



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:01 PM UTC

PDB ID : 3G0C / pdb_00003g0c
Title : Crystal structure of dipeptidyl peptidase IV in complex with a pyrimidinedione inhibitor 1
Authors : Zhang, Z.; Wallace, M.B.; Feng, J.; Stafford, J.A.; Kaldor, S.W.; Shi, L.; Skene, R.J.; Aertgeerts, K.; Lee, B.; Jennings, A.; Xu, R.; Kassel, D.; Webb, D.R.; Gwaltney, S.L.
Deposited on : 2009-01-27
Resolution : 2.69 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](#) ①) were used in the production of this report:

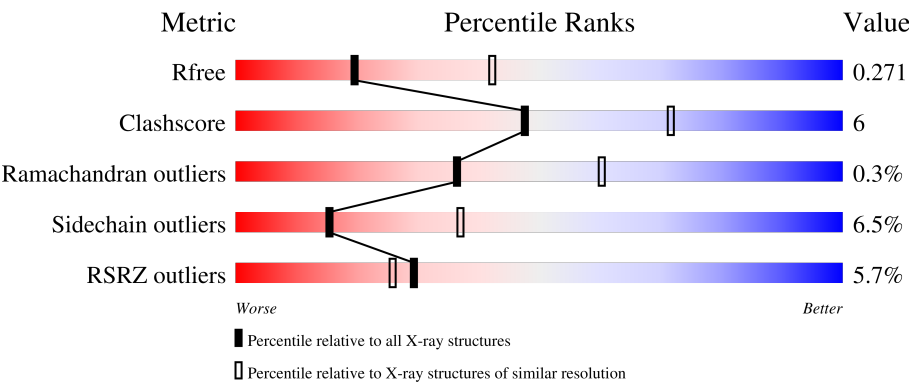
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.69 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	740	
1	B	740	
1	C	740	
1	D	740	
2	E	2	

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Mol	Chain	Length	Quality of chain
2	F	2	50% 50%
2	G	2	100%
2	H	2	50% 50%
2	I	2	100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24940 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	723	Total	C	N	O	S	0	1	0
			5920	3804	972	1118	26			
1	B	729	Total	C	N	O	S	0	1	0
			5972	3834	986	1126	26			
1	C	724	Total	C	N	O	S	0	1	0
			5929	3809	974	1120	26			
1	D	724	Total	C	N	O	S	0	0	0
			5929	3809	974	1120	26			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	expression tag	UNP P27487
A	28	ASP	-	expression tag	UNP P27487
A	29	PRO	-	expression tag	UNP P27487
A	30	GLY	-	expression tag	UNP P27487
A	31	GLY	-	expression tag	UNP P27487
A	32	SER	-	expression tag	UNP P27487
A	33	HIS	-	expression tag	UNP P27487
A	34	HIS	-	expression tag	UNP P27487
A	35	HIS	-	expression tag	UNP P27487
A	36	HIS	-	expression tag	UNP P27487
A	37	HIS	-	expression tag	UNP P27487
A	38	HIS	-	expression tag	UNP P27487
B	27	ALA	-	expression tag	UNP P27487
B	28	ASP	-	expression tag	UNP P27487
B	29	PRO	-	expression tag	UNP P27487
B	30	GLY	-	expression tag	UNP P27487
B	31	GLY	-	expression tag	UNP P27487
B	32	SER	-	expression tag	UNP P27487
B	33	HIS	-	expression tag	UNP P27487
B	34	HIS	-	expression tag	UNP P27487
B	35	HIS	-	expression tag	UNP P27487

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Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	expression tag	UNP P27487
B	37	HIS	-	expression tag	UNP P27487
B	38	HIS	-	expression tag	UNP P27487
C	27	ALA	-	expression tag	UNP P27487
C	28	ASP	-	expression tag	UNP P27487
C	29	PRO	-	expression tag	UNP P27487
C	30	GLY	-	expression tag	UNP P27487
C	31	GLY	-	expression tag	UNP P27487
C	32	SER	-	expression tag	UNP P27487
C	33	HIS	-	expression tag	UNP P27487
C	34	HIS	-	expression tag	UNP P27487
C	35	HIS	-	expression tag	UNP P27487
C	36	HIS	-	expression tag	UNP P27487
C	37	HIS	-	expression tag	UNP P27487
C	38	HIS	-	expression tag	UNP P27487
D	27	ALA	-	expression tag	UNP P27487
D	28	ASP	-	expression tag	UNP P27487
D	29	PRO	-	expression tag	UNP P27487
D	30	GLY	-	expression tag	UNP P27487
D	31	GLY	-	expression tag	UNP P27487
D	32	SER	-	expression tag	UNP P27487
D	33	HIS	-	expression tag	UNP P27487
D	34	HIS	-	expression tag	UNP P27487
D	35	HIS	-	expression tag	UNP P27487
D	36	HIS	-	expression tag	UNP P27487
D	37	HIS	-	expression tag	UNP P27487
D	38	HIS	-	expression tag	UNP P27487

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



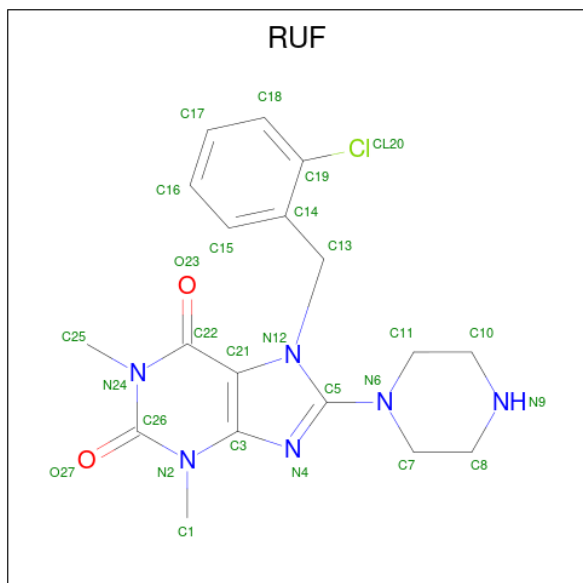
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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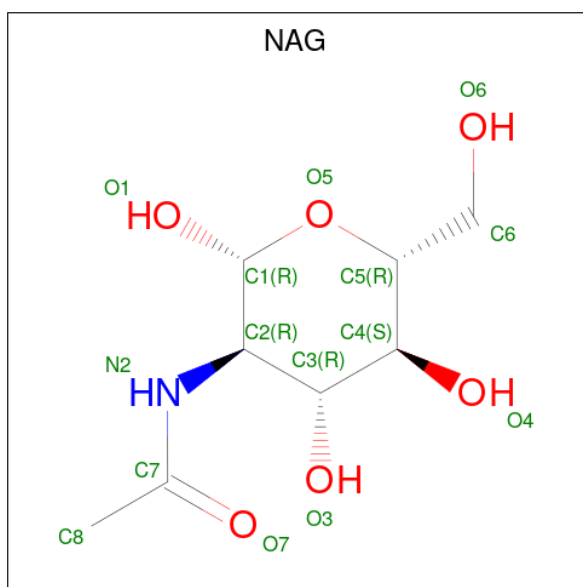
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 7-(2-chlorobenzyl)-1,3-dimethyl-8-piperazin-1-yl-3,7-dihydro-1H-purine-2,6-dione (CCD ID: RUF) (formula: $C_{18}H_{21}ClN_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0
			27	18	1	6	2	
3	B	1	Total	C	Cl	N	O	0
			27	18	1	6	2	
3	C	1	Total	C	Cl	N	O	0
			27	18	1	6	2	
3	D	1	Total	C	Cl	N	O	0
			27	18	1	6	2	

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



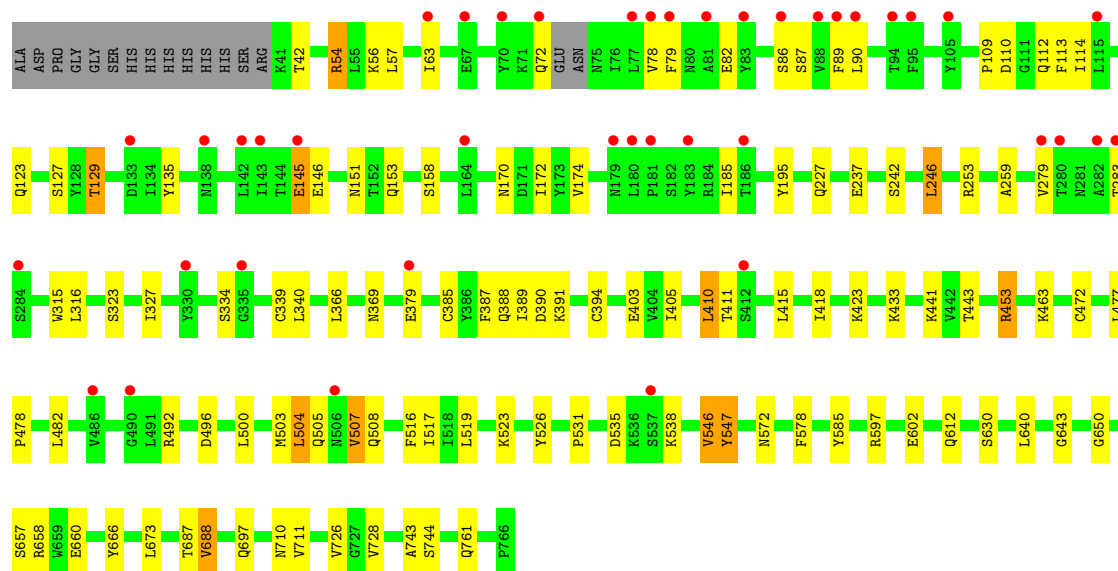
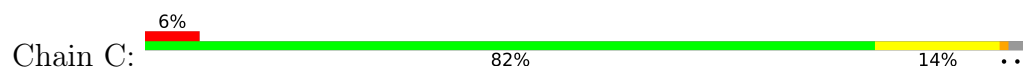
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1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

- Molecule 5 is water.

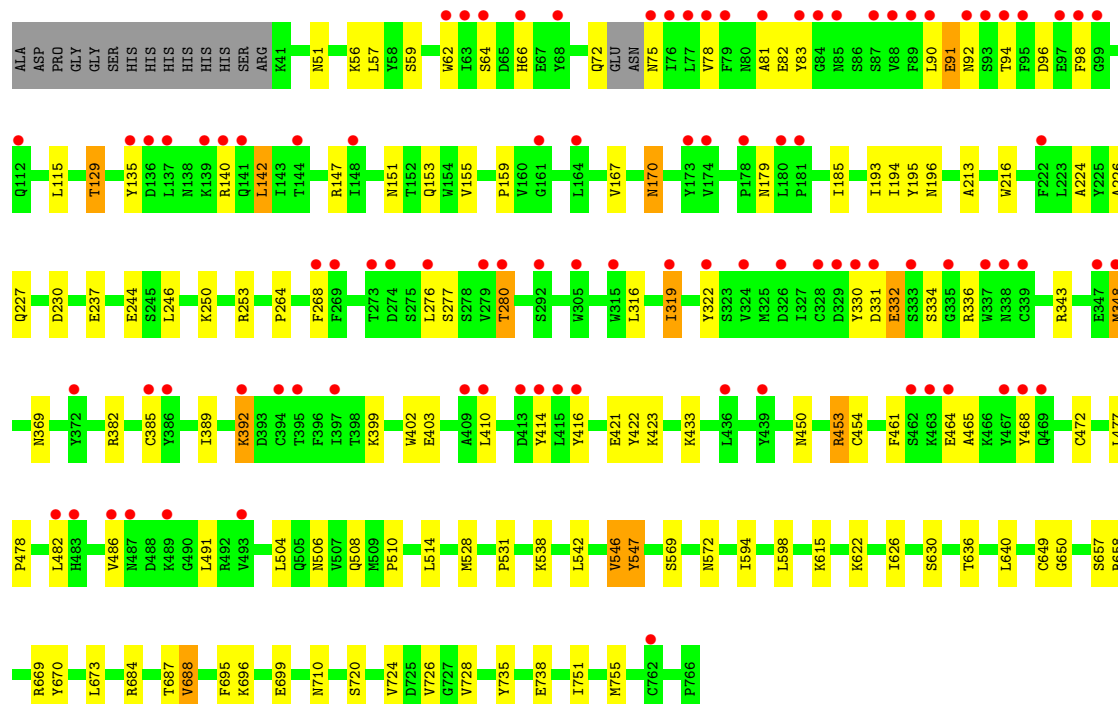
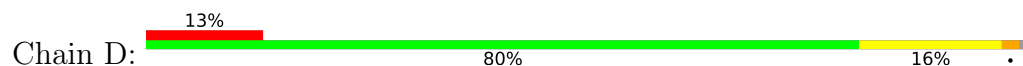
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	231	Total 231	O 231	0	0
5	B	237	Total 237	O 237	0	0
5	C	196	Total 196	O 196	0	0
5	D	110	Total 110	O 110	0	0



• Molecule 1: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4



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

Chain E:  50% 50%

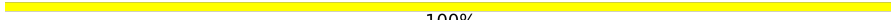
MAG1
MAG2

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

Chain F:  50% 50%

MAG1
MAG2

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

Chain G:  100%

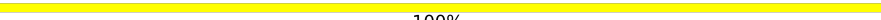
MAG1
MAG2

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

Chain H:  50% 50%

MAG1
MAG2

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

Chain I:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.84Å 122.77Å 145.11Å 90.00° 114.68° 90.00°	Depositor
Resolution (Å)	50.00 – 2.69 50.00 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.69) 99.5 (50.00-2.69)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.195 , 0.248 0.234 , 0.271	Depositor DCC
R_{free} test set	5412 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	24940	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.53	0/6091	0.83	3/8284 (0.0%)
1	B	0.55	1/6149 (0.0%)	0.84	4/8362 (0.0%)
1	C	0.55	0/6100	0.81	1/8296 (0.0%)
1	D	0.55	2/6100 (0.0%)	0.82	3/8296 (0.0%)
All	All	0.55	3/24440 (0.0%)	0.83	11/33238 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	531	PRO	CA-C	5.70	1.55	1.51
1	D	332	GLU	CD-OE1	5.40	1.35	1.25
1	D	332	GLU	CD-OE2	5.35	1.35	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	546	VAL	N-CA-C	7.22	118.88	108.48
1	B	530	LEU	CA-C-N	6.55	124.44	119.66
1	B	530	LEU	C-N-CA	6.55	124.44	119.66
1	C	546	VAL	N-CA-C	5.83	116.88	108.48
1	A	630	SER	CB-CA-C	-5.81	109.33	117.23
1	D	630	SER	CB-CA-C	-5.80	109.34	117.23
1	D	62	TRP	N-CA-C	5.29	116.76	109.15
1	A	546	VAL	N-CA-C	5.27	116.07	108.48
1	B	141	GLN	N-CA-C	5.26	116.52	108.42
1	A	436	LEU	N-CA-C	5.19	117.67	111.71
1	B	659	TRP	N-CA-C	5.07	118.24	111.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	5920	0	5638	68	0
1	B	5972	0	5681	77	0
1	C	5929	0	5649	53	0
1	D	5929	0	5650	60	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
3	A	27	0	21	2	0
3	B	27	0	21	2	0
3	C	27	0	21	4	0
3	D	27	0	21	2	0
4	A	56	0	52	0	0
4	B	56	0	52	0	0
4	C	28	0	26	0	0
4	D	28	0	26	1	0
5	A	231	0	0	3	0
5	B	237	0	0	4	0
5	C	196	0	0	2	0
5	D	110	0	0	1	0
All	All	24940	0	22983	264	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 6.

All (264) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:GLN:HE22	1:A:170:ASN:H	1.15	0.91
1:C:153:GLN:HE22	1:C:170:ASN:H	1.10	0.90
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.15	0.90
1:A:325:MET:HE1	1:A:371:PHE:CZ	2.09	0.88
1:D:90:LEU:HD12	1:D:140:ARG:HH21	1.39	0.87
1:C:54:ARG:HG2	1:C:54:ARG:HH21	1.41	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:GLN:HE22	1:B:170:ASN:H	1.27	0.79
1:B:327:ILE:HD13	1:B:389:ILE:HG13	1.66	0.77
1:D:277:SER:HB3	1:D:280:THR:HG22	1.70	0.73
1:B:78:VAL:HG22	1:B:89:PHE:HB2	1.70	0.73
1:D:658:ARG:HB2	1:D:687:THR:HG22	1.72	0.72
1:B:391:LYS:HE3	1:B:391:LYS:HA	1.73	0.69
1:D:153:GLN:HE22	1:D:170:ASN:H	1.38	0.69
1:B:82:GLU:HG2	1:B:467:TYR:OH	1.91	0.69
1:C:327:ILE:HD13	1:C:389:ILE:HD12	1.75	0.68
1:B:98:PHE:CE1	1:B:100:HIS:HB2	2.30	0.67
1:A:658:ARG:HB2	1:A:687:THR:HG22	1.76	0.65
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.78	0.65
1:B:36:HIS:CD2	1:B:37:HIS:H	2.14	0.64
1:B:338:ASN:OD1	1:B:340:LEU:HD12	1.97	0.64
1:C:237:GLU:HG2	1:C:253:ARG:HG2	1.80	0.63
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.79	0.63
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.81	0.62
1:B:98:PHE:HE1	1:B:100:HIS:HB2	1.64	0.62
1:B:179:ASN:H	1:B:179:ASN:HD22	1.45	0.61
1:B:597:ARG:HH11	1:B:682:HIS:HB2	1.65	0.61
1:A:399:LYS:HD2	1:A:400:GLY:N	2.16	0.61
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.82	0.60
1:A:358[A]:ARG:HD2	5:A:903:HOH:O	2.01	0.60
1:B:710:ASN:C	1:B:710:ASN:HD22	2.09	0.60
1:D:237:GLU:HG2	1:D:253:ARG:HG2	1.84	0.60
1:B:658:ARG:HB2	1:B:687:THR:HG22	1.83	0.60
1:A:325:MET:HE3	1:A:327:ILE:HD11	1.84	0.59
1:D:450:ASN:O	1:D:454:CYS:HB2	2.03	0.59
1:B:391:LYS:HD3	1:B:392:LYS:H	1.68	0.58
1:A:546:VAL:HG12	1:A:627:TRP:O	2.03	0.57
1:A:170:ASN:N	1:A:170:ASN:HD22	2.02	0.57
1:D:129:THR:HG23	1:D:151:ASN:HA	1.85	0.57
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.85	0.57
1:C:114:ILE:HG23	1:C:135:TYR:HB3	1.86	0.57
1:C:129:THR:HG23	1:C:151:ASN:HA	1.85	0.57
1:D:461:PHE:CD2	1:D:468:TYR:HB3	2.39	0.57
1:D:422:TYR:CE1	1:D:423:LYS:HE2	2.40	0.57
1:D:461:PHE:CD2	1:D:465:ALA:HB1	2.40	0.57
1:A:129:THR:HG23	1:A:151:ASN:HA	1.86	0.57
1:B:334:SER:HB3	1:B:336:ARG:HG3	1.87	0.56
1:C:531:PRO:HB3	1:C:572:ASN:ND2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:GLN:HB2	1:D:75:ASN:HB2	1.87	0.56
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.87	0.56
3:A:800:RUF:C13	3:A:800:RUF:H11	2.36	0.56
1:C:54:ARG:HH21	1:C:54:ARG:CG	2.18	0.55
1:B:455:GLN:HB2	1:B:475:PRO:HD3	1.89	0.54
1:B:283:THR:HG22	5:B:849:HOH:O	2.07	0.54
1:B:415:LEU:HB2	1:B:436:LEU:HD11	1.89	0.54
1:A:516:PHE:CD1	1:A:523:LYS:HG2	2.42	0.54
1:B:41:LYS:HE2	1:B:506:ASN:HB3	1.90	0.54
1:C:112:GLN:HG3	1:C:113:PHE:CD2	2.42	0.54
3:C:800:RUF:H13A	3:C:800:RUF:H11	1.90	0.54
3:A:800:RUF:H11	3:A:800:RUF:H13A	1.88	0.54
1:A:487:ASN:OD1	1:A:489:LYS:HG2	2.08	0.54
1:A:364:PHE:HE2	1:A:389:ILE:HD11	1.74	0.53
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.90	0.53
3:C:800:RUF:H11	3:C:800:RUF:C13	2.37	0.53
1:A:399:LYS:HD2	1:A:400:GLY:H	1.73	0.53
1:C:54:ARG:HG2	1:C:54:ARG:NH2	2.17	0.53
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.92	0.53
1:A:477:LEU:HD12	1:A:477:LEU:H	1.73	0.53
1:D:147:ARG:HE	4:D:801:NAG:H83	1.73	0.53
1:C:535:ASP:HB3	1:C:538:LYS:HG3	1.90	0.52
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.91	0.52
1:D:330:TYR:CE2	1:D:332:GLU:HA	2.44	0.52
1:A:407:ILE:HG23	1:A:415:LEU:CD1	2.38	0.52
1:B:242:SER:HB3	1:B:246:LEU:HD12	1.90	0.52
1:B:657:SER:HA	1:B:688:VAL:HG13	1.90	0.52
1:A:325:MET:HE1	1:A:371:PHE:CE2	2.45	0.52
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.45	0.51
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.75	0.51
1:C:174:VAL:HG23	1:C:185:ILE:HD11	1.93	0.51
3:B:800:RUF:C21	3:B:800:RUF:H15	2.40	0.51
1:C:643:GLY:HA2	1:C:697:GLN:HE22	1.75	0.51
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.91	0.51
1:B:72:GLN:HB2	1:B:75:ASN:HB2	1.93	0.51
1:C:505:GLN:HG2	5:C:849:HOH:O	2.10	0.51
1:D:531:PRO:HB3	1:D:572:ASN:HD22	1.75	0.51
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.92	0.51
1:B:608:GLU:O	1:B:612:GLN:HG2	2.11	0.51
1:D:751:ILE:HG12	1:D:755:MET:HE2	1.92	0.51
1:C:410:LEU:HD22	1:C:411:THR:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:ASP:HB3	1:D:334:SER:HB2	1.93	0.50
1:D:657:SER:HA	1:D:688:VAL:HG13	1.93	0.50
1:B:159:PRO:HD3	1:B:216:TRP:HB3	1.93	0.50
1:C:403:GLU:OE2	1:C:585:TYR:HA	2.12	0.50
3:D:800:RUF:C13	3:D:800:RUF:H11	2.42	0.50
1:C:172:ILE:HG22	1:C:185:ILE:HD12	1.94	0.50
1:C:129:THR:HG22	5:C:777:HOH:O	2.11	0.50
1:D:81:ALA:C	1:D:83:TYR:H	2.19	0.50
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.93	0.50
1:B:649:CYS:HB3	1:B:699:GLU:HB2	1.94	0.50
1:B:598:LEU:HD22	1:B:671:MET:HG2	1.93	0.49
1:A:175:LYS:NZ	1:A:180:LEU:O	2.43	0.49
1:A:710:ASN:HD22	1:A:710:ASN:C	2.21	0.49
1:B:386:TYR:O	1:B:394:CYS:HB2	2.12	0.49
1:D:196:ASN:OD1	1:D:227:GLN:HG3	2.13	0.49
1:D:508:GLN:HG2	5:D:823:HOH:O	2.12	0.49
1:D:695:PHE:HB3	1:D:728:VAL:HG11	1.95	0.49
1:D:382:ARG:H	1:D:403:GLU:HG2	1.76	0.49
1:D:91:GLU:HB3	1:D:94:THR:H	1.77	0.49
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.95	0.49
1:C:145:GLU:HG2	1:C:146:GLU:HG2	1.95	0.49
1:C:453:ARG:NH2	1:C:477:LEU:O	2.41	0.49
1:A:407:ILE:HG23	1:A:415:LEU:HD11	1.94	0.48
1:B:90:LEU:HD21	1:B:95:PHE:HE2	1.77	0.48
1:D:322:TYR:HA	1:D:348:MET:HB3	1.95	0.48
1:B:544:LEU:HD23	1:B:626:ILE:HD12	1.94	0.48
1:C:500:LEU:HA	1:C:503:MET:HE2	1.93	0.48
1:C:526:TYR:HB3	1:C:578:PHE:HD1	1.78	0.48
1:A:80:ASN:HD22	1:A:82:GLU:H	1.61	0.48
1:B:135:TYR:CE1	1:B:141:GLN:HA	2.49	0.48
1:A:129:THR:HG21	1:A:151:ASN:HD22	1.78	0.48
1:A:415:LEU:HD12	1:A:416:TYR:N	2.27	0.48
1:A:471:ARG:HG3	1:A:480:TYR:CE1	2.49	0.48
1:C:315:TRP:O	1:C:323:SER:HB2	2.14	0.48
1:D:482:LEU:HD22	1:D:491:LEU:HD12	1.96	0.48
1:D:75:ASN:HA	1:D:91:GLU:HG3	1.96	0.48
1:A:332:GLU:OE2	1:A:332:GLU:HA	2.14	0.48
1:A:333:SER:O	1:A:334:SER:HB3	2.13	0.47
3:D:800:RUF:H11	3:D:800:RUF:C14	2.44	0.47
1:A:82:GLU:HA	1:A:82:GLU:OE1	2.14	0.47
1:B:471[A]:ARG:HG3	1:B:480:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:VAL:O	1:B:639:VAL:HG23	2.14	0.47
1:D:392:LYS:H	1:D:392:LYS:HD2	1.79	0.47
1:C:504:LEU:HA	1:C:507:VAL:HG13	1.96	0.47
1:A:455:GLN:HE21	1:A:557:THR:HG21	1.79	0.47
1:C:517:ILE:HD13	1:C:612:GLN:HG3	1.97	0.47
1:D:461:PHE:CE2	1:D:468:TYR:HB3	2.49	0.47
1:C:710:ASN:C	1:C:710:ASN:HD22	2.23	0.47
1:A:82:GLU:HG2	1:A:467:TYR:OH	2.15	0.47
1:B:741:GLY:O	1:B:742:ILE:C	2.57	0.47
1:C:174:VAL:CG2	1:C:185:ILE:HD11	2.45	0.47
1:B:472:CYS:O	1:B:478:PRO:HA	2.14	0.46
1:D:91:GLU:HB3	1:D:94:THR:N	2.30	0.46
1:D:135:TYR:CZ	1:D:142:LEU:HB2	2.50	0.46
1:D:369:ASN:O	1:D:389:ILE:HG12	2.16	0.46
1:A:268:PHE:CD2	1:A:313:LEU:HD21	2.50	0.46
1:A:598:LEU:HB2	1:A:671:MET:SD	2.55	0.46
1:A:414:TYR:CE2	1:A:433:LYS:HD3	2.50	0.46
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.80	0.46
1:A:657:SER:HA	1:A:688:VAL:HG13	1.97	0.46
1:A:669:ARG:HD2	1:A:670:TYR:CZ	2.51	0.46
1:D:193:ILE:HG22	1:D:194:ILE:HG12	1.97	0.46
1:D:657:SER:HA	1:D:688:VAL:CG1	2.46	0.46
1:B:109:PRO:HG2	1:B:158:SER:O	2.15	0.46
1:D:115:LEU:HD21	1:D:155:VAL:HG21	1.98	0.46
1:C:643:GLY:HA2	1:C:697:GLN:NE2	2.31	0.46
1:A:102:ILE:HD12	1:A:102:ILE:H	1.80	0.46
1:A:306:ALA:HB3	1:A:310:ARG:HG2	1.98	0.46
1:B:129:THR:HG22	5:B:890:HOH:O	2.16	0.46
1:A:547:TYR:CD1	1:A:547:TYR:C	2.94	0.45
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.98	0.45
1:B:242:SER:OG	1:B:243:ASP:N	2.47	0.45
1:A:312:SER:HA	1:A:326:ASP:O	2.17	0.45
3:B:800:RUF:C14	3:B:800:RUF:H11	2.46	0.45
1:D:696:LYS:HG3	1:D:728:VAL:HG22	1.97	0.45
1:B:491:LEU:O	1:B:492:ARG:HB3	2.17	0.45
1:C:369:ASN:C	1:C:389:ILE:HG12	2.41	0.45
1:C:547:TYR:C	1:C:547:TYR:CD1	2.94	0.45
1:D:319:ILE:H	1:D:319:ILE:HG13	1.55	0.45
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.46	0.45
1:A:156:THR:HG23	1:A:216:TRP:HE1	1.82	0.45
1:B:170:ASN:N	1:B:170:ASN:HD22	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:CYS:HB3	1:B:387:PHE:CE2	2.52	0.45
1:B:547:TYR:CD1	1:B:547:TYR:C	2.94	0.45
1:D:343:ARG:HG2	1:D:389:ILE:HG22	1.99	0.45
1:A:571:GLU:HA	1:A:571:GLU:OE2	2.16	0.45
1:B:56:LYS:HE3	1:B:495:GLU:OE2	2.17	0.45
1:B:134:ILE:HD13	1:B:178:PRO:HB3	1.98	0.44
1:B:340:LEU:HB2	1:B:343:ARG:HG3	2.00	0.44
1:B:302:ASP:HB3	1:B:314:GLN:HB2	2.00	0.44
1:D:213:ALA:HB1	1:D:226:ALA:HB3	1.99	0.44
1:A:388:GLN:NE2	5:A:974:HOH:O	2.50	0.44
1:C:109:PRO:HG2	1:C:158:SER:O	2.18	0.44
1:D:640:LEU:HD11	1:D:650:GLY:HA3	2.00	0.44
1:C:242:SER:HB3	1:C:246:LEU:HD12	1.99	0.44
1:A:253:ARG:HH21	1:B:253:ARG:NH2	1.98	0.43
1:B:258:LYS:O	1:B:259:ALA:C	2.59	0.43
1:A:414:TYR:CD2	1:A:433:LYS:HD3	2.53	0.43
1:A:115:LEU:HD21	1:A:155:VAL:HG21	2.00	0.43
1:B:751:ILE:HG12	1:B:755:MET:HE2	1.99	0.43
1:A:513:LYS:O	1:A:527:GLN:HA	2.18	0.43
1:B:153:GLN:NE2	1:B:167:VAL:HG12	2.33	0.43
1:C:110:ASP:OD2	1:C:112:GLN:HG2	2.19	0.43
1:A:415:LEU:HD12	1:A:415:LEU:C	2.44	0.43
1:B:92:ASN:ND2	5:B:980:HOH:O	2.51	0.43
1:D:230:ASP:OD1	1:D:264:PRO:HB3	2.18	0.43
1:A:89:PHE:O	1:A:90:LEU:HG	2.19	0.43
1:B:70:TYR:HB3	1:B:79:PHE:CE1	2.53	0.43
1:B:127:SER:HB3	1:B:211:TYR:CG	2.54	0.43
1:B:167:VAL:HG11	1:B:198:ILE:HG12	2.01	0.43
1:B:263:ASN:ND2	1:B:299:TYR:OH	2.51	0.43
1:D:402:TRP:CD2	1:D:421:GLU:HB2	2.54	0.43
1:D:720:SER:O	1:D:724:VAL:HG23	2.19	0.43
1:C:657:SER:HA	1:C:688:VAL:HG13	2.00	0.43
1:A:382:ARG:NH2	5:A:1:HOH:O	2.52	0.42
1:C:259:ALA:HB3	1:C:660:GLU:HA	2.01	0.42
1:B:127:SER:HB3	1:B:211:TYR:CD2	2.53	0.42
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.49	0.42
1:A:98:PHE:CE1	1:A:100:HIS:HB2	2.54	0.42
1:B:72:GLN:HG3	1:B:77:LEU:CD2	2.50	0.42
1:D:416:TYR:CE1	1:D:433:LYS:HE2	2.55	0.42
1:B:167:VAL:HA	1:B:171:ASP:O	2.20	0.42
1:B:306:ALA:HB3	1:B:310:ARG:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.50	0.42
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.54	0.42
1:A:403:GLU:OE2	1:A:585:TYR:HA	2.19	0.42
1:A:461:PHE:CD2	1:A:468:TYR:HB3	2.55	0.42
1:B:175:LYS:HG3	1:B:182:SER:HB3	2.02	0.42
1:D:453:ARG:NH2	1:D:477:LEU:O	2.49	0.42
1:C:42:THR:HG22	1:C:508:GLN:HG3	2.02	0.42
1:C:516:PHE:CG	1:C:523:LYS:HE3	2.54	0.42
1:D:96:ASP:C	1:D:98:PHE:H	2.27	0.42
1:D:195:TYR:O	1:D:227:GLN:HA	2.20	0.42
1:D:669:ARG:HD2	1:D:670:TYR:CZ	2.55	0.42
1:B:54:ARG:HG3	5:B:884:HOH:O	2.20	0.42
1:B:95:PHE:HE1	1:B:135:TYR:CD1	2.37	0.42
1:C:388:GLN:HB2	1:C:391:LYS:HG2	2.02	0.42
1:D:626:ILE:HG23	1:D:636:THR:HG23	2.01	0.42
1:A:456:TYR:HB2	1:A:557:THR:OG1	2.20	0.41
1:D:472:CYS:O	1:D:478:PRO:HA	2.20	0.41
1:C:472:CYS:O	1:C:478:PRO:HA	2.19	0.41
1:D:649:CYS:HB3	1:D:699:GLU:HB2	2.02	0.41
1:A:436:LEU:HD12	1:A:436:LEU:HA	1.90	0.41
1:D:735:TYR:HB3	1:D:738:GLU:HG3	2.02	0.41
1:C:387:PHE:CD1	1:C:394:CYS:HB3	2.55	0.41
1:C:726:VAL:HG23	1:C:728:VAL:HG23	2.01	0.41
1:D:64:SER:C	1:D:66:HIS:H	2.28	0.41
1:B:36:HIS:CG	1:B:37:HIS:H	2.38	0.41
1:C:405:ILE:HB	1:C:418:ILE:HG22	2.01	0.41
1:A:157:TRP:CE3	1:A:164:LEU:HD13	2.55	0.41
1:B:688:VAL:HG22	1:B:719:ILE:HG12	2.01	0.41
1:B:744:SER:HB2	1:B:747:ALA:HB3	2.03	0.41
1:C:711:VAL:HG23	3:C:800:RUF:H17	2.02	0.41
1:D:547:TYR:C	1:D:547:TYR:CD2	2.97	0.41
1:C:666:TYR:CD1	3:C:800:RUF:H11A	2.56	0.41
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.56	0.41
1:C:79:PHE:CE2	1:C:86:SER:HB3	2.56	0.41
1:C:123:GLN:HB3	1:C:127:SER:OG	2.20	0.41
1:B:506:ASN:HD22	1:B:506:ASN:HA	1.60	0.41
1:D:153:GLN:NE2	1:D:167:VAL:HG12	2.36	0.41
1:C:602:GLU:OE1	1:C:602:GLU:N	2.51	0.40
1:D:726:VAL:HG23	1:D:728:VAL:HG23	2.03	0.40
1:B:164:LEU:HB3	1:B:175:LYS:HB2	2.04	0.40
1:B:326:ASP:OD2	1:B:344:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:GLY:HA2	1:B:476:GLY:O	2.21	0.40
1:C:492:ARG:HB3	1:C:492:ARG:NH2	2.37	0.40
1:D:510:PRO:HD3	1:D:569:SER:HB2	2.03	0.40
1:D:542:LEU:HD23	1:D:542:LEU:C	2.47	0.40
1:A:512:LYS:HA	1:A:528:MET:O	2.21	0.40
1:C:78:VAL:HG23	1:C:89:PHE:HB2	2.03	0.40
1:A:155:VAL:HG12	1:A:166:TYR:HB3	2.02	0.40
1:D:414:TYR:CD2	1:D:433:LYS:HG2	2.56	0.40
1:B:751:ILE:O	1:B:755:MET:HG3	2.21	0.40
1:C:195:TYR:O	1:C:227:GLN:HA	2.21	0.40
1:C:658:ARG:HG3	1:C:687:THR:HG22	2.03	0.40
1:C:743:ALA:O	1:C:744:SER:C	2.64	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	719/740 (97%)	684 (95%)	31 (4%)	4 (1%)	21	44
1	B	726/740 (98%)	698 (96%)	27 (4%)	1 (0%)	48	73
1	C	720/740 (97%)	679 (94%)	39 (5%)	2 (0%)	36	60
1	D	720/740 (97%)	664 (92%)	55 (8%)	1 (0%)	48	73
All	All	2885/2960 (98%)	2725 (94%)	152 (5%)	8 (0%)	36	60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	GLU
1	A	140	ARG
1	A	334	SER

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Mol	Chain	Res	Type
1	A	463	LYS
1	C	423	LYS
1	C	334	SER
1	D	244	GLU
1	B	742	ILE

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	648/662 (98%)	606 (94%)	42 (6%)	15	37
1	B	653/662 (99%)	607 (93%)	46 (7%)	14	34
1	C	649/662 (98%)	610 (94%)	39 (6%)	17	41
1	D	649/662 (98%)	606 (93%)	43 (7%)	15	36
All	All	2599/2648 (98%)	2429 (94%)	170 (6%)	15	37

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LYS
1	A	63	ILE
1	A	78	VAL
1	A	80	ASN
1	A	82	GLU
1	A	129	THR
1	A	143	ILE
1	A	170	ASN
1	A	179	ASN
1	A	182	SER
1	A	243	ASP
1	A	246	LEU
1	A	276	LEU
1	A	283	THR
1	A	313	LEU
1	A	316	LEU

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Mol	Chain	Res	Type
1	A	341	VAL
1	A	370	SER
1	A	385	CYS
1	A	392	LYS
1	A	399	LYS
1	A	413	ASP
1	A	415	LEU
1	A	436	LEU
1	A	440	THR
1	A	448	GLU
1	A	453	ARG
1	A	482	LEU
1	A	504	LEU
1	A	505	GLN
1	A	506	ASN
1	A	507	VAL
1	A	514	LEU
1	A	519	LEU
1	A	542	LEU
1	A	547	TYR
1	A	594	ILE
1	A	597	ARG
1	A	598	LEU
1	A	673	LEU
1	A	677	GLU
1	A	688	VAL
1	B	41	LYS
1	B	46	THR
1	B	59	SER
1	B	61	ARG
1	B	63	ILE
1	B	72	GLN
1	B	78	VAL
1	B	82	GLU
1	B	94	THR
1	B	129	THR
1	B	145	GLU
1	B	170	ASN
1	B	179	ASN
1	B	246	LEU
1	B	276	LEU
1	B	295	ILE

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Mol	Chain	Res	Type
1	B	313	LEU
1	B	316	LEU
1	B	336	ARG
1	B	343	ARG
1	B	344	GLN
1	B	385	CYS
1	B	389	ILE
1	B	391	LYS
1	B	410	LEU
1	B	415	LEU
1	B	436	LEU
1	B	448	GLU
1	B	453	ARG
1	B	463	LYS
1	B	472	CYS
1	B	482	LEU
1	B	504	LEU
1	B	506	ASN
1	B	514	LEU
1	B	536	LYS
1	B	538	LYS
1	B	547	TYR
1	B	575	VAL
1	B	594	ILE
1	B	598	LEU
1	B	614	SER
1	B	660	GLU
1	B	673	LEU
1	B	677	GLU
1	B	688	VAL
1	C	54	ARG
1	C	56	LYS
1	C	57	LEU
1	C	63	ILE
1	C	72	GLN
1	C	82	GLU
1	C	87	SER
1	C	90	LEU
1	C	129	THR
1	C	145	GLU
1	C	246	LEU
1	C	279	VAL

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Mol	Chain	Res	Type
1	C	283	THR
1	C	316	LEU
1	C	339	CYS
1	C	340	LEU
1	C	366	LEU
1	C	379	GLU
1	C	385	CYS
1	C	390	ASP
1	C	410	LEU
1	C	415	LEU
1	C	433	LYS
1	C	441	LYS
1	C	443	THR
1	C	453	ARG
1	C	463	LYS
1	C	482	LEU
1	C	496	ASP
1	C	504	LEU
1	C	507	VAL
1	C	519	LEU
1	C	546	VAL
1	C	547	TYR
1	C	597	ARG
1	C	630	SER
1	C	673	LEU
1	C	688	VAL
1	C	761	GLN
1	D	51	ASN
1	D	56	LYS
1	D	57	LEU
1	D	59	SER
1	D	78	VAL
1	D	82	GLU
1	D	91	GLU
1	D	92	ASN
1	D	129	THR
1	D	142	LEU
1	D	170	ASN
1	D	179	ASN
1	D	185	ILE
1	D	246	LEU
1	D	250	LYS

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Mol	Chain	Res	Type
1	D	276	LEU
1	D	280	THR
1	D	316	LEU
1	D	319	ILE
1	D	336	ARG
1	D	348	MET
1	D	385	CYS
1	D	392	LYS
1	D	399	LYS
1	D	410	LEU
1	D	453	ARG
1	D	464	GLU
1	D	486	VAL
1	D	504	LEU
1	D	506	ASN
1	D	514	LEU
1	D	528	MET
1	D	538	LYS
1	D	546	VAL
1	D	547	TYR
1	D	594	ILE
1	D	598	LEU
1	D	615	LYS
1	D	622	LYS
1	D	673	LEU
1	D	684	ARG
1	D	688	VAL
1	D	710	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	80	ASN
1	A	138	ASN
1	A	141	GLN
1	A	151	ASN
1	A	153	GLN
1	A	169	ASN
1	A	170	ASN
1	A	179	ASN
1	A	196	ASN

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Mol	Chain	Res	Type
1	A	227	GLN
1	A	338	ASN
1	A	344	GLN
1	A	345	HIS
1	A	455	GLN
1	A	508	GLN
1	A	572	ASN
1	A	586	GLN
1	A	592	HIS
1	A	710	ASN
1	A	731	GLN
1	B	36	HIS
1	B	112	GLN
1	B	123	GLN
1	B	141	GLN
1	B	153	GLN
1	B	170	ASN
1	B	179	ASN
1	B	227	GLN
1	B	435	GLN
1	B	455	GLN
1	B	505	GLN
1	B	506	ASN
1	B	572	ASN
1	B	592	HIS
1	B	710	ASN
1	C	66	HIS
1	C	112	GLN
1	C	138	ASN
1	C	141	GLN
1	C	153	GLN
1	C	170	ASN
1	C	344	GLN
1	C	369	ASN
1	C	435	GLN
1	C	572	ASN
1	C	606	GLN
1	C	685	ASN
1	C	697	GLN
1	D	75	ASN
1	D	80	ASN
1	D	100	HIS

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Mol	Chain	Res	Type
1	D	153	GLN
1	D	169	ASN
1	D	170	ASN
1	D	219	ASN
1	D	272	ASN
1	D	344	GLN
1	D	388	GLN
1	D	455	GLN
1	D	572	ASN
1	D	592	HIS
1	D	710	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 ⓘ

10 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	$\# Z > 2$
2	NAG	E	1	2,1	14,14,15	0.53	0	17,19,21	1.01	2 (11%)
2	NAG	E	2	2	14,14,15	0.49	0	17,19,21	0.98	0
2	NAG	F	1	2,1	14,14,15	0.59	0	17,19,21	1.85	5 (29%)
2	NAG	F	2	2	14,14,15	0.59	0	17,19,21	0.90	0
2	NAG	G	1	2,1	14,14,15	0.69	0	17,19,21	1.11	2 (11%)
2	NAG	G	2	2	14,14,15	0.44	0	17,19,21	1.66	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	H	1	2,1	14,14,15	0.56	0	17,19,21	1.17	1 (5%)
2	NAG	H	2	2	14,14,15	0.51	0	17,19,21	0.69	0
2	NAG	I	1	2,1	14,14,15	0.55	0	17,19,21	1.17	1 (5%)
2	NAG	I	2	2	14,14,15	0.56	0	17,19,21	1.23	2 (11%)

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
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	C1-O5-C5	5.80	119.96	112.19
2	F	1	NAG	C1-O5-C5	4.50	118.22	112.19
2	F	1	NAG	C1-C2-N2	3.30	115.63	110.43
2	I	1	NAG	O5-C1-C2	-3.24	106.28	111.29
2	H	1	NAG	C4-C3-C2	3.21	115.72	111.02
2	F	1	NAG	C2-N2-C7	-2.76	119.20	122.90
2	G	1	NAG	C4-C3-C2	2.74	115.03	111.02
2	I	2	NAG	C1-O5-C5	2.67	115.77	112.19
2	G	1	NAG	C2-N2-C7	-2.67	119.32	122.90
2	E	1	NAG	O5-C1-C2	-2.52	107.39	111.29
2	F	1	NAG	C4-C3-C2	-2.32	107.62	111.02
2	F	1	NAG	O5-C1-C2	-2.16	107.95	111.29
2	E	1	NAG	C4-C3-C2	2.08	114.06	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2	NAG	O4-C4-C5	2.03	114.31	109.32

There are no chirality outliers.

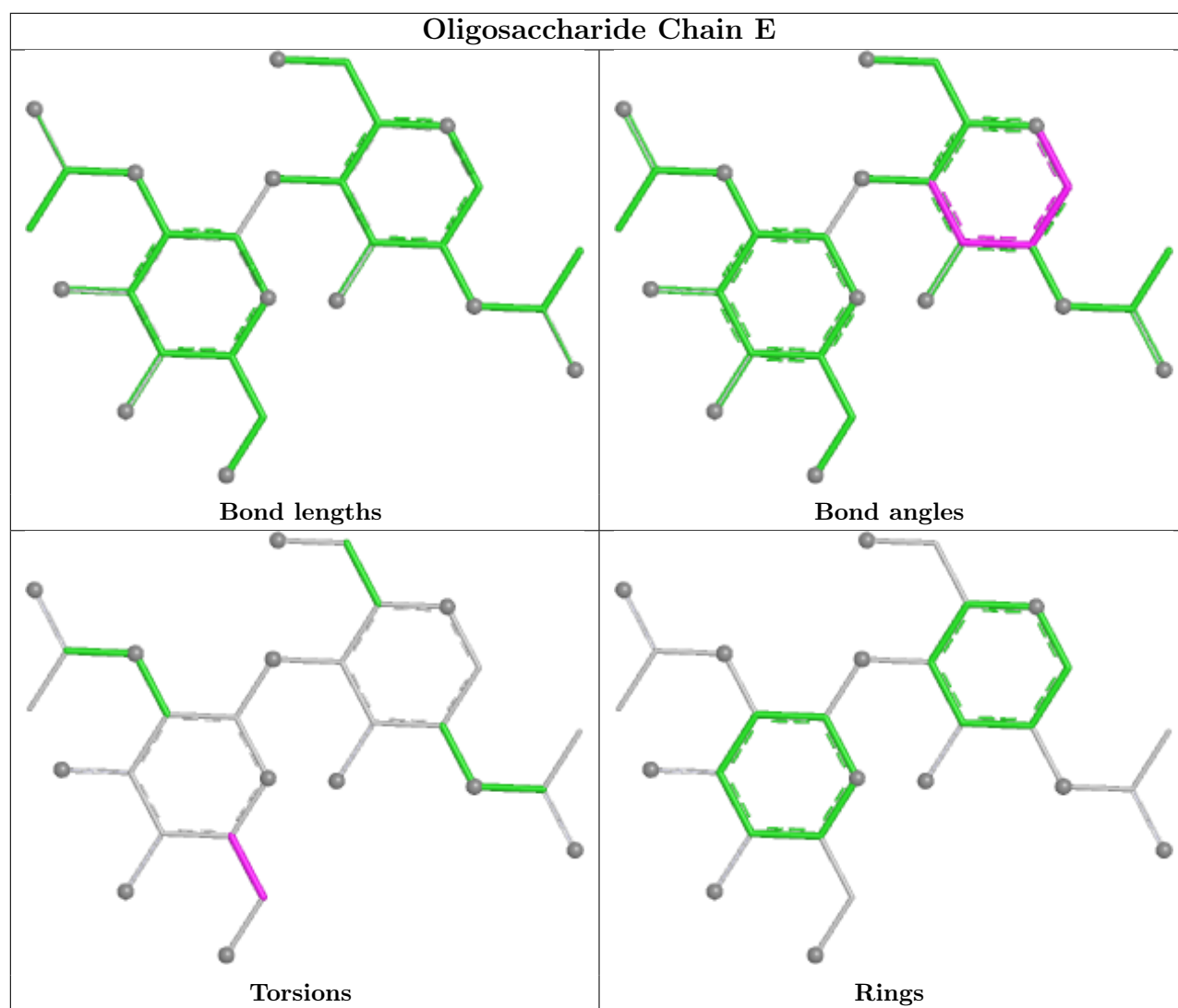
All (22) torsion outliers are listed below:

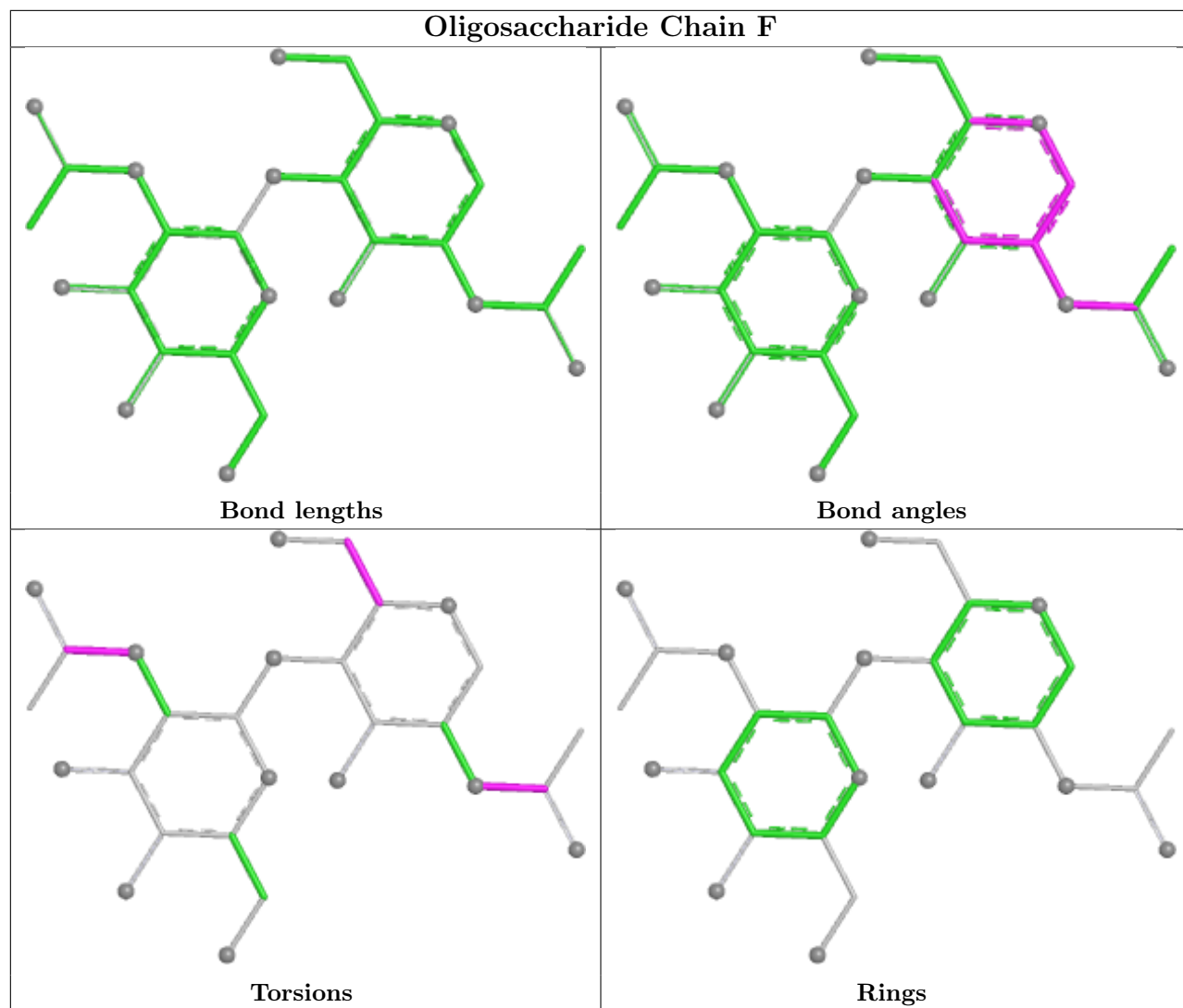
Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C8-C7-N2-C2
2	H	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	G	1	NAG	O7-C7-N2-C2
2	I	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C4-C5-C6-O6

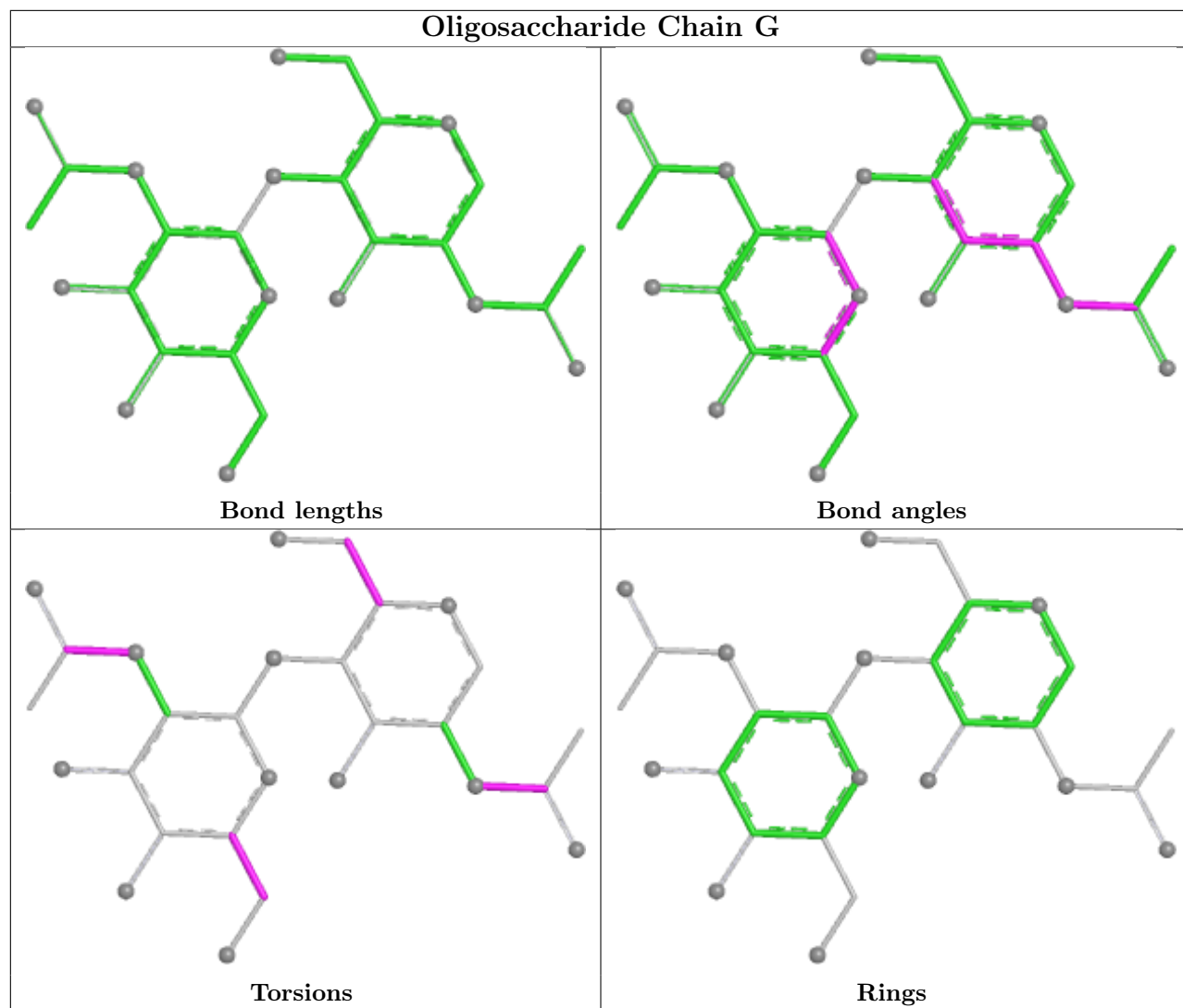
There are no ring outliers.

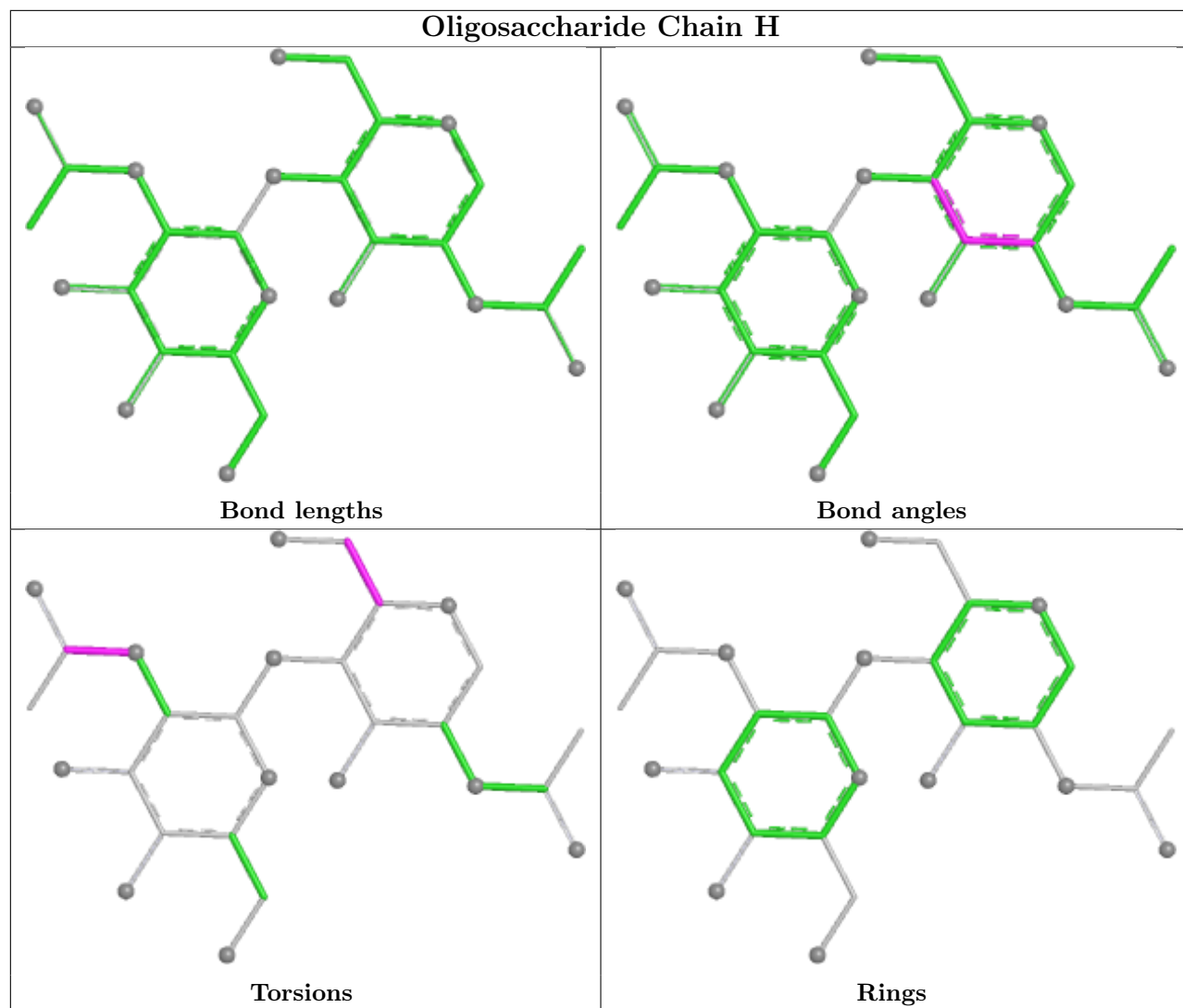
No monomer is involved in short contacts.

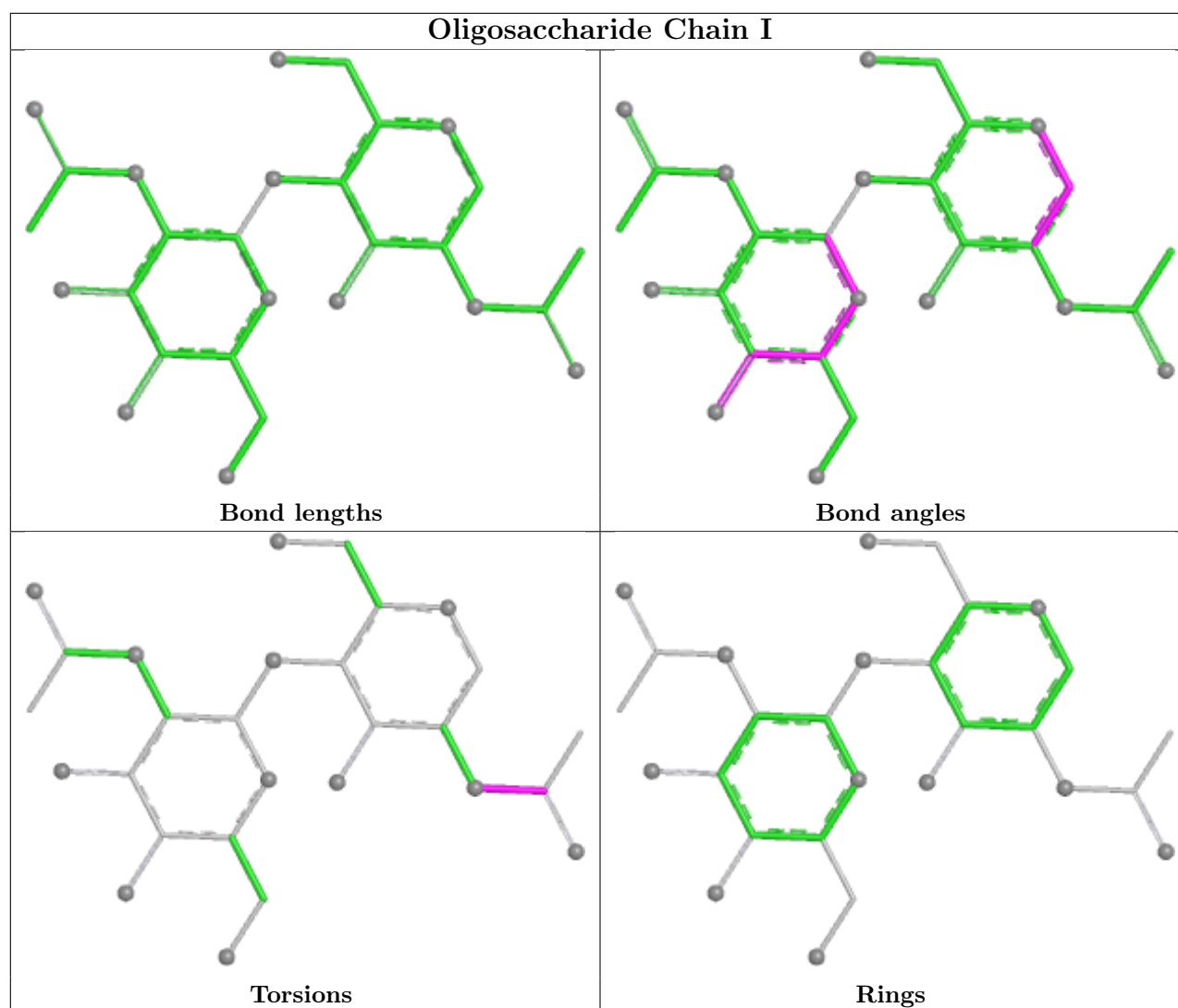
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	803	1	14,14,15	0.81	1 (7%)	17,19,21	1.26	1 (5%)
4	NAG	A	802	1	14,14,15	0.63	0	17,19,21	1.24	1 (5%)
4	NAG	B	806	1	14,14,15	0.56	0	17,19,21	1.15	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	802	1	14,14,15	0.74	0	17,19,21	1.40	2 (11%)
4	NAG	B	803	1	14,14,15	0.58	0	17,19,21	1.45	1 (5%)
4	NAG	A	801	1	14,14,15	0.64	0	17,19,21	1.24	1 (5%)
3	RUF	D	800	-	30,30,30	0.70	1 (3%)	43,44,44	2.41	14 (32%)
3	RUF	B	800	-	30,30,30	0.78	1 (3%)	43,44,44	2.65	12 (27%)
4	NAG	D	801	1	14,14,15	0.59	0	17,19,21	1.19	1 (5%)
4	NAG	C	801	1	14,14,15	0.56	0	17,19,21	1.34	1 (5%)
3	RUF	C	800	-	30,30,30	0.84	1 (3%)	43,44,44	2.50	16 (37%)
4	NAG	B	801	1	14,14,15	0.88	1 (7%)	17,19,21	1.60	4 (23%)
4	NAG	B	802	1	14,14,15	0.59	0	17,19,21	1.05	1 (5%)
3	RUF	A	800	-	30,30,30	0.80	0	43,44,44	2.60	14 (32%)
4	NAG	A	808	1	14,14,15	0.65	0	17,19,21	0.89	0
4	NAG	D	804	1	14,14,15	0.74	1 (7%)	17,19,21	1.69	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	803	1	-	2/6/23/26	0/1/1/1
4	NAG	A	802	1	-	4/6/23/26	0/1/1/1
4	NAG	B	806	1	-	4/6/23/26	0/1/1/1
4	NAG	C	802	1	-	2/6/23/26	0/1/1/1
4	NAG	B	803	1	-	2/6/23/26	0/1/1/1
4	NAG	A	801	1	-	3/6/23/26	0/1/1/1
3	RUF	D	800	-	-	0/8/16/16	0/4/4/4
3	RUF	B	800	-	-	0/8/16/16	0/4/4/4
4	NAG	D	801	1	-	0/6/23/26	0/1/1/1
4	NAG	C	801	1	-	0/6/23/26	0/1/1/1
3	RUF	C	800	-	-	1/8/16/16	0/4/4/4
4	NAG	B	801	1	-	4/6/23/26	0/1/1/1
4	NAG	B	802	1	-	0/6/23/26	0/1/1/1
3	RUF	A	800	-	-	1/8/16/16	0/4/4/4
4	NAG	A	808	1	-	0/6/23/26	0/1/1/1
4	NAG	D	804	1	-	4/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801	NAG	C1-C2	2.50	1.55	1.52
3	C	800	RUF	C22-N24	-2.35	1.35	1.40
3	D	800	RUF	C22-N24	-2.16	1.36	1.40
3	B	800	RUF	C22-N24	-2.13	1.36	1.40
4	A	803	NAG	C1-C2	2.09	1.55	1.52
4	D	804	NAG	C1-C2	2.03	1.55	1.52

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	RUF	C5-N4-C3	8.45	111.67	102.71
3	B	800	RUF	C5-N4-C3	8.31	111.53	102.71
3	C	800	RUF	C5-N4-C3	8.26	111.47	102.71
3	D	800	RUF	C5-N4-C3	7.53	110.70	102.71
3	B	800	RUF	C14-C13-N12	-6.95	104.74	113.14
3	A	800	RUF	N2-C3-N4	5.42	134.44	125.59
3	B	800	RUF	N12-C5-N4	-5.41	107.61	113.77
3	A	800	RUF	N12-C5-N4	-5.41	107.61	113.77
3	A	800	RUF	C14-C13-N12	-5.34	106.69	113.14
3	B	800	RUF	N2-C3-N4	5.26	134.18	125.59
3	C	800	RUF	N12-C5-N4	-5.10	107.97	113.77
3	D	800	RUF	N2-C3-N4	5.04	133.82	125.59
3	C	800	RUF	N2-C3-N4	4.97	133.72	125.59
3	B	800	RUF	C21-C3-N4	-4.91	106.76	112.77
3	A	800	RUF	C21-C3-N4	-4.89	106.78	112.77
3	D	800	RUF	N12-C5-N4	-4.88	108.22	113.77
3	C	800	RUF	C21-C3-N4	-4.59	107.14	112.77
4	D	804	NAG	C1-O5-C5	4.30	117.95	112.19
3	C	800	RUF	C21-C22-N24	4.23	119.81	112.06
3	D	800	RUF	C21-C3-N4	-4.22	107.60	112.77
3	B	800	RUF	C21-C22-N24	4.20	119.75	112.06
3	D	800	RUF	C14-C13-N12	-4.16	108.11	113.14
4	A	801	NAG	C1-O5-C5	4.12	117.70	112.19
3	A	800	RUF	C21-C22-N24	4.07	119.52	112.06
3	D	800	RUF	C21-C22-N24	4.05	119.48	112.06
3	D	800	RUF	N24-C26-N2	4.03	122.18	117.14
4	B	803	NAG	C1-O5-C5	4.00	117.54	112.19
3	A	800	RUF	N24-C26-N2	4.00	122.13	117.14
4	C	801	NAG	C1-O5-C5	3.92	117.44	112.19
3	C	800	RUF	C14-C13-N12	-3.90	108.42	113.14
4	D	801	NAG	C1-O5-C5	3.89	117.39	112.19
4	D	804	NAG	C2-N2-C7	3.83	128.04	122.90
3	B	800	RUF	O23-C22-C21	-3.66	118.88	126.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	NAG	C4-C3-C2	3.66	116.38	111.02
4	C	802	NAG	C4-C3-C2	3.54	116.20	111.02
3	B	800	RUF	N24-C26-N2	3.53	121.55	117.14
3	C	800	RUF	N24-C26-N2	3.46	121.46	117.14
4	A	802	NAG	C1-O5-C5	3.44	116.80	112.19
3	A	800	RUF	O23-C22-C21	-3.38	119.46	126.38
4	B	806	NAG	C1-O5-C5	3.37	116.70	112.19
3	D	800	RUF	C22-N24-C26	-3.35	120.21	125.66
3	C	800	RUF	C22-C21-C3	-3.29	118.78	122.92
3	A	800	RUF	C22-N24-C26	-3.27	120.34	125.66
3	B	800	RUF	C22-N24-C26	-3.22	120.43	125.66
4	B	801	NAG	C1-O5-C5	3.16	116.42	112.19
4	B	801	NAG	C4-C3-C2	3.08	115.53	111.02
3	D	800	RUF	O23-C22-C21	-3.01	120.21	126.38
3	C	800	RUF	C22-N24-C26	-2.92	120.92	125.66
4	B	801	NAG	C2-N2-C7	2.85	126.72	122.90
4	B	802	NAG	C1-O5-C5	2.82	115.97	112.19
3	B	800	RUF	C22-C21-C3	-2.72	119.49	122.92
3	A	800	RUF	C22-C21-C3	-2.65	119.58	122.92
3	C	800	RUF	C22-C21-N12	2.58	135.00	131.35
3	D	800	RUF	C22-C21-C3	-2.48	119.79	122.92
3	C	800	RUF	C1-N2-C26	2.48	121.65	117.33
3	C	800	RUF	O23-C22-C21	-2.44	121.39	126.38
3	B	800	RUF	C3-C21-N12	2.43	106.89	104.93
3	A	800	RUF	C21-N12-C5	2.34	107.26	105.31
3	A	800	RUF	O27-C26-N24	-2.33	118.11	121.33
3	D	800	RUF	C1-N2-C26	2.32	121.37	117.33
4	C	802	NAG	C2-N2-C7	2.27	125.94	122.90
3	B	800	RUF	C21-N12-C5	2.26	107.19	105.31
3	D	800	RUF	C21-N12-C5	2.25	107.19	105.31
3	C	800	RUF	C21-N12-C5	2.25	107.18	105.31
4	B	801	NAG	O7-C7-C8	-2.22	118.11	122.05
3	A	800	RUF	C3-C21-N12	2.15	106.67	104.93
3	C	800	RUF	C10-C11-N6	2.15	113.84	109.61
3	C	800	RUF	O27-C26-N24	-2.10	118.43	121.33
3	D	800	RUF	C21-C3-N2	-2.07	118.59	121.74
3	A	800	RUF	C1-N2-C26	2.07	120.94	117.33
3	C	800	RUF	C25-N24-C26	2.06	120.92	117.33
3	D	800	RUF	O27-C26-N24	-2.02	118.54	121.33

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	NAG	C8-C7-N2-C2
4	A	803	NAG	O7-C7-N2-C2
4	B	801	NAG	C3-C2-N2-C7
4	B	801	NAG	C8-C7-N2-C2
4	B	801	NAG	O7-C7-N2-C2
4	B	803	NAG	C8-C7-N2-C2
4	B	803	NAG	O7-C7-N2-C2
4	B	806	NAG	C8-C7-N2-C2
4	B	806	NAG	O7-C7-N2-C2
4	C	802	NAG	C8-C7-N2-C2
4	C	802	NAG	O7-C7-N2-C2
4	A	801	NAG	O5-C5-C6-O6
4	D	804	NAG	O5-C5-C6-O6
4	D	804	NAG	C8-C7-N2-C2
4	D	804	NAG	O7-C7-N2-C2
4	A	801	NAG	C4-C5-C6-O6
4	D	804	NAG	C4-C5-C6-O6
4	A	802	NAG	C8-C7-N2-C2
4	A	802	NAG	O7-C7-N2-C2
4	A	802	NAG	C4-C5-C6-O6
4	B	806	NAG	C4-C5-C6-O6
4	A	802	NAG	O5-C5-C6-O6
4	B	806	NAG	O5-C5-C6-O6
3	A	800	RUF	N12-C5-N6-C11
3	C	800	RUF	N12-C5-N6-C11
4	B	801	NAG	O5-C5-C6-O6
4	A	801	NAG	C8-C7-N2-C2

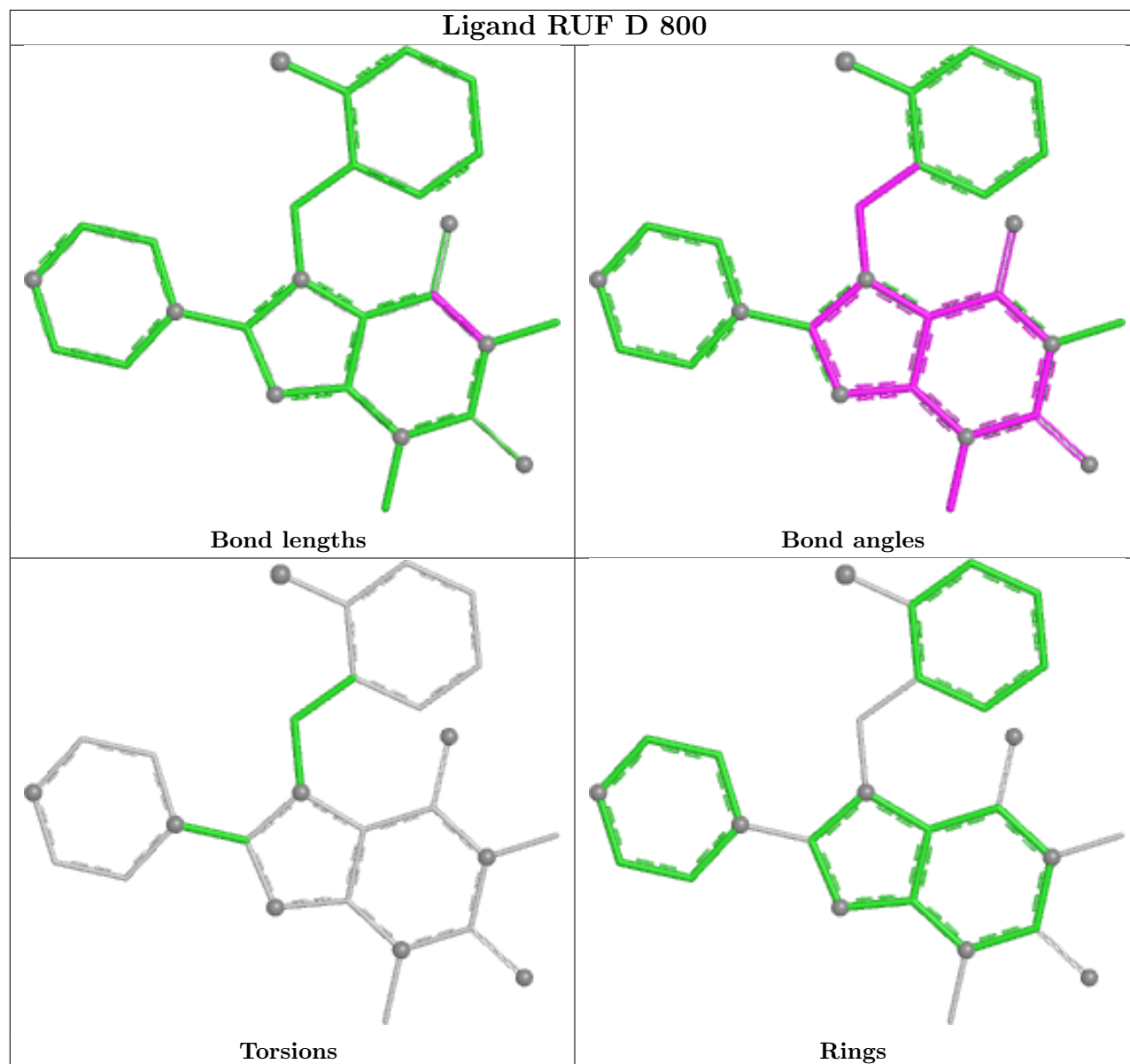
There are no ring outliers.

5 monomers are involved in 11 short contacts:

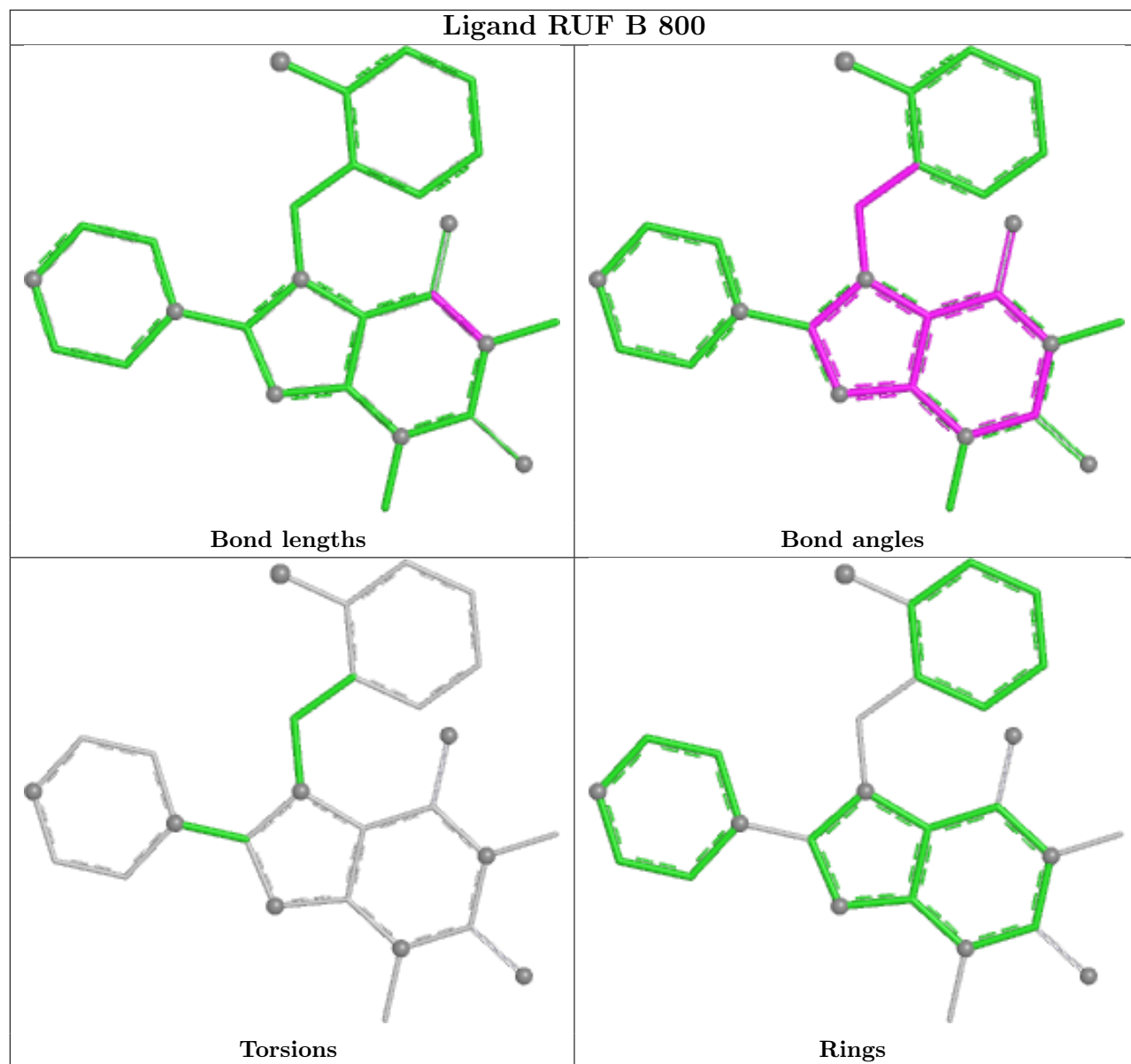
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	800	RUF	2	0
3	B	800	RUF	2	0
4	D	801	NAG	1	0
3	C	800	RUF	4	0
3	A	800	RUF	2	0

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

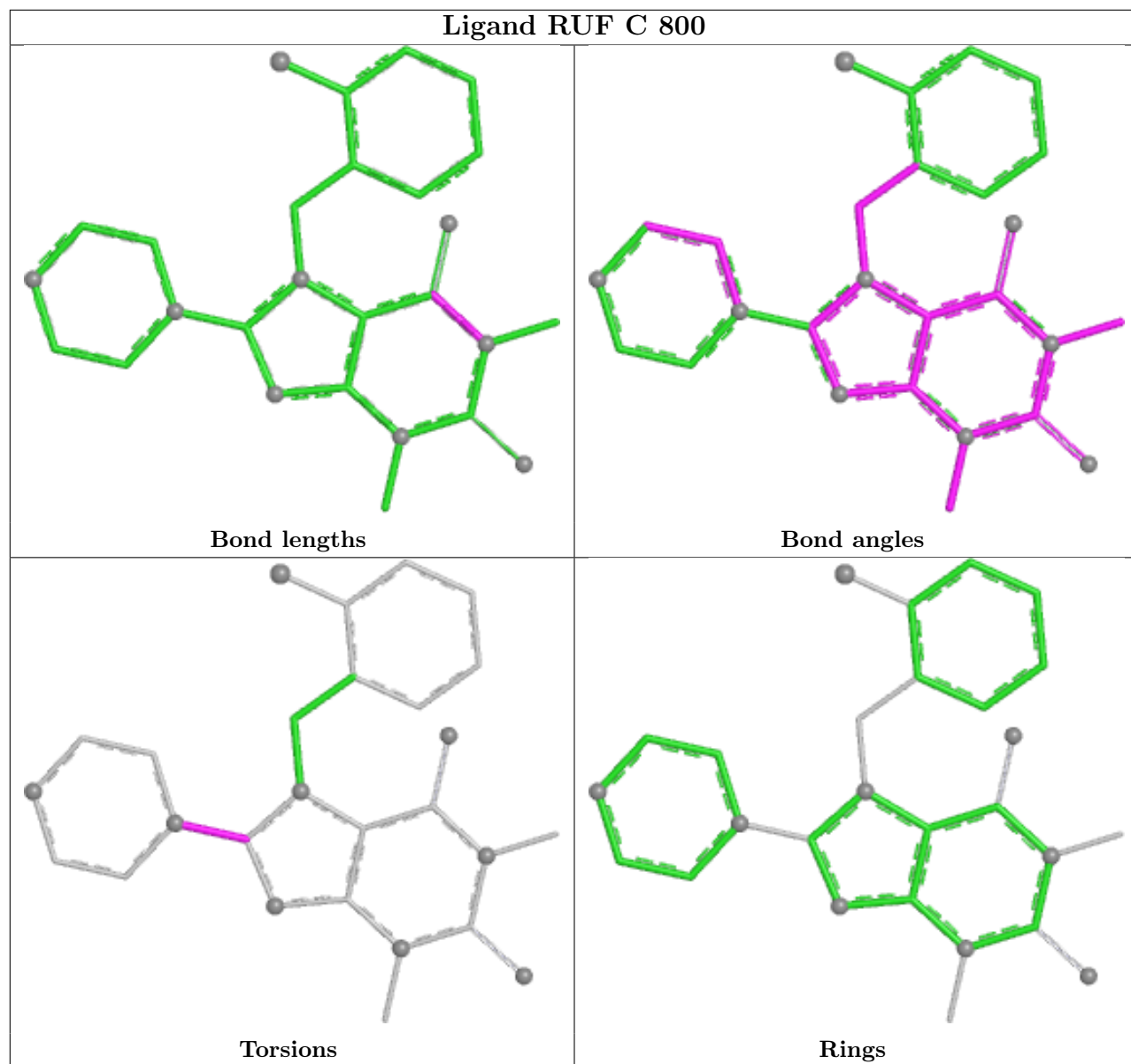
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

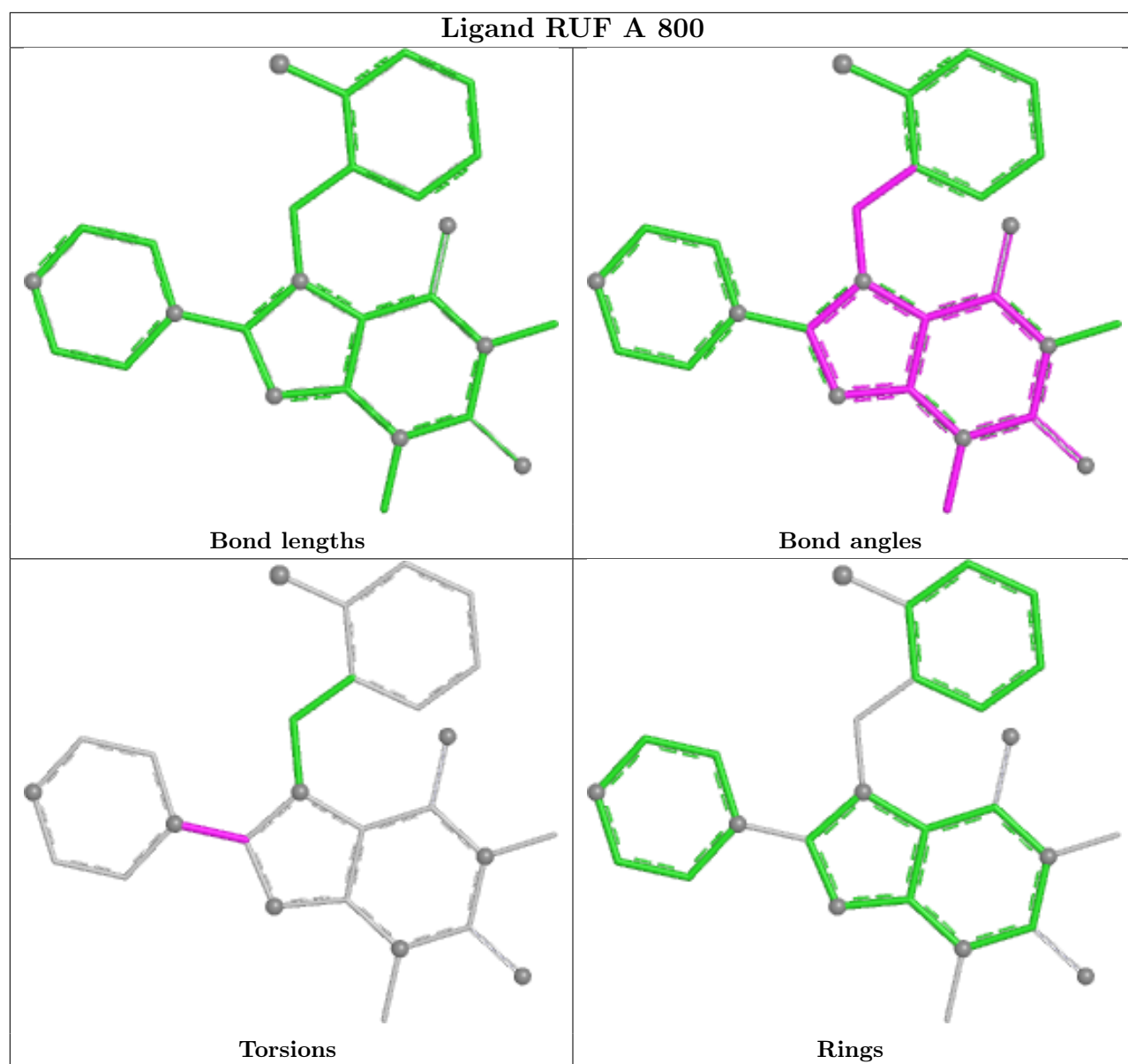


Ligand RUF B 800



Ligand RUF C 800





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	723/740 (97%)	0.40	15 (2%) 63 61	35, 46, 62, 81	1 (0%)
1	B	729/740 (98%)	0.32	13 (1%) 67 65	27, 46, 63, 85	1 (0%)
1	C	724/740 (97%)	0.54	41 (5%) 29 26	37, 46, 64, 82	0
1	D	724/740 (97%)	0.87	95 (13%) 7 6	35, 47, 63, 92	0
All	All	2900/2960 (97%)	0.54	164 (5%) 29 26	27, 46, 63, 92	2 (0%)

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	88	VAL	6.1
1	D	335	GLY	4.2
1	D	415	LEU	4.1
1	D	78	VAL	4.1
1	D	322	TYR	3.8
1	C	89	PHE	3.8
1	D	467	TYR	3.7
1	D	93	SER	3.7
1	D	333	SER	3.7
1	D	330	TYR	3.6
1	D	328	CYS	3.4
1	D	77	LEU	3.3
1	D	92	ASN	3.3
1	D	385	CYS	3.3
1	C	81	ALA	3.2
1	D	416	TYR	3.2
1	C	78	VAL	3.2
1	A	105	TYR	3.1
1	B	75	ASN	3.1
1	D	87	SER	3.0
1	C	330	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	348	MET	3.0
1	A	138	ASN	3.0
1	D	95	PHE	3.0
1	D	62	TRP	2.9
1	D	135	TYR	2.9
1	C	335	GLY	2.9
1	A	399	LYS	2.9
1	D	464	GLU	2.9
1	C	179	ASN	2.9
1	D	468	TYR	2.9
1	C	88	VAL	2.9
1	D	305	TRP	2.9
1	D	397	ILE	2.9
1	D	315	TRP	2.8
1	D	436	LEU	2.8
1	C	79	PHE	2.8
1	D	178	PRO	2.8
1	D	347	GLU	2.8
1	A	90	LEU	2.8
1	D	326	ASP	2.8
1	D	372	TYR	2.8
1	D	273	THR	2.7
1	D	85	ASN	2.7
1	D	89	PHE	2.7
1	D	222	PHE	2.7
1	D	339	CYS	2.7
1	D	483	HIS	2.7
1	D	75	ASN	2.7
1	D	338	ASN	2.7
1	D	394	CYS	2.7
1	A	165	ALA	2.7
1	D	319	ILE	2.6
1	D	486	VAL	2.6
1	D	83	TYR	2.6
1	D	79	PHE	2.6
1	A	274	ASP	2.6
1	C	105	TYR	2.6
1	D	81	ALA	2.6
1	D	413	ASP	2.5
1	D	76	ILE	2.5
1	A	489	LYS	2.5
1	D	97	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	279	VAL	2.5
1	C	83	TYR	2.5
1	D	414	TYR	2.5
1	B	72	GLN	2.5
1	D	324	VAL	2.5
1	A	332	GLU	2.4
1	A	490	GLY	2.4
1	C	279	VAL	2.4
1	B	63	ILE	2.4
1	D	90	LEU	2.4
1	D	337	TRP	2.4
1	C	115	LEU	2.4
1	D	148	ILE	2.4
1	B	328	CYS	2.4
1	B	766	PRO	2.4
1	C	72	GLN	2.4
1	C	486	VAL	2.4
1	D	140	ARG	2.4
1	C	143	ILE	2.4
1	D	329	ASP	2.4
1	B	208	PHE	2.4
1	D	180	LEU	2.3
1	D	276	LEU	2.3
1	D	63	ILE	2.3
1	D	94	THR	2.3
1	D	66	HIS	2.3
1	D	469	GLN	2.3
1	C	95	PHE	2.3
1	D	137	LEU	2.3
1	D	64	SER	2.3
1	D	136	ASP	2.3
1	D	462	SER	2.3
1	C	63	ILE	2.3
1	D	280	THR	2.3
1	A	92	ASN	2.3
1	D	161	GLY	2.3
1	D	395	THR	2.3
1	D	173	TYR	2.3
1	A	86	SER	2.3
1	C	180	LEU	2.3
1	D	164	LEU	2.3
1	D	392	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	70	TYR	2.2
1	D	487	ASN	2.2
1	D	292	SER	2.2
1	B	98	PHE	2.2
1	C	186	THR	2.2
1	C	490	GLY	2.2
1	A	102	ILE	2.2
1	D	98	PHE	2.2
1	C	67	GLU	2.2
1	D	68	TYR	2.2
1	C	133	ASP	2.2
1	D	99	GLY	2.2
1	D	268	PHE	2.2
1	C	282	ALA	2.2
1	C	94	THR	2.2
1	B	301	CYS	2.2
1	C	138	ASN	2.2
1	D	139	LYS	2.2
1	C	77	LEU	2.2
1	C	142	LEU	2.2
1	D	410	LEU	2.2
1	D	331	ASP	2.2
1	A	744	SER	2.2
1	D	279	VAL	2.2
1	D	269	PHE	2.2
1	D	409	ALA	2.1
1	D	144	THR	2.1
1	D	439	TYR	2.1
1	C	90	LEU	2.1
1	C	164	LEU	2.1
1	C	284	SER	2.1
1	D	181	PRO	2.1
1	D	84	GLY	2.1
1	B	95	PHE	2.1
1	C	86	SER	2.1
1	C	412	SER	2.1
1	C	145	GLU	2.1
1	C	379	GLU	2.1
1	B	505	GLN	2.1
1	D	482	LEU	2.1
1	C	506	ASN	2.1
1	C	183	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	274	ASP	2.1
1	D	141	GLN	2.1
1	D	762	CYS	2.1
1	C	70	TYR	2.1
1	D	493	VAL	2.1
1	D	463	LYS	2.0
1	D	489	LYS	2.0
1	C	280	THR	2.0
1	A	488	ASP	2.0
1	B	391	LYS	2.0
1	C	537	SER	2.0
1	C	181	PRO	2.0
1	C	283	THR	2.0
1	D	112	GLN	2.0
1	B	179	ASN	2.0
1	D	174	VAL	2.0
1	D	386	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

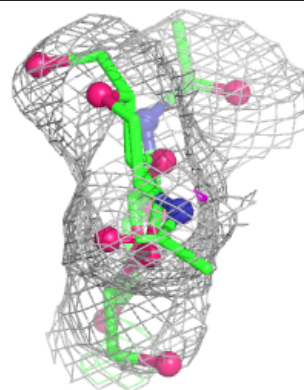
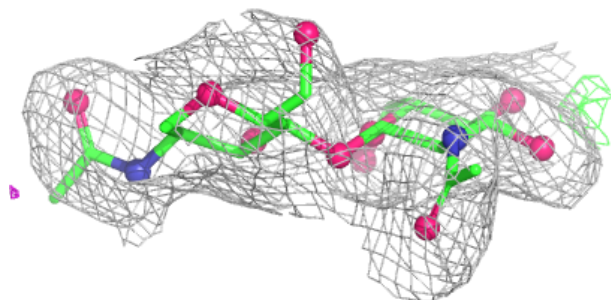
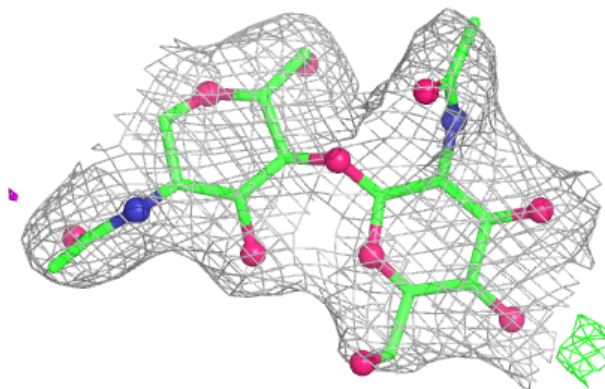
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	G	2	14/15	0.71	0.13	74,76,78,79	0
2	NAG	F	2	14/15	0.72	0.14	74,75,76,77	0
2	NAG	H	2	14/15	0.73	0.12	74,76,78,79	0
2	NAG	F	1	14/15	0.74	0.14	63,67,69,71	0
2	NAG	I	2	14/15	0.81	0.13	61,64,66,67	0
2	NAG	H	1	14/15	0.86	0.10	60,63,67,71	0
2	NAG	G	1	14/15	0.87	0.09	55,61,65,70	0
2	NAG	E	2	14/15	0.90	0.10	61,62,64,65	0
2	NAG	I	1	14/15	0.91	0.09	51,53,55,58	0
2	NAG	E	1	14/15	0.92	0.10	52,54,57,59	0

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

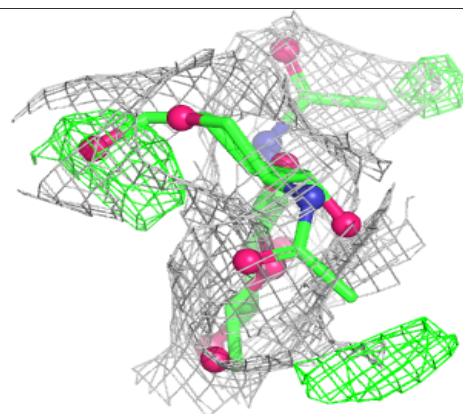
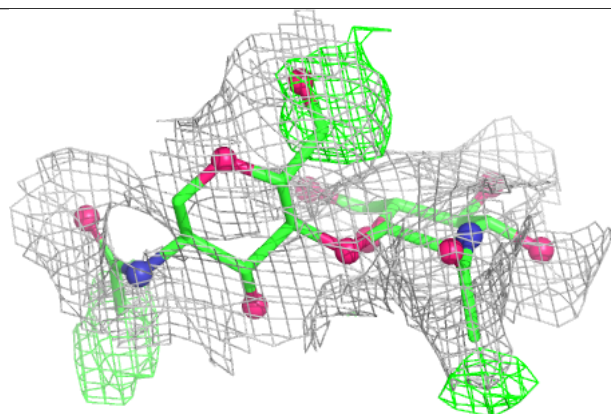
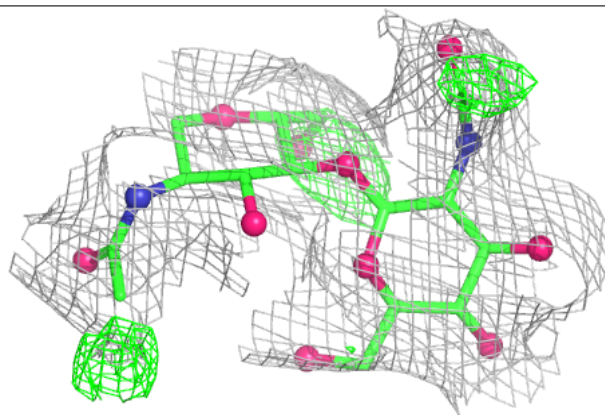
Electron density around Chain E:

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



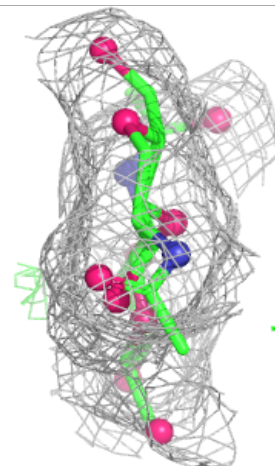
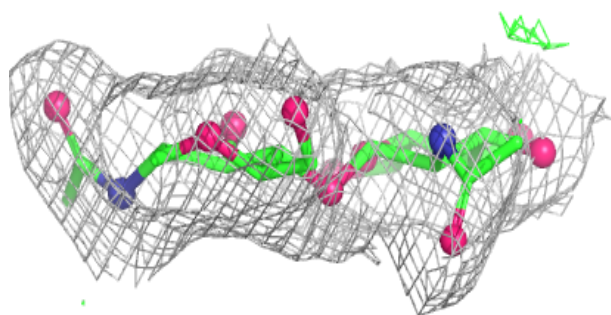
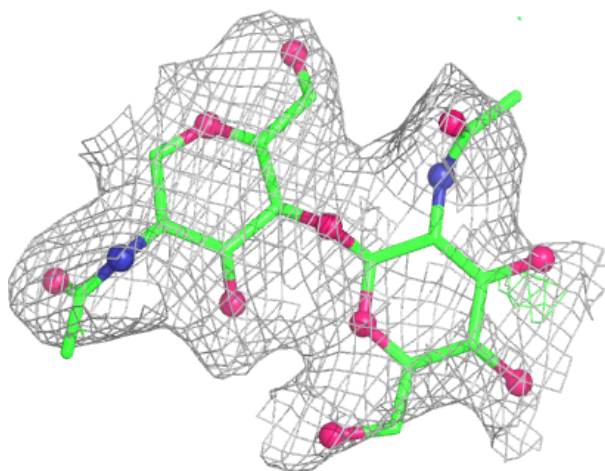
Electron density around Chain F:

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



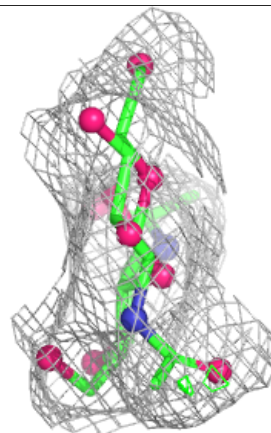
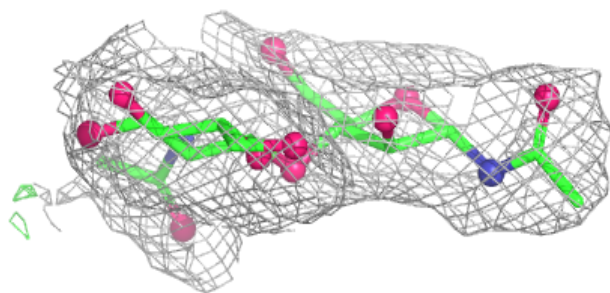
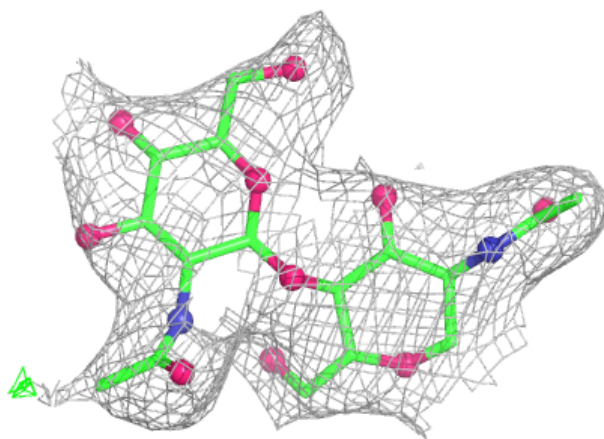
Electron density around Chain G:

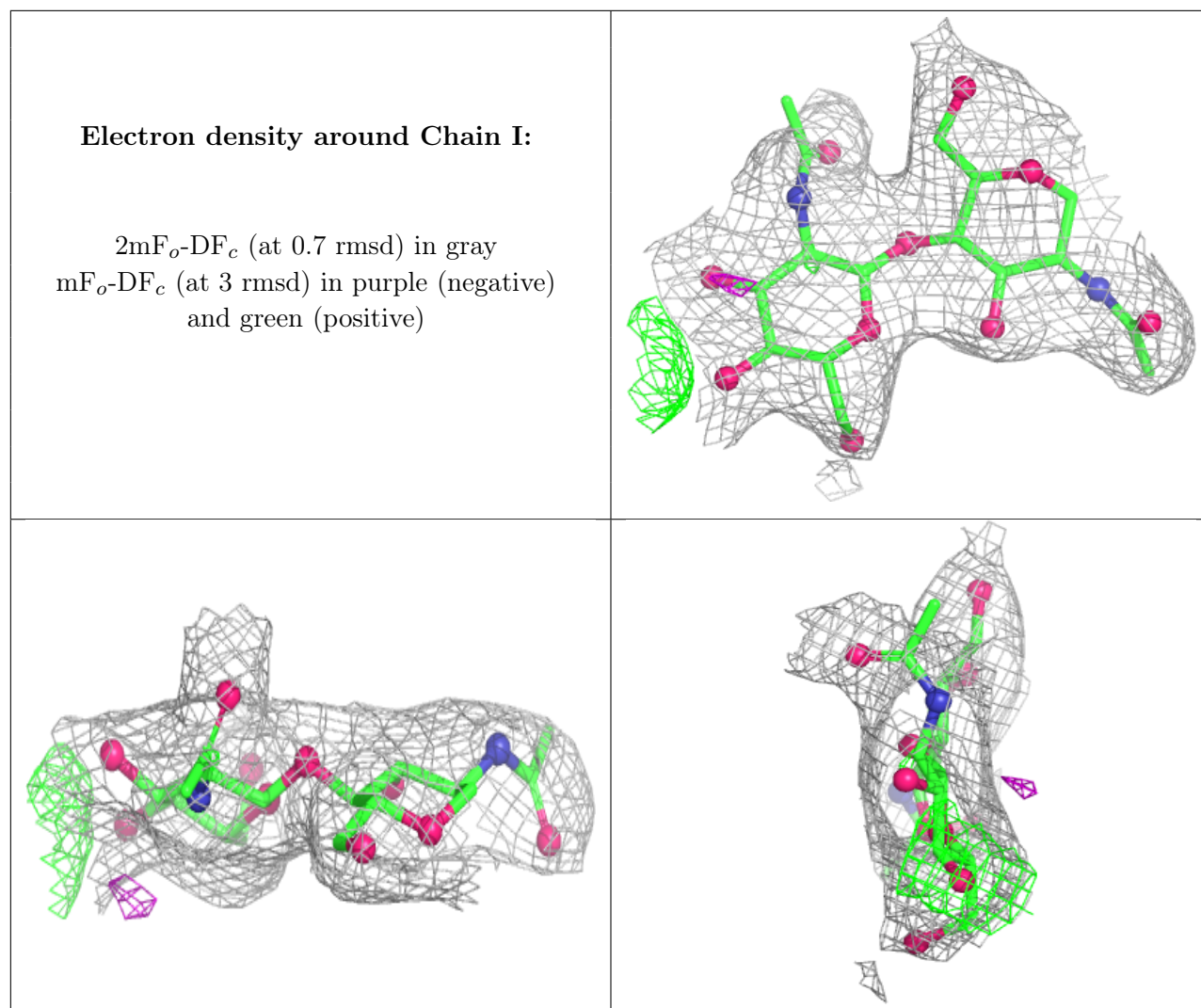
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

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





6.4 Ligands [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.

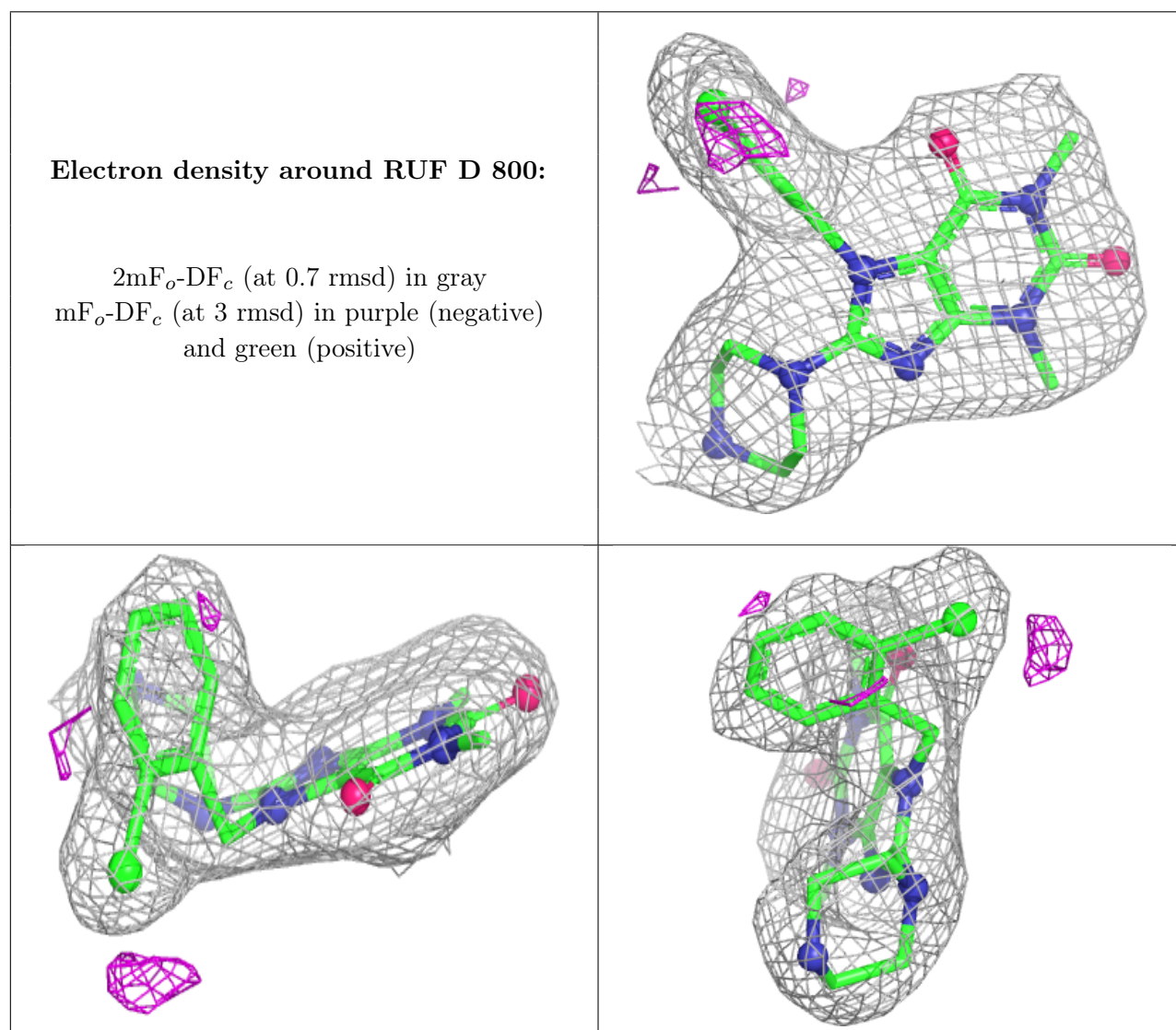
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	B	801	14/15	0.63	0.15	68,70,71,71	0
4	NAG	D	801	14/15	0.67	0.14	55,57,57,58	0
4	NAG	A	803	14/15	0.70	0.14	61,64,69,69	0
4	NAG	D	804	14/15	0.70	0.14	73,76,78,78	0
4	NAG	C	801	14/15	0.72	0.13	52,53,55,56	0
4	NAG	B	803	14/15	0.74	0.14	58,61,64,64	0
4	NAG	A	801	14/15	0.75	0.12	58,60,61,61	0
4	NAG	A	802	14/15	0.81	0.11	65,68,68,69	0

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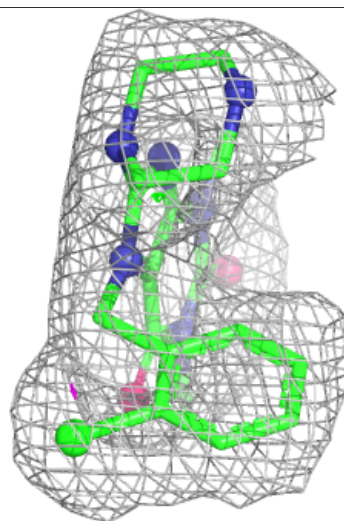
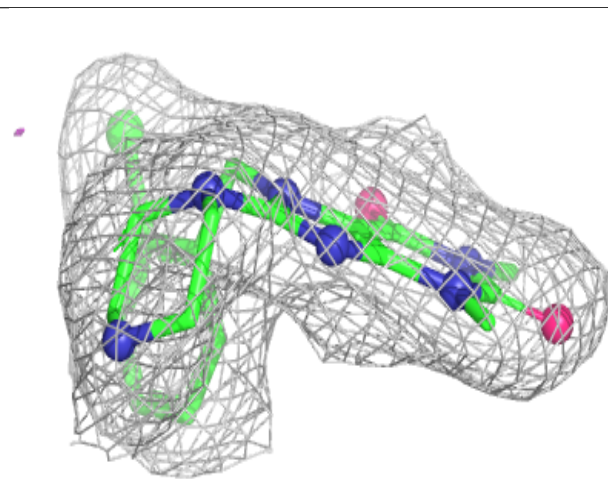
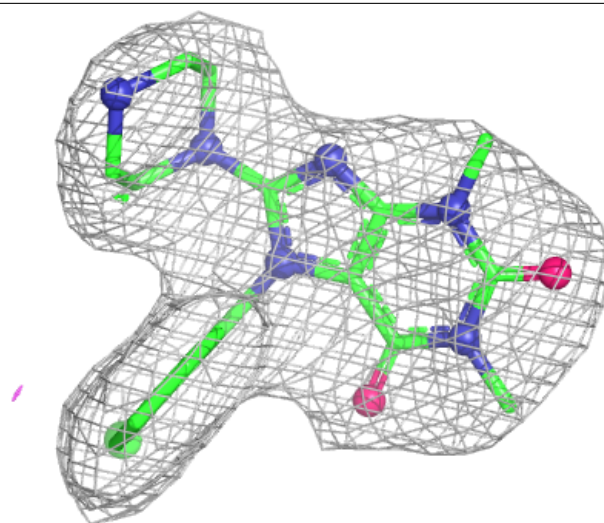
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	802	14/15	0.81	0.11	56,60,62,64	0
4	NAG	B	806	14/15	0.82	0.11	61,63,66,66	0
4	NAG	C	802	14/15	0.82	0.12	58,61,64,64	0
4	NAG	A	808	14/15	0.87	0.10	54,58,60,60	0
3	RUF	D	800	27/27	0.90	0.14	51,53,54,55	0
3	RUF	A	800	27/27	0.93	0.12	52,55,58,59	0
3	RUF	C	800	27/27	0.94	0.12	53,55,55,56	0
3	RUF	B	800	27/27	0.95	0.12	54,55,59,59	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.



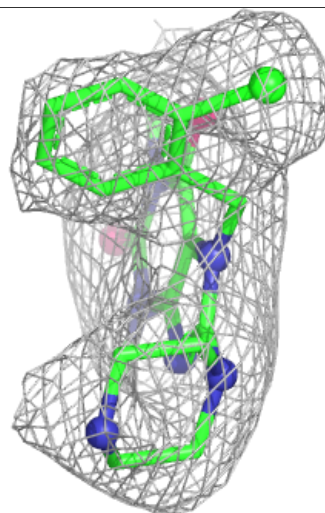
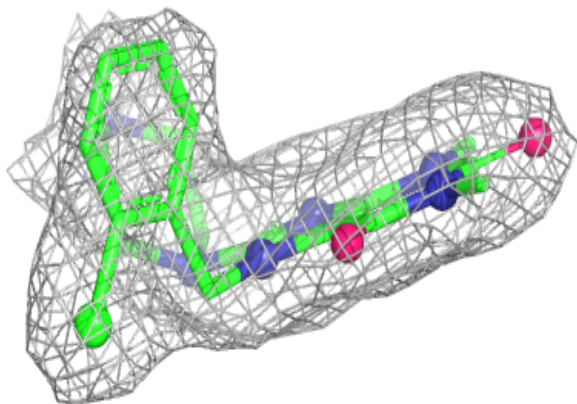
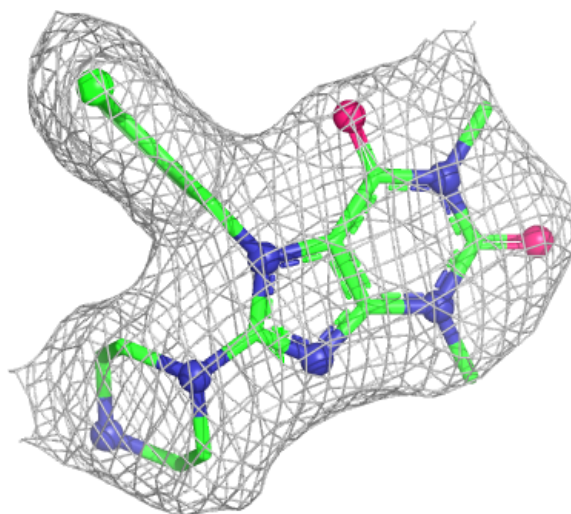
Electron density around RUF A 800:

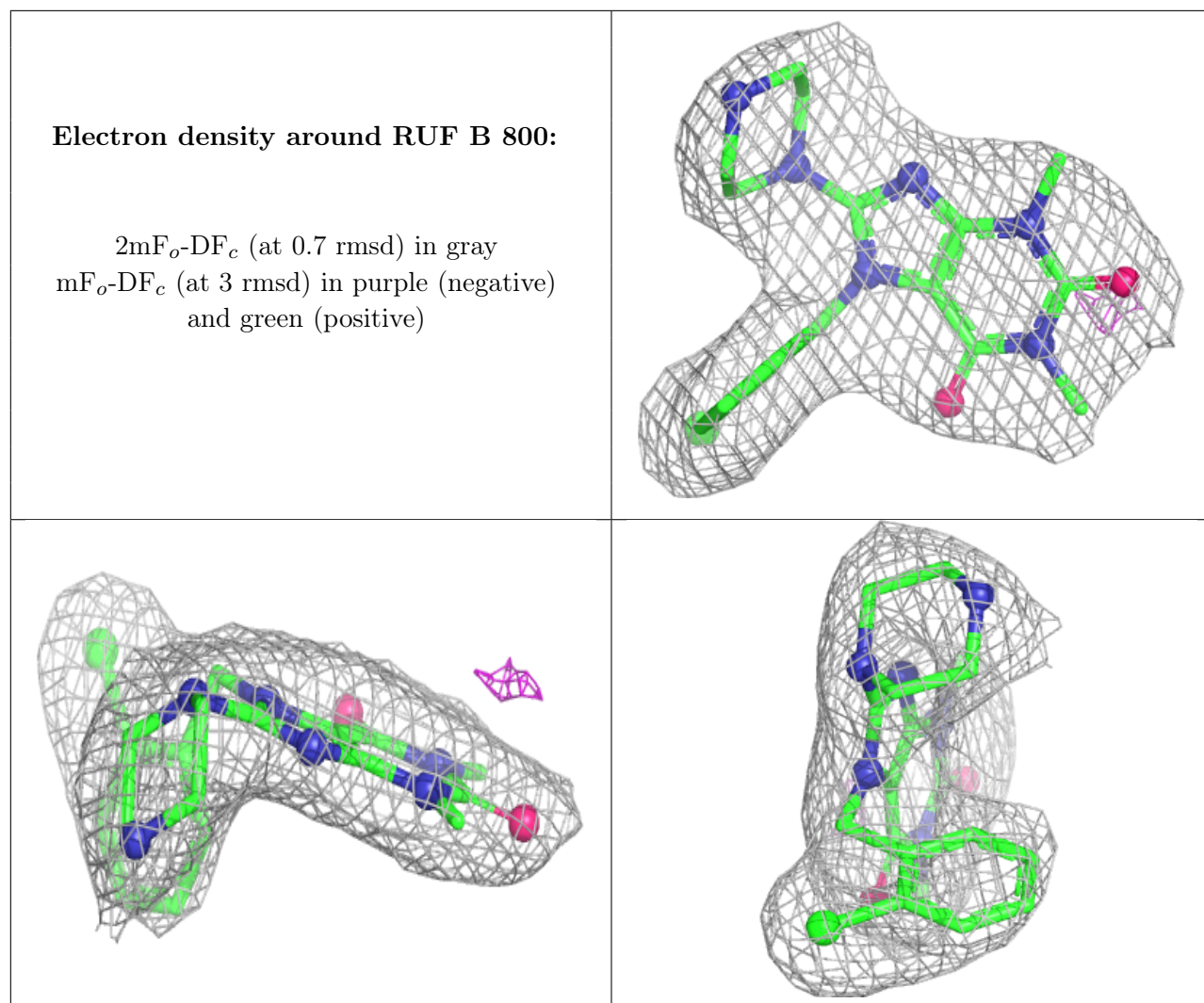
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around RUF C 800:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.