



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2024 – 12:11 AM EDT

PDB ID : 7TCT
Title : Integrin alpha IIB beta3 complex with UR2922
Authors : Zhu, J.; Lin, F.-Y.; Zhu, J.; Springer, T.A.
Deposited on : 2021-12-28
Resolution : 2.50 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:

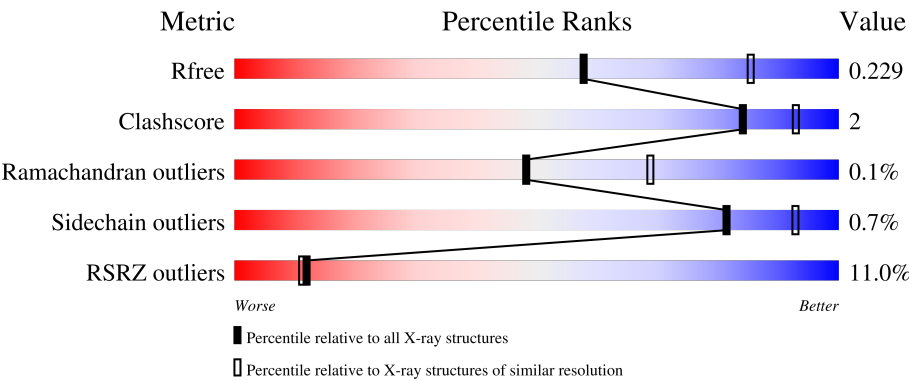
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.50 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	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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>2%</div><div>94%</div><div>5%</div><div></div></div>
1	C	457	<div><div>2%</div><div>91%</div><div>8%</div><div></div></div>
2	B	472	<div><div>10%</div><div>93%</div><div>6%</div><div></div></div>
2	D	472	<div><div>7%</div><div>92%</div><div>8%</div><div></div></div>
3	E	221	<div><div>36%</div><div>88%</div><div>9%</div><div></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 14 unique types of molecules in this entry. The entry contains 22118 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	453	Total	C	N	O	S	0	5	0
			3503	2227	604	664	8			
1	C	453	Total	C	N	O	S	1	3	0
			3493	2219	602	664	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	4	0
			3620	2256	618	712	34			
2	D	471	Total	C	N	O	S	1	1	0
			3631	2260	620	716	35			

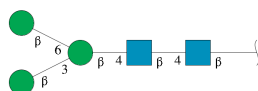
- Molecule 3 is a protein called Fab heavy chain.

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 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 beta-D-mannopyranose-(1-3)-[beta-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 beta-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 CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Ca	0	0
			2	2		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

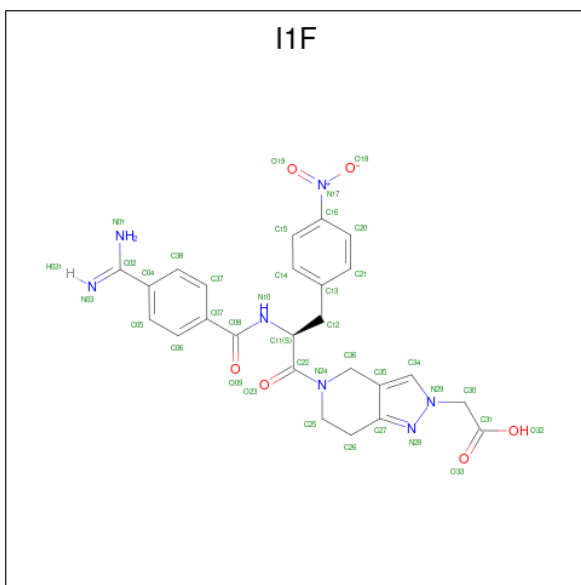
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Mg	0	0
			1	1		
10	D	1	Total	Mg	0	0
			1	1		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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 {5-[N-(4-carbamimidoylbenzoyl)-4-nitro-L-phenylalanyl]-4,5,6,7-tetrahydro-2H-pyrazolo[4,3-c]pyridin-2-yl}acetic acid (three-letter code: I1F) (formula: C₂₅H₂₅N₇O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	N	O	0	0
			38	25	7	6		
12	D	1	Total	C	N	O	0	0
			38	25	7	6		

- Molecule 13 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	1	Total	Cl	0	0
			1	1		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	334	Total	O	0	0
			334	334		
14	B	145	Total	O	0	0
			145	145		
14	C	231	Total	O	0	0
			231	231		
14	D	166	Total	O	0	0
			166	166		
14	E	18	Total	O	0	0
			18	18		
14	F	17	Total	O	0	0
			17	17		

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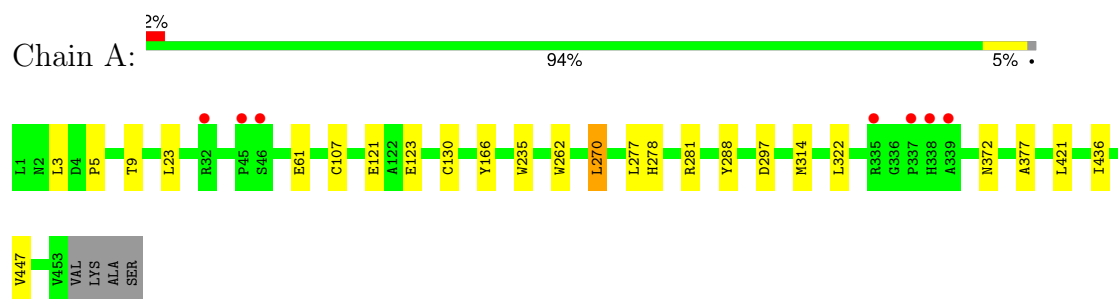
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	H	44	Total 44	O 44	0	0
14	L	43	Total 43	O 43	0	0

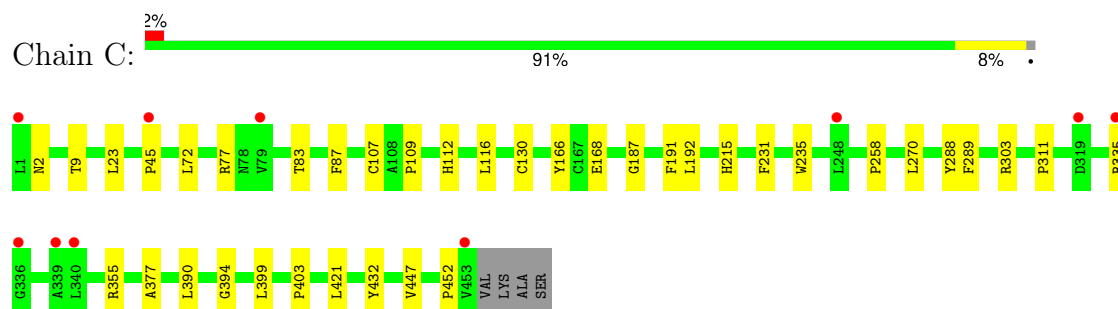
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

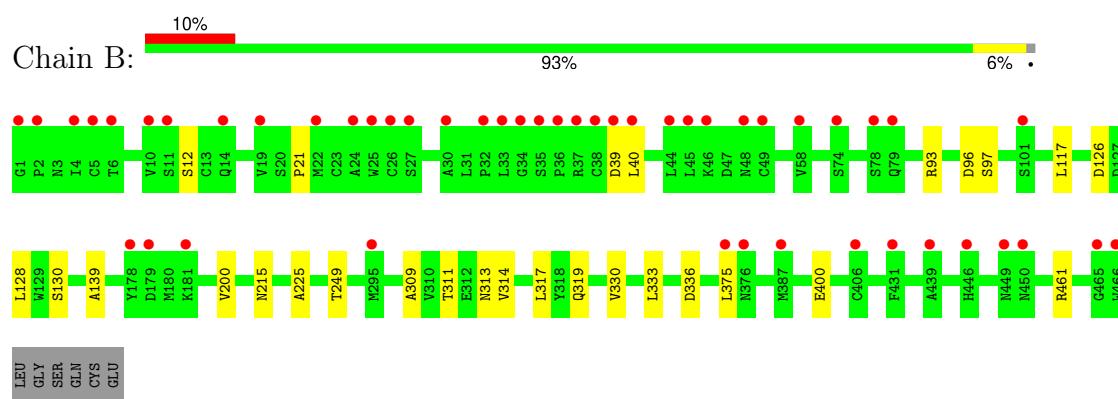
- Molecule 1: Integrin alpha-IIb heavy chain



- Molecule 1: Integrin alpha-IIb heavy chain

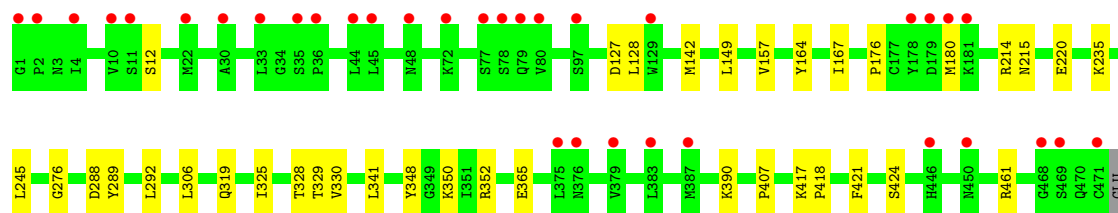


- Molecule 2: Isoform Beta-3C of Integrin beta-3

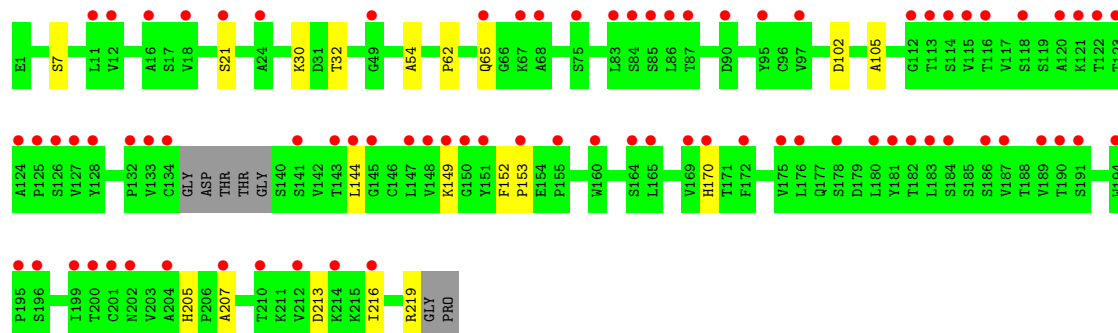
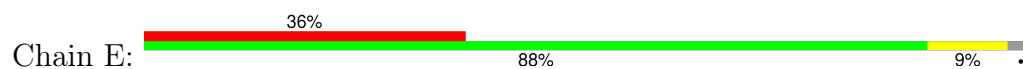


- Molecule 2: Isoform Beta-3C of Integrin beta-3

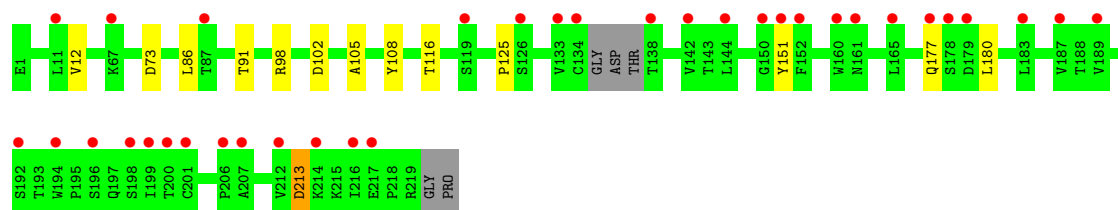
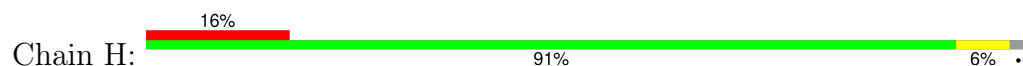




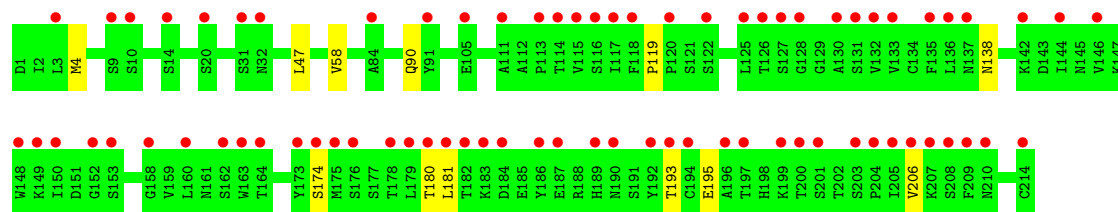
● Molecule 3: Fab heavy chain



● Molecule 3: Fab heavy chain



● Molecule 4: Fab light chain

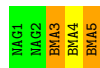


● Molecule 4: Fab light chain



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

Chain G:  40% 20% 40%



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

Chain I:  50% 50%



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

Chain K:  100%



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

Chain J:  75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	259.16Å 143.84Å 104.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.28 – 2.50 49.28 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.28-2.50) 99.4 (49.28-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.195 , 0.227 0.196 , 0.229	Depositor DCC
R_{free} test set	133809 reflections (1.48%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22118	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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: MG, SO4, I1F, CL, NAG, BMA, CA

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	0.26	0/3612	0.47	0/4922
1	C	0.25	0/3596	0.46	0/4900
2	B	0.24	0/3690	0.43	0/5002
2	D	0.25	0/3698	0.44	0/5013
3	E	0.25	0/1673	0.45	0/2290
3	H	0.25	0/1684	0.46	0/2305
4	F	0.25	0/1673	0.44	0/2269
4	L	0.25	0/1673	0.45	0/2269
All	All	0.25	0/21299	0.45	0/28970

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	3503	0	3348	12	0
1	C	3493	0	3327	20	0
2	B	3620	0	3546	15	0
2	D	3631	0	3548	20	0
3	E	1631	0	1590	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	0	1600	8	0
4	F	1637	0	1553	7	0
4	L	1637	0	1553	3	0
5	G	61	0	52	2	0
6	I	28	0	25	1	0
6	K	28	0	25	0	0
7	J	50	0	43	0	0
8	A	4	0	0	0	0
8	B	2	0	0	0	0
8	C	4	0	0	0	0
8	D	2	0	0	0	0
9	A	25	0	0	0	0
9	C	15	0	0	0	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
11	B	14	0	13	0	0
11	D	14	0	13	0	0
12	B	38	0	0	0	0
12	D	38	0	0	0	0
13	C	1	0	0	0	0
14	A	334	0	0	0	0
14	B	145	0	0	0	0
14	C	231	0	0	0	0
14	D	166	0	0	2	0
14	E	18	0	0	0	0
14	F	17	0	0	0	0
14	H	44	0	0	0	0
14	L	43	0	0	0	0
All	All	22118	0	20236	91	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 (91) 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:417:LYS:HG3	2:D:424:SER:HB3	1.74	0.67
2:D:365:GLU:N	2:D:365:GLU:OE1	2.26	0.66
2:D:292:LEU:HD22	2:D:325:ILE:HD11	1.83	0.59
3:E:62:PRO:HA	3:E:65:GLN:HG2	1.85	0.59
3:H:12:VAL:HG21	3:H:86:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:CYS:HA	1:A:130:CYS:HA	1.88	0.55
2:D:306:LEU:HB3	2:D:328:THR:HG22	1.87	0.55
2:D:176:PRO:O	2:D:214:ARG:NH1	2.40	0.53
2:B:39:ASP:OD1	2:B:40:LEU:N	2.36	0.53
4:F:193:THR:HG23	4:F:206:VAL:HG13	1.89	0.53
3:E:30:LYS:HG3	3:E:54:ALA:HA	1.90	0.53
1:A:281:ARG:HD2	5:G:4:BMA:H62	1.90	0.52
1:C:83:THR:HB	1:C:116:LEU:HB2	1.92	0.52
1:C:107:CYS:HA	1:C:130:CYS:HA	1.92	0.51
3:H:125:PRO:HB3	3:H:151:TYR:HB3	1.93	0.50
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.94	0.50
3:H:91:THR:HG23	3:H:116:THR:HA	1.94	0.50
3:H:177:GLN:N	3:H:180:LEU:O	2.44	0.50
2:B:126:ASP:OD1	2:B:126:ASP:N	2.43	0.50
3:E:102:ASP:HB3	3:E:105:ALA:HB2	1.94	0.50
1:A:262:TRP:HB3	2:B:317:LEU:HD13	1.94	0.49
1:A:436:ILE:HG22	1:A:447:VAL:HG22	1.94	0.49
2:D:319:GLN:HA	2:D:330:VAL:HG21	1.95	0.49
3:E:149:LYS:NZ	4:F:180:THR:HG21	2.28	0.49
1:A:9:THR:HB	1:A:447:VAL:HB	1.94	0.48
2:D:12:SER:HB3	2:D:461:ARG:HD3	1.95	0.48
3:E:144:LEU:HD13	3:E:216:ILE:HG21	1.95	0.48
2:D:418:PRO:HB2	2:D:421:PHE:CD1	2.49	0.47
4:F:195:GLU:HG2	4:F:206:VAL:HG22	1.95	0.47
1:C:235:TRP:CZ2	1:C:270:LEU:HD11	2.48	0.47
1:C:394:GLY:HA2	1:C:399:LEU:HD23	1.96	0.47
2:B:12:SER:HB3	2:B:461:ARG:HD3	1.96	0.47
2:D:390:LYS:NZ	3:H:73:ASP:OD1	2.47	0.47
2:B:21:PRO:O	2:B:93:ARG:NH1	2.48	0.46
2:B:319[A]:GLN:HA	2:B:330:VAL:HG21	1.97	0.46
1:A:377:ALA:HB2	1:A:421:LEU:HD11	1.97	0.46
3:H:102:ASP:HB3	3:H:105:ALA:HB2	1.97	0.46
2:D:235:LYS:HE3	2:D:276:GLY:O	2.15	0.46
2:B:319[B]:GLN:HA	2:B:330:VAL:HG21	1.98	0.46
1:C:187:GLY:HA2	1:C:191:PHE:HA	1.97	0.46
2:B:130:SER:OG	2:B:336:ASP:O	2.34	0.45
2:D:329:THR:O	14:D:2101:HOH:O	2.21	0.45
3:H:98:ARG:HG3	3:H:108:TYR:HB2	1.97	0.45
4:L:4:MET:HE1	4:L:90:GLN:HB3	1.99	0.45
5:G:3:BMA:H62	5:G:5:BMA:H2	1.58	0.44
2:B:139:ALA:HB2	2:B:200:VAL:HG11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:213:ASP:OD1	3:H:213:ASP:N	2.47	0.44
1:C:390:LEU:HD23	1:C:403:PRO:HG3	1.99	0.44
1:C:9:THR:HB	1:C:447:VAL:HB	2.00	0.44
2:D:164:TYR:O	2:D:215:ASN:HB2	2.18	0.44
1:A:277:LEU:O	1:A:278[B]:HIS:ND1	2.50	0.44
2:B:313:ASN:ND2	2:B:314:VAL:HG13	2.33	0.43
2:D:329:THR:HG23	2:D:350:LYS:HD2	1.99	0.43
3:E:7:SER:HB3	3:E:21:SER:HB3	2.00	0.43
3:E:219:ARG:CZ	4:F:119:PRO:HG2	2.48	0.43
2:B:311:THR:HA	2:B:333:LEU:O	2.18	0.43
4:L:195:GLU:HG2	4:L:206:VAL:HG22	1.99	0.43
1:C:87:PHE:HB2	1:C:112:HIS:HB2	2.01	0.43
1:C:377:ALA:HB2	1:C:421:LEU:HD11	2.00	0.43
2:D:288:ASP:OD1	2:D:289:TYR:N	2.50	0.43
1:C:303:ARG:HH22	1:C:335:ARG:HE	1.67	0.43
3:E:152:PHE:HA	3:E:153:PRO:HA	1.74	0.43
2:B:96:ASP:OD1	2:B:97:SER:N	2.44	0.42
4:F:4:MET:HE1	4:F:90:GLN:HB3	2.01	0.42
2:B:117:LEU:HD11	2:B:225:ALA:HB1	2.01	0.42
2:B:249:THR:HA	2:B:309:ALA:O	2.19	0.42
2:B:400:GLU:HB2	6:I:1:NAG:H83	2.02	0.42
2:D:365:GLU:OE2	2:D:407:PRO:HB3	2.19	0.42
1:A:3:LEU:O	1:A:5:PRO:HD3	2.19	0.42
1:C:45:PRO:HD3	1:C:72:LEU:HD12	2.02	0.42
2:D:157:VAL:O	2:D:220:GLU:HB3	2.20	0.42
2:D:142:MET:HB2	2:D:149:LEU:HD22	2.02	0.42
1:C:215:HIS:CE1	3:E:32:THR:HG22	2.55	0.41
1:C:77:ARG:NH2	3:E:102:ASP:OD2	2.45	0.41
1:A:314:MET:HB3	1:A:322:LEU:HB3	2.02	0.41
1:C:2:ASN:N	1:C:2:ASN:OD1	2.54	0.41
1:C:311:PRO:O	1:C:355:ARG:HA	2.20	0.41
1:C:432:TYR:CZ	1:C:452:PRO:HA	2.55	0.41
2:D:352:ARG:NH1	14:D:2113:HOH:O	2.51	0.41
3:E:213:ASP:OD1	3:E:213:ASP:N	2.53	0.41
1:C:109:PRO:O	1:C:168:GLU:HA	2.20	0.41
2:D:245:LEU:HD11	2:D:348:TYR:HD1	1.86	0.41
3:E:205:HIS:CE1	3:E:207:ALA:HB3	2.56	0.41
1:A:297:ASP:O	1:A:372:ASN:HB2	2.21	0.41
1:C:112:HIS:CD2	2:D:167:ILE:HD11	2.56	0.41
4:F:47:LEU:HA	4:F:58:VAL:HG21	2.02	0.41
1:A:121:GLU:HG3	1:A:123:GLU:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:TRP:CZ2	1:A:270:LEU:HD11	2.55	0.40
1:C:258:PRO:HA	1:C:289:PHE:O	2.21	0.40
1:C:192:LEU:HD11	1:C:231:PHE:CD1	2.57	0.40
3:E:170:HIS:CE1	4:F:174:SER:HG	2.39	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	456/457 (100%)	444 (97%)	12 (3%)	0	100	100
1	C	454/457 (99%)	438 (96%)	16 (4%)	0	100	100
2	B	468/472 (99%)	446 (95%)	21 (4%)	1 (0%)	44	64
2	D	470/472 (100%)	452 (96%)	18 (4%)	0	100	100
3	E	210/221 (95%)	197 (94%)	13 (6%)	0	100	100
3	H	212/221 (96%)	203 (96%)	9 (4%)	0	100	100
4	F	212/214 (99%)	201 (95%)	10 (5%)	1 (0%)	25	44
4	L	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
All	All	2694/2728 (99%)	2587 (96%)	105 (4%)	2 (0%)	48	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	375	LEU
4	F	138	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	366/364 (100%)	361 (99%)	5 (1%)	62	83
1	C	364/364 (100%)	361 (99%)	3 (1%)	79	91
2	B	416/417 (100%)	414 (100%)	2 (0%)	86	95
2	D	417/417 (100%)	413 (99%)	4 (1%)	73	88
3	E	186/190 (98%)	186 (100%)	0	100	100
3	H	187/190 (98%)	186 (100%)	1 (0%)	86	95
4	F	188/188 (100%)	187 (100%)	1 (0%)	86	95
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2312/2318 (100%)	2296 (99%)	16 (1%)	81	93

All (16) 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	270	LEU
1	A	288	TYR
2	B	128	LEU
2	B	215	ASN
1	C	23	LEU
1	C	166	TYR
1	C	288	TYR
2	D	127	ASP
2	D	128	LEU
2	D	180	MET
2	D	341	LEU
4	F	181	LEU
3	H	213	ASP

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

Mol	Chain	Res	Type
1	A	197	GLN
2	B	301	GLN
1	C	197	GLN
1	C	219	GLN
2	D	301	GLN
2	D	408	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	0.34	0	17,19,21	0.49	0
5	NAG	G	2	5	14,14,15	0.20	0	17,19,21	0.53	0
5	BMA	G	3	5	11,11,12	1.45	2 (18%)	15,15,17	1.67	2 (13%)
5	BMA	G	4	5	11,11,12	0.99	0	15,15,17	1.10	0
5	BMA	G	5	5	11,11,12	0.97	1 (9%)	15,15,17	1.20	1 (6%)
6	NAG	I	1	6,2	14,14,15	0.24	0	17,19,21	0.45	0
6	NAG	I	2	6	14,14,15	0.27	0	17,19,21	0.41	0
7	NAG	J	1	7,2	14,14,15	0.30	0	17,19,21	0.49	0
7	NAG	J	2	7	14,14,15	0.21	0	17,19,21	0.58	0
7	BMA	J	3	7	11,11,12	0.96	0	15,15,17	1.33	1 (6%)
7	BMA	J	4	7	11,11,12	0.81	0	15,15,17	1.05	0
6	NAG	K	1	6,2	14,14,15	0.32	0	17,19,21	0.47	0
6	NAG	K	2	6	14,14,15	0.25	0	17,19,21	0.44	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	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	-	2/2/19/22	0/1/1/1
5	BMA	G	4	5	-	0/2/19/22	0/1/1/1
5	BMA	G	5	5	-	2/2/19/22	0/1/1/1
6	NAG	I	1	6,2	-	1/6/23/26	0/1/1/1
6	NAG	I	2	6	-	4/6/23/26	0/1/1/1
7	NAG	J	1	7,2	-	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	BMA	J	4	7	-	0/2/19/22	0/1/1/1
6	NAG	K	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	3	BMA	O5-C5	3.13	1.49	1.43
5	G	3	BMA	C2-C3	2.32	1.56	1.52
5	G	5	BMA	C4-C5	2.29	1.57	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	3	BMA	O3-C3-C2	4.21	118.64	110.05
7	J	3	BMA	O3-C3-C2	4.03	118.28	110.05
5	G	3	BMA	O5-C5-C6	3.45	114.38	107.66
5	G	5	BMA	C1-C2-C3	-3.05	105.20	109.64

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	3	BMA	O5-C5-C6-O6
5	G	5	BMA	C4-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6

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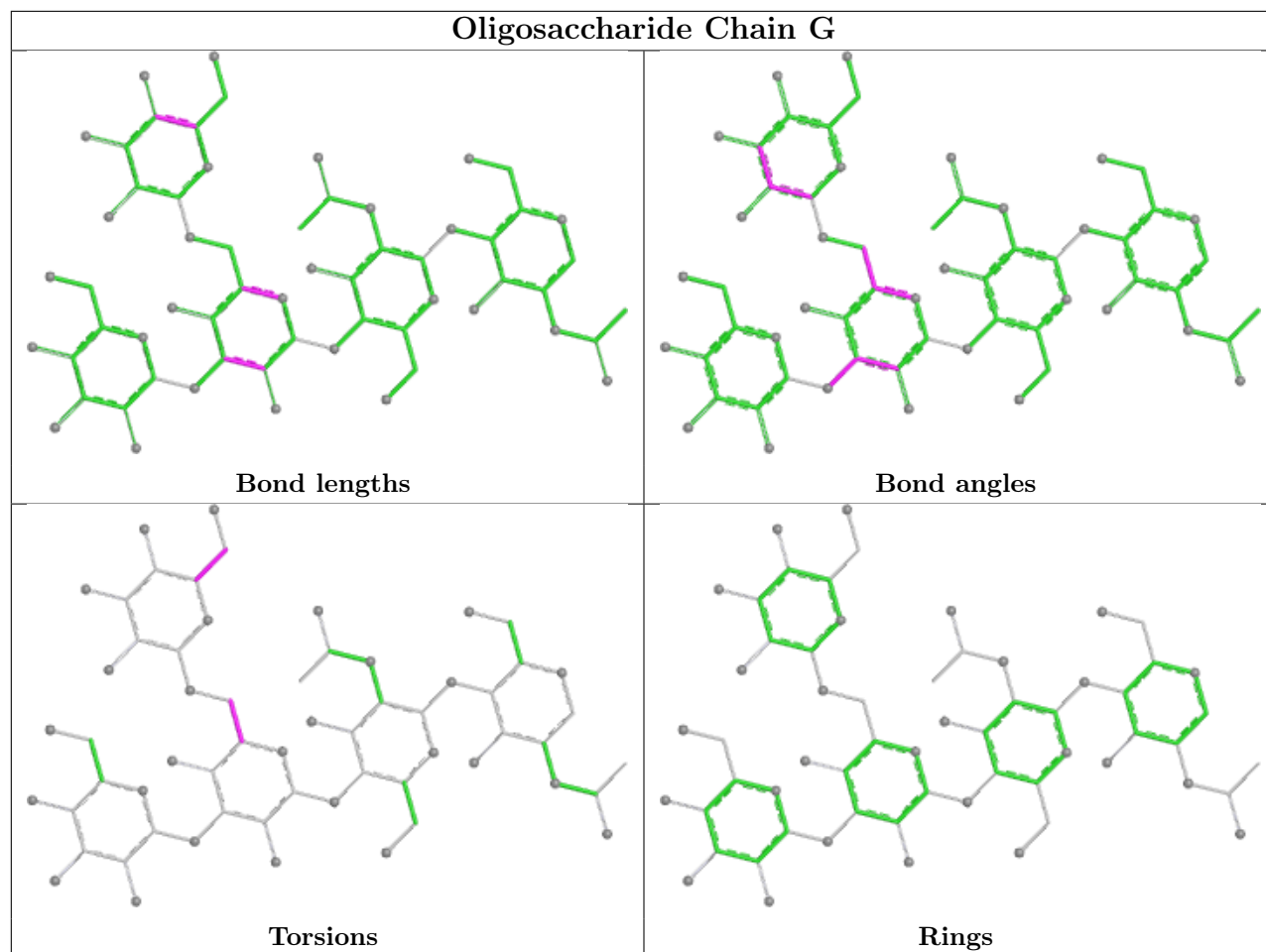
Mol	Chain	Res	Type	Atoms
5	G	5	BMA	O5-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
6	I	2	NAG	O5-C5-C6-O6
7	J	3	BMA	O5-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
6	I	1	NAG	C1-C2-N2-C7

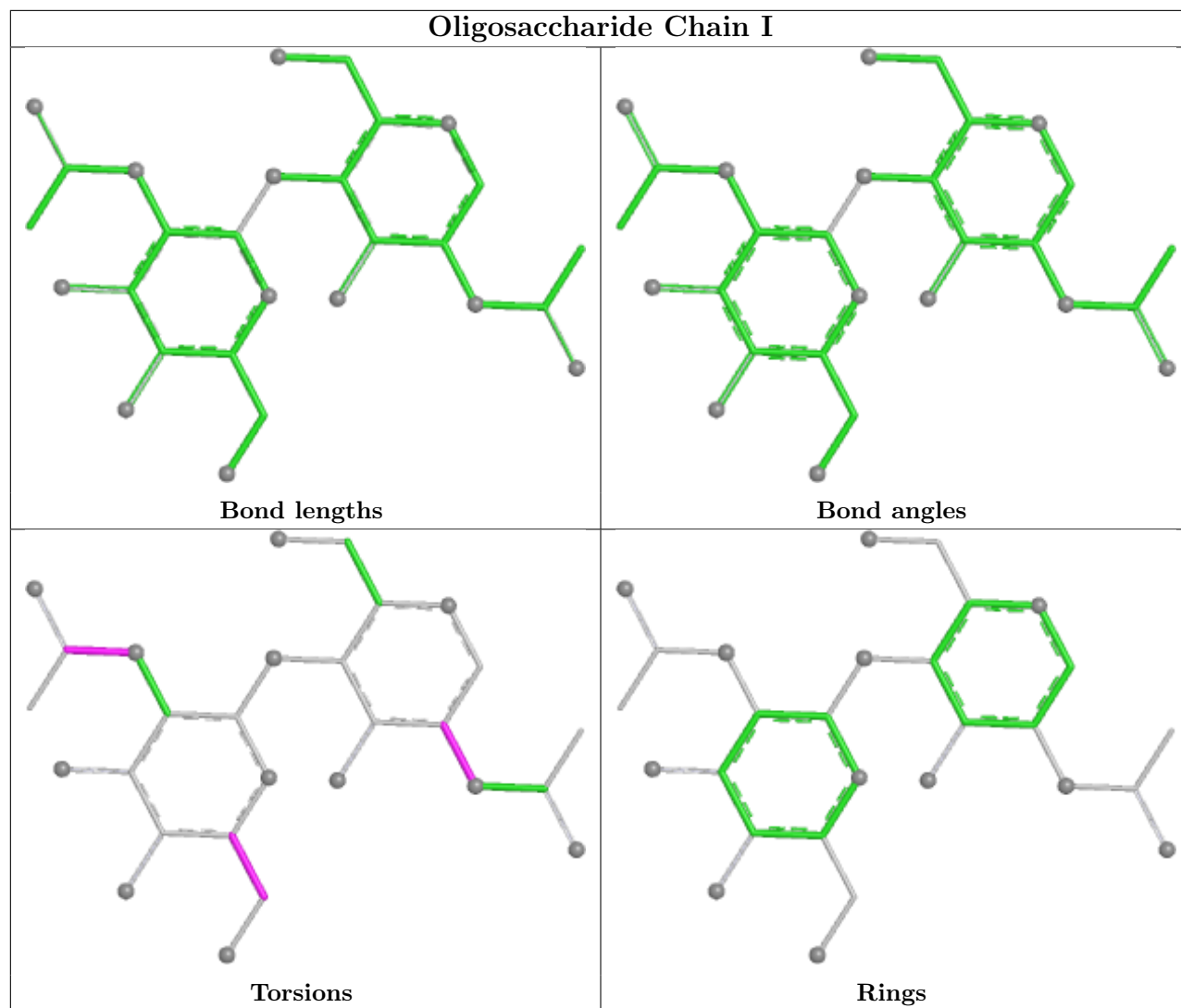
There are no ring outliers.

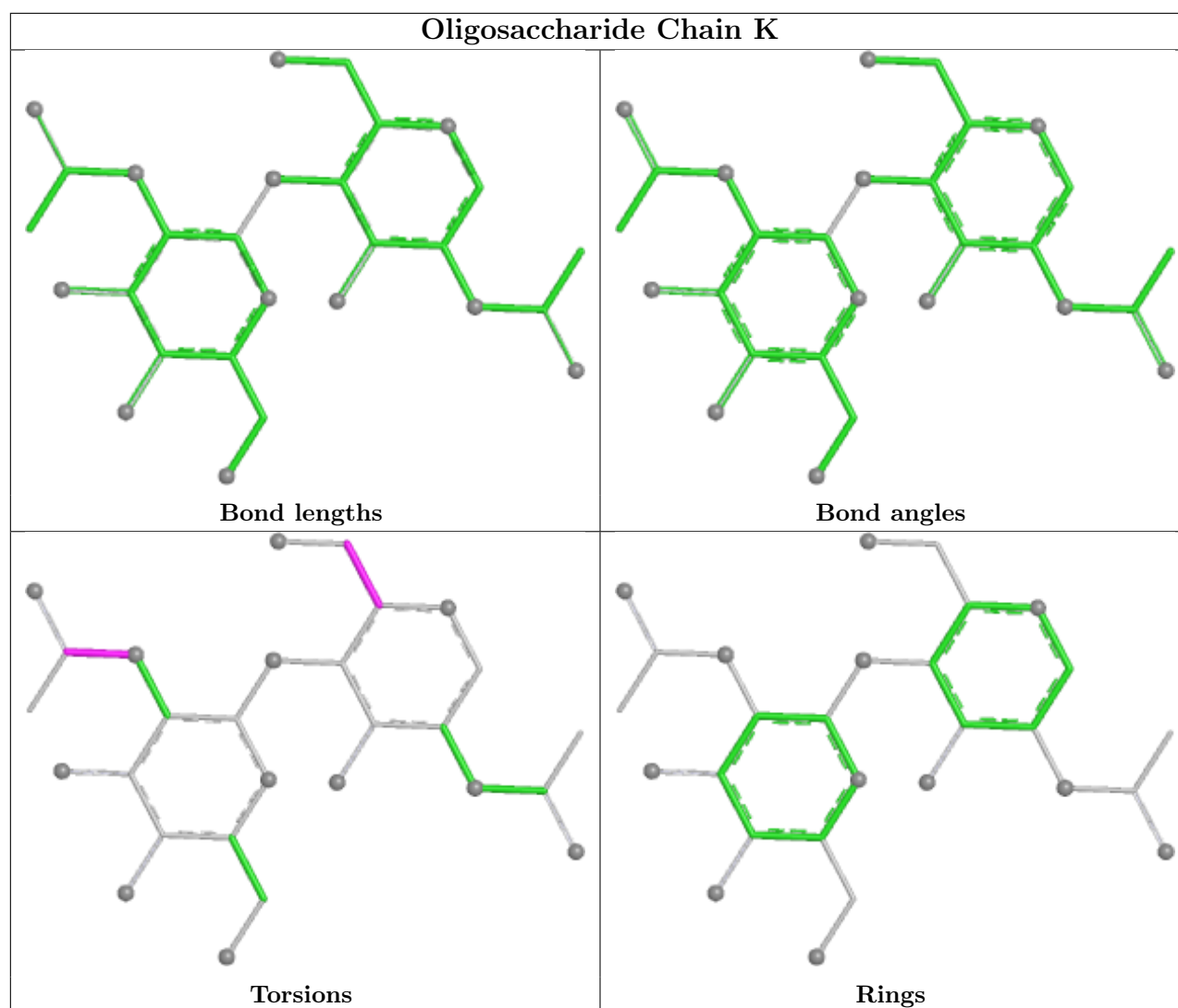
4 monomers are involved in 3 short contacts:

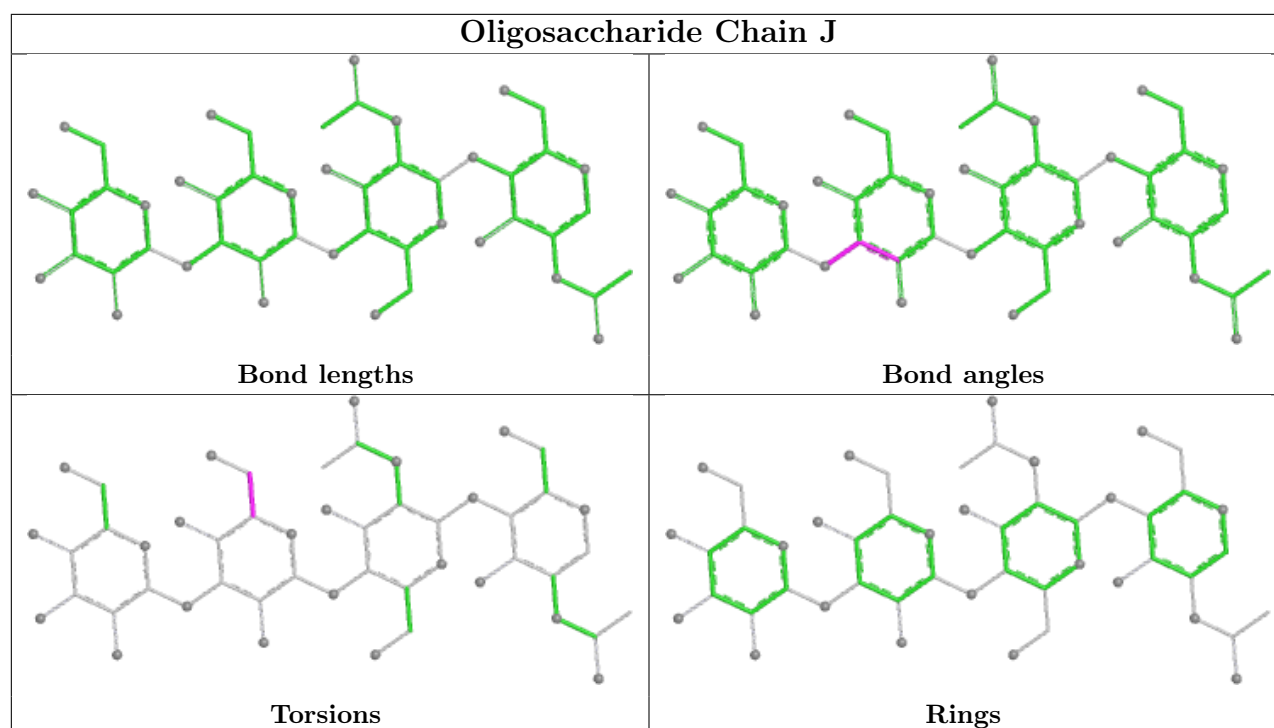
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	3	BMA	1	0
5	G	4	BMA	1	0
6	I	1	NAG	1	0
5	G	5	BMA	1	0

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









5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 15 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
9	SO4	C	508	-	4,4,4	0.24	0	6,6,6	0.10	0
9	SO4	A	509	-	4,4,4	0.24	0	6,6,6	0.10	0
9	SO4	C	506	-	4,4,4	0.24	0	6,6,6	0.08	0
12	I1F	B	2005	10	39,41,41	5.16	20 (51%)	45,58,58	2.52	7 (15%)
11	NAG	D	2004	2	14,14,15	0.35	0	17,19,21	0.54	0
9	SO4	A	507	-	4,4,4	0.24	0	6,6,6	0.07	0
9	SO4	A	508	-	4,4,4	0.24	0	6,6,6	0.07	0
9	SO4	A	505	-	4,4,4	0.24	0	6,6,6	0.06	0
9	SO4	C	507	-	4,4,4	0.24	0	6,6,6	0.06	0
12	I1F	D	2005	10	39,41,41	5.20	20 (51%)	45,58,58	2.55	7 (15%)
9	SO4	A	506	-	4,4,4	0.22	0	6,6,6	0.07	0
11	NAG	B	2004	2	14,14,15	0.42	0	17,19,21	0.54	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
12	I1F	D	2005	10	-	2/30/41/41	0/4/4/4
11	NAG	D	2004	2	-	2/6/23/26	0/1/1/1
11	NAG	B	2004	2	-	0/6/23/26	0/1/1/1
12	I1F	B	2005	10	-	4/30/41/41	0/4/4/4

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	2005	I1F	C27-N28	12.74	1.51	1.34
12	B	2005	I1F	C27-N28	12.72	1.51	1.34
12	D	2005	I1F	C34-C35	11.99	1.51	1.37
12	B	2005	I1F	C34-C35	11.82	1.51	1.37
12	D	2005	I1F	C35-C27	10.78	1.57	1.40
12	B	2005	I1F	C35-C27	10.77	1.57	1.40
12	D	2005	I1F	C15-C14	8.74	1.52	1.38
12	D	2005	I1F	O19-N17	8.62	1.37	1.22
12	B	2005	I1F	O19-N17	8.62	1.37	1.22
12	B	2005	I1F	C15-C14	8.59	1.52	1.38
12	D	2005	I1F	C06-C05	8.43	1.52	1.38
12	D	2005	I1F	C38-C04	8.27	1.51	1.39
12	B	2005	I1F	C38-C04	8.22	1.51	1.39
12	B	2005	I1F	C06-C05	8.14	1.52	1.38
12	D	2005	I1F	C37-C07	8.12	1.51	1.39
12	B	2005	I1F	C37-C07	8.11	1.51	1.39
12	B	2005	I1F	C20-C16	7.45	1.52	1.38
12	D	2005	I1F	C20-C16	7.43	1.52	1.38
12	D	2005	I1F	C21-C13	6.76	1.52	1.38
12	B	2005	I1F	C21-C13	6.75	1.52	1.38
12	D	2005	I1F	C22-N24	6.63	1.44	1.35
12	B	2005	I1F	C22-N24	6.46	1.44	1.35
12	D	2005	I1F	C26-C27	-5.36	1.42	1.50
12	B	2005	I1F	C26-C27	-5.20	1.43	1.50
12	D	2005	I1F	C08-N10	3.96	1.43	1.34
12	B	2005	I1F	C08-N10	3.86	1.43	1.34
12	D	2005	I1F	C36-C35	3.86	1.59	1.51
12	B	2005	I1F	C36-C35	3.76	1.59	1.51
12	D	2005	I1F	C36-N24	3.20	1.51	1.46
12	B	2005	I1F	C36-N24	3.14	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	2005	I1F	C04-C02	2.99	1.53	1.47
12	B	2005	I1F	C25-C26	-2.87	1.46	1.51
12	B	2005	I1F	C04-C02	2.82	1.52	1.47
12	D	2005	I1F	C25-C26	-2.77	1.46	1.51
12	B	2005	I1F	C06-C07	-2.64	1.35	1.39
12	B	2005	I1F	C05-C04	-2.58	1.35	1.39
12	D	2005	I1F	C06-C07	-2.47	1.35	1.39
12	D	2005	I1F	C05-C04	-2.46	1.35	1.39
12	B	2005	I1F	C38-C37	-2.13	1.35	1.38
12	D	2005	I1F	C38-C37	-2.13	1.35	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	2005	I1F	C26-C25-N24	11.23	121.61	110.03
12	B	2005	I1F	C26-C25-N24	10.20	120.55	110.03
12	B	2005	I1F	C34-N29-N28	7.00	116.93	111.45
12	B	2005	I1F	C30-N29-C34	-6.57	121.22	129.38
12	D	2005	I1F	C30-N29-C34	-6.42	121.41	129.38
12	D	2005	I1F	C34-N29-N28	6.41	116.47	111.45
12	B	2005	I1F	C35-C36-N24	-5.98	102.51	111.56
12	D	2005	I1F	C35-C36-N24	-5.02	103.96	111.56
12	D	2005	I1F	C35-C34-N29	3.82	112.04	107.61
12	B	2005	I1F	C35-C34-N29	3.42	111.58	107.61
12	B	2005	I1F	C36-C35-C34	3.04	137.43	129.19
12	D	2005	I1F	C36-C35-C34	3.01	137.34	129.19
12	D	2005	I1F	O32-C31-C30	2.48	120.53	112.21
12	B	2005	I1F	O32-C31-C30	2.26	119.78	112.21

There are no chirality outliers.

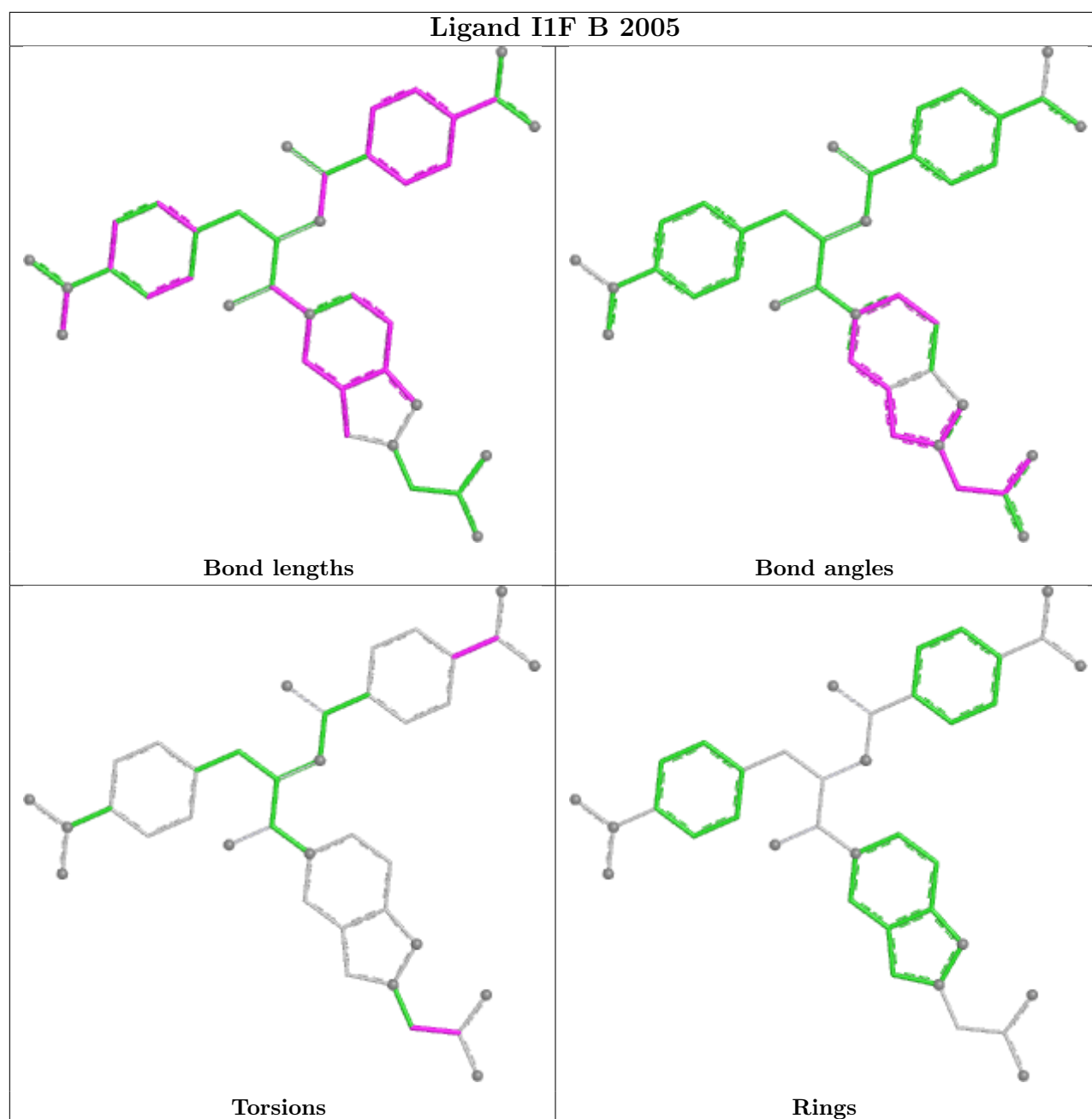
All (8) torsion outliers are listed below:

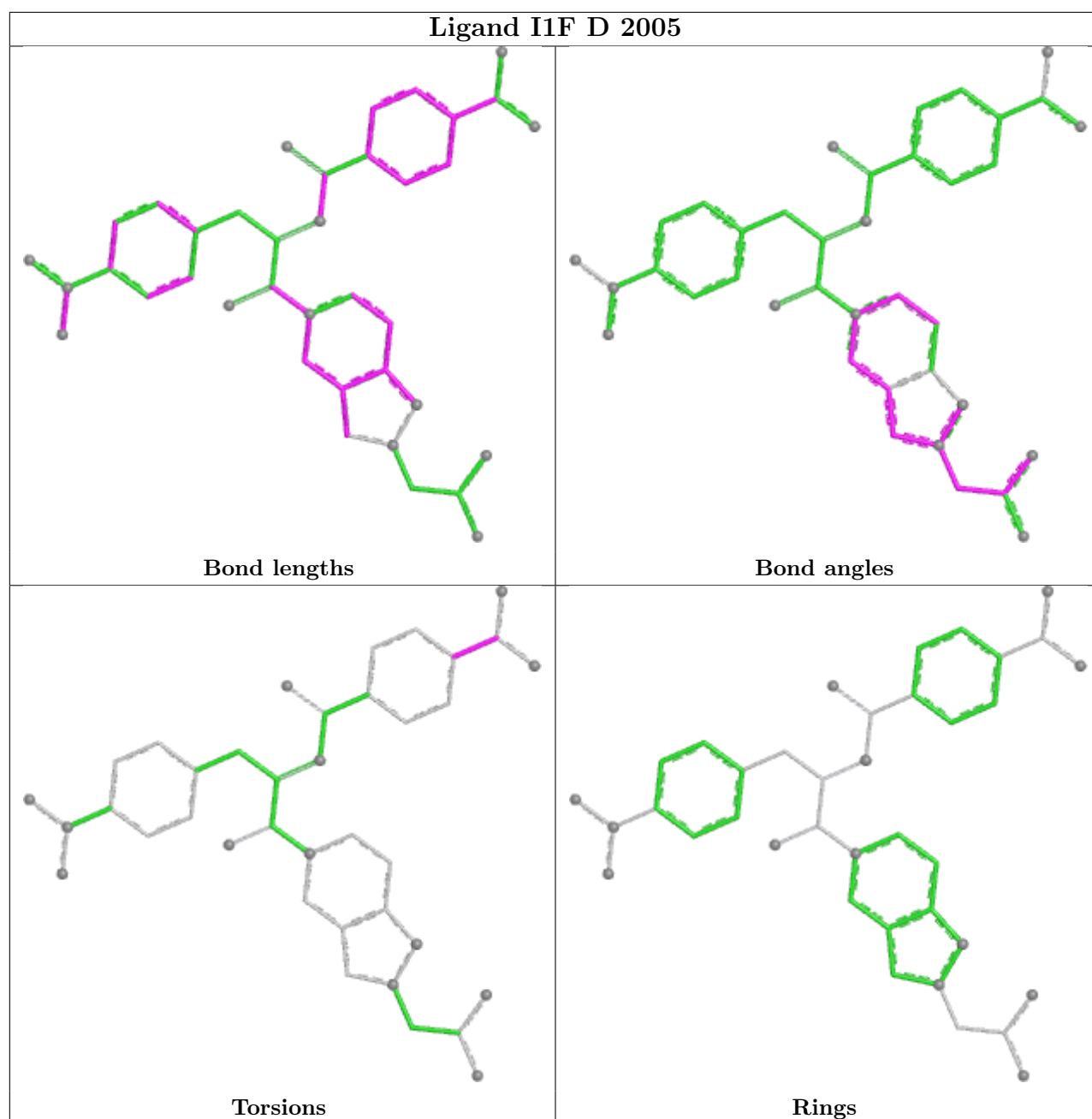
Mol	Chain	Res	Type	Atoms
12	B	2005	I1F	N01-C02-C04-C05
12	B	2005	I1F	N01-C02-C04-C38
12	D	2005	I1F	N01-C02-C04-C05
12	D	2005	I1F	N01-C02-C04-C38
11	D	2004	NAG	O5-C5-C6-O6
11	D	2004	NAG	C4-C5-C6-O6
12	B	2005	I1F	N29-C30-C31-O33
12	B	2005	I1F	N29-C30-C31-O32

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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, 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	453/457 (99%)	-0.26	7 (1%) 71 68	19, 34, 57, 93	6 (1%)
1	C	453/457 (99%)	0.16	10 (2%) 62 59	23, 46, 75, 110	4 (0%)
2	B	466/472 (98%)	0.61	49 (10%) 13 12	17, 62, 128, 152	5 (1%)
2	D	471/472 (99%)	0.67	34 (7%) 23 21	21, 58, 107, 142	2 (0%)
3	E	214/221 (96%)	1.73	80 (37%) 1 1	52, 92, 121, 149	0
3	H	216/221 (97%)	1.00	35 (16%) 5 5	41, 72, 122, 131	0
4	F	214/214 (100%)	1.71	75 (35%) 1 1	59, 89, 160, 173	0
4	L	214/214 (100%)	0.62	7 (3%) 49 46	43, 64, 92, 140	0
All	All	2701/2728 (99%)	0.61	297 (10%) 12 11	17, 57, 121, 173	17 (0%)

All (297) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	125	LEU	5.3
3	E	133	VAL	5.0
4	F	209	PHE	4.9
2	B	450	ASN	4.8
2	B	181	LYS	4.5
2	B	4	ILE	4.4
2	B	375	LEU	4.3
3	E	212	VAL	4.2
4	F	181	LEU	4.2
4	F	144	ILE	4.2
1	C	1	LEU	4.1
2	B	36	PRO	4.1
4	F	126	THR	4.1
3	E	134	CYS	4.0
3	H	138	THR	4.0
4	F	176	SER	4.0

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Mol	Chain	Res	Type	RSRZ
3	E	165	LEU	3.9
3	H	160	TRP	3.9
3	E	132	PRO	3.8
2	B	295	MET	3.8
2	B	466	TRP	3.8
2	D	44	LEU	3.8
4	F	146	VAL	3.8
3	H	201	CYS	3.8
3	H	177	GLN	3.7
3	E	85	SER	3.6
4	F	127	SER	3.6
4	F	133	VAL	3.6
4	F	192	TYR	3.6
3	E	127	VAL	3.6
2	D	376	ASN	3.6
4	F	158	GLY	3.6
2	B	44	LEU	3.5
4	F	135	PHE	3.5
3	H	178	SER	3.5
4	F	193	THR	3.5
4	F	148	TRP	3.5
3	H	212	VAL	3.5
3	H	150	GLY	3.4
2	B	10	VAL	3.4
2	B	78	SER	3.4
2	D	10	VAL	3.4
2	B	35	SER	3.4
2	D	2	PRO	3.4
3	E	149	LYS	3.4
2	B	25	TRP	3.4
3	E	141	SER	3.3
2	B	37	ARG	3.3
2	B	46	LYS	3.3
2	B	27	SER	3.3
3	E	83	LEU	3.3
1	A	339	ALA	3.3
3	E	183	LEU	3.3
3	H	200	THR	3.3
4	F	130	ALA	3.3
1	C	339	ALA	3.2
4	F	131	SER	3.2
3	H	216	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
4	F	186	TYR	3.2
2	D	79	GLN	3.2
4	F	136	LEU	3.2
4	F	132	VAL	3.2
2	B	11	SER	3.2
2	B	39	ASP	3.1
1	C	453	VAL	3.1
4	F	200	THR	3.1
4	F	105	GLU	3.1
4	F	9	SER	3.1
4	F	174	SER	3.1
3	E	199	ILE	3.1
2	B	49	CYS	3.1
3	E	21	SER	3.1
4	F	208	SER	3.1
3	E	115	VAL	3.1
3	E	204	ALA	3.1
3	H	144	LEU	3.1
2	D	48	ASN	3.1
2	B	439	ALA	3.1
3	E	128	TYR	3.1
2	B	40	LEU	3.0
3	E	11	LEU	3.0
4	F	179	LEU	3.0
2	D	179	ASP	3.0
2	B	22	MET	3.0
2	D	77	SER	3.0
3	E	150	GLY	3.0
2	D	129	TRP	3.0
4	F	187	GLU	3.0
3	E	207	ALA	3.0
2	B	30	ALA	2.9
3	E	16	ALA	2.9
4	F	164	THR	2.9
2	D	1	GLY	2.9
2	D	36	PRO	2.9
3	E	214	LYS	2.9
2	B	465	GLY	2.9
3	H	198	SER	2.9
2	D	4	ILE	2.9
3	E	196	SER	2.9
4	F	175	MET	2.9

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Mol	Chain	Res	Type	RSRZ
3	E	124	ALA	2.9
4	F	117	ILE	2.8
2	B	32	PRO	2.8
3	E	186	SER	2.8
4	F	153	SER	2.8
2	B	79	GLN	2.8
3	E	169	VAL	2.8
4	F	180	THR	2.8
4	F	210	ASN	2.8
3	H	196	SER	2.8
3	E	187	VAL	2.8
2	B	33	LEU	2.8
3	E	87	THR	2.8
3	H	199	ILE	2.8
3	E	84	SER	2.8
3	E	118	SER	2.8
4	F	111	ALA	2.8
3	E	176	LEU	2.7
1	C	335	ARG	2.7
4	F	150	ILE	2.7
4	F	205	ILE	2.7
3	E	181	TYR	2.7
2	B	26	CYS	2.7
3	E	90	ASP	2.7
4	L	184	ASP	2.7
4	F	113	PRO	2.7
4	F	152	GLY	2.7
4	F	116	SER	2.7
3	E	12	VAL	2.7
3	H	142	VAL	2.7
3	H	165	LEU	2.7
3	E	123	THR	2.7
3	H	194	TRP	2.7
2	D	469	SER	2.7
3	E	151	TYR	2.7
2	D	181	LYS	2.7
3	E	86	LEU	2.6
2	B	179	ASP	2.6
4	F	194	CYS	2.6
3	E	200	THR	2.6
2	B	24	ALA	2.6
3	E	201	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
3	H	87	THR	2.6
2	D	450	ASN	2.6
4	F	160	LEU	2.6
2	D	446	HIS	2.6
3	E	160	TRP	2.6
2	B	34	GLY	2.6
2	B	48	ASN	2.6
2	D	471	CYS	2.6
3	E	67	LYS	2.5
3	E	121	LYS	2.5
3	E	18	VAL	2.5
3	E	178	SER	2.5
4	L	111	ALA	2.5
4	F	137	ASN	2.5
3	H	67	LYS	2.5
4	F	206	VAL	2.5
2	B	101	SER	2.5
3	E	68	ALA	2.5
3	E	191	SER	2.5
2	B	2	PRO	2.5
2	D	383	LEU	2.5
3	E	170	HIS	2.5
4	F	163	TRP	2.5
3	E	153	PRO	2.5
4	F	120	PRO	2.5
3	E	216	ILE	2.5
2	D	387	MET	2.5
3	H	214	LYS	2.5
4	F	91	TYR	2.5
1	A	338	HIS	2.5
3	E	148	VAL	2.5
3	E	189	VAL	2.5
3	H	189	VAL	2.5
1	A	337	PRO	2.5
4	F	178	THR	2.5
4	F	182	THR	2.5
4	F	207	LYS	2.5
2	B	45	LEU	2.4
2	B	446	HIS	2.4
4	F	189	HIS	2.4
2	B	19	VAL	2.4
2	B	14	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
3	E	184	SER	2.4
3	E	194	TRP	2.4
4	F	31	SER	2.4
3	E	122	THR	2.4
1	C	340	LEU	2.4
3	H	152	PHE	2.4
4	F	118	PHE	2.4
2	B	178	TYR	2.4
2	D	80	VAL	2.4
3	H	206	PRO	2.4
4	F	115	VAL	2.4
3	E	120	ALA	2.4
4	F	10	SER	2.4
4	F	162	SER	2.4
3	E	182	THR	2.4
2	D	375	LEU	2.4
3	E	202	ASN	2.4
3	H	134	CYS	2.4
2	B	74	SER	2.4
1	C	336	GLY	2.4
4	F	3	LEU	2.3
1	A	45	PRO	2.3
2	B	38	CYS	2.3
3	E	175	VAL	2.3
2	B	1	GLY	2.3
3	E	113	THR	2.3
3	E	147	LEU	2.3
3	E	97	VAL	2.3
2	D	11	SER	2.3
2	D	78	SER	2.3
4	F	128	GLY	2.3
2	D	45	LEU	2.3
3	E	180	LEU	2.3
3	E	210	THR	2.3
4	F	114	THR	2.3
3	E	172	PHE	2.3
4	L	135	PHE	2.3
4	F	190	ASN	2.3
4	L	212	ASN	2.3
2	D	180	MET	2.3
2	B	406	CYS	2.3
2	D	33	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	97	SER	2.3
3	E	49	GLY	2.3
2	B	6	THR	2.3
4	F	199	LYS	2.3
4	F	184	ASP	2.3
2	B	376	ASN	2.3
2	B	449	ASN	2.3
2	D	178	TYR	2.3
4	L	214	CYS	2.3
3	E	144	LEU	2.2
3	H	11	LEU	2.2
2	D	35	SER	2.2
3	E	190	THR	2.2
4	F	14	SER	2.2
3	E	195	PRO	2.2
2	D	379	VAL	2.2
3	H	151	TYR	2.2
2	D	30	ALA	2.2
3	H	207	ALA	2.2
4	F	84	ALA	2.2
4	F	122	SER	2.2
4	F	201	SER	2.2
2	B	431	PHE	2.2
3	H	179	ASP	2.2
3	E	65	GLN	2.2
3	E	112	GLY	2.2
3	E	145	GLY	2.2
2	B	5	CYS	2.2
3	E	116	THR	2.2
3	H	119	SER	2.2
4	F	20	SER	2.2
2	B	58	VAL	2.2
2	D	22	MET	2.2
1	A	46	SER	2.2
3	E	114	SER	2.2
3	H	126	SER	2.2
1	C	45	PRO	2.2
4	F	32	ASN	2.2
4	F	173	TYR	2.1
2	B	387	MET	2.1
1	A	32[A]	ARG	2.1
4	F	197	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	75	SER	2.1
3	H	192	SER	2.1
3	E	125	PRO	2.1
3	H	217	GLU	2.1
4	L	105	GLU	2.1
3	H	187	VAL	2.1
1	A	335	ARG	2.1
3	H	133	VAL	2.1
3	E	24	ALA	2.1
3	E	155	PRO	2.1
4	F	183	LYS	2.1
4	L	190	ASN	2.1
1	C	79	VAL	2.1
1	C	248	LEU	2.1
2	D	72	LYS	2.1
4	F	142	LYS	2.1
3	H	161	ASN	2.1
3	H	183	LEU	2.0
4	F	196	ALA	2.0
2	D	468	GLY	2.0
3	E	95	TYR	2.0
3	E	143	THR	2.0
4	F	204	PRO	2.0
3	E	164	SER	2.0
4	F	214	CYS	2.0
1	C	319	ASP	2.0
4	F	149	LYS	2.0
3	E	126	SER	2.0
4	F	203	SER	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 ⓘ

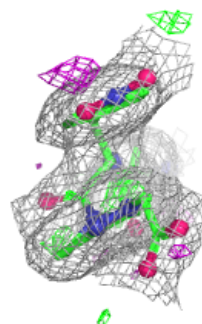
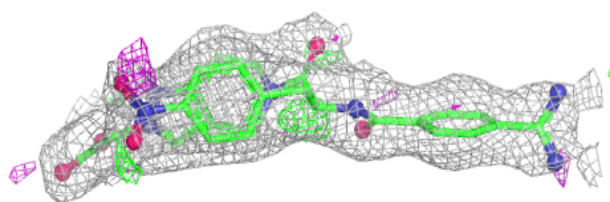
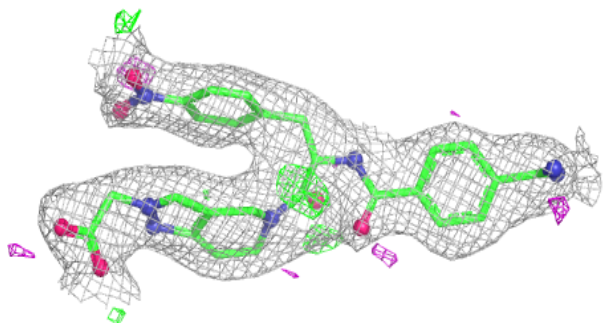
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	NAG	D	2004	14/15	0.71	0.17	84,103,109,115	0
9	SO4	C	507	5/5	0.73	0.14	88,98,100,104	0
9	SO4	C	506	5/5	0.74	0.19	76,85,90,93	0
11	NAG	B	2004	14/15	0.80	0.13	90,105,118,120	0
13	CL	C	501	1/1	0.84	0.20	92,92,92,92	0
9	SO4	C	508	5/5	0.87	0.10	66,68,74,83	5
9	SO4	A	506	5/5	0.89	0.14	69,70,73,80	0
9	SO4	A	507	5/5	0.89	0.13	62,80,86,88	0
9	SO4	A	508	5/5	0.90	0.16	80,84,88,94	0
12	IIF	D	2005	38/38	0.91	0.13	28,42,71,74	0
9	SO4	A	509	5/5	0.91	0.13	50,58,63,67	0
9	SO4	A	505	5/5	0.92	0.17	68,72,77,83	0
12	IIF	B	2005	38/38	0.94	0.09	21,37,53,68	0
10	MG	B	2001	1/1	0.95	0.06	21,21,21,21	0
8	CA	A	503	1/1	0.95	0.05	28,28,28,28	0
8	CA	B	2002	1/1	0.96	0.06	43,43,43,43	0
8	CA	D	2002	1/1	0.96	0.05	40,40,40,40	0
10	MG	D	2001	1/1	0.97	0.05	23,23,23,23	0
8	CA	C	505	1/1	0.97	0.05	52,52,52,52	0
8	CA	A	502	1/1	0.98	0.03	31,31,31,31	0
8	CA	C	504	1/1	0.98	0.04	56,56,56,56	0
8	CA	D	2003	1/1	0.98	0.07	34,34,34,34	0
8	CA	C	503	1/1	0.99	0.04	58,58,58,58	0
8	CA	A	504	1/1	0.99	0.03	31,31,31,31	0
8	CA	A	501	1/1	0.99	0.03	41,41,41,41	0
8	CA	B	2003	1/1	0.99	0.02	32,32,32,32	0
8	CA	C	502	1/1	0.99	0.03	60,60,60,60	0

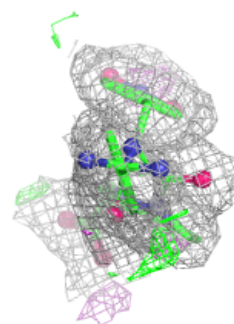
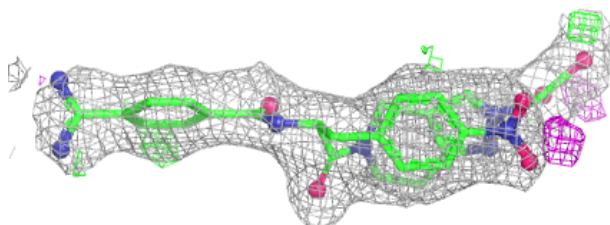
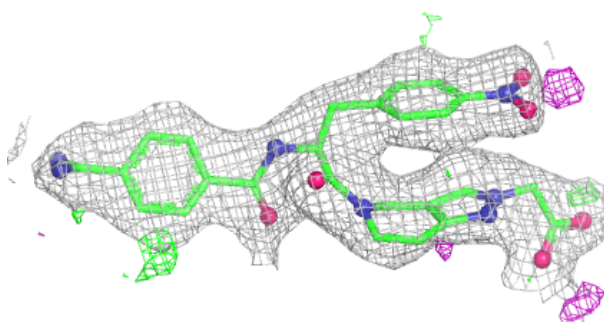
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around I1F 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 I1F 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.