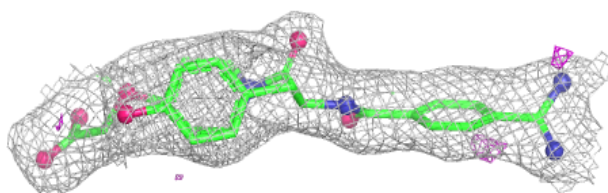
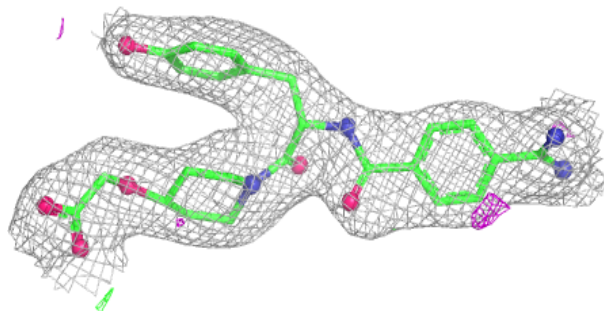
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	NAG	D	2004	14/15	0.61	0.18	85,85,85,85	0
13	NAG	B	2004	14/15	0.62	0.16	86,86,86,86	0
8	SO4	A	508	5/5	0.74	0.19	52,52,52,52	0
8	SO4	C	501	5/5	0.78	0.26	65,65,65,65	0
8	SO4	C	502	5/5	0.82	0.21	70,70,70,70	0
8	SO4	A	501	5/5	0.84	0.31	61,61,61,61	0
9	GOL	A	503	6/6	0.85	0.14	48,48,48,48	0
8	SO4	L	301	5/5	0.88	0.22	71,71,71,71	0
11	CL	C	505	1/1	0.89	0.16	67,67,67,67	0
14	NB9	D	2005	34/34	0.92	0.10	48,48,48,48	0
10	CA	B	2002	1/1	0.93	0.15	52,52,52,52	0
11	CL	C	504	1/1	0.93	0.10	56,56,56,56	0
14	NB9	B	2005	34/34	0.93	0.10	38,38,38,38	0
8	SO4	C	503	5/5	0.93	0.12	61,61,61,61	5
8	SO4	A	502	5/5	0.95	0.10	50,50,50,50	0
11	CL	A	509	1/1	0.95	0.08	53,53,53,53	0
10	CA	D	2002	1/1	0.97	0.06	53,53,53,53	0
10	CA	A	507	1/1	0.97	0.04	36,36,36,36	0
10	CA	A	506	1/1	0.97	0.04	36,36,36,36	0
10	CA	C	506	1/1	0.97	0.05	64,64,64,64	0
12	MG	D	2001	1/1	0.98	0.07	40,40,40,40	0
10	CA	D	2003	1/1	0.98	0.04	42,42,42,42	0
10	CA	C	507	1/1	0.98	0.04	56,56,56,56	0
10	CA	C	508	1/1	0.98	0.04	51,51,51,51	0
10	CA	A	504	1/1	0.98	0.04	48,48,48,48	0
10	CA	A	505	1/1	0.99	0.03	38,38,38,38	0
10	CA	C	509	1/1	0.99	0.03	49,49,49,49	0
10	CA	B	2003	1/1	0.99	0.03	33,33,33,33	0
12	MG	B	2001	1/1	1.00	0.08	28,28,28,28	0

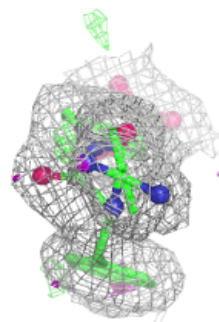
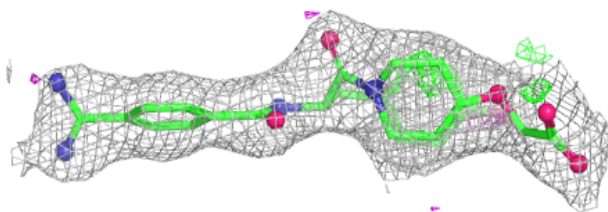
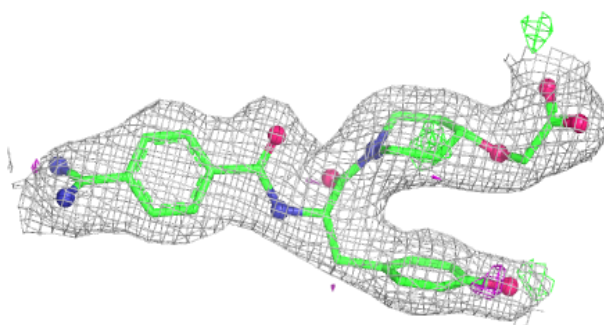
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NB9 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)

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.