



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2024 – 12:34 AM EDT

PDB ID : 7UDH  
Title : Integrin alpha IIB beta3 complex with BMS4-3  
Authors : Lin, F.-Y.; Zhu, J.; Zhu, J.; Springer, T.A.  
Deposited on : 2022-03-19  
Resolution : 2.00 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](mailto: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:

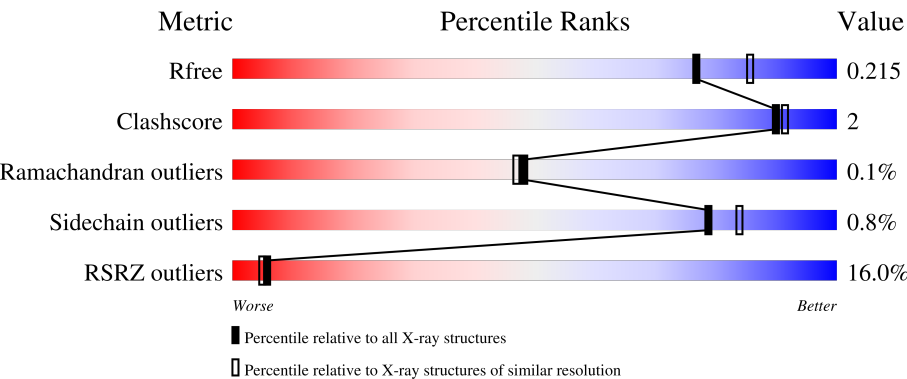
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh &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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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 <sub>free</sub>	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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  $\geq 3$ , 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>2%</div><div>95%</div><div>..</div></div>
1	C	457	<div><div>5%</div><div>96%</div><div>..</div></div>
2	B	472	<div><div>13%</div><div>93%</div><div>6% .</div></div>
2	D	472	<div><div>16%</div><div>94%</div><div>5%</div></div>
3	E	221	<div><div>40%</div><div>94%</div><div>..</div></div>

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	4	
6	I	2	
6	K	2	
7	J	5	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	I	1	-	-	X	-
7	NAG	J	1	-	-	X	-

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 22567 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	4	0
			3499	2226	601	664	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	3	0
			3610	2248	616	712	34			
2	D	471	Total	C	N	O	S	3	0	0
			3623	2255	619	715	34			

- 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)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



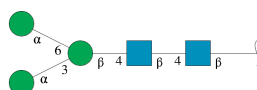
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	4	Total	C	N	O	0	0	0
			50	28	2	20			

- 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)-[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
7	J	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	4	Total	Ca	0	0
			4	4		
9	C	4	Total	Ca	0	0
			4	4		

- Molecule 10 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

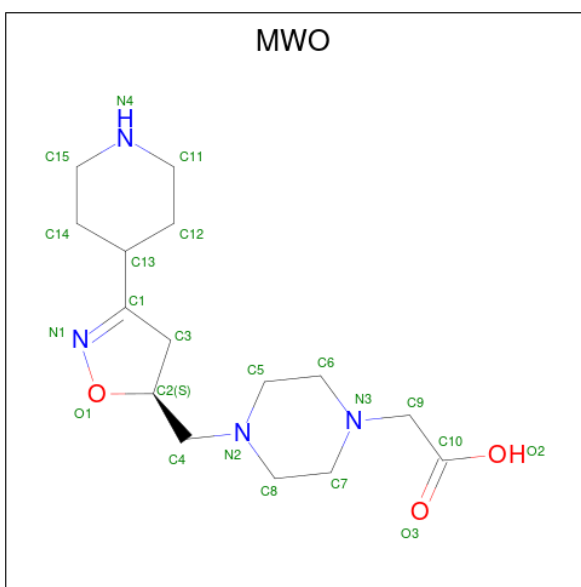
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	3	Total	Mn	0	0
			3	3		
10	D	3	Total	Mn	0	0
			3	3		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



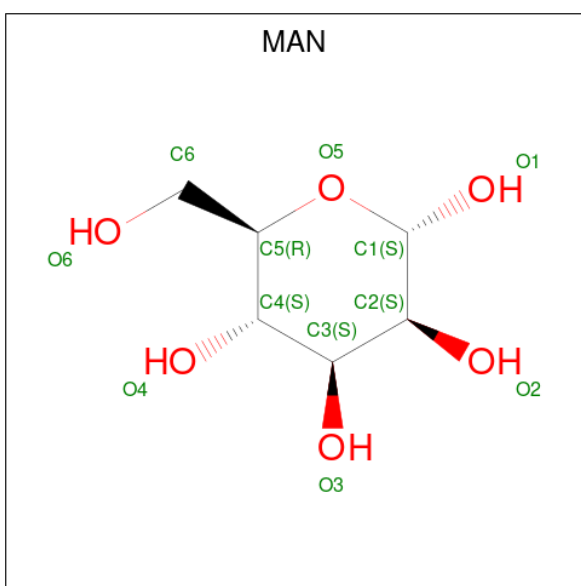
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 12 is (4-{[(5S)-3-(piperidin-4-yl)-4,5-dihydro-1,2-oxazol-5-yl]methyl}piperazin-1-yl)acetic acid (three-letter code: MWO) (formula:  $C_{15}H_{26}N_4O_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	N	O	0	0
			22	15	4	3		
12	D	1	Total	C	N	O	0	0
			22	15	4	3		

- Molecule 13 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 14 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	2	Total	Cl	0	0
			2	2		
14	D	1	Total	Cl	0	0
			1	1		

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	542	Total	O	0	0
			542	542		
15	B	319	Total	O	0	0
			319	319		
15	C	232	Total	O	0	0
			232	232		
15	D	200	Total	O	0	0
			200	200		
15	E	29	Total	O	0	0
			29	29		
15	F	20	Total	O	0	0
			20	20		
15	H	45	Total	O	0	0
			45	45		
15	L	87	Total	O	0	0
			87	87		

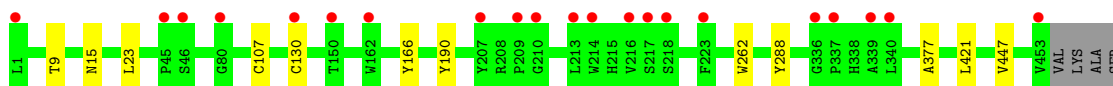
### 3 Residue-property plots

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.

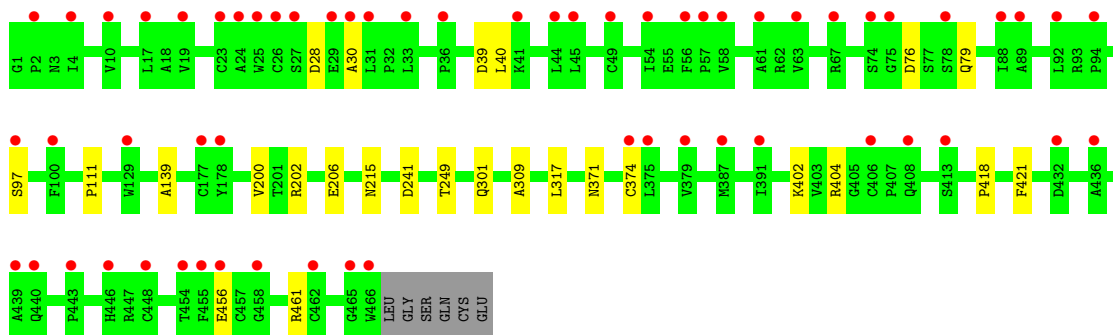
- Molecule 1: Integrin alpha-IIb heavy chain



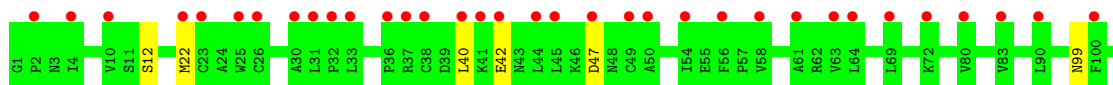
- Molecule 1: Integrin alpha-IIb heavy chain

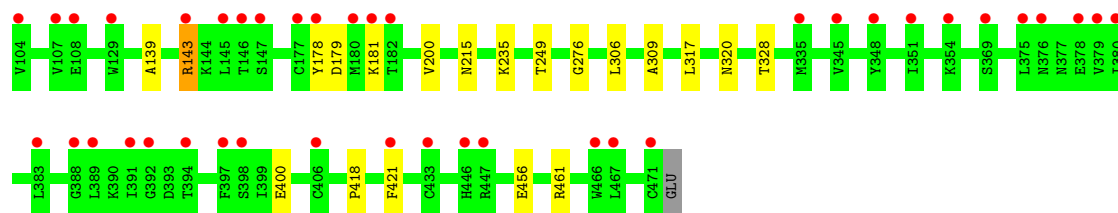


- Molecule 2: Isoform Beta-3C of Integrin beta-3

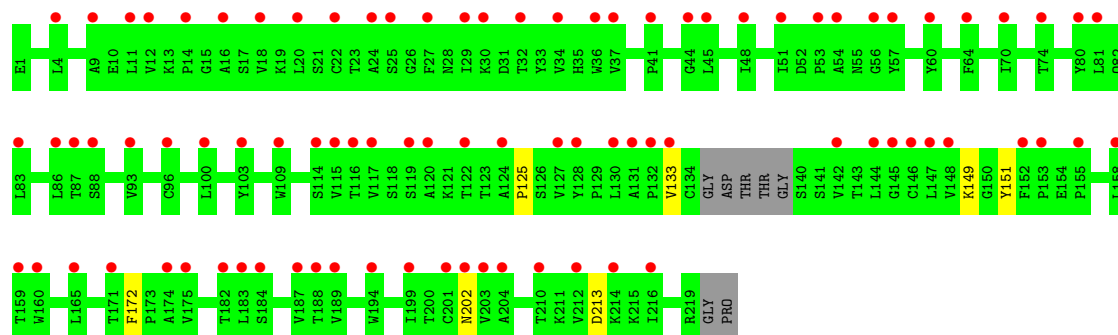
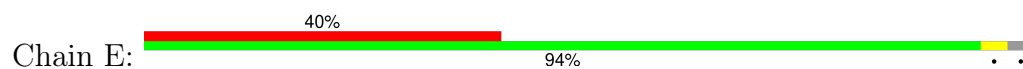


- Molecule 2: Isoform Beta-3C of Integrin beta-3

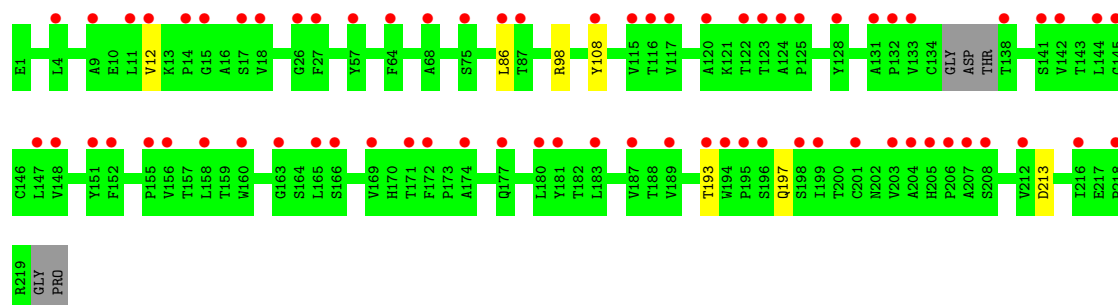




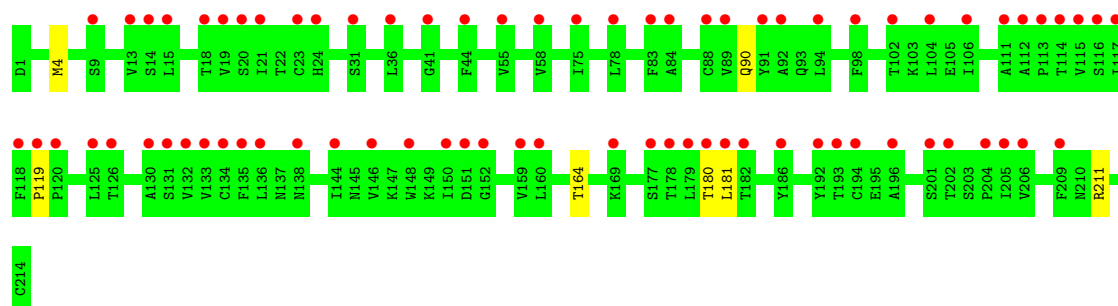
• Molecule 3: 10E5 Fab heavy chain



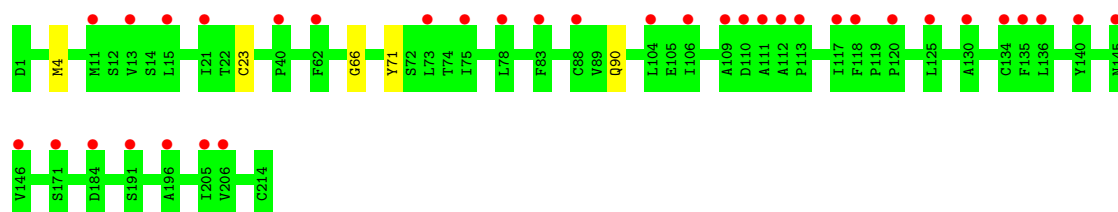
• Molecule 3: 10E5 Fab heavy chain



• Molecule 4: 10E5 Fab light chain



• Molecule 4: 10E5 Fab light chain



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



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



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



- Molecule 7: 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	258.33Å 144.67Å 105.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.99 – 2.00 48.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.99-2.00) 97.4 (48.99-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.185 , 0.214 0.187 , 0.215	Depositor DCC
$R_{free}$ test set	262774 reflections (0.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.2	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 64.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	22567	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BMA, SO4, NAG, CA, MWO, CL, MAN, MN

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	0.30	0/3608	0.53	0/4918
1	C	0.27	0/3605	0.50	0/4912
2	B	0.28	0/3680	0.48	0/4989
2	D	0.26	0/3690	0.47	0/5003
3	E	0.24	0/1673	0.45	0/2290
3	H	0.25	0/1684	0.48	0/2305
4	F	0.24	0/1673	0.44	0/2269
4	L	0.25	0/1673	0.47	0/2269
All	All	0.27	0/21286	0.48	0/28955

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	3499	0	3345	9	0
1	C	3502	0	3334	4	0
2	B	3610	0	3531	19	0
2	D	3623	0	3541	28	0
3	E	1631	0	1590	5	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	4	0
4	F	1637	0	1553	5	0
4	L	1637	0	1553	3	0
5	G	50	0	42	0	0
6	I	28	0	25	7	0
6	K	28	0	25	1	0
7	J	61	0	52	8	0
8	A	20	0	0	0	0
8	C	20	0	0	0	0
8	L	5	0	0	0	0
9	A	4	0	0	0	0
9	C	4	0	0	0	0
10	B	3	0	0	0	0
10	D	3	0	0	0	0
11	B	14	0	13	0	0
11	D	14	0	13	5	0
12	B	22	0	0	0	0
12	D	22	0	0	0	0
13	C	11	0	10	0	0
14	C	2	0	0	0	0
14	D	1	0	0	0	0
15	A	542	0	0	3	1
15	B	319	0	0	2	0
15	C	232	0	0	0	1
15	D	200	0	0	2	0
15	E	29	0	0	0	0
15	F	20	0	0	1	0
15	H	45	0	0	0	0
15	L	87	0	0	1	0
All	All	22567	0	20227	72	1

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 (72) 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:320:ASN:HD21	7:J:1:NAG:C1	0.99	1.59
2:D:99:ASN:ND2	11:D:2004:NAG:C1	1.68	1.56
2:B:371:ASN:HD21	6:I:1:NAG:C1	0.97	1.53
2:B:371:ASN:ND2	6:I:1:NAG:C1	1.73	1.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:320:ASN:ND2	7:J:1:NAG:C1	1.76	1.45
2:B:371:ASN:HD21	6:I:1:NAG:C2	1.63	1.10
2:B:371:ASN:ND2	6:I:1:NAG:C2	2.16	1.07
2:D:320:ASN:HD21	7:J:1:NAG:C2	1.75	1.00
2:D:99:ASN:CG	11:D:2004:NAG:C1	2.39	0.91
2:B:371:ASN:CG	6:I:1:NAG:C1	2.41	0.88
2:D:320:ASN:CG	7:J:1:NAG:C1	2.44	0.85
2:D:99:ASN:ND2	11:D:2004:NAG:O5	2.10	0.82
2:B:371:ASN:ND2	6:I:1:NAG:H2	1.96	0.81
4:L:23:CYS:SG	15:L:457:HOH:O	2.47	0.72
2:D:320:ASN:ND2	7:J:1:NAG:C2	2.45	0.71
2:D:99:ASN:ND2	11:D:2004:NAG:C2	2.53	0.70
4:F:211:ARG:NH2	15:F:301:HOH:O	2.26	0.69
2:D:181:LYS:NZ	15:D:2101:HOH:O	2.26	0.67
2:D:143:ARG:NH1	15:D:2103:HOH:O	2.30	0.64
2:B:301:GLN:NE2	15:B:2103:HOH:O	2.29	0.63
2:B:371:ASN:OD1	6:I:1:NAG:C1	2.48	0.62
2:B:404:ARG:NH1	15:B:2105:HOH:O	2.33	0.62
2:D:320:ASN:ND2	7:J:1:NAG:O5	2.30	0.60
2:D:99:ASN:OD1	11:D:2004:NAG:C1	2.51	0.59
2:D:306:LEU:HB3	2:D:328:THR:HG22	1.85	0.59
2:D:320:ASN:OD1	7:J:1:NAG:C1	2.51	0.58
1:A:335:ARG:NH2	15:A:607:HOH:O	2.37	0.57
2:B:202:ARG:NH2	2:B:206:GLU:OE2	2.40	0.55
2:B:97:SER:HB3	2:B:402:LYS:HG2	1.92	0.52
2:D:22:MET:HG2	2:D:40:LEU:HD22	1.94	0.50
1:A:9:THR:HB	1:A:447:VAL:HB	1.95	0.49
3:E:202:ASN:HA	3:E:213:ASP:HB3	1.94	0.49
1:C:262:TRP:HB3	2:D:317:LEU:HD13	1.95	0.48
2:D:456:GLU:OE2	2:D:461:ARG:NH1	2.47	0.48
1:A:32:ARG:NH2	15:A:616:HOH:O	2.47	0.47
1:A:262:TRP:HB3	2:B:317:LEU:HD13	1.97	0.47
3:H:213:ASP:OD1	3:H:213:ASP:N	2.47	0.47
1:A:27:LYS:HG2	1:A:33:VAL:HG22	1.97	0.47
3:E:133:VAL:HG22	4:F:119:PRO:HD3	1.96	0.47
2:B:456:GLU:OE2	2:B:461:ARG:NH1	2.49	0.46
2:D:418:PRO:HB2	2:D:421:PHE:CD1	2.52	0.45
3:E:172:PHE:CD2	4:F:164:THR:HG23	2.52	0.45
2:D:178:TYR:CG	2:D:179:ASP:N	2.85	0.44
2:B:249:THR:HA	2:B:309:ALA:O	2.17	0.44
2:B:28:ASP:OD1	2:B:30:ALA:N	2.51	0.43

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:ASP:OD1	2:B:40:LEU:N	2.48	0.43
2:D:249:THR:HA	2:D:309:ALA:O	2.17	0.43
1:C:9:THR:HB	1:C:447:VAL:HB	2.00	0.43
2:D:12:SER:HB3	2:D:461:ARG:HD3	1.98	0.43
3:H:12:VAL:HG21	3:H:86:LEU:HD13	2.00	0.43
2:D:235:LYS:HE3	2:D:276:GLY:O	2.18	0.43
2:D:42:GLU:OE2	2:D:42:GLU:N	2.51	0.43
4:L:4:MET:HE2	4:L:90:GLN:HB3	2.01	0.43
4:L:66:GLY:HA3	4:L:71:TYR:HA	2.01	0.43
1:C:107:CYS:HA	1:C:130:CYS:HA	2.01	0.43
1:A:15:ASN:HD22	1:A:16:GLY:N	2.17	0.43
1:A:122:ALA:O	1:A:123:GLU:HB2	2.19	0.43
2:B:111:PRO:HG2	2:B:241:ASP:O	2.18	0.43
2:B:139:ALA:HB2	2:B:200:VAL:HG11	2.01	0.42
4:F:4:MET:HE2	4:F:90:GLN:HB3	2.00	0.42
1:C:377:ALA:HB2	1:C:421:LEU:HD11	2.00	0.42
2:D:320:ASN:ND2	7:J:1:NAG:H2	2.30	0.42
3:E:149:LYS:NZ	4:F:180:THR:HG21	2.35	0.42
1:A:41:ARG:NH1	15:A:623:HOH:O	2.49	0.42
2:D:139:ALA:HB2	2:D:200:VAL:HG11	2.02	0.41
2:D:400:GLU:HB2	6:K:1:NAG:H83	2.02	0.41
3:H:193:THR:O	3:H:197:GLN:N	2.50	0.41
1:A:258:PRO:HA	1:A:289:PHE:O	2.21	0.41
2:B:418:PRO:HB2	2:B:421:PHE:CD1	2.55	0.41
3:H:98:ARG:HG3	3:H:108:TYR:HB2	2.03	0.41
2:D:249:THR:HG22	2:D:309:ALA:HB3	2.03	0.40
3:E:125:PRO:HB3	3:E:151:TYR:HB3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1035:HOH:O	15:C:786:HOH:O[1_554]	2.11	0.09

## 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	456/457 (100%)	440 (96%)	15 (3%)	1 (0%)	44	42
1	C	455/457 (100%)	441 (97%)	14 (3%)	0	100	100
2	B	467/472 (99%)	452 (97%)	14 (3%)	1 (0%)	44	42
2	D	469/472 (99%)	451 (96%)	18 (4%)	0	100	100
3	E	210/221 (95%)	196 (93%)	14 (7%)	0	100	100
3	H	212/221 (96%)	203 (96%)	9 (4%)	0	100	100
4	F	212/214 (99%)	199 (94%)	13 (6%)	0	100	100
4	L	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
All	All	2693/2728 (99%)	2587 (96%)	104 (4%)	2 (0%)	48	47

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	76	ASP

### 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	366/364 (100%)	359 (98%)	7 (2%)	52	57
1	C	365/364 (100%)	360 (99%)	5 (1%)	62	68
2	B	415/417 (100%)	412 (99%)	3 (1%)	81	86
2	D	416/417 (100%)	413 (99%)	3 (1%)	81	86
3	E	186/190 (98%)	186 (100%)	0	100	100
3	H	187/190 (98%)	187 (100%)	0	100	100
4	F	188/188 (100%)	187 (100%)	1 (0%)	86	90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2311/2318 (100%)	2292 (99%)	19 (1%)	79	84

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	23	LEU
1	A	166	TYR
1	A	190	TYR
1	A	219	GLN
1	A	288	TYR
1	A	395	GLN
2	B	79	GLN
2	B	215	ASN
2	B	374	CYS
1	C	15	ASN
1	C	23	LEU
1	C	166	TYR
1	C	190	TYR
1	C	288	TYR
2	D	47	ASP
2	D	143	ARG
2	D	215	ASN
4	F	181	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
2	B	280	HIS
2	B	301	GLN
2	B	371	ASN
2	D	82	GLN
2	D	301	GLN
2	D	320	ASN

### 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	5,2	14,14,15	0.24	0	17,19,21	0.41	0
5	NAG	G	2	5	14,14,15	0.33	0	17,19,21	0.36	0
5	BMA	G	3	5	11,11,12	1.01	1 (9%)	15,15,17	0.95	1 (6%)
5	MAN	G	4	5	11,11,12	0.64	0	15,15,17	1.03	2 (13%)
6	NAG	I	1	6	14,14,15	0.23	0	17,19,21	0.48	0
6	NAG	I	2	6	14,14,15	0.29	0	17,19,21	0.39	0
7	NAG	J	1	7	14,14,15	0.30	0	17,19,21	0.47	0
7	NAG	J	2	7	14,14,15	0.31	0	17,19,21	0.42	0
7	BMA	J	3	7	11,11,12	0.96	0	15,15,17	0.70	0
7	MAN	J	4	7	11,11,12	0.76	0	15,15,17	0.93	2 (13%)
7	MAN	J	5	7	11,11,12	0.77	1 (9%)	15,15,17	1.13	2 (13%)
6	NAG	K	1	6	14,14,15	0.24	0	17,19,21	0.39	0
6	NAG	K	2	6	14,14,15	0.22	0	17,19,21	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	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
6	NAG	I	1	6	-	1/6/23/26	0/1/1/1
6	NAG	I	2	6	-	4/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	J	1	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	-	1/2/19/22	0/1/1/1
7	MAN	J	4	7	-	2/2/19/22	0/1/1/1
7	MAN	J	5	7	-	1/2/19/22	0/1/1/1
6	NAG	K	1	6	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	3	BMA	O5-C1	-2.35	1.39	1.43
7	J	5	MAN	C1-C2	2.03	1.57	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	5	MAN	C1-O5-C5	3.45	116.81	112.19
5	G	4	MAN	C1-O5-C5	2.49	115.52	112.19
7	J	4	MAN	C1-O5-C5	2.33	115.31	112.19
5	G	4	MAN	O2-C2-C3	-2.22	105.55	110.15
7	J	4	MAN	O2-C2-C3	-2.19	105.61	110.15
5	G	3	BMA	C3-C4-C5	2.17	114.17	110.23
7	J	5	MAN	O2-C2-C3	-2.01	105.98	110.15

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	J	4	MAN	O5-C5-C6-O6
7	J	4	MAN	C4-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
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
6	K	2	NAG	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
7	J	5	MAN	O5-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

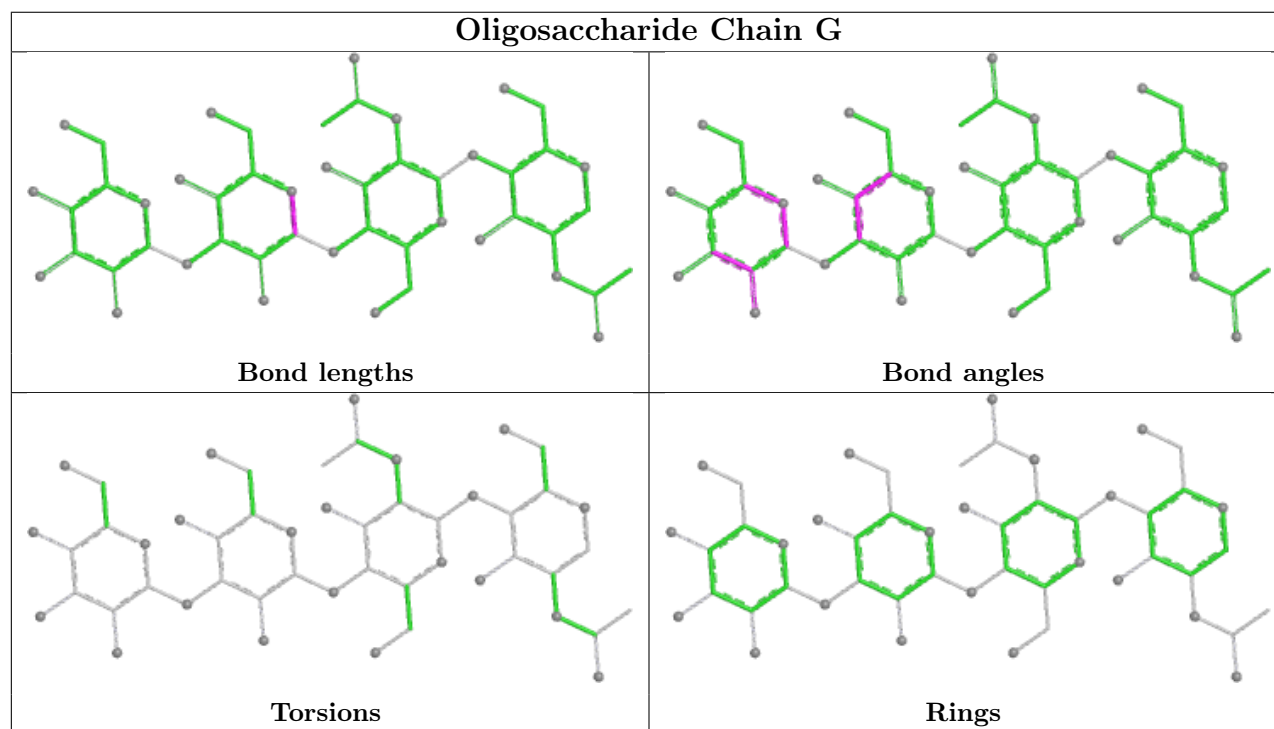
Mol	Chain	Res	Type	Atoms
7	J	3	BMA	O5-C5-C6-O6

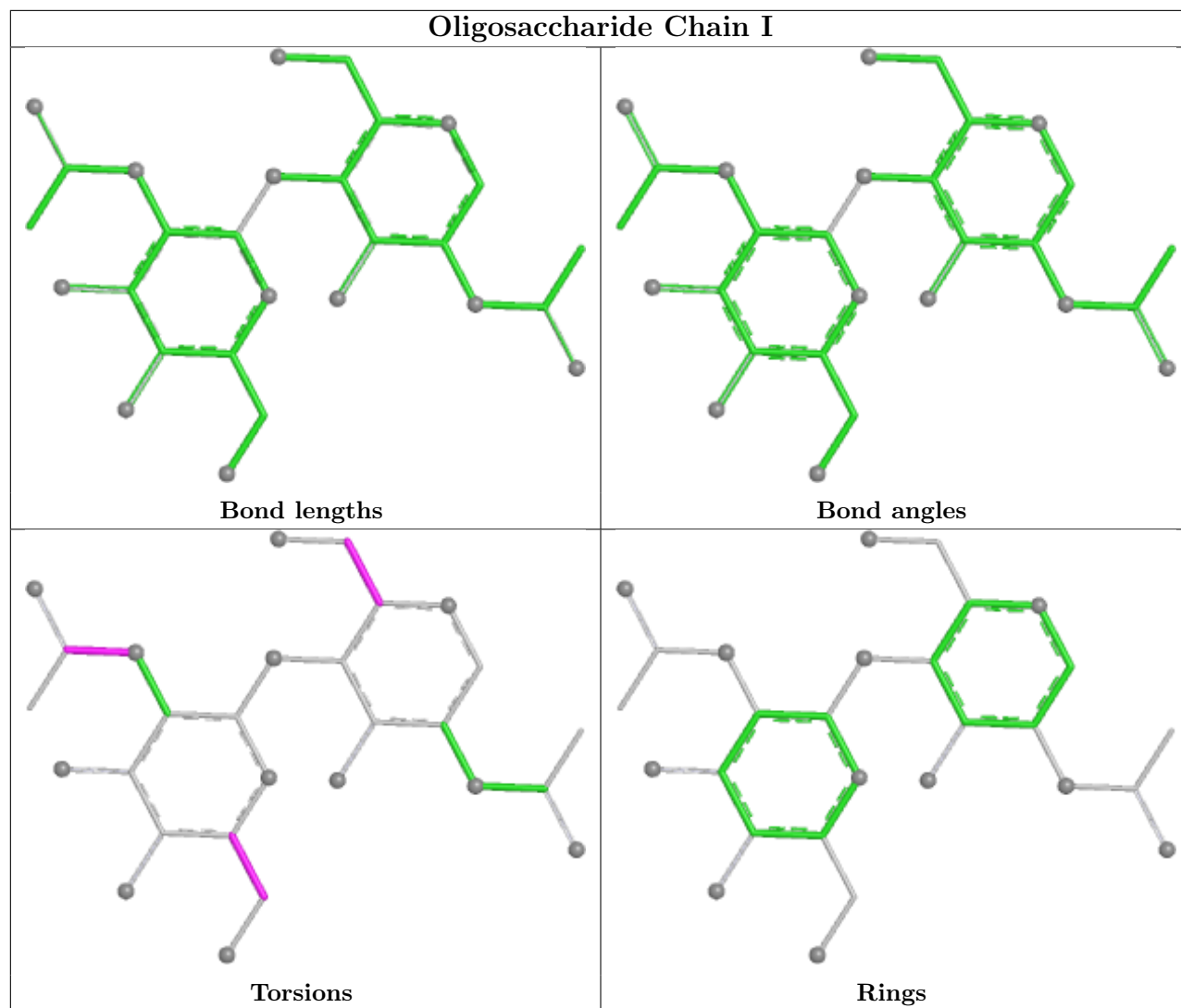
There are no ring outliers.

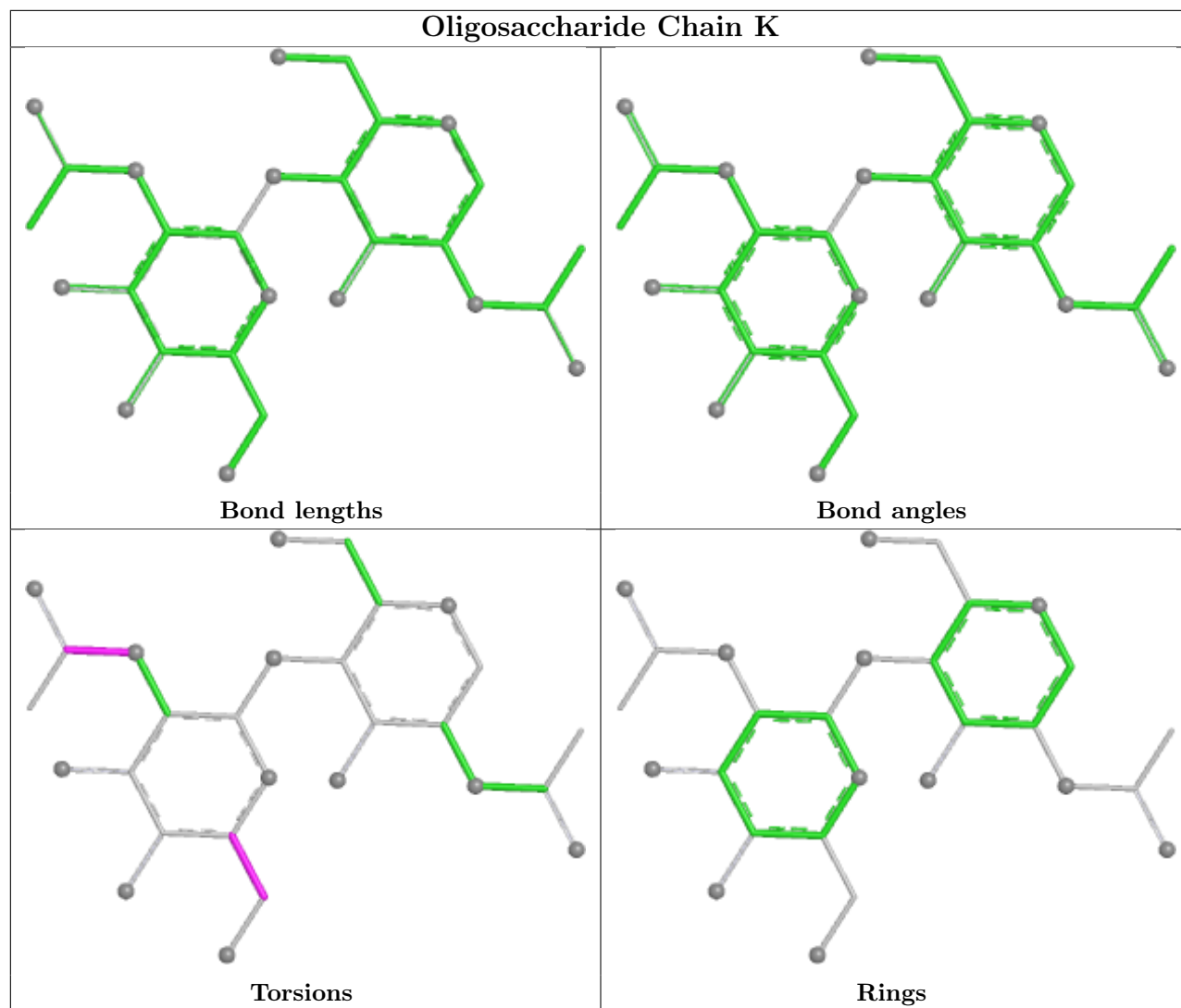
3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	1	NAG	7	0
6	K	1	NAG	1	0
7	J	1	NAG	8	0

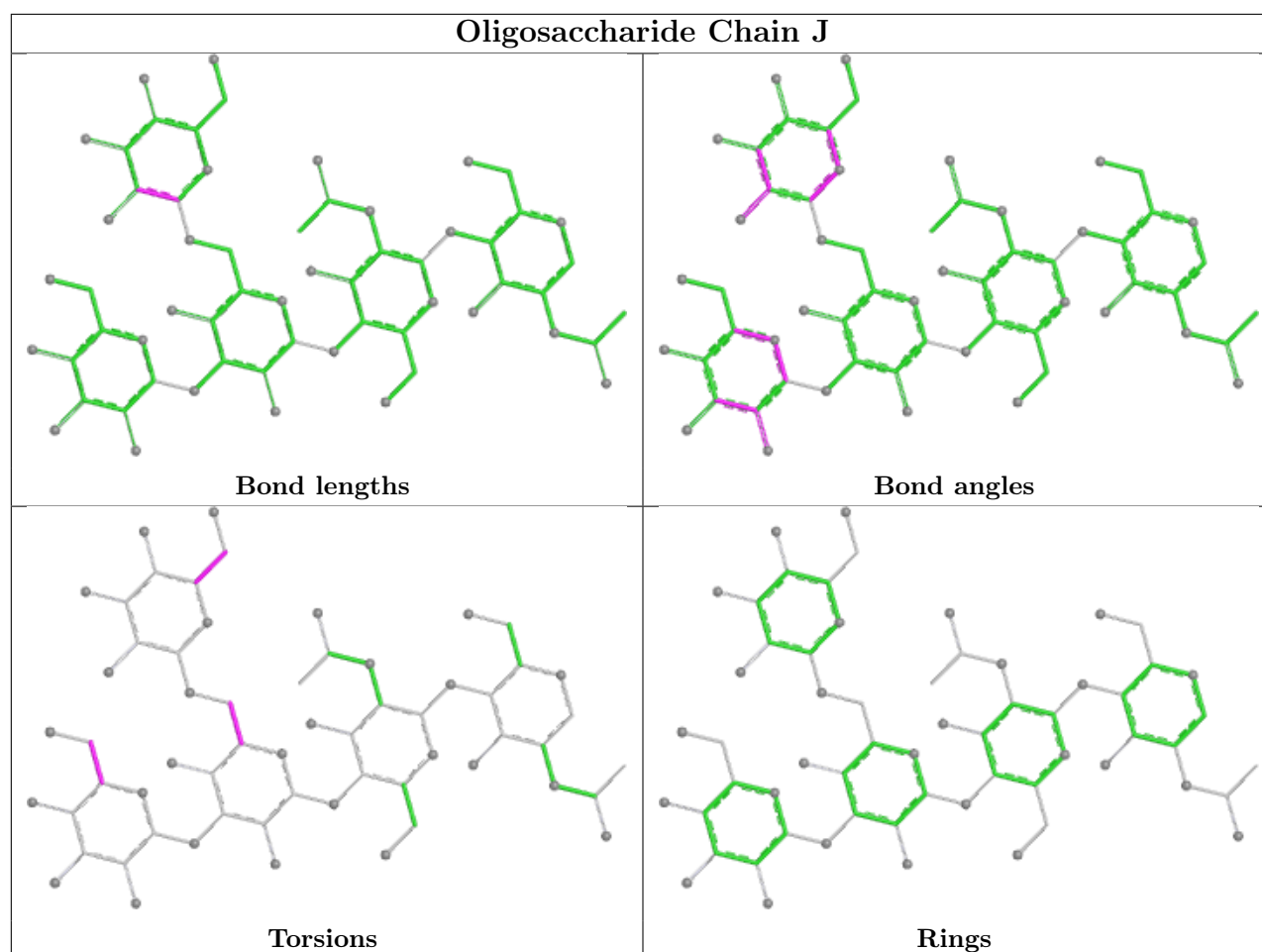
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 17 are monoatomic - leaving 14 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	$\# Z  > 2$
13	MAN	C	501	-	11,11,12	0.77	0	15,15,17	1.01	1 (6%)
8	SO4	A	507	-	4,4,4	0.23	0	6,6,6	0.11	0
8	SO4	A	501	-	4,4,4	0.25	0	6,6,6	0.09	0
12	MWO	B	2005	10	23,24,24	3.07	9 (39%)	25,32,32	2.17	5 (20%)
11	NAG	B	2004	2	14,14,15	0.16	0	17,19,21	0.46	0
11	NAG	D	2004	-	14,14,15	0.22	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	SO4	C	504	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	A	508	-	4,4,4	0.23	0	6,6,6	0.08	0
8	SO4	L	301	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	C	503	-	4,4,4	0.24	0	6,6,6	0.06	0
8	SO4	C	511	-	4,4,4	0.24	0	6,6,6	0.08	0
12	MWO	D	2006	10	23,24,24	3.06	9 (39%)	25,32,32	2.23	7 (28%)
8	SO4	A	502	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	C	502	-	4,4,4	0.23	0	6,6,6	0.09	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	MAN	C	501	-	-	2/2/19/22	0/1/1/1
12	MWO	B	2005	10	-	3/12/39/39	0/3/3/3
11	NAG	B	2004	2	-	2/6/23/26	0/1/1/1
12	MWO	D	2006	10	-	3/12/39/39	0/3/3/3
11	NAG	D	2004	-	-	0/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	2006	MWO	C4-N2	-7.70	1.31	1.47
12	B	2005	MWO	C4-N2	-7.65	1.31	1.47
12	B	2005	MWO	O1-C2	-7.11	1.36	1.46
12	D	2006	MWO	O1-C2	-7.01	1.36	1.46
12	D	2006	MWO	C5-N2	-5.21	1.32	1.46
12	B	2005	MWO	C5-N2	-5.19	1.32	1.46
12	D	2006	MWO	C8-N2	-5.19	1.32	1.46
12	B	2005	MWO	C8-N2	-5.10	1.33	1.46
12	B	2005	MWO	C3-C1	4.72	1.59	1.50
12	D	2006	MWO	C3-C1	4.57	1.59	1.50
12	B	2005	MWO	O1-N1	-2.69	1.38	1.42
12	B	2005	MWO	C1-N1	2.60	1.29	1.27
12	D	2006	MWO	O1-N1	-2.59	1.38	1.42
12	D	2006	MWO	C1-N1	2.44	1.29	1.27
12	D	2006	MWO	C14-C13	-2.37	1.47	1.53
12	B	2005	MWO	C14-C13	-2.32	1.47	1.53
12	D	2006	MWO	C12-C13	-2.28	1.47	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2005	MWO	C12-C13	-2.24	1.47	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	2005	MWO	C3-C1-N1	-7.25	109.89	114.37
12	D	2006	MWO	C3-C1-N1	-6.27	110.50	114.37
12	D	2006	MWO	O1-C2-C3	5.56	109.41	104.37
12	B	2005	MWO	O1-C2-C3	4.27	108.24	104.37
12	B	2005	MWO	C12-C13-C14	-3.26	103.14	110.00
12	D	2006	MWO	C12-C13-C1	-3.17	105.46	111.99
12	D	2006	MWO	C12-C13-C14	-3.14	103.37	110.00
12	D	2006	MWO	C14-C13-C1	-2.95	105.92	111.99
12	B	2005	MWO	C12-C13-C1	-2.84	106.14	111.99
12	B	2005	MWO	C14-C13-C1	-2.83	106.17	111.99
12	D	2006	MWO	O1-N1-C1	2.63	111.50	109.23
13	C	501	MAN	C1-O5-C5	2.36	115.35	112.19
12	D	2006	MWO	O2-C10-C9	2.15	121.87	113.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	2005	MWO	N1-C1-C13-C12
12	B	2005	MWO	C3-C2-C4-N2
12	B	2005	MWO	O1-C2-C4-N2
12	D	2006	MWO	C3-C2-C4-N2
12	D	2006	MWO	O1-C2-C4-N2
11	B	2004	NAG	O5-C5-C6-O6
11	B	2004	NAG	C4-C5-C6-O6
13	C	501	MAN	O5-C5-C6-O6
13	C	501	MAN	C4-C5-C6-O6
12	D	2006	MWO	C3-C1-C13-C14

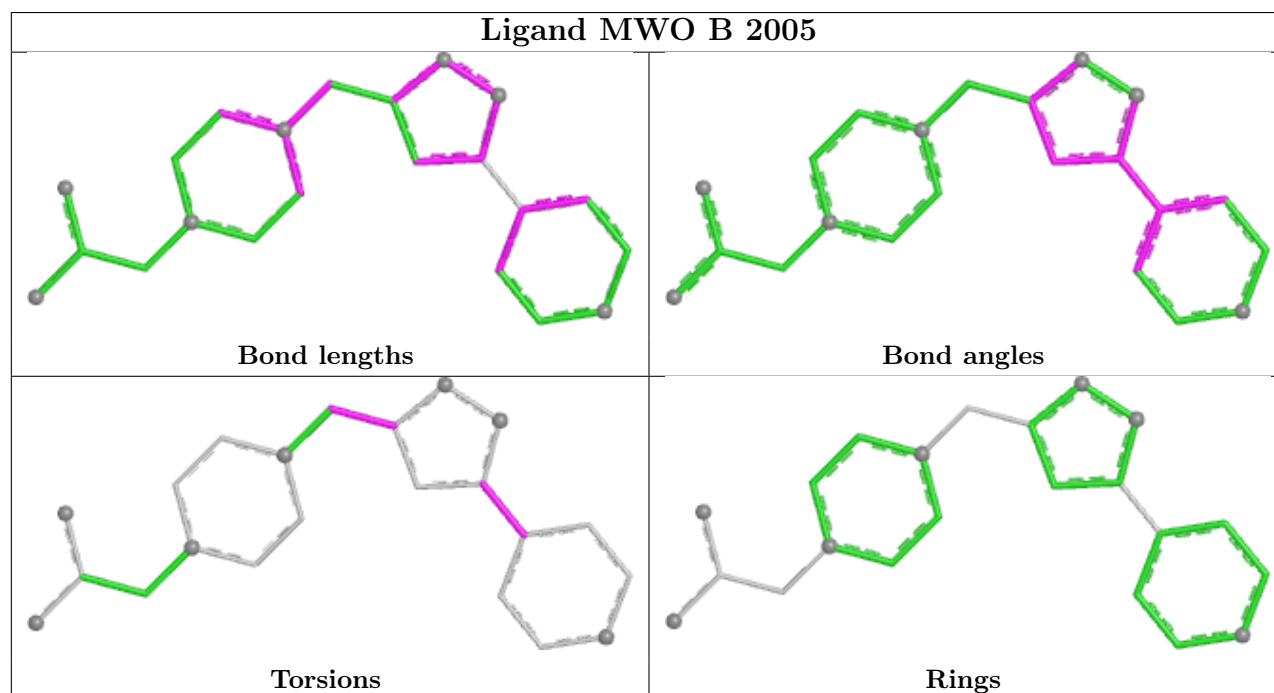
There are no ring outliers.

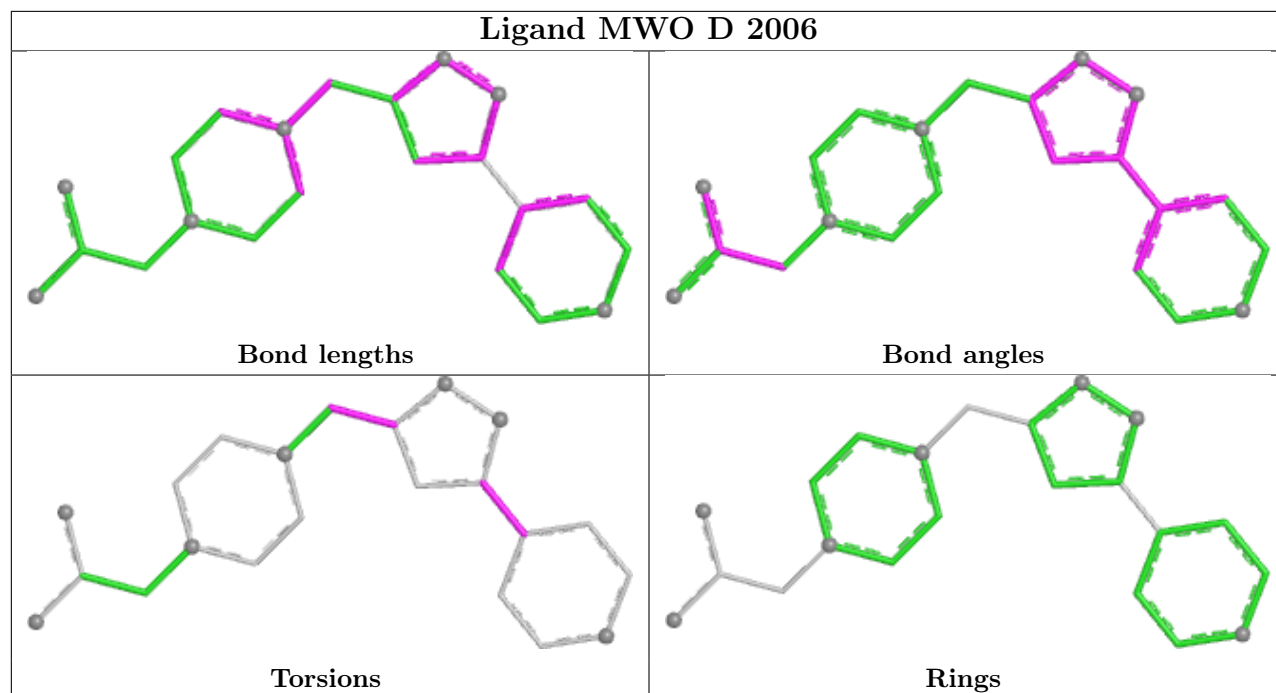
1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	2004	NAG	5	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.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	454/457 (99%)	-0.02	9 (1%) 64 63	23, 43, 74, 136	4 (0%)
1	C	453/457 (99%)	0.55	21 (4%) 38 36	28, 57, 90, 138	4 (0%)
2	B	466/472 (98%)	0.64	60 (12%) 9 7	20, 65, 152, 196	4 (0%)
2	D	471/472 (99%)	1.04	74 (15%) 6 5	40, 74, 147, 199	1 (0%)
3	E	214/221 (96%)	1.95	88 (41%) 1 1	71, 135, 197, 233	0
3	H	216/221 (97%)	1.62	71 (32%) 1 1	49, 102, 162, 187	0
4	F	214/214 (100%)	1.67	75 (35%) 1 1	69, 125, 193, 226	0
4	L	214/214 (100%)	1.28	35 (16%) 5 5	53, 85, 117, 210	0
All	All	2702/2728 (99%)	0.90	433 (16%) 6 5	20, 72, 164, 233	13 (0%)

All (433) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	147	LEU	7.2
1	A	454	VAL	5.4
1	A	217	SER	5.0
3	H	189	VAL	5.0
3	E	165	LEU	4.7
3	E	203	VAL	4.7
4	F	125	LEU	4.6
2	B	44	LEU	4.6
3	H	207	ALA	4.6
3	E	212	VAL	4.5
3	E	11	LEU	4.4
2	D	391	ILE	4.4
3	E	29	ILE	4.2
4	F	178	THR	4.2
2	D	375	LEU	4.2
3	E	189	VAL	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	E	160	TRP	4.1
4	F	132	VAL	4.1
3	E	199	ILE	4.0
4	F	179	LEU	4.0
3	H	195	PRO	4.0
2	D	467	LEU	4.0
2	D	30	ALA	3.9
2	D	44	LEU	3.9
2	B	465	GLY	3.9
4	F	209	PHE	3.9
4	L	125	LEU	3.9
4	F	130	ALA	3.9
2	B	455	PHE	3.8
3	E	183	LEU	3.8
3	E	146	CYS	3.8
2	D	129	TRP	3.8
3	E	184	SER	3.7
2	D	45	LEU	3.7
4	F	181	LEU	3.7
3	H	194	TRP	3.7
3	E	187	VAL	3.7
2	B	446	HIS	3.7
2	D	145	LEU	3.7
3	E	54	ALA	3.7
3	H	120	ALA	3.7
3	H	142	VAL	3.7
2	D	69	LEU	3.6
3	E	81	LEU	3.6
2	B	25	TRP	3.6
3	H	181	TYR	3.6
3	E	130	LEU	3.6
4	L	78	LEU	3.6
4	F	115	VAL	3.6
3	E	9	ALA	3.6
3	E	144	LEU	3.5
3	E	127	VAL	3.5
4	F	136	LEU	3.5
3	H	206	PRO	3.5
3	H	212	VAL	3.5
2	D	49	CYS	3.5
2	D	471	CYS	3.5
3	E	14	PRO	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	H	11	LEU	3.4
2	D	61	ALA	3.4
1	C	217	SER	3.4
2	B	129	TRP	3.4
4	F	133	VAL	3.4
2	D	178	TYR	3.4
4	F	117	ILE	3.4
4	L	106	ILE	3.4
4	F	196	ALA	3.3
3	E	4	LEU	3.3
3	H	158	LEU	3.3
3	E	174	ALA	3.3
4	F	204	PRO	3.3
4	F	21	ILE	3.3
3	H	18	VAL	3.3
1	A	45	PRO	3.3
2	D	2	PRO	3.2
4	F	78	LEU	3.2
3	E	36	TRP	3.2
2	B	178	TYR	3.2
3	E	128	TYR	3.2
2	D	446	HIS	3.2
3	E	16	ALA	3.2
4	L	111	ALA	3.2
2	D	104	VAL	3.2
3	E	201	CYS	3.2
3	E	216	ILE	3.2
1	C	453	VAL	3.1
3	E	86	LEU	3.1
4	F	160	LEU	3.1
3	E	182	THR	3.1
3	E	194	TRP	3.1
3	H	169	VAL	3.1
3	H	171	THR	3.1
3	H	199	ILE	3.1
4	L	15	LEU	3.1
3	H	187	VAL	3.1
3	H	151	TYR	3.0
3	H	204	ALA	3.0
4	F	135	PHE	3.0
3	H	165	LEU	3.0
2	B	61	ALA	3.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	H	196	SER	3.0
2	D	90	LEU	3.0
2	B	63	VAL	3.0
2	D	26	CYS	3.0
2	B	57	PRO	3.0
2	B	4	ILE	3.0
3	H	203	VAL	3.0
2	B	26	CYS	3.0
2	B	374	CYS	3.0
3	E	124	ALA	2.9
4	F	205	ILE	2.9
4	L	112	ALA	2.9
2	D	56	PHE	2.9
2	D	389	LEU	2.9
3	E	20	LEU	2.9
3	E	27	PHE	2.9
4	F	206	VAL	2.9
2	D	54	ILE	2.9
4	F	192	TYR	2.9
2	B	56	PHE	2.9
2	D	466	TRP	2.9
4	L	113	PRO	2.9
3	E	120	ALA	2.9
2	D	182	THR	2.9
3	E	115	VAL	2.9
3	H	160	TRP	2.9
4	F	134	CYS	2.9
3	E	30	LYS	2.9
3	H	9	ALA	2.9
4	F	193	THR	2.8
3	E	57	TYR	2.8
3	E	132	PRO	2.8
2	B	30	ALA	2.8
2	B	466	TRP	2.8
2	B	432	ASP	2.8
4	F	186	TYR	2.8
2	D	379	VAL	2.8
4	F	146	VAL	2.8
4	L	146	VAL	2.8
2	B	436	ALA	2.8
3	E	116	THR	2.8
3	H	87	THR	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	130	CYS	2.8
4	F	150	ILE	2.8
3	H	166	SER	2.8
1	C	340	LEU	2.7
2	B	443	PRO	2.7
2	D	83	VAL	2.7
3	E	12	VAL	2.7
2	B	439	ALA	2.7
3	E	145	GLY	2.7
2	D	40	LEU	2.7
1	C	209	PRO	2.7
4	F	113	PRO	2.7
4	L	120	PRO	2.7
2	B	100	PHE	2.7
4	L	135	PHE	2.7
1	A	339	ALA	2.7
1	C	339	ALA	2.7
4	F	202	THR	2.7
2	B	458	GLY	2.7
2	D	143	ARG	2.7
2	B	33	LEU	2.7
2	D	64	LEU	2.7
3	E	45	LEU	2.7
3	E	83	LEU	2.7
3	H	144	LEU	2.7
1	C	162	TRP	2.7
2	D	25	TRP	2.7
3	E	109	TRP	2.7
4	F	19	VAL	2.7
4	F	159	VAL	2.7
1	C	150	THR	2.7
3	E	171	THR	2.7
2	D	433	CYS	2.7
3	H	163	GLY	2.7
2	D	47	ASP	2.7
3	H	4	LEU	2.7
3	H	183	LEU	2.7
3	E	64	PHE	2.6
3	E	133	VAL	2.6
4	F	102	THR	2.6
4	F	114	THR	2.6
4	L	206	VAL	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	46	SER	2.6
2	B	74	SER	2.6
4	F	75	ILE	2.6
2	D	32	PRO	2.6
2	D	181	LYS	2.6
3	E	158	LEU	2.6
4	F	15	LEU	2.6
2	D	376	ASN	2.6
1	C	46	SER	2.6
3	E	159	THR	2.6
2	D	63	VAL	2.6
2	D	4	ILE	2.6
3	H	218	PRO	2.6
4	F	106	ILE	2.6
3	E	100	LEU	2.6
1	C	218	SER	2.6
3	H	152	PHE	2.6
4	F	83	PHE	2.6
2	D	42	GLU	2.6
2	D	23	CYS	2.6
1	C	45	PRO	2.6
2	B	45	LEU	2.6
1	C	336	GLY	2.6
3	E	44	GLY	2.6
3	E	74	THR	2.6
1	C	207	TYR	2.5
1	C	1	LEU	2.5
2	B	92	LEU	2.5
2	D	33	LEU	2.5
3	H	75	SER	2.5
2	D	392	GLY	2.5
3	H	116	THR	2.5
4	F	180	THR	2.5
4	L	11	MET	2.5
1	C	216	VAL	2.5
3	E	37	VAL	2.5
3	H	148	VAL	2.5
4	L	13	VAL	2.5
4	L	118	PHE	2.5
3	H	128	TYR	2.5
4	F	194	CYS	2.5
3	H	125	PRO	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	H	86	LEU	2.5
4	F	104	LEU	2.5
2	D	41	LYS	2.5
2	D	146	THR	2.5
2	D	394	THR	2.5
3	E	188	THR	2.5
2	B	58	VAL	2.5
2	B	379	VAL	2.5
2	D	107	VAL	2.5
4	L	83	PHE	2.5
4	F	119	PRO	2.5
1	C	213	LEU	2.5
3	E	51	ILE	2.5
3	E	56	GLY	2.5
3	H	193	THR	2.5
3	E	24	ALA	2.5
3	E	204	ALA	2.5
2	B	408	GLN	2.5
3	H	201	CYS	2.4
4	F	88	CYS	2.4
4	L	40	PRO	2.4
2	D	398	SER	2.4
2	D	22	MET	2.4
3	H	15	GLY	2.4
4	F	148	TRP	2.4
2	B	17	LEU	2.4
3	H	216	ILE	2.4
4	L	205	ILE	2.4
3	E	131	ALA	2.4
4	L	109	ALA	2.4
3	E	53	PRO	2.4
4	F	169	LYS	2.4
4	F	201	SER	2.4
4	F	23	CYS	2.4
2	B	89	ALA	2.4
3	H	131	ALA	2.4
3	E	148	VAL	2.4
3	H	115	VAL	2.4
3	H	117	VAL	2.4
4	F	13	VAL	2.4
4	F	58	VAL	2.4
3	H	177	GLN	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	F	91	TYR	2.4
4	F	126	THR	2.4
3	E	48	ILE	2.4
4	L	75	ILE	2.4
3	H	205	HIS	2.4
1	C	337	PRO	2.4
3	E	142	VAL	2.4
3	E	175	VAL	2.4
1	C	130	CYS	2.4
2	B	49	CYS	2.4
2	D	406	CYS	2.4
3	H	122	THR	2.4
2	B	31	LEU	2.3
2	D	31	LEU	2.3
2	D	38	CYS	2.3
2	B	454	THR	2.3
3	E	80	TYR	2.3
2	D	180	MET	2.3
2	B	375	LEU	2.3
3	H	180	LEU	2.3
2	B	97	SER	2.3
2	B	36	PRO	2.3
1	A	216	VAL	2.3
2	D	345	VAL	2.3
2	B	41	LYS	2.3
3	H	208	SER	2.3
2	B	24	ALA	2.3
2	D	351	ILE	2.3
3	H	124	ALA	2.3
4	F	111	ALA	2.3
4	F	112	ALA	2.3
2	B	75	GLY	2.3
4	F	152	GLY	2.3
4	L	145	ASN	2.3
1	C	214	TRP	2.3
2	D	80	VAL	2.3
3	E	117	VAL	2.3
2	D	397	PHE	2.3
2	D	378	GLU	2.3
2	B	78	SER	2.3
2	D	383	LEU	2.3
3	E	103	TYR	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	H	108	TYR	2.3
4	F	131	SER	2.3
3	H	147	LEU	2.3
4	F	36	LEU	2.3
3	E	70	ILE	2.2
1	A	337	PRO	2.2
3	E	210	THR	2.2
4	F	24	HIS	2.2
2	B	19	VAL	2.2
2	D	58	VAL	2.2
3	H	156	VAL	2.2
3	E	22	CYS	2.2
4	F	44	PHE	2.2
4	F	98	PHE	2.2
2	B	27	SER	2.2
2	B	413	SER	2.2
3	E	119	SER	2.2
3	E	60	TYR	2.2
4	L	140	TYR	2.2
1	C	210	GLY	2.2
2	B	54	ILE	2.2
4	F	41	GLY	2.2
4	L	117	ILE	2.2
4	F	120	PRO	2.2
3	H	138	THR	2.2
4	F	151	ASP	2.2
4	L	184	ASP	2.2
2	D	147	SER	2.2
4	L	171	SER	2.2
3	H	64	PHE	2.2
1	C	80	GLY	2.2
3	H	26	GLY	2.2
4	L	136	LEU	2.2
4	L	130	ALA	2.2
4	L	196	ALA	2.2
3	H	14	PRO	2.2
3	H	155	PRO	2.2
4	F	144	ILE	2.2
2	B	440	GLN	2.2
2	D	108	GLU	2.2
3	E	114	SER	2.2
3	H	141	SER	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	F	89	VAL	2.2
2	B	177	CYS	2.2
2	B	448	CYS	2.2
2	D	177	CYS	2.2
4	F	84	ALA	2.2
2	B	2	PRO	2.2
2	D	36	PRO	2.2
2	D	348	TYR	2.2
3	E	153	PRO	2.2
3	H	132	PRO	2.2
2	B	88	ILE	2.2
2	B	391	ILE	2.2
2	D	380	ILE	2.2
3	E	87	THR	2.1
4	F	18	THR	2.1
2	D	369	SER	2.1
3	H	17	SER	2.1
4	F	20	SER	2.1
4	F	31	SER	2.1
3	E	18	VAL	2.1
3	E	96	CYS	2.1
4	F	55	VAL	2.1
2	D	100	PHE	2.1
3	E	152	PHE	2.1
3	H	27	PHE	2.1
3	H	174	ALA	2.1
3	E	155	PRO	2.1
3	H	57	TYR	2.1
4	L	110	ASP	2.1
3	E	88	SER	2.1
3	H	123	THR	2.1
4	F	182	THR	2.1
2	B	387	MET	2.1
2	D	335	MET	2.1
2	B	456	GLU	2.1
3	E	34	VAL	2.1
3	H	12	VAL	2.1
2	B	94	PRO	2.1
2	D	354	LYS	2.1
3	E	122	THR	2.1
4	L	191	SER	2.1
2	B	29	GLU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	67	ARG	2.1
2	B	10	VAL	2.1
2	B	406	CYS	2.1
4	L	88	CYS	2.1
1	C	223	PHE	2.1
2	D	421	PHE	2.1
4	F	94	LEU	2.1
4	F	118	PHE	2.1
4	L	73	LEU	2.1
3	E	25	SER	2.1
4	F	9	SER	2.1
4	L	21	ILE	2.1
3	E	32	THR	2.1
3	E	202	ASN	2.1
2	B	23	CYS	2.0
3	H	133	VAL	2.0
4	L	134	CYS	2.0
3	E	41	PRO	2.0
4	F	92	ALA	2.0
1	A	177	GLN	2.0
2	D	72	LYS	2.0
3	H	172	PHE	2.0
3	H	198	SER	2.0
4	F	14	SER	2.0
4	F	116	SER	2.0
4	F	138	ASN	2.0
2	D	37	ARG	2.0
2	D	388	GLY	2.0
3	H	145	GLY	2.0
2	B	462	CYS	2.0
2	D	10	VAL	2.0
2	D	50	ALA	2.0
3	E	93	VAL	2.0
3	E	214	LYS	2.0
3	H	68	ALA	2.0
4	F	177	SER	2.0
4	L	104	LEU	2.0
2	D	447	ARG	2.0
4	L	62	PHE	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, 95<sup>th</sup> 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
8	SO4	C	503	5/5	0.62	0.20	177,178,178,180	0
11	NAG	D	2004	14/15	0.62	0.14	99,110,119,120	0
11	NAG	B	2004	14/15	0.65	0.12	114,130,138,139	0
13	MAN	C	501	11/12	0.65	0.12	134,136,140,140	0
8	SO4	C	511	5/5	0.75	0.17	170,170,171,171	0
8	SO4	C	502	5/5	0.78	0.21	156,157,159,160	0
8	SO4	L	301	5/5	0.80	0.12	144,145,145,146	0
8	SO4	A	507	5/5	0.80	0.19	167,169,171,171	0
14	CL	D	2005	1/1	0.82	0.24	110,110,110,110	0
8	SO4	A	508	5/5	0.84	0.17	137,140,144,144	0
8	SO4	C	504	5/5	0.88	0.12	132,133,133,141	0
14	CL	C	506	1/1	0.89	0.21	129,129,129,129	0
8	SO4	A	501	5/5	0.89	0.16	117,118,120,123	0
14	CL	C	505	1/1	0.91	0.20	108,108,108,108	0
8	SO4	A	502	5/5	0.94	0.08	72,73,75,77	0
12	MWO	B	2005	22/22	0.94	0.12	36,66,85,88	0
12	MWO	D	2006	22/22	0.95	0.13	52,77,103,106	0
9	CA	A	505	1/1	0.97	0.04	37,37,37,37	0
10	MN	B	2002	1/1	0.97	0.15	74,74,74,74	0
9	CA	C	510	1/1	0.98	0.05	51,51,51,51	0
9	CA	A	504	1/1	0.98	0.04	39,39,39,39	0
9	CA	A	503	1/1	0.98	0.04	47,47,47,47	0
9	CA	C	507	1/1	0.98	0.04	73,73,73,73	0
9	CA	C	508	1/1	0.98	0.04	60,60,60,60	0
9	CA	A	506	1/1	0.99	0.04	39,39,39,39	0
9	CA	C	509	1/1	0.99	0.03	57,57,57,57	0
10	MN	D	2001	1/1	0.99	0.03	48,48,48,48	0

*Continued on next page...*

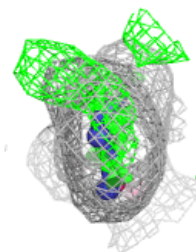
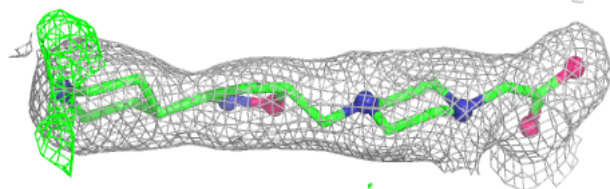
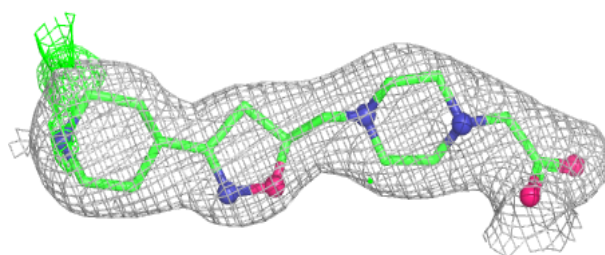
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	MN	D	2002	1/1	0.99	0.09	61,61,61,61	0
10	MN	D	2003	1/1	1.00	0.06	50,50,50,50	0
10	MN	B	2001	1/1	1.00	0.01	36,36,36,36	0
10	MN	B	2003	1/1	1.00	0.06	37,37,37,37	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.

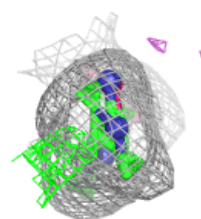
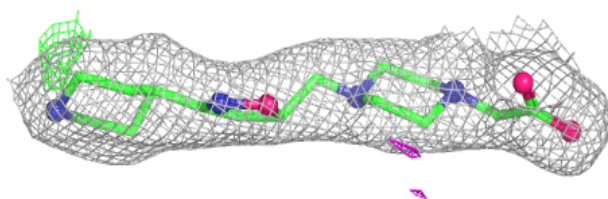
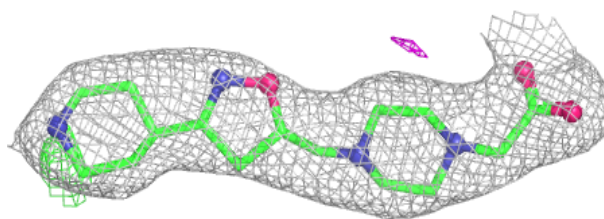
**Electron density around MWO B 2005:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MWO D 2006:**

$2mF_o - DF_c$  (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.