Full wwPDB X-ray Structure Validation Report ⓘ

Apr 12, 2022 – 08:06 AM EDT

PDB ID	:	2QJR
Title	:	dipepdyl peptidase IV in complex with inhibitor PZF
Authors	:	Shenping, L.
Deposited on	:	2007-07-09
Resolution	:	2.20 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 following versions of software and data (see references ⓘ) were used in the production of this report:

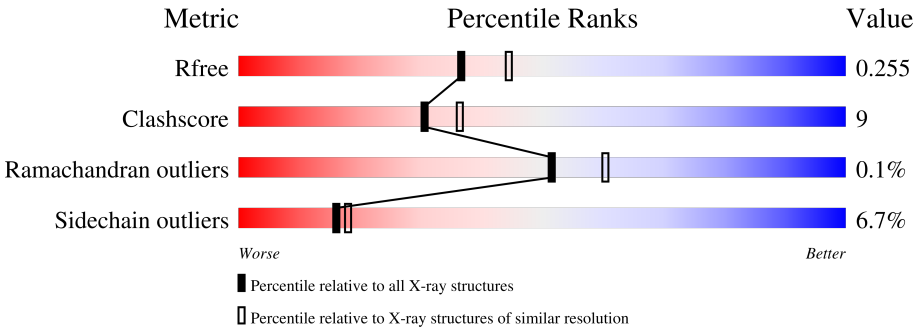
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	748	75% 20%
1	B	748	69% 23% 5%
2	C	2	100%
2	E	2	100%
2	F	2	50% 50%
2	G	2	100%
2	H	2	50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	4	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	G	1	X	-	-	-
2	NAG	H	1	X	-	-	-
3	LGU	D	3	X	-	-	-
6	LGU	A	803	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12532 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 membrane form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5957	3825	980	1126	26			
1	B	728	Total	C	N	O	S	0	0	0
			5957	3825	980	1126	26			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	767	LEU	-	expression tag	UNP P27487
A	768	VAL	-	expression tag	UNP P27487
A	769	PRO	-	expression tag	UNP P27487
A	770	ARG	-	expression tag	UNP P27487
A	771	GLY	-	expression tag	UNP P27487
A	772	SER	-	expression tag	UNP P27487
A	773	HIS	-	expression tag	UNP P27487
A	774	HIS	-	expression tag	UNP P27487
A	775	HIS	-	expression tag	UNP P27487
A	776	HIS	-	expression tag	UNP P27487
A	777	HIS	-	expression tag	UNP P27487
A	778	HIS	-	expression tag	UNP P27487
B	767	LEU	-	expression tag	UNP P27487
B	768	VAL	-	expression tag	UNP P27487
B	769	PRO	-	expression tag	UNP P27487
B	770	ARG	-	expression tag	UNP P27487
B	771	GLY	-	expression tag	UNP P27487
B	772	SER	-	expression tag	UNP P27487
B	773	HIS	-	expression tag	UNP P27487
B	774	HIS	-	expression tag	UNP P27487
B	775	HIS	-	expression tag	UNP P27487
B	776	HIS	-	expression tag	UNP P27487
B	777	HIS	-	expression tag	UNP P27487
B	778	HIS	-	expression tag	UNP P27487

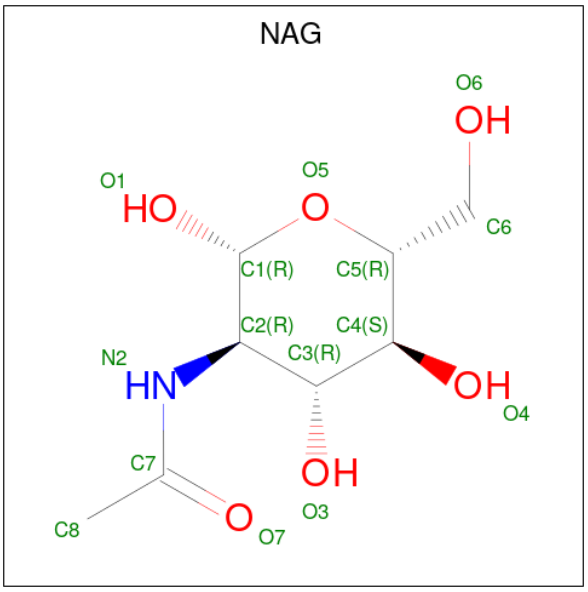
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

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

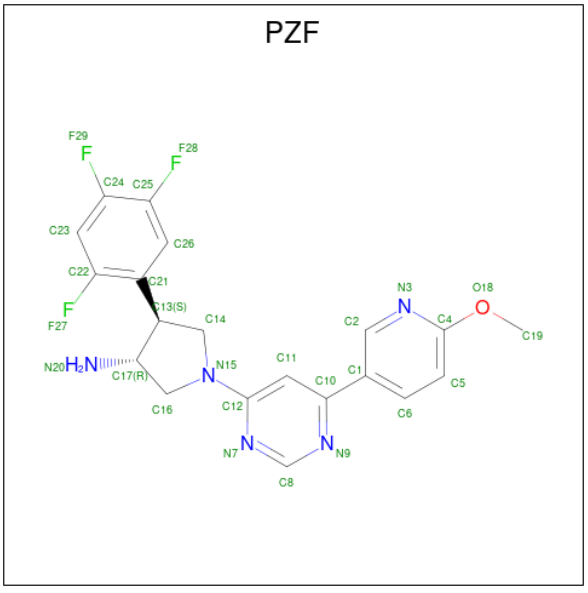
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: 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	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is (3R,4S)-1-[6-(6-METHOXYPYRIDIN-3-YL)PYRIMIDIN-4-YL]-4-(2,4,5-TRIFLUOROPHENYL)PYRROLIDIN-3-AMINE (three-letter code: PZF) (formula: $C_{20}H_{18}F_3N_5O$).



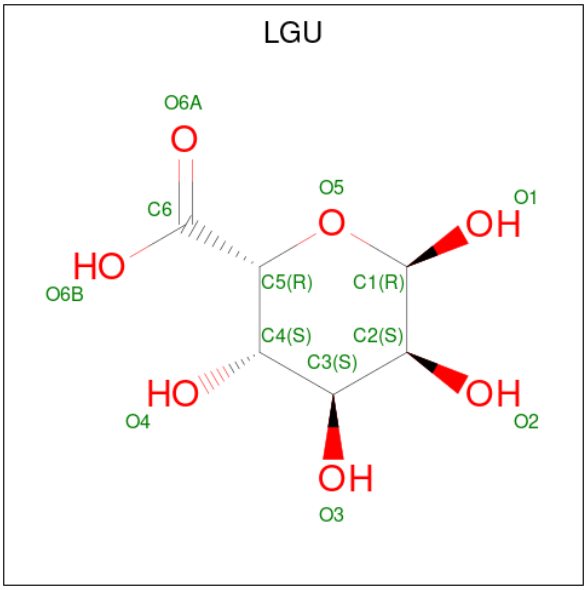
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	0	0
			29	20	3	5	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	F	N	O	0	0
			29	20	3	5	1		

- Molecule 6 is alpha-L-gulopyranuronic acid (three-letter code: LGU) (formula: $C_6H_{10}O_7$).



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

- Molecule 7 is water.

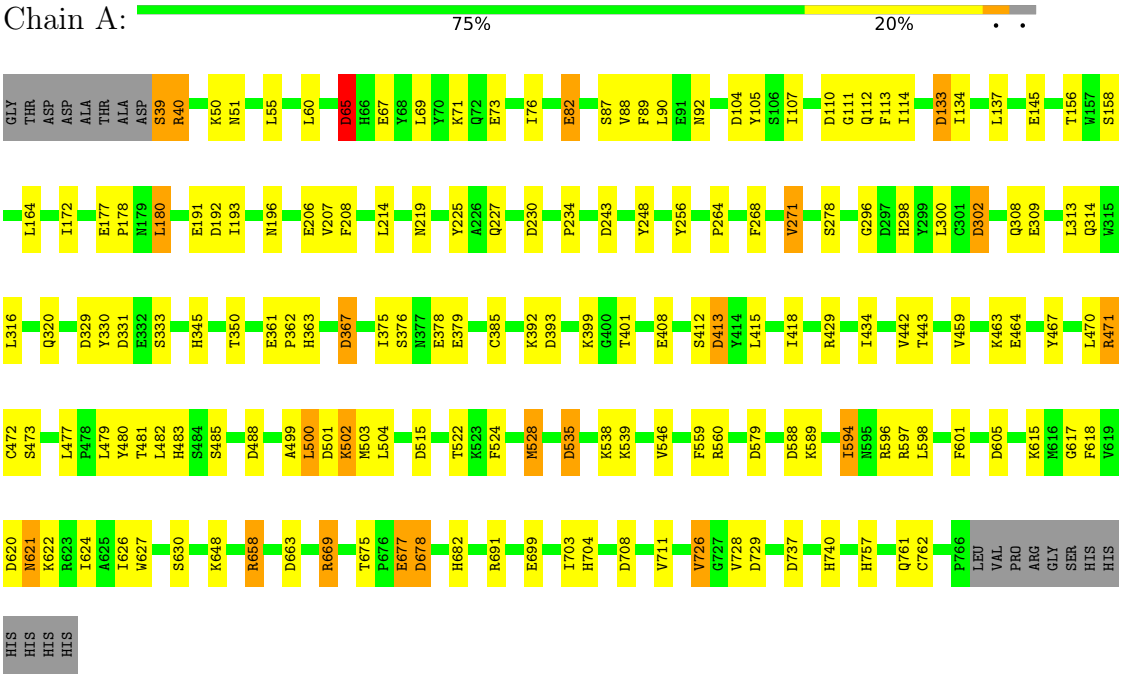
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	105	Total	O	0	0
			105	105		
7	B	226	Total	O	0	0
			226	226		

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. 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. 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.

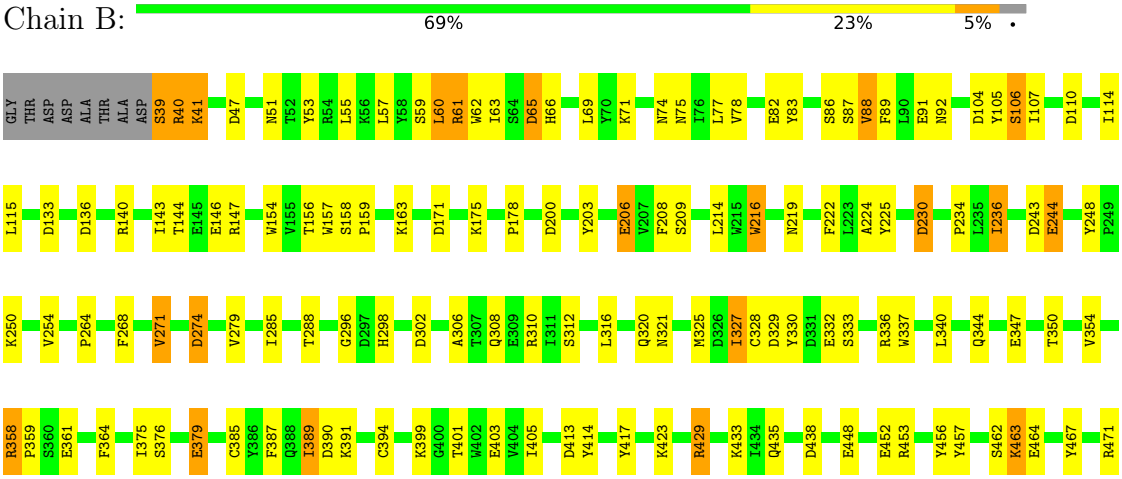
• Molecule 1: Dipeptidyl peptidase 4 membrane form

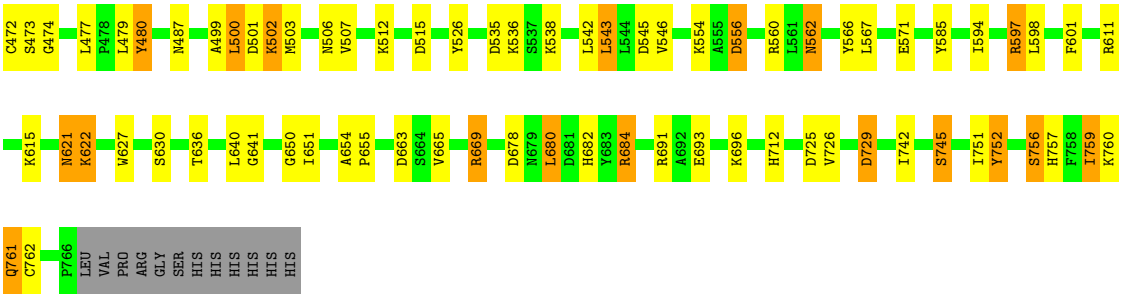
Chain A:



• Molecule 1: Dipeptidyl peptidase 4 membrane form

Chain B:



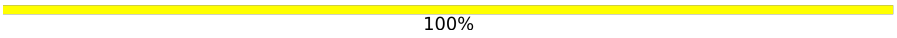


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

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

Chain E:



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

Chain F:

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

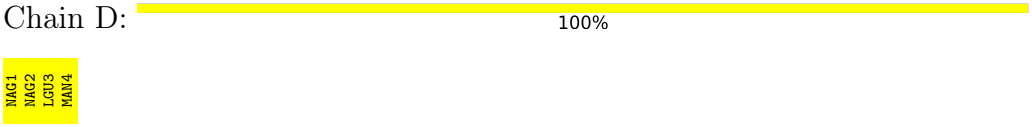
Chain G:

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

Chain H:

• Molecule 3: alpha-D-mannopyranose-(1-3)-alpha-L-gulopyranuronic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.47Å 68.80Å 422.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.90 – 2.20 41.90 – 2.19	Depositor EDS
% Data completeness (in resolution range)	85.7 (41.90-2.20) 85.4 (41.90-2.19)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.65 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.191 , 0.253 0.200 , 0.255	Depositor DCC
R_{free} test set	4280 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.929	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 67.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.055 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12532	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.12	6/6129 (0.1%)	1.09	33/8336 (0.4%)
1	B	1.43	42/6129 (0.7%)	1.24	43/8336 (0.5%)
All	All	1.29	48/12258 (0.4%)	1.17	76/16672 (0.5%)

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	385	CYS	CB-SG	-8.03	1.68	1.82
1	B	250	LYS	CD-CE	6.76	1.68	1.51
1	B	244	GLU	CD-OE1	6.63	1.32	1.25
1	B	83	TYR	CE1-CZ	6.46	1.47	1.38
1	B	82	GLU	CD-OE1	6.43	1.32	1.25
1	A	658	ARG	NE-CZ	6.40	1.41	1.33
1	B	463	LYS	CE-NZ	6.37	1.65	1.49
1	B	669	ARG	CD-NE	-6.30	1.35	1.46
1	B	417	TYR	CD1-CE1	-6.29	1.29	1.39
1	B	480	TYR	CE2-CZ	-6.19	1.30	1.38
1	B	203	TYR	CE1-CZ	6.14	1.46	1.38
1	B	429	ARG	NE-CZ	6.03	1.40	1.33
1	B	347	GLU	CD-OE1	5.92	1.32	1.25
1	B	61	ARG	CG-CD	5.88	1.66	1.51
1	B	271	VAL	CB-CG2	-5.88	1.40	1.52
1	A	379	GLU	CD-OE2	5.84	1.32	1.25
1	B	473	SER	CB-OG	-5.82	1.34	1.42
1	B	752	TYR	CD1-CE1	5.79	1.48	1.39
1	B	216	TRP	CG-CD1	5.76	1.44	1.36
1	B	254	VAL	CB-CG1	5.70	1.64	1.52
1	A	39	SER	CA-CB	5.66	1.61	1.52
1	B	423	LYS	CE-NZ	5.63	1.63	1.49
1	B	745	SER	CB-OG	-5.56	1.35	1.42
1	A	256	TYR	CE1-CZ	-5.48	1.31	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	354	VAL	CB-CG2	-5.48	1.41	1.52
1	B	82	GLU	CD-OE2	5.46	1.31	1.25
1	B	106	SER	CB-OG	5.45	1.49	1.42
1	B	403	GLU	CD-OE2	5.39	1.31	1.25
1	B	86	SER	CB-OG	-5.37	1.35	1.42
1	B	225	TYR	CD1-CE1	-5.30	1.31	1.39
1	B	756	SER	CB-OG	5.29	1.49	1.42
1	B	312	SER	CB-OG	-5.27	1.35	1.42
1	B	88	VAL	CB-CG1	-5.26	1.41	1.52
1	A	82	GLU	CD-OE2	5.24	1.31	1.25
1	B	526	TYR	CD1-CE1	-5.23	1.31	1.39
1	B	452	GLU	CD-OE1	5.22	1.31	1.25
1	B	222	PHE	CD1-CE1	5.21	1.49	1.39
1	B	154	TRP	CE3-CZ3	5.17	1.47	1.38
1	B	585	TYR	CE1-CZ	-5.11	1.31	1.38
1	B	391	LYS	CE-NZ	5.11	1.61	1.49
1	B	467	TYR	CE1-CZ	-5.10	1.31	1.38
1	A	589	LYS	CE-NZ	5.08	1.61	1.49
1	B	347	GLU	CD-OE2	5.07	1.31	1.25
1	B	379	GLU	CD-OE1	5.06	1.31	1.25
1	B	453	ARG	CZ-NH1	-5.05	1.26	1.33
1	B	456	TYR	CZ-OH	5.05	1.46	1.37
1	B	474	GLY	C-O	-5.03	1.15	1.23
1	B	457	TYR	CD2-CE2	5.00	1.46	1.39

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	669	ARG	NE-CZ-NH2	-12.46	114.07	120.30
1	A	669	ARG	NE-CZ-NH1	12.26	126.43	120.30
1	B	453	ARG	NE-CZ-NH1	-10.82	114.89	120.30
1	B	61	ARG	NE-CZ-NH2	-10.66	114.97	120.30
1	A	658	ARG	NE-CZ-NH1	10.27	125.44	120.30
1	B	453	ARG	NE-CZ-NH2	9.92	125.26	120.30
1	A	329	ASP	CB-CG-OD2	8.99	126.39	118.30
1	B	429	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	A	501	ASP	CB-CG-OD2	8.88	126.30	118.30
1	B	302	ASP	CB-CG-OD2	8.68	126.11	118.30
1	A	579	ASP	CB-CG-OD2	8.51	125.96	118.30
1	B	515	ASP	CB-CG-OD2	8.18	125.66	118.30
1	A	367	ASP	CB-CG-OD2	8.17	125.65	118.30
1	B	678	ASP	CB-CG-OD2	8.13	125.61	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	230	ASP	CB-CG-OD2	8.10	125.59	118.30
1	A	691	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	B	316	LEU	CB-CG-CD1	7.99	124.58	111.00
1	B	60	LEU	CA-CB-CG	7.98	133.66	115.30
1	B	725	ASP	CB-CG-OD2	7.96	125.46	118.30
1	A	393	ASP	CB-CG-OD2	7.75	125.27	118.30
1	A	133	ASP	CB-CG-OD2	7.46	125.01	118.30
1	A	515	ASP	CB-CG-OD2	7.41	124.97	118.30
1	A	560	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	678	ASP	CB-CG-OD2	7.18	124.76	118.30
1	A	65	ASP	CB-CG-OD2	7.08	124.67	118.30
1	A	401	THR	OG1-CB-CG2	-7.04	93.80	110.00
1	B	271	VAL	CB-CA-C	-7.02	98.06	111.40
1	A	535	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	302	ASP	CB-CG-OD2	6.98	124.58	118.30
1	B	729	ASP	CB-CG-OD2	6.96	124.56	118.30
1	B	556	ASP	CB-CG-OD2	6.94	124.55	118.30
1	A	104	ASP	CB-CG-OD1	6.92	124.53	118.30
1	B	61	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	B	438	ASP	CB-CG-OD2	6.67	124.31	118.30
1	A	243	ASP	CB-CG-OD1	6.63	124.27	118.30
1	B	133	ASP	CB-CG-OD2	6.63	124.27	118.30
1	B	47	ASP	CB-CG-OD2	6.63	124.26	118.30
1	B	390	ASP	CB-CG-OD2	6.61	124.25	118.30
1	B	316	LEU	CB-CG-CD2	-6.59	99.79	111.00
1	B	501	ASP	CB-CG-OD2	6.52	124.17	118.30
1	B	321	ASN	CB-CA-C	-6.51	97.37	110.40
1	A	691	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	B	669	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	A	669	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	413	ASP	CB-CG-OD2	6.16	123.84	118.30
1	B	65	ASP	CB-CG-OD2	6.14	123.82	118.30
1	A	443	THR	OG1-CB-CG2	-6.09	96.00	110.00
1	B	385	CYS	CA-CB-SG	-6.03	103.16	114.00
1	A	331	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	329	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	737	ASP	CB-CG-OD1	5.75	123.48	118.30
1	B	171	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	243	ASP	CB-CG-OD1	5.66	123.39	118.30
1	B	560	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	708	ASP	CB-CG-OD1	5.65	123.39	118.30
1	B	104	ASP	CB-CG-OD2	5.65	123.38	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	560	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	67	GLU	OE1-CD-OE2	-5.61	116.57	123.30
1	A	620	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	588	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	605	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	501	ASP	CB-CG-OD1	-5.46	113.38	118.30
1	B	60	LEU	CB-CG-CD2	5.44	120.25	111.00
1	B	759	ILE	CG1-CB-CG2	-5.44	99.44	111.40
1	B	394	CYS	N-CA-C	-5.33	96.61	111.00
1	B	274	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	546	VAL	CG1-CB-CG2	-5.28	102.46	110.90
1	A	110	ASP	CB-CG-OD2	5.27	123.05	118.30
1	B	115	LEU	CA-CB-CG	5.26	127.39	115.30
1	B	206	GLU	CB-CA-C	-5.25	99.90	110.40
1	B	560	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	271	VAL	CB-CA-C	-5.21	101.50	111.40
1	B	110	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	321	ASN	N-CA-CB	-5.14	101.35	110.60
1	B	78	VAL	CB-CA-C	-5.12	101.68	111.40
1	A	488	ASP	CB-CG-OD2	5.11	122.90	118.30

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	5957	0	5672	94	0
1	B	5957	0	5672	125	0
2	C	28	0	25	1	0
2	E	28	0	25	0	0
2	F	28	0	25	1	0
2	G	28	0	25	2	0
2	H	28	0	25	1	0
3	D	50	0	40	0	0
4	A	14	0	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	14	0	13	1	0
5	A	29	0	18	1	0
5	B	29	0	18	0	0
6	A	11	0	7	0	0
7	A	105	0	0	10	0
7	B	226	0	0	22	0
All	All	12532	0	11578	219	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 9.

All (219) 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:39:SER:O	1:A:40:ARG:CZ	1.79	1.29
1:B:40:ARG:N	1:B:40:ARG:HD3	1.64	1.12
1:B:39:SER:HB2	1:B:40:ARG:HD2	1.31	1.08
1:B:597:ARG:HD3	7:B:992:HOH:O	1.56	1.02
1:A:621:ASN:C	1:A:621:ASN:HD22	1.64	0.99
1:B:39:SER:HB2	1:B:40:ARG:CD	1.91	0.99
1:B:74:ASN:HB2	7:B:1034:HOH:O	1.63	0.94
1:B:401:THR:HG22	1:B:401:THR:O	1.74	0.87
1:B:39:SER:O	7:B:901:HOH:O	1.93	0.87
1:B:40:ARG:HD3	1:B:40:ARG:H	1.29	0.87
1:B:147:ARG:HD3	7:B:905:HOH:O	1.75	0.87
1:A:434:ILE:HD12	1:A:442:VAL:HG22	1.59	0.85
1:A:630:SER:OG	1:A:740:HIS:NE2	2.09	0.84
1:B:499:ALA:O	1:B:502:LYS:HG2	1.78	0.84
1:B:65:ASP:OD1	1:B:463:LYS:O	1.95	0.83
1:B:236:ILE:HG12	1:B:712:HIS:CE1	2.13	0.82
1:A:39:SER:O	1:A:40:ARG:NH1	2.14	0.80
1:A:39:SER:O	1:A:40:ARG:NH2	2.16	0.79
1:B:598:LEU:O	1:B:682:HIS:HE1	1.65	0.79
1:B:219:ASN:HB2	1:B:308:GLN:OE1	1.85	0.75
1:B:61:ARG:HD3	7:B:1068:HOH:O	1.85	0.75
1:A:345:HIS:HD2	7:A:969:HOH:O	1.70	0.74
1:B:66:HIS:HD2	7:B:1105:HOH:O	1.71	0.74
1:B:306:ALA:HB3	1:B:310:ARG:HG2	1.70	0.73
1:B:389:ILE:O	7:B:902:HOH:O	2.06	0.73
1:A:658:ARG:NE	7:A:901:HOH:O	1.93	0.72
1:B:66:HIS:CD2	7:B:1105:HOH:O	2.42	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:LEU:HD22	1:B:500:LEU:HD13	1.73	0.71
1:A:463:LYS:O	1:A:464:GLU:HB2	1.91	0.70
1:A:177:GLU:HB2	1:A:180:LEU:HD22	1.73	0.70
1:A:499:ALA:O	1:A:502:LYS:HG3	1.91	0.69
1:B:74:ASN:O	1:B:75:ASN:OD1	2.10	0.69
1:A:206:GLU:OE2	1:A:663:ASP:OD2	2.11	0.68
1:B:55:LEU:HD23	1:B:500:LEU:CD1	2.23	0.68
1:A:89:PHE:CE2	1:A:107:ILE:HD13	2.29	0.68
1:B:57:LEU:HD23	7:B:958:HOH:O	1.94	0.68
1:A:71:LYS:NZ	1:A:92:ASN:HD21	1.92	0.68
1:B:89:PHE:CE2	1:B:107:ILE:HD13	2.30	0.67
1:B:71:LYS:NZ	1:B:74:ASN:HA	2.09	0.67
1:A:761:GLN:NE2	7:A:903:HOH:O	2.26	0.66
1:B:39:SER:CB	1:B:40:ARG:HH11	2.09	0.66
1:A:621:ASN:HD22	1:A:622:LYS:N	1.93	0.65
1:B:503:MET:O	1:B:506:ASN:HB2	1.97	0.65
1:B:147:ARG:NH1	7:B:905:HOH:O	2.29	0.64
1:A:345:HIS:CD2	7:A:969:HOH:O	2.46	0.64
1:A:621:ASN:C	1:A:621:ASN:ND2	2.42	0.63
1:B:680:LEU:HD22	1:B:684:ARG:HD3	1.80	0.63
1:B:89:PHE:HE2	1:B:107:ILE:HD13	1.64	0.63
1:B:429:ARG:NE	7:B:903:HOH:O	2.18	0.63
1:A:298:HIS:HE1	7:A:970:HOH:O	1.81	0.63
1:B:414:TYR:CD1	1:B:433:LYS:HD2	2.32	0.63
1:B:598:LEU:O	1:B:682:HIS:CE1	2.49	0.63
1:A:111:GLY:O	1:A:137:LEU:HD12	2.00	0.62
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.65	0.62
1:B:358:ARG:HB2	1:B:359:PRO:HD2	1.80	0.62
1:B:621:ASN:HD22	1:B:621:ASN:C	2.02	0.62
1:A:500:LEU:HD22	1:A:504:LEU:HG	1.82	0.62
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.80	0.62
1:A:361:GLU:OE2	1:A:363:HIS:HE1	1.83	0.61
1:B:71:LYS:HZ1	1:B:74:ASN:HA	1.65	0.61
1:B:40:ARG:N	1:B:40:ARG:CD	2.48	0.61
1:B:163:LYS:NZ	1:B:274:ASP:OD1	2.31	0.61
1:B:39:SER:HB2	1:B:40:ARG:HD3	1.80	0.60
4:B:801:NAG:C4	7:B:910:HOH:O	2.49	0.60
1:B:401:THR:O	1:B:401:THR:CG2	2.44	0.60
1:B:40:ARG:CB	1:B:506:ASN:O	2.50	0.59
1:A:39:SER:O	1:A:40:ARG:NE	2.32	0.59
1:A:434:ILE:HD12	1:A:442:VAL:CG2	2.32	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:680:LEU:HD22	1:B:684:ARG:CD	2.32	0.58
1:A:76:ILE:HD12	1:A:90:LEU:HB3	1.85	0.58
1:B:405:ILE:HG13	1:B:429:ARG:CD	2.33	0.58
1:A:71:LYS:HZ1	1:A:92:ASN:HD21	1.52	0.57
1:B:55:LEU:HD23	1:B:500:LEU:HD12	1.85	0.57
1:A:470:LEU:HD12	1:A:483:HIS:CE1	2.40	0.57
1:A:528:MET:HE1	1:A:618:PHE:CZ	2.39	0.57
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.88	0.57
1:B:535:ASP:OD2	1:B:538:LYS:NZ	2.38	0.57
1:B:55:LEU:HD23	1:B:500:LEU:HD11	1.87	0.56
1:B:39:SER:OG	1:B:40:ARG:NH1	2.39	0.56
1:B:562:ASN:C	1:B:562:ASN:HD22	2.08	0.56
1:A:89:PHE:HE2	1:A:107:ILE:HD13	1.71	0.55
1:B:597:ARG:CD	7:B:992:HOH:O	2.30	0.55
1:A:207:VAL:HG12	1:A:208:PHE:CD1	2.42	0.55
1:A:134:ILE:HD11	1:A:164:LEU:CD1	2.37	0.54
1:B:40:ARG:HB2	1:B:506:ASN:O	2.07	0.54
1:B:296:GLY:O	1:B:298:HIS:HD2	1.90	0.54
7:B:1032:HOH:O	2:G:1:NAG:H82	2.07	0.54
1:B:325:MET:HE1	1:B:327:ILE:HD11	1.88	0.53
1:A:65:ASP:OD1	1:A:65:ASP:N	2.27	0.53
1:B:399:LYS:NZ	7:B:915:HOH:O	2.42	0.53
1:A:314:GLN:HE22	1:A:362:PRO:HD3	1.73	0.53
1:A:726:VAL:CG1	1:A:728:VAL:HG23	2.39	0.53
1:A:219:ASN:HB2	1:A:308:GLN:OE1	2.08	0.53
1:A:320:GLN:OE1	1:A:669:ARG:HD3	2.10	0.52
1:A:624:ILE:HD12	7:A:916:HOH:O	2.07	0.52
1:A:675:THR:HB	1:A:677:GLU:OE1	2.09	0.52
1:A:594:ILE:CD1	1:A:601:PHE:HB2	2.40	0.52
1:A:191:GLU:O	1:A:192:ASP:HB2	2.10	0.51
1:A:230:ASP:OD1	1:A:264:PRO:HB3	2.09	0.51
1:A:378:GLU:CG	7:A:906:HOH:O	2.58	0.51
1:A:546:VAL:HG21	1:A:626:ILE:HD11	1.93	0.51
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.92	0.51
1:B:693:GLU:CD	1:B:726:VAL:HG21	2.32	0.51
1:A:528:MET:HE1	1:A:618:PHE:HZ	1.74	0.50
1:A:296:GLY:O	1:A:298:HIS:HD2	1.94	0.50
1:A:596:ARG:NH2	1:A:678:ASP:OD1	2.42	0.50
1:B:463:LYS:O	1:B:464:GLU:HB2	2.12	0.50
1:B:87:SER:OG	2:F:1:NAG:O7	2.29	0.50
1:B:621:ASN:HD22	1:B:622:LYS:N	2.09	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:MET:CE	1:B:327:ILE:HD11	2.43	0.49
1:B:594:ILE:CD1	1:B:601:PHE:HB2	2.42	0.49
1:B:146:GLU:O	1:B:175:LYS:NZ	2.42	0.49
1:A:40:ARG:NE	1:A:40:ARG:HA	2.24	0.49
7:B:1124:HOH:O	2:H:1:NAG:H83	2.12	0.49
1:B:477:LEU:CD2	1:B:500:LEU:HD13	2.42	0.49
1:B:611:ARG:O	1:B:615:LYS:HG2	2.13	0.49
1:B:200:ASP:OD2	1:B:264:PRO:HG3	2.12	0.49
1:B:206:GLU:HG3	1:B:665:VAL:HB	1.95	0.49
1:A:594:ILE:HG23	1:A:594:ILE:O	2.13	0.49
1:B:463:LYS:O	1:B:464:GLU:CB	2.58	0.48
1:B:41:LYS:HE2	1:B:53:TYR:OH	2.13	0.48
1:A:473:SER:OG	7:A:902:HOH:O	2.20	0.48
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.48	0.48
1:A:757:HIS:HD2	1:B:729:ASP:OD2	1.97	0.48
1:A:726:VAL:HG13	1:A:728:VAL:HG23	1.94	0.48
1:A:477:LEU:HD22	1:A:500:LEU:HD13	1.95	0.48
1:A:522:THR:HG22	1:A:524:PHE:CE2	2.50	0.47
1:B:39:SER:C	1:B:40:ARG:HD3	2.32	0.47
1:A:502:LYS:HE2	1:A:503:MET:HG3	1.95	0.47
1:A:408:GLU:HG3	1:A:418:ILE:HD12	1.97	0.47
1:B:39:SER:CB	1:B:40:ARG:CD	2.81	0.46
1:A:69:LEU:HD13	1:A:107:ILE:HD12	1.98	0.46
1:B:39:SER:N	1:B:40:ARG:HH11	2.14	0.46
1:B:310:ARG:HA	1:B:328:CYS:O	2.15	0.46
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.97	0.46
1:A:413:ASP:OD2	1:A:413:ASP:N	2.49	0.46
1:A:361:GLU:OE2	1:A:363:HIS:CE1	2.68	0.46
1:A:55:LEU:HD21	1:A:559:PHE:HE2	1.80	0.46
1:B:693:GLU:O	1:B:696:LYS:HG3	2.15	0.46
1:A:429:ARG:NE	7:A:911:HOH:O	2.43	0.46
1:A:134:ILE:HD11	1:A:164:LEU:HD11	1.97	0.46
1:B:358:ARG:HB2	1:B:359:PRO:CD	2.46	0.45
1:A:206:GLU:CD	5:A:802:PZF:H202	2.20	0.45
1:B:414:TYR:CE1	1:B:433:LYS:HD2	2.50	0.45
1:B:751:ILE:HG23	1:B:752:TYR:N	2.32	0.45
1:B:636:THR:HG21	1:B:651:ILE:O	2.15	0.45
1:B:41:LYS:CE	1:B:53:TYR:OH	2.65	0.45
1:A:375:ILE:HG23	7:A:994:HOH:O	2.17	0.45
1:A:528:MET:HE3	1:A:618:PHE:CE1	2.52	0.45
1:A:415:LEU:HD23	1:A:415:LEU:C	2.37	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:SER:HB2	1:B:159:PRO:CD	2.47	0.45
1:B:143:ILE:HD13	1:B:178:PRO:HB2	2.00	0.44
1:B:756:SER:O	1:B:760:LYS:HG3	2.18	0.44
1:B:144:THR:HG22	7:B:1120:HOH:O	2.17	0.44
1:B:306:ALA:CB	1:B:310:ARG:HG2	2.44	0.44
1:A:648:LYS:NZ	1:A:699:GLU:OE1	2.50	0.44
1:A:214:LEU:HD23	1:A:225:TYR:HB3	2.00	0.44
1:A:471:ARG:HD2	1:A:480:TYR:CE2	2.53	0.44
1:B:325:MET:O	1:B:344:GLN:HA	2.18	0.44
1:B:359:PRO:HA	7:B:908:HOH:O	2.18	0.44
1:B:545:ASP:OD1	1:B:554:LYS:NZ	2.40	0.44
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.98	0.44
1:A:268:PHE:CZ	1:A:313:LEU:HD21	2.54	0.43
1:B:206:GLU:OE2	1:B:663:ASP:OD2	2.36	0.43
1:A:192:ASP:C	1:A:193:ILE:HG13	2.39	0.43
1:B:654:ALA:N	1:B:655:PRO:CD	2.81	0.43
1:A:375:ILE:HG22	1:A:376:SER:N	2.33	0.43
1:A:535:ASP:OD2	1:A:538:LYS:HG2	2.18	0.43
1:A:598:LEU:O	1:A:682:HIS:NE2	2.39	0.43
1:B:63:ILE:HG21	1:B:69:LEU:CD1	2.48	0.43
1:B:144:THR:CG2	7:B:1120:HOH:O	2.66	0.43
1:B:641:GLY:O	1:B:691:ARG:HB3	2.17	0.43
1:B:759:ILE:HG23	1:B:759:ILE:HD12	1.66	0.43
1:A:134:ILE:CD1	1:A:164:LEU:HD11	2.49	0.43
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.54	0.43
1:B:158:SER:HA	1:B:216:TRP:CD1	2.53	0.43
1:B:332:GLU:OE1	2:G:2:NAG:O3	2.36	0.43
1:A:729:ASP:OD2	1:B:757:HIS:HD2	2.02	0.43
1:B:106:SER:HG	1:B:157:TRP:HD1	1.67	0.43
1:A:309:GLU:HB3	1:A:330:TYR:HB3	2.00	0.42
1:A:648:LYS:NZ	1:A:699:GLU:OE2	2.52	0.42
2:C:1:NAG:H61	2:C:2:NAG:C7	2.49	0.42
1:A:172:ILE:HD13	1:A:214:LEU:HD21	2.01	0.42
1:A:418:ILE:HD11	1:A:459:VAL:HG12	2.01	0.42
1:B:627:TRP:HB2	1:B:651:ILE:HB	2.02	0.42
1:A:69:LEU:CD1	1:A:107:ILE:HD12	2.50	0.42
1:A:82:GLU:HB2	1:A:467:TYR:OH	2.19	0.41
1:B:364:PHE:CE2	1:B:389:ILE:HD11	2.51	0.41
1:B:571:GLU:CD	1:B:760:LYS:HD3	2.40	0.41
1:A:711:VAL:CG2	1:A:740:HIS:CE1	3.03	0.41
1:B:71:LYS:HZ3	1:B:74:ASN:HA	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:GLU:OE1	1:B:448:GLU:HA	2.20	0.41
1:B:320:GLN:OE1	1:B:669:ARG:HD3	2.21	0.41
1:B:375:ILE:CD1	1:B:387:PHE:HZ	2.34	0.41
1:B:543:LEU:HD12	1:B:567:LEU:HD13	2.01	0.41
1:A:112:GLN:HB3	1:A:113:PHE:CE2	2.55	0.41
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.56	0.41
1:A:477:LEU:HD22	1:A:500:LEU:CD1	2.51	0.41
1:B:208:PHE:O	1:B:209:SER:C	2.58	0.41
1:B:330:TYR:HB2	1:B:337:TRP:CH2	2.55	0.41
1:B:761:GLN:C	1:B:761:GLN:OE1	2.59	0.41
1:B:405:ILE:HG13	1:B:429:ARG:HD3	2.03	0.41
1:B:487:ASN:N	7:B:907:HOH:O	2.34	0.41
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.21	0.41
1:A:703:ILE:HD13	1:A:703:ILE:HG21	1.78	0.41
1:B:512:LYS:NZ	1:B:556:ASP:O	2.49	0.41
1:B:742:ILE:HG22	1:B:742:ILE:O	2.20	0.41
1:A:177:GLU:HA	1:A:178:PRO:HD3	1.94	0.41
1:A:539:LYS:HE2	1:A:617:GLY:O	2.21	0.41
1:B:62:TRP:CG	1:B:462:SER:HA	2.56	0.41
1:B:39:SER:CB	1:B:40:ARG:HD3	2.49	0.41
1:B:236:ILE:HG12	1:B:712:HIS:ND1	2.34	0.41
1:B:471:ARG:HG3	1:B:480:TYR:CE2	2.56	0.41
1:A:481:THR:OG1	1:A:483:HIS:CE1	2.71	0.40
1:B:435:GLN:NE2	7:B:934:HOH:O	2.51	0.40
1:B:285:ILE:HG23	1:B:336:ARG:HH11	1.85	0.40
1:B:669:ARG:HD2	7:B:1085:HOH:O	2.20	0.40
1:B:136:ASP:C	1:B:136:ASP:OD1	2.60	0.40
1:B:562:ASN:C	1:B:562:ASN:ND2	2.73	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	726/748 (97%)	694 (96%)	31 (4%)	1 (0%)	51 60
1	B	726/748 (97%)	689 (95%)	36 (5%)	1 (0%)	51 60
All	All	1452/1496 (97%)	1383 (95%)	67 (5%)	2 (0%)	51 60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	B	630	SER

5.3.2 Protein sidechains (i)

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	651/669 (97%)	610 (94%)	41 (6%)	18 20
1	B	651/669 (97%)	605 (93%)	46 (7%)	14 16
All	All	1302/1338 (97%)	1215 (93%)	87 (7%)	16 18

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	50	LYS
1	A	51	ASN
1	A	60	LEU
1	A	65	ASP
1	A	87	SER
1	A	88	VAL
1	A	133	ASP
1	A	145	GLU
1	A	156	THR
1	A	158	SER
1	A	180	LEU
1	A	271	VAL
1	A	278	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	300	LEU
1	A	316	LEU
1	A	333	SER
1	A	350	THR
1	A	367	ASP
1	A	385	CYS
1	A	392	LYS
1	A	399	LYS
1	A	412	SER
1	A	413	ASP
1	A	471	ARG
1	A	472	CYS
1	A	479	LEU
1	A	482	LEU
1	A	485	SER
1	A	500	LEU
1	A	502	LYS
1	A	528	MET
1	A	594	ILE
1	A	597	ARG
1	A	615	LYS
1	A	621	ASN
1	A	627	TRP
1	A	677	GLU
1	A	704	HIS
1	A	726	VAL
1	A	762	CYS
1	B	39	SER
1	B	40	ARG
1	B	41	LYS
1	B	51	ASN
1	B	59	SER
1	B	60	LEU
1	B	77	LEU
1	B	88	VAL
1	B	91	GLU
1	B	92	ASN
1	B	140	ARG
1	B	156	THR
1	B	214	LEU
1	B	230	ASP
1	B	236	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	244	GLU
1	B	271	VAL
1	B	279	VAL
1	B	288	THR
1	B	327	ILE
1	B	333	SER
1	B	340	LEU
1	B	350	THR
1	B	358	ARG
1	B	361	GLU
1	B	376	SER
1	B	379	GLU
1	B	389	ILE
1	B	472	CYS
1	B	479	LEU
1	B	500	LEU
1	B	502	LYS
1	B	507	VAL
1	B	536	LYS
1	B	542	LEU
1	B	543	LEU
1	B	562	ASN
1	B	566	TYR
1	B	597	ARG
1	B	621	ASN
1	B	622	LYS
1	B	680	LEU
1	B	684	ARG
1	B	745	SER
1	B	761	GLN
1	B	762	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	92	ASN
1	A	169	ASN
1	A	247	GLN
1	A	263	ASN
1	A	298	HIS
1	A	314	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	338	ASN
1	A	363	HIS
1	A	483	HIS
1	A	533	HIS
1	A	621	ASN
1	A	748	HIS
1	A	757	HIS
1	B	75	ASN
1	B	123	GLN
1	B	169	ASN
1	B	263	ASN
1	B	298	HIS
1	B	383	HIS
1	B	487	ASN
1	B	562	ASN
1	B	586	GLN
1	B	621	ASN
1	B	682	HIS
1	B	697	GLN
1	B	757	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

14 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	C	1	2,1	14,14,15	1.50	3 (21%)	17,19,21	1.64	4 (23%)
2	NAG	C	2	2	14,14,15	0.86	0	17,19,21	1.94	6 (35%)
3	NAG	D	1	3,1	14,14,15	1.30	2 (14%)	17,19,21	2.20	9 (52%)
3	NAG	D	2	3	14,14,15	0.91	0	17,19,21	1.15	1 (5%)
3	LGU	D	3	3,6	11,11,13	0.84	1 (9%)	15,15,19	2.44	6 (40%)
3	MAN	D	4	3	11,11,12	1.10	1 (9%)	15,15,17	1.77	1 (6%)
2	NAG	E	1	2,1	14,14,15	0.73	0	17,19,21	2.60	6 (35%)
2	NAG	E	2	2	14,14,15	0.81	1 (7%)	17,19,21	1.37	2 (11%)
2	NAG	F	1	2,1	14,14,15	1.21	1 (7%)	17,19,21	2.24	4 (23%)
2	NAG	F	2	2	14,14,15	1.21	1 (7%)	17,19,21	1.72	5 (29%)
2	NAG	G	1	2,1	14,14,15	1.13	1 (7%)	17,19,21	1.88	4 (23%)
2	NAG	G	2	2	14,14,15	0.53	0	17,19,21	1.53	2 (11%)
2	NAG	H	1	2,1	14,14,15	0.90	1 (7%)	17,19,21	1.77	2 (11%)
2	NAG	H	2	2	14,14,15	0.65	0	17,19,21	1.81	5 (29%)

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	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	LGU	D	3	3,6	1/1/4/6	2/2/19/24	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
2	NAG	G	1	2,1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	NAG	H	1	2,1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	NAG	O5-C1	-3.60	1.38	1.43
3	D	1	NAG	O5-C1	-3.55	1.38	1.43
2	C	1	NAG	O5-C1	-3.19	1.38	1.43
2	C	1	NAG	C2-N2	-3.18	1.40	1.46
2	H	1	NAG	O5-C1	-2.74	1.39	1.43
3	D	4	MAN	O5-C1	-2.73	1.39	1.43
2	G	1	NAG	C1-C2	2.46	1.56	1.52
2	F	1	NAG	C2-N2	-2.36	1.42	1.46
3	D	1	NAG	O5-C5	-2.33	1.38	1.43
3	D	3	LGU	C4-C5	2.16	1.57	1.53
2	E	2	NAG	C1-C2	2.09	1.55	1.52
2	C	1	NAG	C1-C2	2.03	1.55	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	NAG	C1-O5-C5	6.95	121.60	112.19
2	F	1	NAG	O5-C1-C2	-6.83	100.50	111.29
3	D	4	MAN	O5-C1-C2	-5.73	101.93	110.77
3	D	3	LGU	C1-O5-C5	5.22	119.27	112.19
2	E	1	NAG	O5-C1-C2	5.11	119.35	111.29
2	C	2	NAG	C1-O5-C5	5.05	119.04	112.19
2	G	1	NAG	O5-C1-C2	5.02	119.22	111.29
2	G	2	NAG	C1-O5-C5	4.93	118.87	112.19
2	H	1	NAG	O5-C1-C2	4.78	118.84	111.29
3	D	3	LGU	C1-C2-C3	-4.77	103.80	109.67
2	H	2	NAG	C1-O5-C5	4.46	118.24	112.19
2	C	1	NAG	C2-N2-C7	4.06	128.69	122.90
3	D	1	NAG	C1-C2-N2	3.90	117.15	110.49
3	D	3	LGU	O2-C2-C1	3.37	116.05	109.15
2	E	1	NAG	O5-C5-C6	3.33	112.43	107.20
2	E	2	NAG	O5-C5-C6	3.23	112.26	107.20
2	G	1	NAG	O4-C4-C3	3.15	117.62	110.35
3	D	1	NAG	O3-C3-C4	-3.08	103.22	110.35
2	F	2	NAG	O5-C1-C2	3.06	116.11	111.29
2	F	2	NAG	C3-C4-C5	3.05	115.67	110.24
3	D	1	NAG	O6-C6-C5	-3.01	100.97	111.29
2	H	1	NAG	O7-C7-N2	3.01	127.48	121.95
2	E	1	NAG	C3-C4-C5	2.99	115.58	110.24
3	D	1	NAG	C3-C4-C5	2.99	115.58	110.24
2	F	2	NAG	O7-C7-N2	2.94	127.36	121.95
2	H	2	NAG	C1-C2-N2	-2.91	105.52	110.49
2	H	2	NAG	O5-C1-C2	2.89	115.86	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1	NAG	O5-C5-C6	-2.83	102.76	107.20
2	E	1	NAG	O5-C5-C4	2.82	117.68	110.83
2	H	2	NAG	O4-C4-C5	2.73	116.08	109.30
3	D	1	NAG	O4-C4-C3	-2.67	104.18	110.35
3	D	2	NAG	O4-C4-C3	-2.63	104.27	110.35
2	H	2	NAG	C3-C4-C5	-2.61	105.58	110.24
2	C	1	NAG	O5-C5-C6	2.58	111.25	107.20
2	F	1	NAG	O3-C3-C2	-2.56	104.17	109.47
2	F	2	NAG	C1-O5-C5	2.53	115.62	112.19
2	F	2	NAG	O4-C4-C3	-2.43	104.73	110.35
2	C	2	NAG	C6-C5-C4	-2.37	107.45	113.00
3	D	3	LGU	O5-C1-C2	2.35	114.40	110.77
2	F	1	NAG	O7-C7-C8	-2.34	117.72	122.06
2	C	2	NAG	O6-C6-C5	-2.32	103.34	111.29
3	D	1	NAG	O5-C5-C4	2.28	116.37	110.83
2	C	2	NAG	O3-C3-C2	2.25	114.12	109.47
3	D	3	LGU	C2-C3-C4	-2.24	107.02	110.89
2	E	2	NAG	C4-C3-C2	2.23	114.29	111.02
2	C	2	NAG	C2-N2-C7	2.22	126.07	122.90
2	C	1	NAG	O5-C5-C4	2.20	116.17	110.83
2	F	1	NAG	C1-O5-C5	2.14	115.10	112.19
2	G	2	NAG	O4-C4-C3	2.14	115.30	110.35
3	D	3	LGU	O5-C5-C4	2.13	116.01	110.83
2	E	1	NAG	O3-C3-C4	-2.11	105.46	110.35
2	C	2	NAG	C3-C4-C5	-2.11	106.47	110.24
3	D	1	NAG	C1-O5-C5	2.07	115.00	112.19
2	C	1	NAG	O5-C1-C2	-2.07	108.02	111.29
2	G	1	NAG	O7-C7-C8	-2.06	118.23	122.06
3	D	1	NAG	C2-N2-C7	-2.05	119.98	122.90
2	G	1	NAG	O3-C3-C2	-2.03	105.27	109.47

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	1	NAG	C1
2	H	1	NAG	C1
3	D	3	LGU	C5

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	3	LGU	C4-C5-C6-O6B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
3	D	3	LGU	O5-C5-C6-O6B
3	D	1	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O5-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	C	2	NAG	C3-C2-N2-C7
2	F	2	NAG	O7-C7-N2-C2
2	H	2	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6

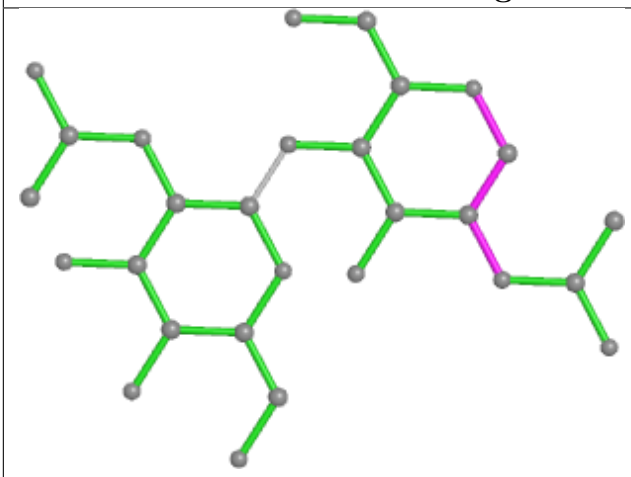
There are no ring outliers.

6 monomers are involved in 5 short contacts:

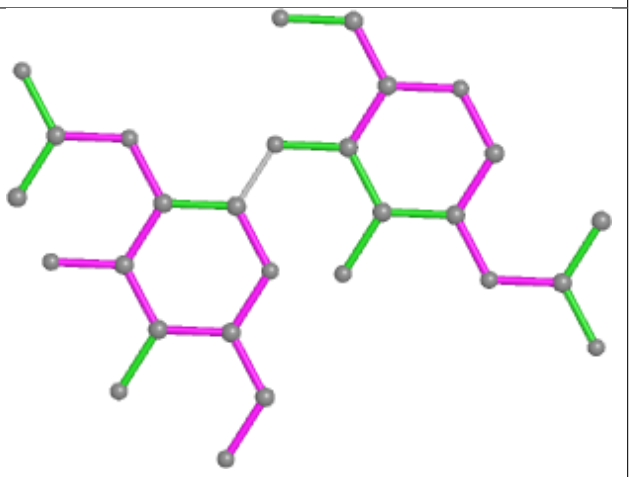
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	1	0
2	C	1	NAG	1	0
2	G	2	NAG	1	0
2	C	2	NAG	1	0
2	H	1	NAG	1	0
2	F	1	NAG	1	0

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

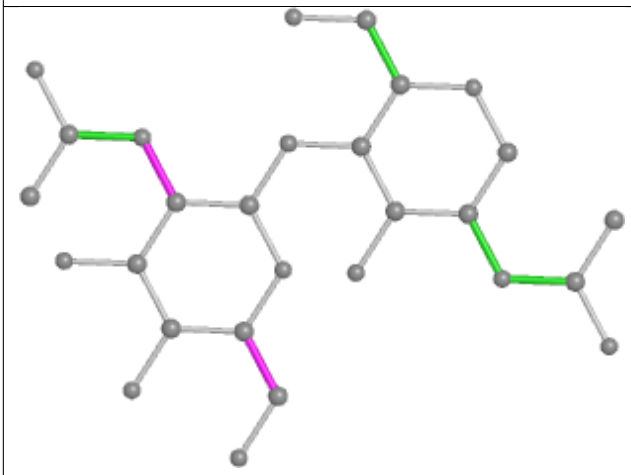
Oligosaccharide Chain C



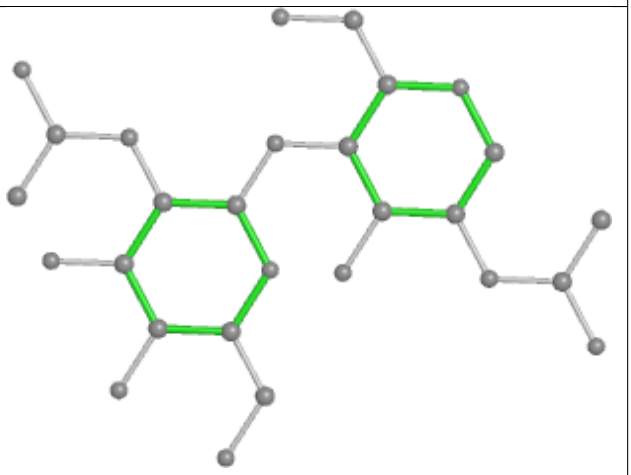
Bond lengths



Bond angles

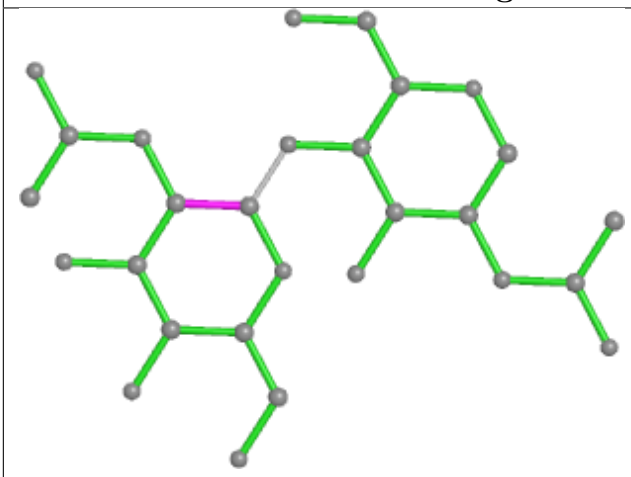


Torsions

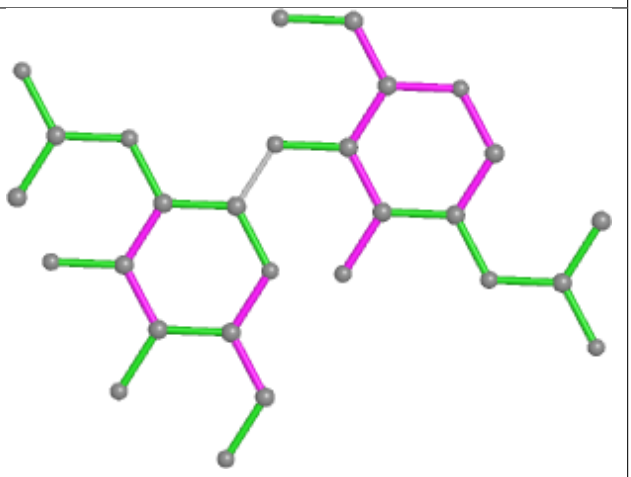


Rings

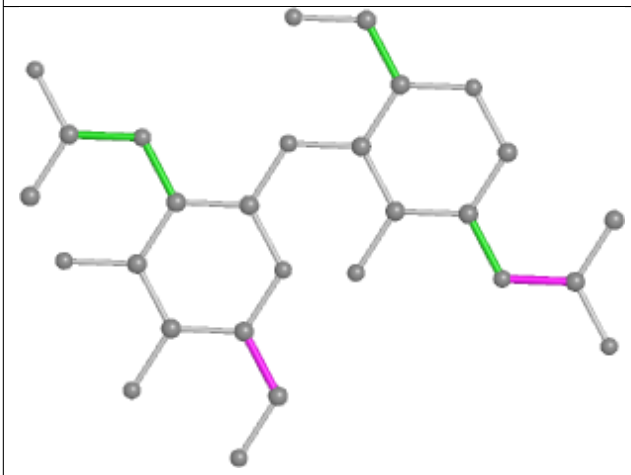
Oligosaccharide Chain E



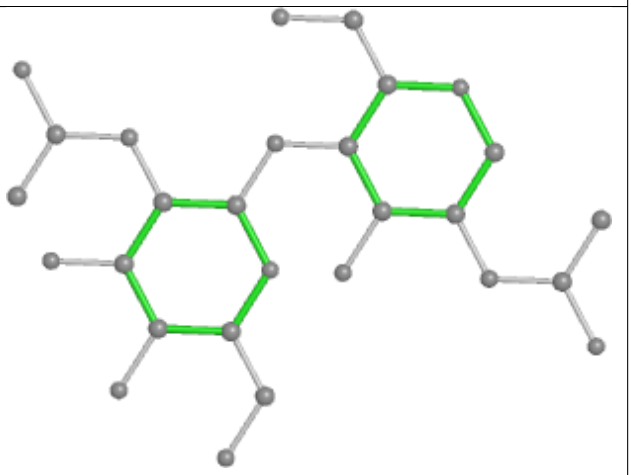
Bond lengths



Bond angles

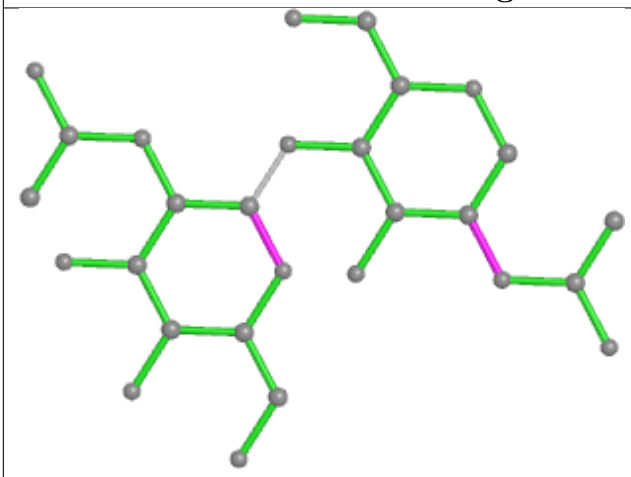


Torsions

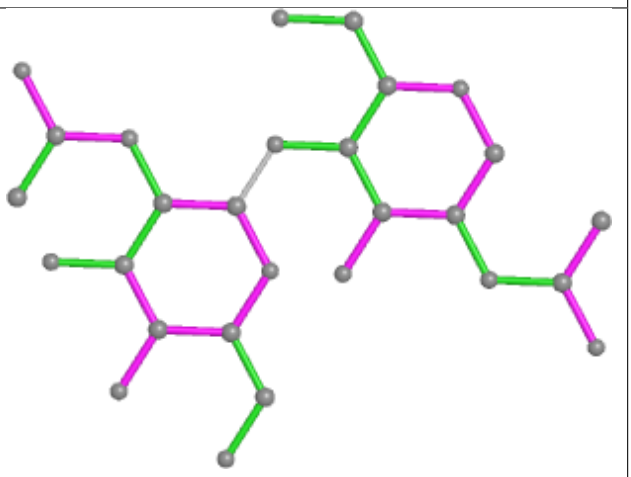


Rings

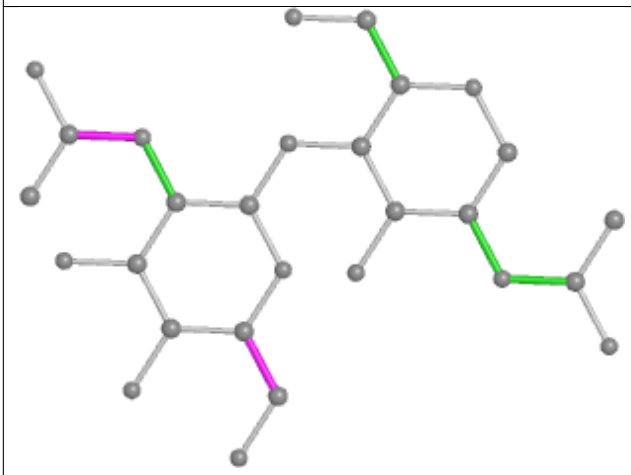
Oligosaccharide Chain F



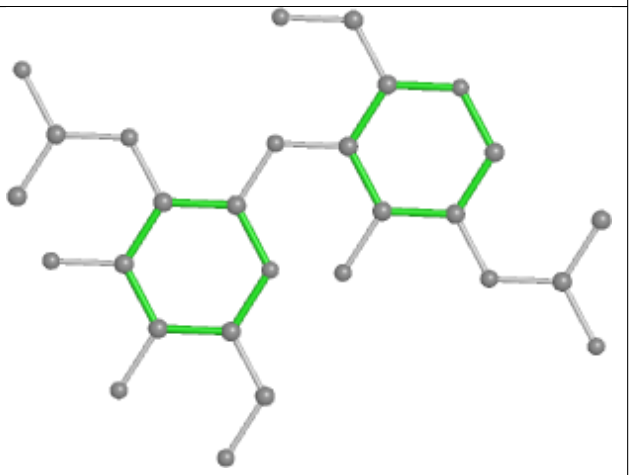
Bond lengths



Bond angles

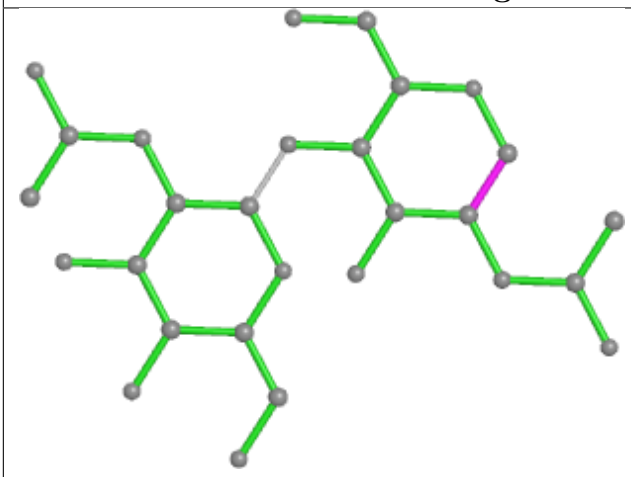


Torsions

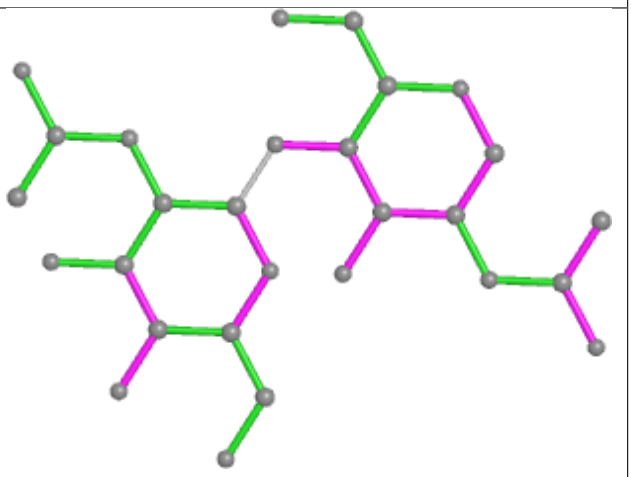


Rings

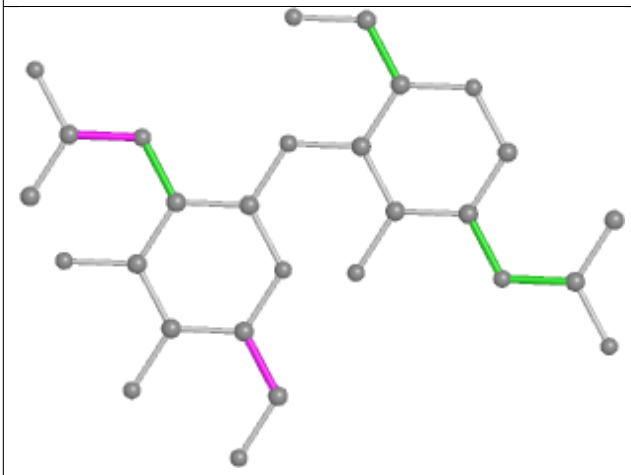
Oligosaccharide Chain G



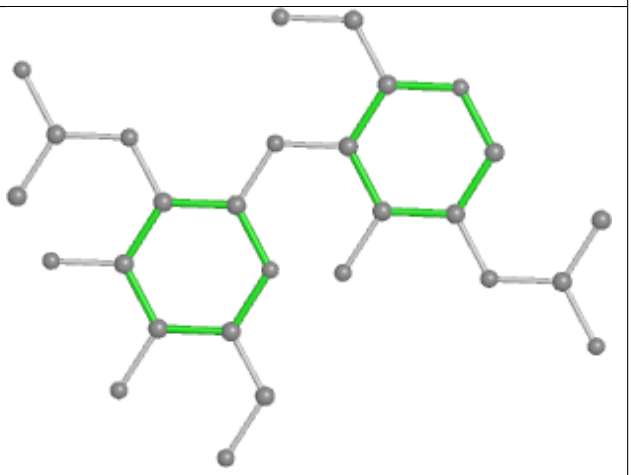
Bond lengths



Bond angles

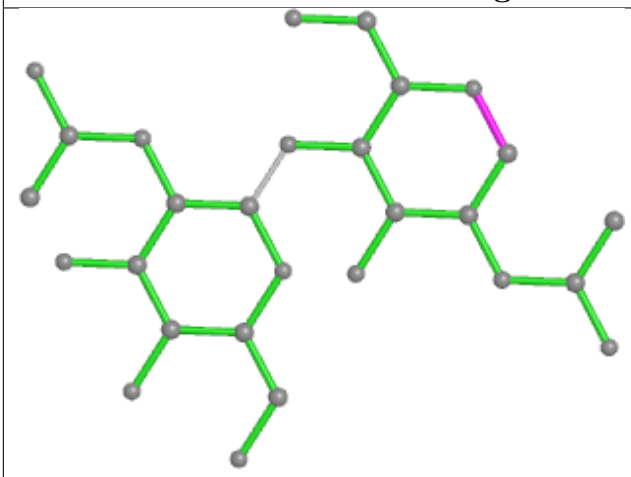


Torsions

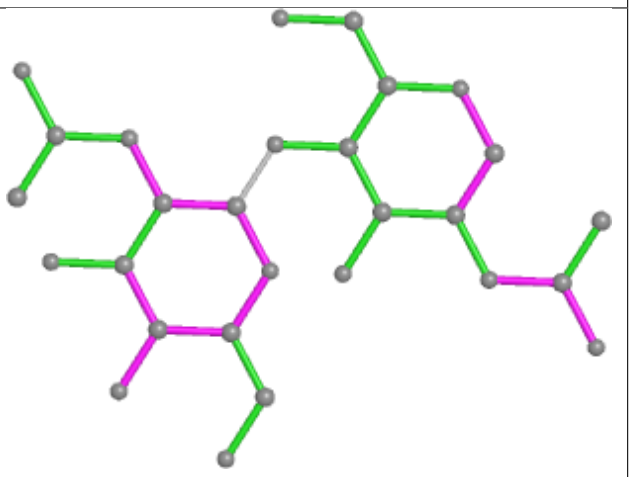


Rings

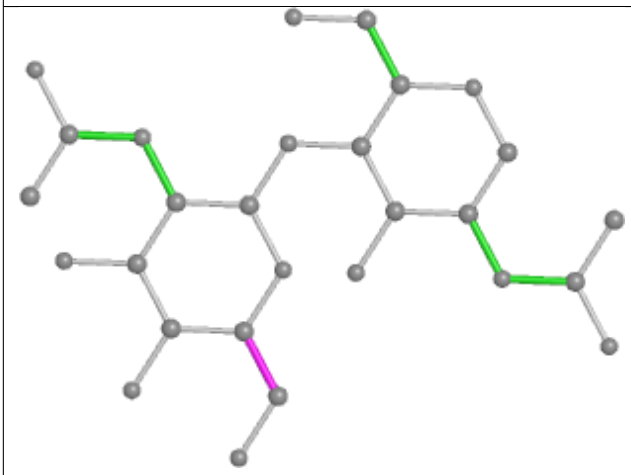
Oligosaccharide Chain H



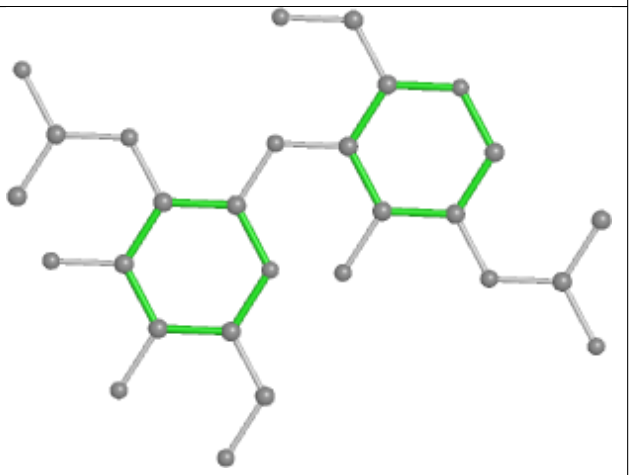
Bond lengths



Bond angles

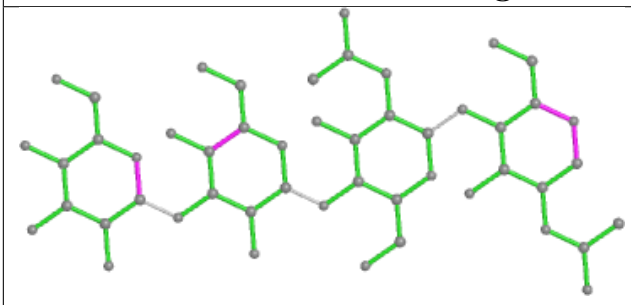


Torsions

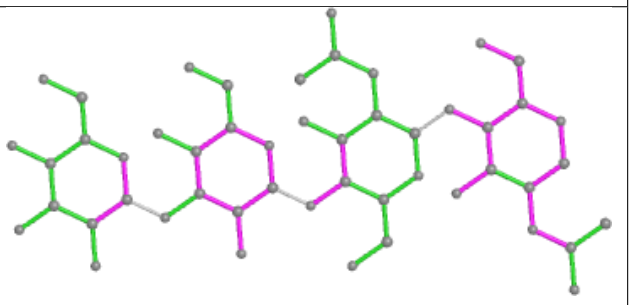


Rings

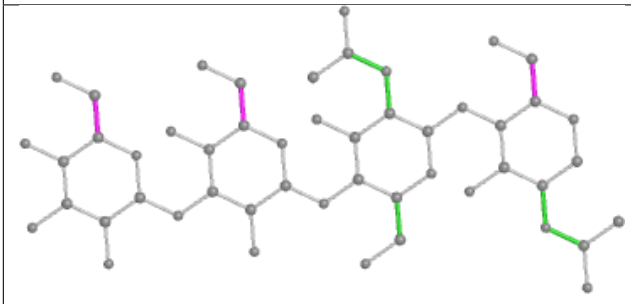
Oligosaccharide Chain D



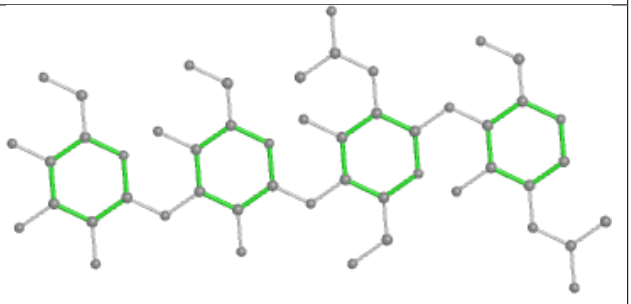
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

5 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	801	1	14,14,15	0.92	1 (7%)	17,19,21	1.50	3 (17%)
5	PZF	A	802	-	32,32,32	0.99	1 (3%)	40,46,46	2.36	16 (40%)
4	NAG	B	801	1	14,14,15	1.16	1 (7%)	17,19,21	2.39	7 (41%)
6	LGU	A	803	3	11,11,13	0.87	0	15,15,19	1.98	5 (33%)
5	PZF	B	802	-	32,32,32	1.50	8 (25%)	40,46,46	2.60	15 (37%)

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	801	1	-	4/6/23/26	0/1/1/1
5	PZF	A	802	-	-	0/14/26/26	0/4/4/4
4	NAG	B	801	1	-	2/6/23/26	0/1/1/1
6	LGU	A	803	3	1/1/4/6	2/2/19/24	0/1/1/1
5	PZF	B	802	-	-	0/14/26/26	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801	NAG	O5-C1	-3.60	1.38	1.43
5	B	802	PZF	C26-C21	-3.33	1.34	1.39
5	B	802	PZF	F29-C24	-2.75	1.28	1.35
5	B	802	PZF	C4-N3	2.57	1.36	1.32
5	B	802	PZF	C14-N15	2.54	1.49	1.46
5	B	802	PZF	C8-N9	2.26	1.38	1.33
5	A	802	PZF	C2-N3	-2.25	1.29	1.34
5	B	802	PZF	C21-C13	-2.24	1.47	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	NAG	O5-C1	-2.09	1.40	1.43
5	B	802	PZF	O18-C4	2.06	1.38	1.35
5	B	802	PZF	C11-C10	2.01	1.42	1.39

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	802	PZF	C8-N7-C12	8.15	122.06	114.94
5	B	802	PZF	C10-C11-C12	6.69	121.42	117.03
5	A	802	PZF	C8-N7-C12	5.90	120.09	114.94
5	A	802	PZF	C8-N9-C10	5.82	123.63	115.74
5	A	802	PZF	N9-C8-N7	-5.34	120.25	128.60
4	B	801	NAG	O4-C4-C5	-5.11	96.60	109.30
5	B	802	PZF	O18-C4-C5	4.64	124.78	116.71
6	A	803	LGU	O5-C1-C2	-4.53	103.78	110.77
5	B	802	PZF	N9-C8-N7	-4.49	121.59	128.60
5	A	802	PZF	C10-C11-C12	4.12	119.73	117.03
5	B	802	PZF	C2-N3-C4	4.10	120.24	116.63
4	B	801	NAG	C3-C4-C5	3.97	117.32	110.24
4	B	801	NAG	C1-O5-C5	3.94	117.53	112.19
5	A	802	PZF	C14-N15-C16	3.93	116.84	111.67
5	A	802	PZF	C11-C10-N9	-3.88	117.11	122.16
6	A	803	LGU	C1-O5-C5	-3.66	107.24	112.19
5	B	802	PZF	C11-C12-N7	-3.54	116.60	122.73
5	B	802	PZF	C8-N9-C10	3.29	120.19	115.74
5	B	802	PZF	C11-C10-N9	-3.23	117.96	122.16
4	B	801	NAG	O5-C5-C6	3.11	112.08	107.20
4	A	801	NAG	C1-O5-C5	3.02	116.28	112.19
5	A	802	PZF	C2-N3-C4	2.95	119.23	116.63
5	B	802	PZF	C5-C4-N3	-2.88	120.58	124.87
5	A	802	PZF	C2-C1-C10	-2.73	116.83	121.22
4	B	801	NAG	O5-C5-C4	2.69	117.37	110.83
5	B	802	PZF	C2-C1-C10	-2.62	117.01	121.22
4	B	801	NAG	C6-C5-C4	-2.60	106.90	113.00
5	A	802	PZF	C14-N15-C12	-2.59	120.43	123.60
4	A	801	NAG	C1-C2-N2	2.45	114.68	110.49
5	B	802	PZF	O18-C4-N3	-2.42	114.61	119.57
6	A	803	LGU	C3-C4-C5	2.41	114.54	110.24
6	A	803	LGU	C2-C3-C4	2.41	115.07	110.89
5	B	802	PZF	C14-C13-C21	2.41	118.17	114.98
5	A	802	PZF	F28-C25-C24	2.39	124.24	118.43
5	A	802	PZF	C21-C26-C25	2.34	122.48	119.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	802	PZF	C23-C22-C21	-2.29	121.09	123.83
5	B	802	PZF	C11-C10-C1	2.27	124.87	121.85
5	B	802	PZF	C21-C26-C25	2.26	122.37	119.23
6	A	803	LGU	O5-C5-C6	2.17	110.60	107.20
5	A	802	PZF	C11-C12-N7	-2.14	119.02	122.73
5	A	802	PZF	C26-C25-C24	-2.13	118.61	121.03
4	A	801	NAG	C2-N2-C7	-2.11	119.91	122.90
5	A	802	PZF	N7-C12-N15	2.09	119.92	116.79
5	A	802	PZF	C26-C21-C22	2.02	118.17	116.48
5	B	802	PZF	C14-N15-C12	2.01	126.06	123.60
4	B	801	NAG	O3-C3-C2	-2.00	105.32	109.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	803	LGU	C5

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	NAG	C8-C7-N2-C2
4	A	801	NAG	O7-C7-N2-C2
6	A	803	LGU	O5-C5-C6-O6B
6	A	803	LGU	C4-C5-C6-O6B
4	B	801	NAG	C4-C5-C6-O6
4	B	801	NAG	O5-C5-C6-O6
4	A	801	NAG	C4-C5-C6-O6
4	A	801	NAG	O5-C5-C6-O6

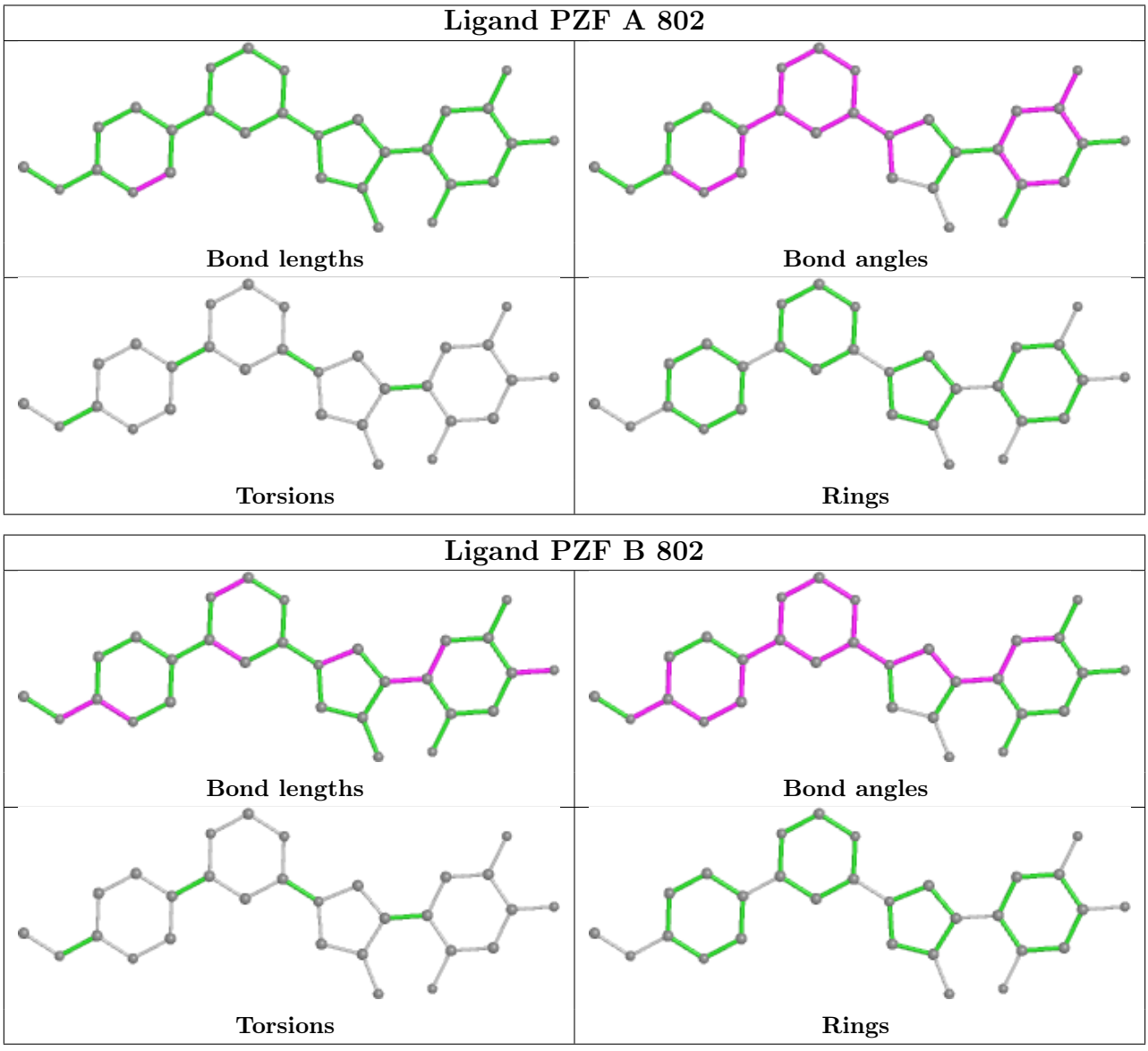
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	802	PZF	1	0
4	B	801	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

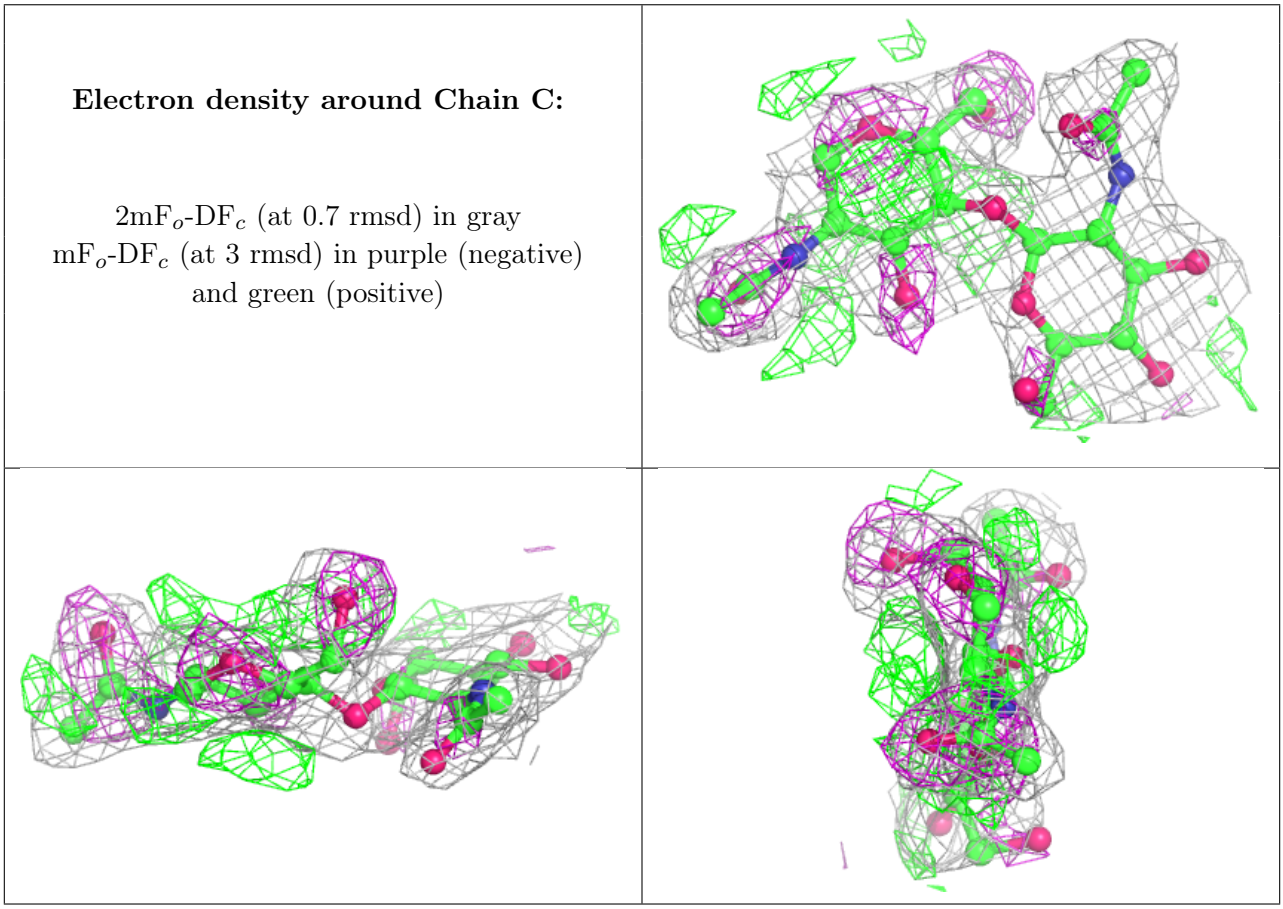
6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

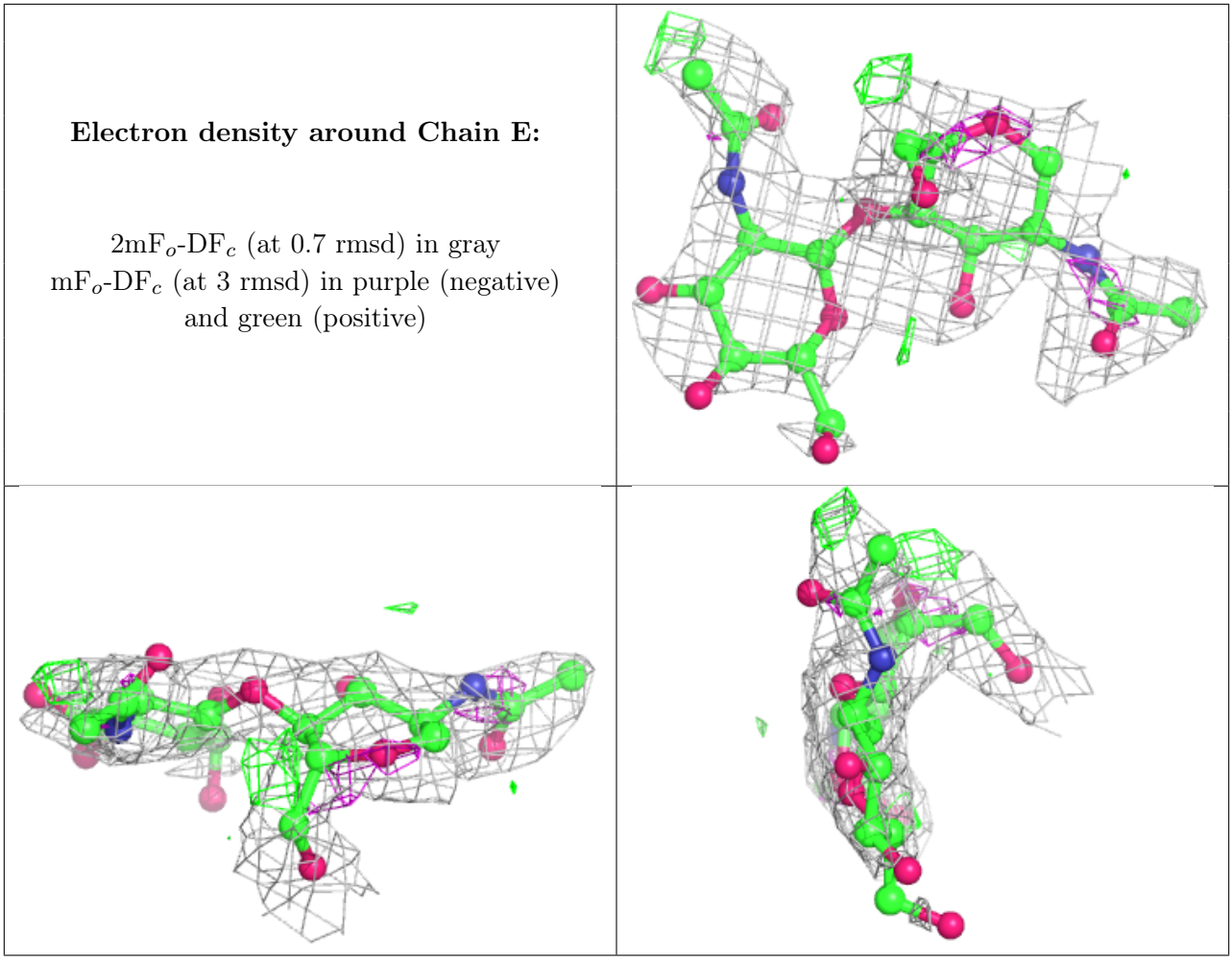
Electron density around Chain C:

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



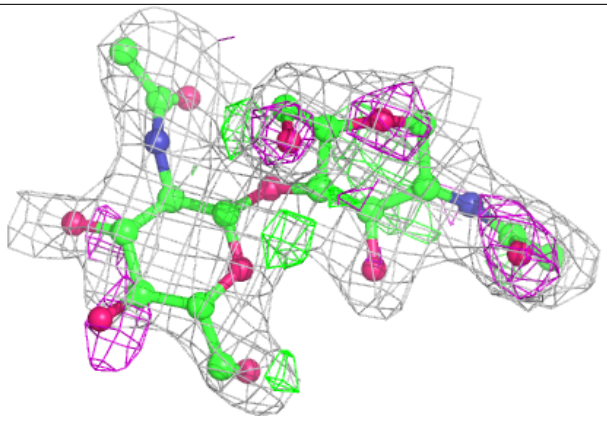
Electron density around Chain E:

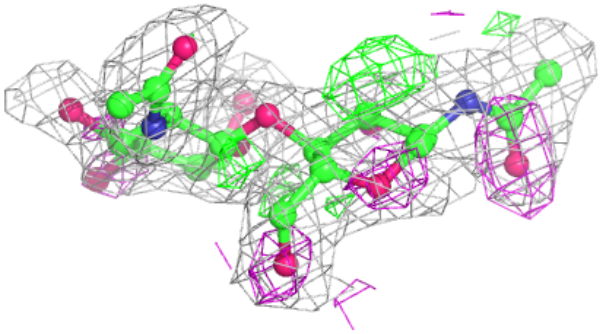
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain F:

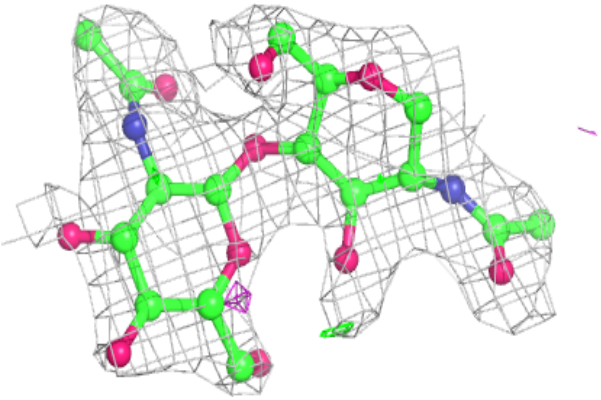
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

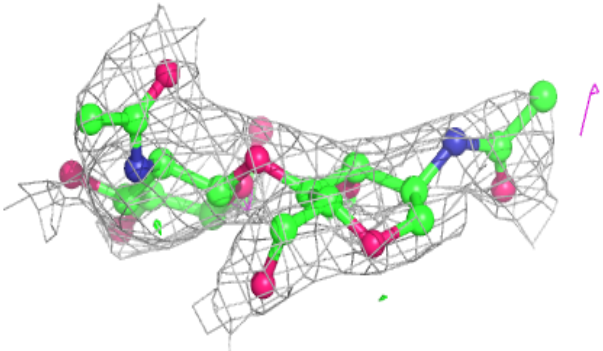


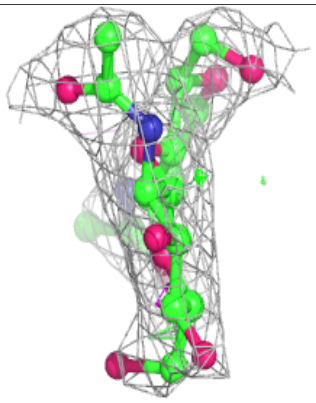


Electron density around Chain G:

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

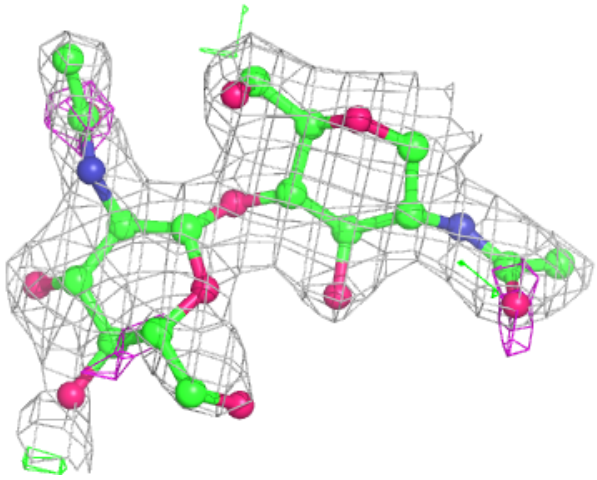


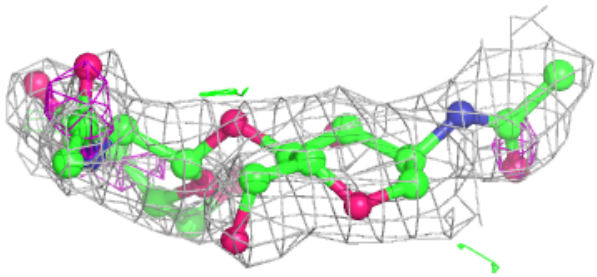


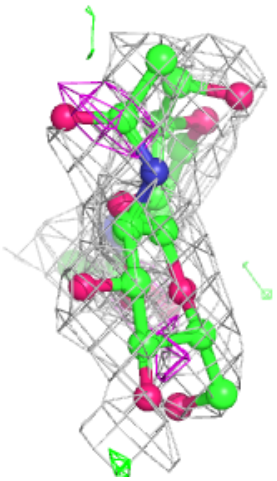


Electron density around Chain H:

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

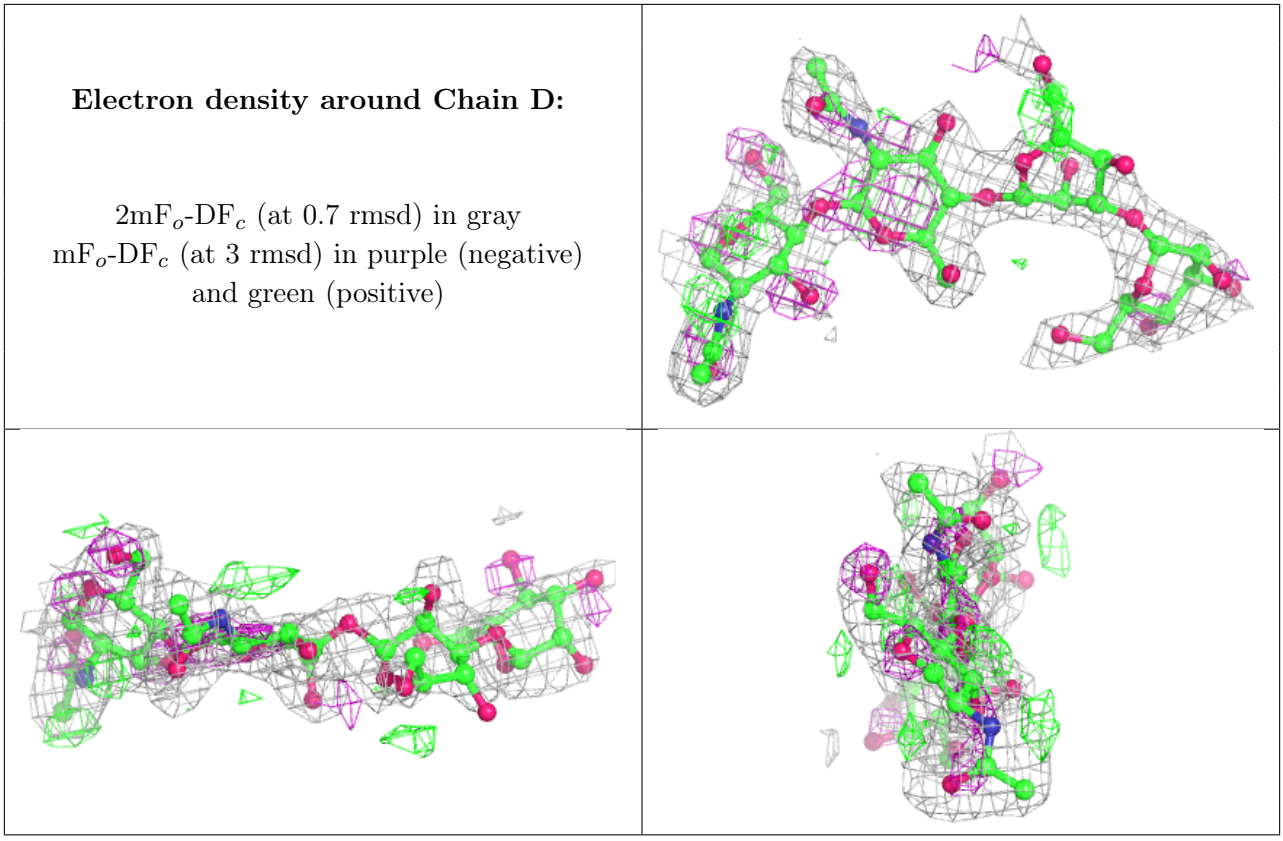






Electron density around Chain D:

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



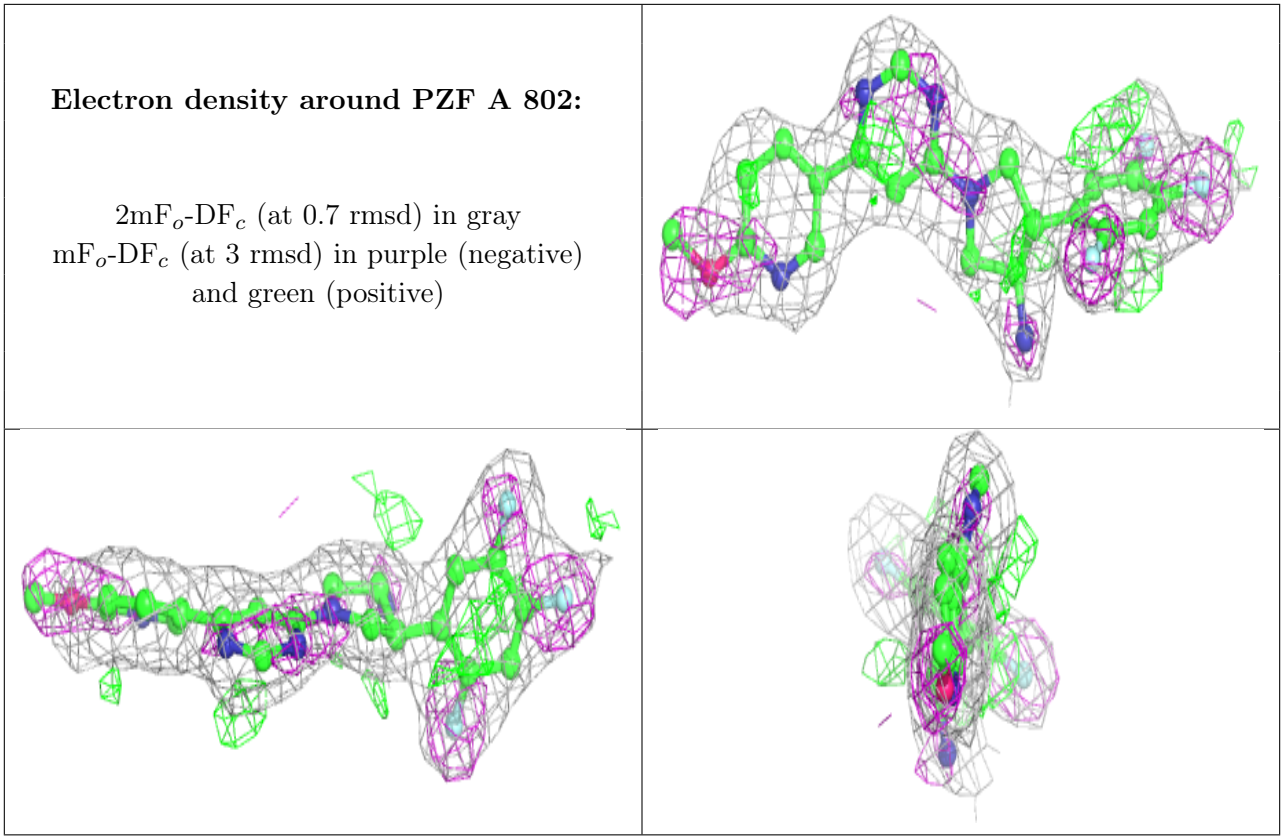
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

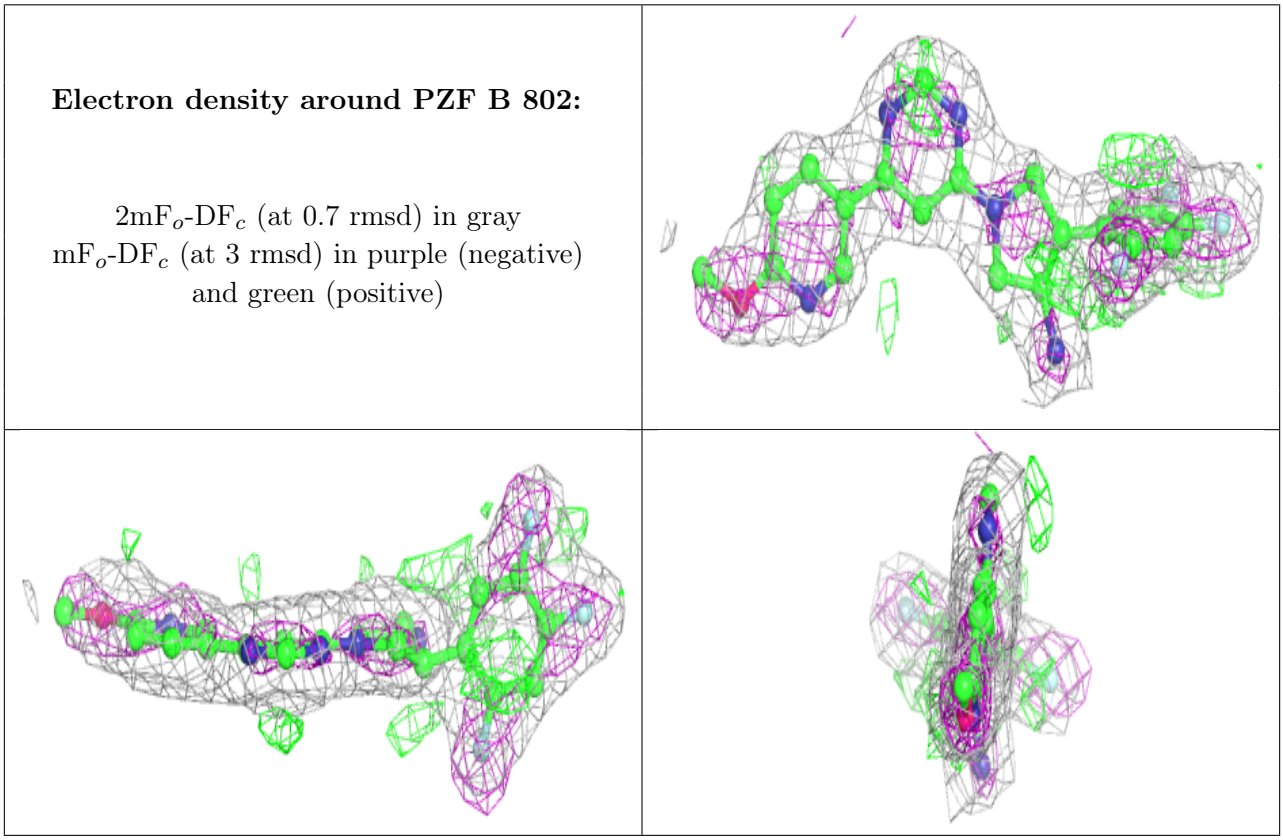
Electron density around PZF A 802:

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



Electron density around PZF B 802:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.