Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 11:06 PM EDT

PDB ID	:	7TBE
Title	:	Crystal structure of Plasmepsin X from Plasmodium vivax in complex with WM4
Authors	:	Hodder, A.N.; Christensen, J.B.; Scally, S.W.; Cowman, A.F.
Deposited on	:	2021-12-21
Resolution	:	3.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

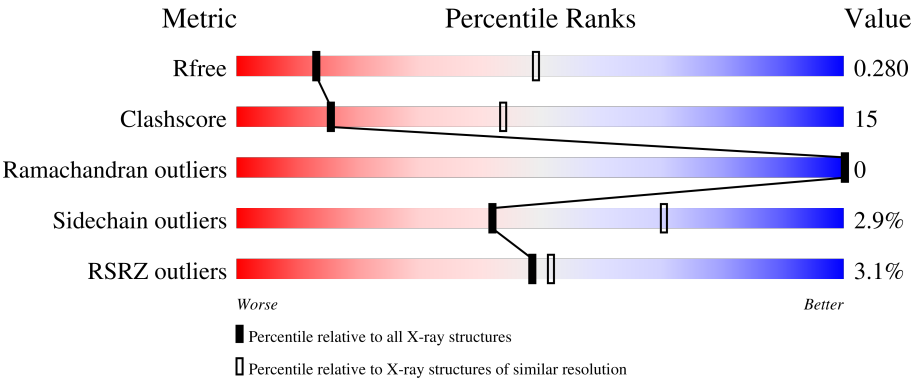
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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% 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	379	3% 71% 23% 6%
1	B	379	3% 65% 28% 6%
1	C	379	3% 58% 31% 10%
1	D	379	2% 61% 27% 10%
2	E	3	67% 33%

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Mol	Chain	Length	Quality of chain
3	F	2	100%
3	G	2	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11096 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 Plasmepsin X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2752	1779	442	517	14			
1	B	357	Total	C	N	O	S	0	0	0
			2725	1761	437	514	13			
1	C	342	Total	C	N	O	S	0	0	0
			2648	1711	420	503	14			
1	D	340	Total	C	N	O	S	0	0	0
			2608	1690	413	491	14			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	546	LEU	-	expression tag	UNP A0A1G4H6I9
A	547	GLU	-	expression tag	UNP A0A1G4H6I9
A	548	ASN	-	expression tag	UNP A0A1G4H6I9
A	549	LEU	-	expression tag	UNP A0A1G4H6I9
A	550	TYR	-	expression tag	UNP A0A1G4H6I9
A	551	PHE	-	expression tag	UNP A0A1G4H6I9
A	552	GLN	-	expression tag	UNP A0A1G4H6I9
A	553	GLY	-	expression tag	UNP A0A1G4H6I9
A	554	ASP	-	expression tag	UNP A0A1G4H6I9
A	555	TYR	-	expression tag	UNP A0A1G4H6I9
A	556	LYS	-	expression tag	UNP A0A1G4H6I9
A	557	ASP	-	expression tag	UNP A0A1G4H6I9
A	558	ASP	-	expression tag	UNP A0A1G4H6I9
A	559	ASP	-	expression tag	UNP A0A1G4H6I9
A	560	ASP	-	expression tag	UNP A0A1G4H6I9
A	561	LYS	-	expression tag	UNP A0A1G4H6I9
A	562	HIS	-	expression tag	UNP A0A1G4H6I9
B	546	LEU	-	expression tag	UNP A0A1G4H6I9
B	547	GLU	-	expression tag	UNP A0A1G4H6I9
B	548	ASN	-	expression tag	UNP A0A1G4H6I9
B	549	LEU	-	expression tag	UNP A0A1G4H6I9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	550	TYR	-	expression tag	UNP A0A1G4H6I9
B	551	PHE	-	expression tag	UNP A0A1G4H6I9
B	552	GLN	-	expression tag	UNP A0A1G4H6I9
B	553	GLY	-	expression tag	UNP A0A1G4H6I9
B	554	ASP	-	expression tag	UNP A0A1G4H6I9
B	555	TYR	-	expression tag	UNP A0A1G4H6I9
B	556	LYS	-	expression tag	UNP A0A1G4H6I9
B	557	ASP	-	expression tag	UNP A0A1G4H6I9
B	558	ASP	-	expression tag	UNP A0A1G4H6I9
B	559	ASP	-	expression tag	UNP A0A1G4H6I9
B	560	ASP	-	expression tag	UNP A0A1G4H6I9
B	561	LYS	-	expression tag	UNP A0A1G4H6I9
B	562	HIS	-	expression tag	UNP A0A1G4H6I9
C	546	LEU	-	expression tag	UNP A0A1G4H6I9
C	547	GLU	-	expression tag	UNP A0A1G4H6I9
C	548	ASN	-	expression tag	UNP A0A1G4H6I9
C	549	LEU	-	expression tag	UNP A0A1G4H6I9
C	550	TYR	-	expression tag	UNP A0A1G4H6I9
C	551	PHE	-	expression tag	UNP A0A1G4H6I9
C	552	GLN	-	expression tag	UNP A0A1G4H6I9
C	553	GLY	-	expression tag	UNP A0A1G4H6I9
C	554	ASP	-	expression tag	UNP A0A1G4H6I9
C	555	TYR	-	expression tag	UNP A0A1G4H6I9
C	556	LYS	-	expression tag	UNP A0A1G4H6I9
C	557	ASP	-	expression tag	UNP A0A1G4H6I9
C	558	ASP	-	expression tag	UNP A0A1G4H6I9
C	559	ASP	-	expression tag	UNP A0A1G4H6I9
C	560	ASP	-	expression tag	UNP A0A1G4H6I9
C	561	LYS	-	expression tag	UNP A0A1G4H6I9
C	562	HIS	-	expression tag	UNP A0A1G4H6I9
D	546	LEU	-	expression tag	UNP A0A1G4H6I9
D	547	GLU	-	expression tag	UNP A0A1G4H6I9
D	548	ASN	-	expression tag	UNP A0A1G4H6I9
D	549	LEU	-	expression tag	UNP A0A1G4H6I9
D	550	TYR	-	expression tag	UNP A0A1G4H6I9
D	551	PHE	-	expression tag	UNP A0A1G4H6I9
D	552	GLN	-	expression tag	UNP A0A1G4H6I9
D	553	GLY	-	expression tag	UNP A0A1G4H6I9
D	554	ASP	-	expression tag	UNP A0A1G4H6I9
D	555	TYR	-	expression tag	UNP A0A1G4H6I9
D	556	LYS	-	expression tag	UNP A0A1G4H6I9
D	557	ASP	-	expression tag	UNP A0A1G4H6I9

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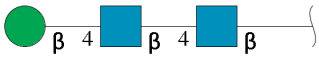
Chain	Residue	Modelled	Actual	Comment	Reference
D	558	ASP	-	expression tag	UNP A0A1G4H6I9
D	559	ASP	-	expression tag	UNP A0A1G4H6I9
D	560	ASP	-	expression tag	UNP A0A1G4H6I9
D	561	LYS	-	expression tag	UNP A0A1G4H6I9
D	562	HIS	-	expression tag	UNP A0A1G4H6I9

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

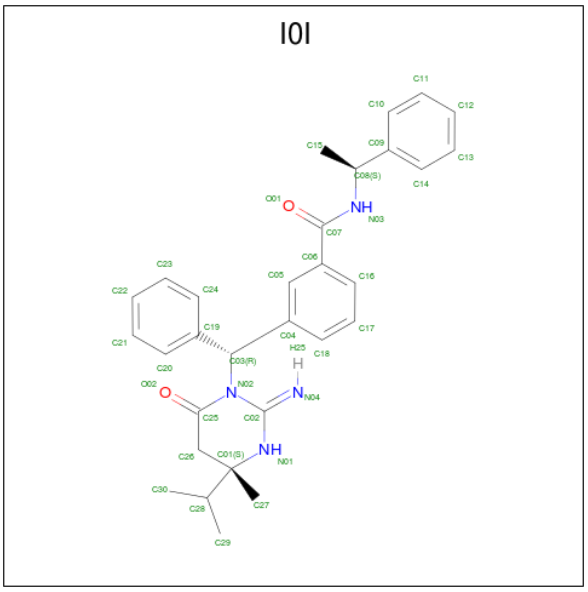


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

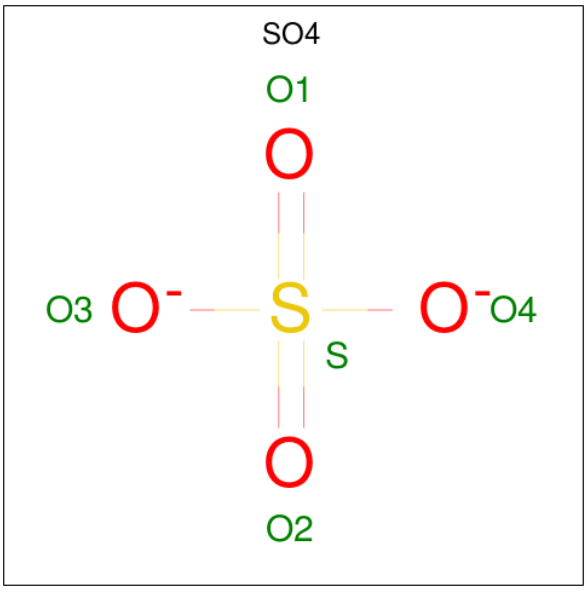
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 3-[(R)-[(2E,4S)-2-imino-4-methyl-6-oxo-4-(propan-2-yl)-1,3-diazinan-1-yl](phenyl)methyl]-N-[(1S)-1-phenylethyl]benzamide (three-letter code: I0I) (formula: $C_{30}H_{34}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 36 30 4 2	0	0
4	B	1	Total C N O 36 30 4 2	0	0
4	C	1	Total C N O 36 30 4 2	0	0
4	D	1	Total C N O 36 30 4 2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is water.

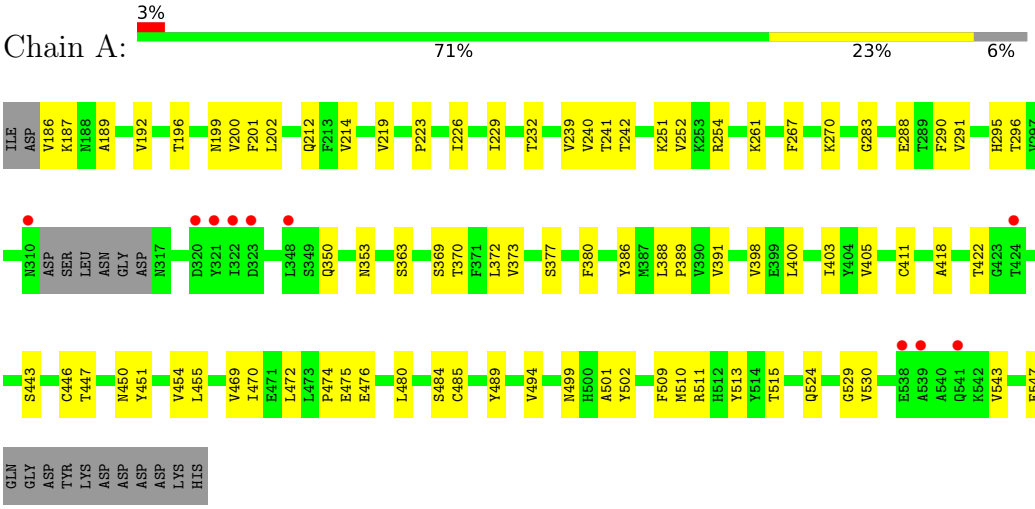
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	46	Total O 46 46	0	0
6	B	30	Total O 30 30	0	0
6	C	21	Total O 21 21	0	0
6	D	22	Total O 22 22	0	0

3 Residue-property plots (i)

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

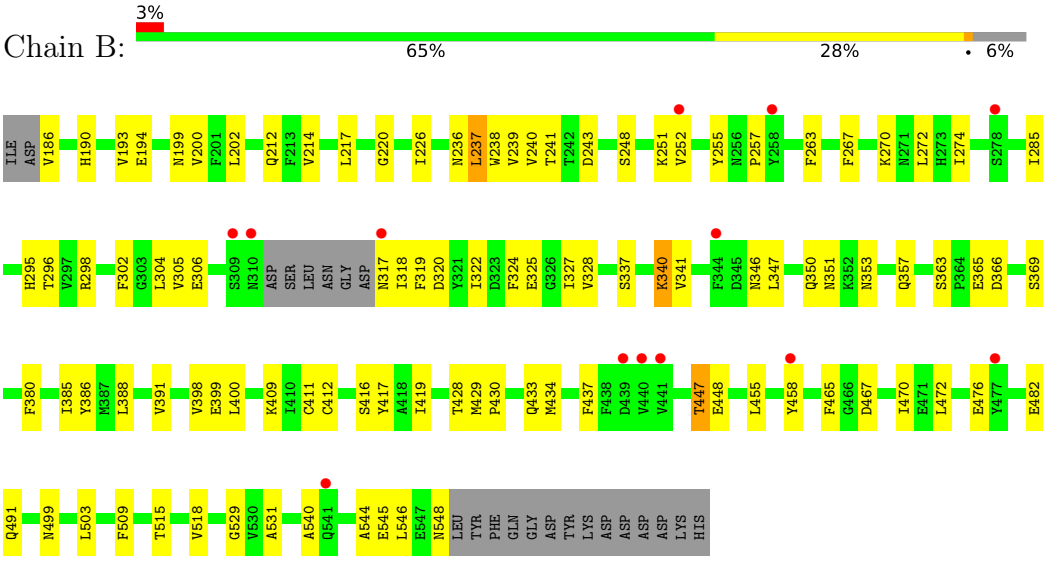
• Molecule 1: Plasmepsin X

Chain A:



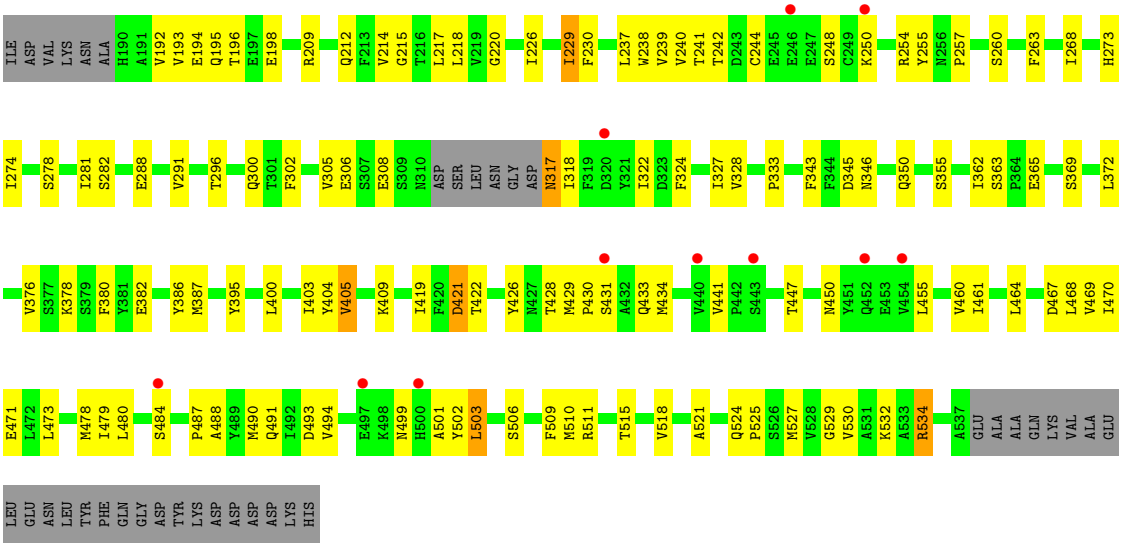
• Molecule 1: Plasmepsin X

Chain B:



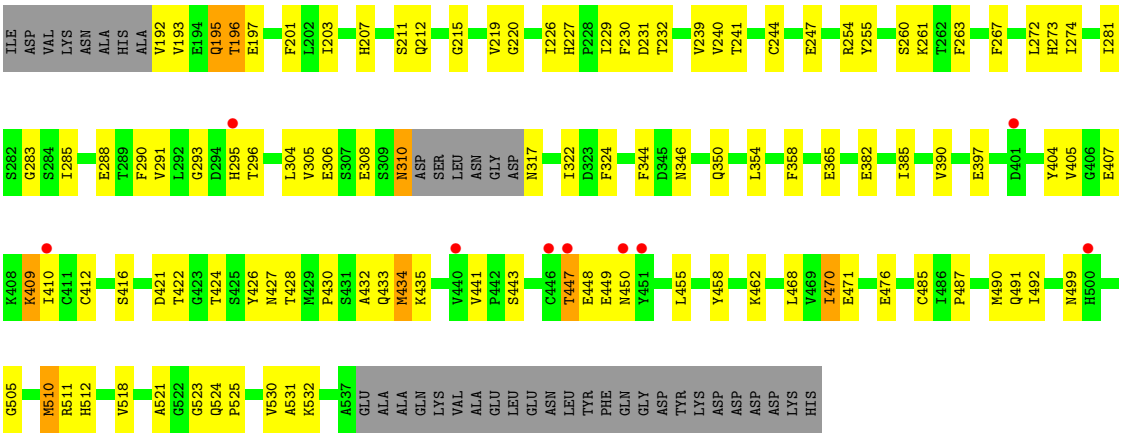
• Molecule 1: Plasmepsin X

Chain C:



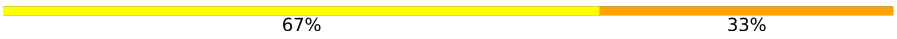
• Molecule 1: Plasmepsin X

Chain D:



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

Chain E:

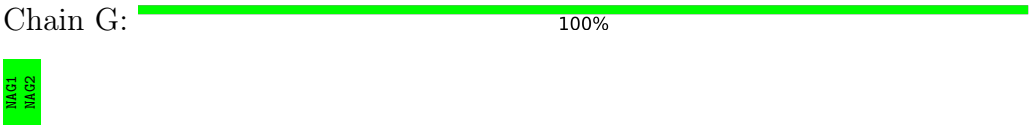


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

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

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	80.50Å 253.28Å 171.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.19 – 3.35 39.19 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.19-3.35) 99.9 (39.19-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.223 , 0.281 0.222 , 0.280	Depositor DCC
R_{free} test set	1286 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	58.3	Xtriage
Anisotropy	0.887	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 57.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	11096	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: I0I, NAG, SO4, BMA

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	0.31	0/2820	0.55	0/3830
1	B	0.32	0/2792	0.55	0/3795
1	C	0.32	0/2716	0.56	0/3691
1	D	0.32	0/2675	0.57	0/3638
All	All	0.32	0/11003	0.56	0/14954

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2752	0	2644	71	1
1	B	2725	0	2594	84	1
1	C	2648	0	2518	91	0
1	D	2608	0	2478	81	0
2	E	39	0	34	1	0
3	F	28	0	25	5	0
3	G	28	0	25	0	0
4	A	36	0	0	0	0
4	B	36	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	36	0	0	1	0
4	D	36	0	0	3	0
5	C	5	0	0	1	0
6	A	46	0	0	2	0
6	B	30	0	0	0	0
6	C	21	0	0	0	0
6	D	22	0	0	1	1
All	All	11096	0	10318	316	2

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 15.

All (316) 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:429:MET:HB2	1:A:434:MET:HE2	1.54	0.88
1:D:427:ASN:ND2	1:D:505:GLY:H	1.74	0.86
1:B:202:LEU:HD21	1:B:540:ALA:HB3	1.60	0.83
1:D:427:ASN:HD22	1:D:505:GLY:H	1.27	0.83
1:A:447:THR:H	1:A:450:ASN:HB3	1.44	0.82
1:D:462:LYS:HG2	1:D:471:GLU:HG2	1.62	0.81
1:C:291:VAL:HG22	1:C:296:THR:HG22	1.60	0.81
1:D:434:MET:HG2	1:D:491:GLN:HB2	1.63	0.80
1:A:455:LEU:HD22	1:A:475:GLU:HA	1.62	0.79
1:A:291:VAL:HG22	1:A:296:THR:HG22	1.65	0.77
1:B:291:VAL:HG22	1:B:296:THR:HG22	1.68	0.76
1:B:236:ASN:HD22	1:B:274:ILE:HD11	1.51	0.75
1:B:272:LEU:HD11	1:B:337:SER:HB3	1.68	0.75
1:D:274:ILE:HB	1:D:281:ILE:HG22	1.69	0.74
1:B:272:LEU:HD22	1:B:285:ILE:HD11	1.69	0.74
3:F:1:NAG:H83	3:F:1:NAG:H3	1.70	0.74
1:C:238:TRP:HZ2	1:C:274:ILE:HD13	1.53	0.73
1:D:291:VAL:HG22	1:D:296:THR:HG22	1.69	0.73
1:A:388:LEU:HB3	1:A:398:VAL:HG11	1.69	0.73
1:B:194:GLU:HA	1:B:544:ALA:HA	1.70	0.73
1:C:429:MET:HB2	1:C:434:MET:HE2	1.72	0.72
1:B:363:SER:H	1:B:369:SER:HB3	1.55	0.72
1:B:238:TRP:HE1	1:B:274:ILE:HD12	1.55	0.70
1:B:467:ASP:HB3	1:C:525:PRO:HG3	1.72	0.70
1:A:192:VAL:HB	1:D:196:THR:HA	1.74	0.70
1:D:193:VAL:HG11	1:D:518:VAL:HG11	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:VAL:HA	1:B:305:VAL:HB	1.75	0.69
1:B:252:VAL:HB	1:B:325:GLU:HG2	1.74	0.69
1:C:318:ILE:O	1:C:322:ILE:HG12	1.93	0.68
1:A:199:ASN:OD1	1:A:353:ASN:HB2	1.94	0.68
1:D:421:ASP:OD2	1:D:424:THR:HG23	1.94	0.67
1:A:386:TYR:CZ	1:D:524:GLN:HB2	2.30	0.67
1:B:391:VAL:HG11	1:B:399:GLU:HG3	1.77	0.67
1:A:446:CYS:HA	1:A:450:ASN:HD22	1.60	0.66
1:A:186:VAL:HG21	1:B:270:LYS:HG3	1.76	0.66
1:B:298:ARG:H	1:B:350:GLN:HE22	1.44	0.66
1:A:226:ILE:HD13	1:A:239:VAL:HG13	1.78	0.65
1:B:226:ILE:HD13	1:B:239:VAL:HG13	1.79	0.64
1:B:388:LEU:HB3	1:B:398:VAL:HG11	1.79	0.64
1:B:236:ASN:ND2	1:B:274:ILE:HD11	2.11	0.64
1:C:192:VAL:HG11	1:C:518:VAL:HG11	1.80	0.64
1:B:455:LEU:HA	1:B:458:TYR:HD2	1.62	0.63
1:C:429:MET:HG2	1:C:502:TYR:HD2	1.63	0.63
1:D:226:ILE:HD13	1:D:239:VAL:HG13	1.80	0.63
1:A:470:ILE:HD11	1:A:530:VAL:HG21	1.81	0.63
1:C:230:PHE:O	1:C:422:THR:OG1	2.15	0.63
1:D:521:ALA:O	1:D:524:GLN:HG2	1.99	0.62
1:B:220:GLY:HA2	1:B:288:GLU:OE2	1.99	0.62
1:D:447:THR:HG22	1:D:450:ASN:H	1.65	0.62
1:D:421:ASP:OD1	4:D:601:I0I:N04	2.33	0.62
1:D:470:ILE:HD11	1:D:530:VAL:HG11	1.80	0.62
1:C:434:MET:HE3	1:C:491:GLN:HA	1.79	0.62
1:D:241:THR:HG22	1:D:255:TYR:HD2	1.65	0.61
1:C:378:LYS:O	1:C:534:ARG:NH2	2.33	0.61
3:F:2:NAG:H3	3:F:2:NAG:H83	1.83	0.61
1:C:308:GLU:O	1:C:317:ASN:ND2	2.34	0.61
1:C:431:SER:HB2	1:C:493:ASP:OD2	2.01	0.61
1:C:428:THR:OG1	1:C:503:LEU:HB2	2.00	0.61
1:B:429:MET:HB2	1:B:434:MET:HE2	1.81	0.61
1:D:308:GLU:O	1:D:317:ASN:ND2	2.32	0.61
1:A:451:TYR:CZ	1:A:455:LEU:HD21	2.35	0.61
1:B:455:LEU:HA	1:B:458:TYR:CD2	2.36	0.60
1:C:240:VAL:HA	1:C:305:VAL:HB	1.83	0.60
1:B:193:VAL:O	1:B:545:GLU:N	2.34	0.60
1:C:365:GLU:OE2	1:C:511:ARG:HD2	2.02	0.60
1:D:230:PHE:O	1:D:422:THR:OG1	2.16	0.60
1:C:273:HIS:ND1	1:C:282:SER:HB3	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:THR:HA	1:C:254:ARG:HH21	1.67	0.58
1:C:195:GLN:HG3	1:C:355:SER:OG	2.04	0.58
1:A:450:ASN:O	1:A:454:VAL:HG23	2.04	0.58
1:D:432:ALA:O	1:D:435:LYS:HG2	2.04	0.58
1:C:192:VAL:HG23	1:C:527:MET:SD	2.44	0.57
1:C:229:ILE:HG12	1:C:327:ILE:HD13	1.86	0.57
1:D:346:ASN:OD1	1:D:350:GLN:NE2	2.37	0.57
1:C:226:ILE:HD13	1:C:239:VAL:HG13	1.85	0.57
1:B:386:TYR:CE2	1:C:192:VAL:HG22	2.39	0.57
1:B:267:PHE:CD1	1:D:532:LYS:HE3	2.40	0.56
1:C:441:VAL:HG12	1:C:487:PRO:HG3	1.87	0.56
1:C:479:ILE:HG13	1:C:488:ALA:HB2	1.88	0.56
1:B:430:PRO:HB3	1:B:499:ASN:HA	1.87	0.56
1:B:341:VAL:HG12	1:B:346:ASN:HB2	1.88	0.56
1:B:419:ILE:HB	1:B:503:LEU:HD23	1.87	0.56
1:A:192:VAL:N	1:D:195:GLN:O	2.28	0.56
1:A:524:GLN:HG2	1:B:340:LYS:HD2	1.87	0.56
1:B:243:ASP:HB3	1:B:306:GLU:HG2	1.87	0.56
1:B:243:ASP:CB	1:B:306:GLU:HG2	2.36	0.56
1:C:220:GLY:HA2	1:C:288:GLU:OE2	2.06	0.56
1:D:476:GLU:HB3	1:D:512:HIS:CE1	2.42	0.55
1:A:202:LEU:HD23	1:A:370:THR:HG21	1.87	0.55
1:A:261:LYS:NZ	6:A:801:HOH:O	2.39	0.55
1:C:242:THR:HA	1:C:254:ARG:NH2	2.21	0.55
1:B:199:ASN:OD1	1:B:353:ASN:HB2	2.07	0.55
1:B:241:THR:HG22	1:B:255:TYR:HD2	1.71	0.55
1:D:385:ILE:HG12	1:D:531:ALA:HB2	1.89	0.55
1:C:405:VAL:HG22	1:C:461:ILE:HG12	1.88	0.55
1:A:447:THR:H	1:A:450:ASN:CB	2.19	0.55
1:B:324:PHE:CZ	1:B:327:ILE:HG13	2.42	0.55
1:C:429:MET:HG2	1:C:502:TYR:CD2	2.43	0.54
1:C:521:ALA:O	1:C:524:GLN:HG2	2.08	0.54
1:D:232:THR:OG1	1:D:422:THR:HG23	2.07	0.54
1:B:237:LEU:HD13	1:B:328:VAL:HA	1.90	0.53
1:D:447:THR:HG23	1:D:449:GLU:H	1.73	0.53
1:B:324:PHE:HZ	1:B:327:ILE:HG13	1.74	0.53
1:D:267:PHE:HB2	1:D:285:ILE:HB	1.91	0.53
1:B:386:TYR:CZ	1:C:524:GLN:HB2	2.44	0.53
1:B:365:GLU:HG2	1:B:366:ASP:N	2.24	0.53
1:C:386:TYR:O	1:C:529:GLY:HA2	2.08	0.53
1:C:317:ASN:N	1:C:317:ASN:OD1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ARG:H	1:B:350:GLN:NE2	2.07	0.52
1:A:443:SER:HA	1:A:485:CYS:O	2.10	0.52
1:C:455:LEU:HD22	1:C:478:MET:HG3	1.90	0.52
1:A:240:VAL:HA	1:A:305:VAL:HB	1.92	0.52
1:C:196:THR:HG22	1:C:376:VAL:HG23	1.90	0.52
1:A:386:TYR:CE2	1:D:525:PRO:HD2	2.45	0.52
1:C:300:GLN:HG2	1:C:343:PHE:HD1	1.75	0.52
1:A:267:PHE:CG	1:C:532:LYS:HD3	2.45	0.52
1:B:380:PHE:CE2	1:B:540:ALA:HB2	2.45	0.52
1:A:524:GLN:CG	1:B:340:LYS:HD2	2.40	0.52
1:B:238:TRP:HB2	1:B:327:ILE:HB	1.92	0.52
1:D:404:TYR:CE2	1:D:409:LYS:HG2	2.44	0.52
1:C:430:PRO:HB3	1:C:499:ASN:HA	1.93	0.51
1:D:365:GLU:OE2	1:D:511:ARG:HD2	2.11	0.51
1:B:428:THR:OG1	1:B:503:LEU:HB2	2.11	0.51
1:D:295:HIS:CD2	1:D:354:LEU:HD11	2.45	0.51
1:D:422:THR:HG22	1:D:510:MET:HE1	1.92	0.51
1:C:470:ILE:HD11	1:C:530:VAL:HG21	1.92	0.51
1:D:310:ASN:H	1:D:310:ASN:ND2	2.09	0.51
1:D:441:VAL:HG12	1:D:487:PRO:HB3	1.93	0.51
1:C:240:VAL:HG12	1:C:254:ARG:HG2	1.93	0.51
1:C:212:GLN:HB3	1:C:214:VAL:HG13	1.93	0.51
1:D:382:GLU:HG3	1:D:532:LYS:HD3	1.93	0.51
1:C:333:PRO:HG3	1:C:345:ASP:OD2	2.10	0.50
1:C:515:THR:HG22	1:C:530:VAL:HG12	1.92	0.50
1:B:365:GLU:HG2	1:B:366:ASP:H	1.75	0.50
1:D:263:PHE:CZ	1:D:304:LEU:HD21	2.45	0.50
1:A:288:GLU:OE1	1:A:288:GLU:HA	2.12	0.50
1:D:207:HIS:NE2	1:D:211:SER:HA	2.26	0.50
1:D:231:ASP:OD2	4:D:601:I0I:N01	2.44	0.50
1:B:429:MET:HE3	1:B:434:MET:HA	1.92	0.50
1:C:346:ASN:OD1	1:C:350:GLN:NE2	2.45	0.50
1:C:460:VAL:HG13	1:C:473:LEU:HD23	1.93	0.50
1:B:428:THR:HA	1:B:490:MET:O	2.12	0.50
1:D:430:PRO:O	1:D:434:MET:HB2	2.12	0.50
1:A:202:LEU:HB3	1:A:370:THR:HG21	1.93	0.50
1:C:244:CYS:HB2	1:C:306:GLU:HA	1.94	0.49
1:D:201:PHE:CE1	1:D:354:LEU:HD21	2.47	0.49
1:C:263:PHE:HA	1:C:288:GLU:OE1	2.12	0.49
1:B:385:ILE:HG12	1:B:531:ALA:HB2	1.93	0.49
1:D:426:TYR:HD2	1:D:490:MET:HB3	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:ILE:HB	1:B:503:LEU:CD2	2.43	0.49
1:A:187:LYS:HD2	1:D:192:VAL:CG2	2.42	0.49
1:B:470:ILE:HG21	1:B:509:PHE:HE1	1.78	0.49
1:B:518:VAL:HG21	1:B:546:LEU:HD22	1.94	0.49
1:C:372:LEU:HD21	1:C:380:PHE:CE2	2.48	0.49
1:D:412:CYS:SG	1:D:416:SER:OG	2.68	0.49
1:D:317:ASN:N	6:D:701:HOH:O	2.45	0.49
1:D:433:GLN:N	1:D:433:GLN:OE1	2.44	0.49
1:C:447:THR:OG1	1:C:450:ASN:HB2	2.13	0.49
1:D:220:GLY:HA3	1:D:260:SER:HB2	1.95	0.49
1:D:244:CYS:HB2	1:D:306:GLU:HA	1.94	0.49
1:D:422:THR:HG22	1:D:510:MET:CE	2.43	0.49
1:A:455:LEU:HA	1:A:474:PRO:HB2	1.94	0.48
1:C:421:ASP:OD1	4:C:701:I0I:N04	2.46	0.48
1:C:494:VAL:HG21	1:C:501:ALA:HB3	1.95	0.48
1:A:200:VAL:HB	1:A:543:VAL:HG21	1.94	0.48
1:C:260:SER:OG	1:C:263:PHE:HB2	2.14	0.48
1:D:247:GLU:H	1:D:247:GLU:CD	2.16	0.48
1:A:212:GLN:HG2	1:A:229:ILE:HD11	1.94	0.48
1:A:223:PRO:HD2	6:A:821:HOH:O	2.13	0.48
1:A:429:MET:HG2	1:A:502:TYR:HD2	1.79	0.48
1:C:241:THR:HG22	1:C:255:TYR:HD2	1.77	0.48
1:A:202:LEU:HB3	1:A:370:THR:CG2	2.44	0.48
1:B:372:LEU:HD21	1:B:380:PHE:HE2	1.78	0.48
1:C:430:PRO:HD2	1:C:502:TYR:CE2	2.48	0.48
1:B:217:LEU:HD23	1:B:226:ILE:HD11	1.96	0.47
1:C:237:LEU:HD13	1:C:328:VAL:HA	1.96	0.47
1:C:238:TRP:CZ2	1:C:274:ILE:HD13	2.40	0.47
1:D:272:LEU:HG	1:D:285:ILE:HD11	1.97	0.47
1:B:412:CYS:SG	1:B:416:SER:HB2	2.55	0.47
1:D:455:LEU:HA	1:D:458:TYR:HD1	1.80	0.47
3:F:1:NAG:H3	3:F:1:NAG:C8	2.44	0.47
1:C:324:PHE:HZ	1:C:327:ILE:HG12	1.80	0.47
1:A:186:VAL:HG21	1:B:270:LYS:CG	2.45	0.47
1:A:470:ILE:HG21	1:A:509:PHE:HE1	1.80	0.47
1:B:190:HIS:HA	1:B:548:ASN:HB2	1.97	0.47
1:B:263:PHE:HA	1:B:288:GLU:OE1	2.14	0.46
1:A:469:VAL:O	1:D:523:GLY:HA3	2.15	0.46
1:C:192:VAL:HG12	1:C:193:VAL:N	2.30	0.46
1:C:288:GLU:HB2	1:C:302:PHE:CE1	2.50	0.46
1:B:380:PHE:CZ	1:B:540:ALA:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:VAL:HG11	1:B:324:PHE:O	2.16	0.46
1:C:395:TYR:HB3	1:C:419:ILE:HG23	1.98	0.46
1:C:433:GLN:OE1	1:C:433:GLN:N	2.48	0.46
1:A:400:LEU:HD21	1:A:403:ILE:HD11	1.98	0.46
1:A:494:VAL:HB	1:A:501:ALA:HB3	1.97	0.46
1:B:429:MET:HB2	1:B:434:MET:CE	2.44	0.46
1:C:215:GLY:HA3	1:C:230:PHE:HE1	1.81	0.46
1:C:480:LEU:HA	1:C:484:SER:O	2.15	0.46
1:A:455:LEU:HD22	1:A:475:GLU:CA	2.41	0.46
1:C:404:TYR:CE2	1:C:409:LYS:HB2	2.51	0.46
1:C:431:SER:N	1:C:493:ASP:OD1	2.42	0.46
1:D:283:GLY:HA3	1:D:304:LEU:O	2.16	0.46
1:D:447:THR:HG22	1:D:450:ASN:HB2	1.97	0.46
1:B:236:ASN:HD21	1:B:337:SER:CB	2.29	0.45
1:C:400:LEU:HD21	1:C:403:ILE:HD11	1.98	0.45
1:A:291:VAL:HA	1:A:295:HIS:O	2.16	0.45
1:A:472:LEU:HA	1:A:476:GLU:OE1	2.16	0.45
1:C:464:LEU:CD2	1:C:469:VAL:HG22	2.46	0.45
1:B:212:GLN:HB3	1:B:214:VAL:HG13	1.97	0.45
1:B:391:VAL:HG21	1:B:417:TYR:CD2	2.51	0.45
1:A:186:VAL:O	1:A:187:LYS:HG3	2.16	0.45
1:B:319:PHE:HA	1:B:322:ILE:HG12	1.98	0.45
1:C:278:SER:HB2	1:C:318:ILE:HG23	1.98	0.45
1:B:434:MET:HE3	1:B:491:GLN:HA	1.98	0.45
1:B:317:ASN:HB3	1:B:320:ASP:OD2	2.16	0.45
1:D:390:VAL:HA	1:D:397:GLU:O	2.17	0.45
1:D:447:THR:HG23	1:D:448:GLU:N	2.31	0.45
1:A:232:THR:OG1	1:A:422:THR:HG23	2.17	0.45
1:B:272:LEU:HD11	1:B:337:SER:CB	2.41	0.45
1:D:443:SER:HA	1:D:485:CYS:O	2.17	0.45
1:A:202:LEU:HG	1:A:372:LEU:HG	1.98	0.45
1:A:242:THR:HA	1:A:254:ARG:HH21	1.82	0.45
1:A:377:SER:HB3	1:A:380:PHE:CD2	2.52	0.45
3:F:2:NAG:H3	3:F:2:NAG:C8	2.46	0.45
1:D:241:THR:HA	1:D:255:TYR:O	2.17	0.44
1:B:327:ILE:HD13	4:B:701:I0I:C29	2.47	0.44
1:A:429:MET:HG2	1:A:502:TYR:CD2	2.53	0.44
1:B:447:THR:HG22	1:B:448:GLU:H	1.82	0.44
1:C:404:TYR:OH	1:C:409:LYS:HE3	2.18	0.44
3:F:2:NAG:H83	3:F:2:NAG:C3	2.47	0.44
1:A:212:GLN:HB3	1:A:214:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:GLU:O	1:A:511:ARG:NH2	2.51	0.44
1:C:255:TYR:O	1:C:257:PRO:HD3	2.18	0.44
1:C:426:TYR:HB2	1:C:490:MET:HE2	2.00	0.44
1:D:344:PHE:CZ	1:D:358:PHE:HD2	2.36	0.44
1:D:405:VAL:HG21	1:D:410:ILE:HD12	1.99	0.44
1:A:283:GLY:HA3	1:A:304:LEU:O	2.18	0.44
1:C:237:LEU:HD12	1:C:327:ILE:O	2.17	0.44
2:E:1:NAG:O7	2:E:1:NAG:C3	2.65	0.44
1:A:389:PRO:O	1:A:398:VAL:HG13	2.18	0.44
1:C:324:PHE:CZ	1:C:327:ILE:HG12	2.53	0.44
1:D:428:THR:HA	1:D:490:MET:O	2.18	0.44
1:D:434:MET:HE3	1:D:434:MET:HA	2.00	0.44
1:A:418:ALA:HA	1:A:502:TYR:O	2.18	0.44
1:C:362:ILE:HB	1:C:511:ARG:HA	2.00	0.44
1:A:242:THR:HA	1:A:254:ARG:NH2	2.33	0.43
1:C:250:LYS:HA	1:C:254:ARG:HE	1.81	0.43
1:A:189:ALA:HB1	1:D:193:VAL:O	2.18	0.43
1:C:363:SER:H	1:C:369:SER:HB3	1.82	0.43
1:A:240:VAL:HG12	1:A:254:ARG:HG2	2.00	0.43
1:A:267:PHE:CD1	1:C:532:LYS:HD3	2.53	0.43
1:B:248:SER:HA	1:B:251:LYS:HE2	2.00	0.43
1:D:240:VAL:HA	1:D:305:VAL:HB	2.01	0.43
1:A:251:LYS:HG3	1:A:252:VAL:HG13	1.99	0.43
1:B:288:GLU:HB2	1:B:302:PHE:CE1	2.53	0.43
1:D:288:GLU:HB3	1:D:290:PHE:CE1	2.53	0.43
1:D:212:GLN:CD	1:D:229:ILE:HD11	2.39	0.43
1:D:322:ILE:HG22	1:D:324:PHE:HB2	2.01	0.43
1:D:240:VAL:CG1	1:D:254:ARG:HG2	2.49	0.43
1:D:430:PRO:HG3	1:D:499:ASN:O	2.18	0.43
1:A:429:MET:HE2	1:A:489:TYR:CD2	2.54	0.43
1:B:257:PRO:HG3	1:B:304:LEU:HD23	2.01	0.43
1:D:241:THR:HG22	1:D:255:TYR:CD2	2.49	0.42
1:A:451:TYR:CE1	1:A:455:LEU:HD21	2.53	0.42
1:C:470:ILE:HG21	1:C:509:PHE:HE1	1.83	0.42
1:A:241:THR:HG21	1:A:304:LEU:HB3	2.02	0.42
1:A:429:MET:HE2	1:A:489:TYR:CE2	2.54	0.42
1:B:515:THR:HA	1:B:529:GLY:O	2.20	0.42
1:D:215:GLY:O	1:D:227:HIS:HA	2.19	0.42
1:B:200:VAL:HA	1:B:373:VAL:O	2.19	0.42
1:C:209:ARG:N	5:C:702:SO4:O3	2.48	0.42
1:C:506:SER:HA	1:C:510:MET:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:VAL:HG13	1:A:290:PHE:CE1	2.54	0.42
1:C:447:THR:H	1:C:450:ASN:HB3	1.84	0.42
1:B:200:VAL:HG22	1:B:374:GLY:C	2.40	0.42
4:D:601:I0I:C18	4:D:601:I0I:C24	2.98	0.42
1:D:455:LEU:HA	1:D:458:TYR:CD1	2.54	0.42
1:B:455:LEU:HD23	1:B:458:TYR:CE2	2.55	0.42
1:B:472:LEU:HA	1:B:476:GLU:OE1	2.19	0.42
1:A:363:SER:H	1:A:369:SER:HB3	1.85	0.41
1:C:387:MET:HE3	1:C:527:MET:HG3	2.01	0.41
1:D:272:LEU:HG	1:D:285:ILE:CD1	2.50	0.41
1:B:433:GLN:OE1	1:B:433:GLN:N	2.53	0.41
1:C:194:GLU:OE1	1:C:376:VAL:HG21	2.21	0.41
1:C:217:LEU:HD23	1:C:226:ILE:HD11	2.02	0.41
1:C:429:MET:HB2	1:C:434:MET:CE	2.48	0.41
1:A:405:VAL:O	1:A:405:VAL:HG13	2.21	0.41
1:B:272:LEU:HD22	1:B:285:ILE:CD1	2.47	0.41
1:B:272:LEU:HD12	1:B:272:LEU:HA	1.83	0.41
1:B:357:GLN:HE21	1:B:518:VAL:HG13	1.86	0.41
1:C:461:ILE:O	1:C:471:GLU:HA	2.21	0.41
1:D:219:VAL:HG12	1:D:288:GLU:HG2	2.01	0.41
1:D:468:LEU:HD12	1:D:468:LEU:HA	1.85	0.41
1:A:201:PHE:CE2	1:A:373:VAL:HB	2.56	0.41
1:B:347:LEU:HD12	1:B:351:ASN:ND2	2.36	0.41
1:C:273:HIS:C	1:C:274:ILE:HD12	2.40	0.41
1:D:231:ASP:HA	1:D:422:THR:OG1	2.21	0.41
1:B:186:VAL:HG23	1:C:467:ASP:HB2	2.01	0.41
1:C:281:ILE:HD11	1:C:305:VAL:HG22	2.02	0.41
1:D:441:VAL:CG1	1:D:487:PRO:HB3	2.51	0.41
1:A:470:ILE:HG23	1:A:513:TYR:CZ	2.56	0.41
1:A:515:THR:HA	1:A:529:GLY:O	2.21	0.41
1:B:291:VAL:HA	1:B:295:HIS:O	2.21	0.41
1:B:400:LEU:HD13	1:B:465:PHE:CE1	2.55	0.41
1:C:468:LEU:HA	1:C:468:LEU:HD12	1.88	0.41
1:D:273:HIS:O	1:D:274:ILE:HD13	2.21	0.41
1:C:248:SER:OG	1:C:308:GLU:OE1	2.19	0.40
1:B:318:ILE:O	1:B:322:ILE:HG12	2.22	0.40
1:A:298:ARG:O	1:A:350:GLN:NE2	2.46	0.40
1:A:422:THR:HG22	1:A:510:MET:HE1	2.03	0.40
1:A:480:LEU:HD12	1:A:484:SER:O	2.22	0.40
1:C:218:LEU:HB2	1:C:291:VAL:HB	2.04	0.40
1:D:203:ILE:HD11	1:D:293:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:GLY:CA	1:D:260:SER:HB2	2.52	0.40
1:A:430:PRO:HB3	1:A:499:ASN:HA	2.03	0.40
1:D:447:THR:HG22	1:D:450:ASN:CB	2.52	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ARG:NH1	1:B:482:GLU:O[1_655]	2.09	0.11
6:D:709:HOH:O	6:D:715:HOH:O[3_554]	2.14	0.06

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	353/379 (93%)	337 (96%)	16 (4%)	0	100	100
1	B	353/379 (93%)	342 (97%)	11 (3%)	0	100	100
1	C	338/379 (89%)	328 (97%)	10 (3%)	0	100	100
1	D	336/379 (89%)	322 (96%)	14 (4%)	0	100	100
All	All	1380/1516 (91%)	1329 (96%)	51 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	295/332 (89%)	290 (98%)	5 (2%)	60 80
1	B	288/332 (87%)	281 (98%)	7 (2%)	49 74
1	C	286/332 (86%)	277 (97%)	9 (3%)	40 69
1	D	279/332 (84%)	267 (96%)	12 (4%)	29 60
All	All	1148/1328 (86%)	1115 (97%)	33 (3%)	42 70

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	THR
1	A	270	LYS
1	A	391	VAL
1	A	411	CYS
1	A	547	GLU
1	B	237	LEU
1	B	340	LYS
1	B	409	LYS
1	B	411	CYS
1	B	437	PHE
1	B	447	THR
1	B	486	ILE
1	C	198	GLU
1	C	229	ILE
1	C	268	ILE
1	C	317	ASN
1	C	382	GLU
1	C	405	VAL
1	C	421	ASP
1	C	503	LEU
1	C	534	ARG
1	D	195	GLN
1	D	196	THR
1	D	197	GLU
1	D	261	LYS
1	D	310	ASN
1	D	407	GLU
1	D	409	LYS
1	D	434	MET
1	D	447	THR
1	D	470	ILE
1	D	492	ILE
1	D	510	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	ASN
1	B	236	ASN
1	C	317	ASN
1	D	199	ASN
1	D	212	GLN
1	D	310	ASN
1	D	317	ASN
1	D	357	GLN
1	D	427	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

7 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	0.65	0	17,19,21	1.25	1 (5%)
2	NAG	E	2	2	14,14,15	0.48	0	17,19,21	1.58	2 (11%)
2	BMA	E	3	2	11,11,12	0.93	1 (9%)	15,15,17	1.01	1 (6%)
3	NAG	F	1	3,1	14,14,15	1.10	2 (14%)	17,19,21	1.34	2 (11%)
3	NAG	F	2	3	14,14,15	0.64	0	17,19,21	2.00	3 (17%)
3	NAG	G	1	3,1	14,14,15	0.41	0	17,19,21	0.59	0
3	NAG	G	2	3	14,14,15	0.46	0	17,19,21	0.68	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	5/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	O5-C1	-3.06	1.38	1.43
3	F	1	NAG	C1-C2	2.39	1.55	1.52
2	E	3	BMA	C1-C2	2.29	1.57	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	2	NAG	C2-N2-C7	5.53	130.77	122.90
3	F	2	NAG	C1-O5-C5	4.71	118.57	112.19
2	E	2	NAG	C1-O5-C5	4.66	118.51	112.19
2	E	1	NAG	C2-N2-C7	4.16	128.83	122.90
3	F	1	NAG	C2-N2-C7	3.97	128.56	122.90
3	F	2	NAG	C1-C2-N2	3.48	116.43	110.49
2	E	2	NAG	C2-N2-C7	3.08	127.28	122.90
3	F	1	NAG	C1-C2-N2	2.21	114.26	110.49
2	E	3	BMA	O5-C5-C6	2.03	110.39	107.20

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C3-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
3	F	2	NAG	C3-C2-N2-C7
3	F	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
2	E	2	NAG	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
3	G	2	NAG	C1-C2-N2-C7
3	F	1	NAG	C3-C2-N2-C7
2	E	3	BMA	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6

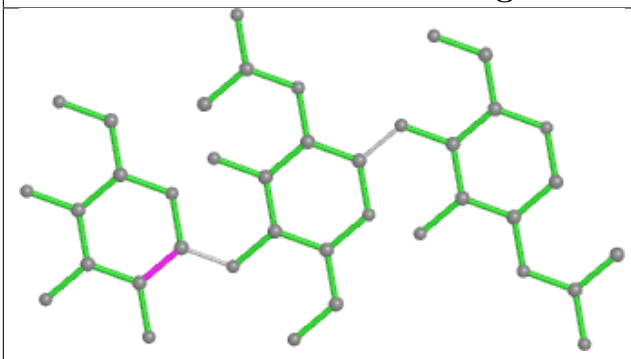
There are no ring outliers.

3 monomers are involved in 6 short contacts:

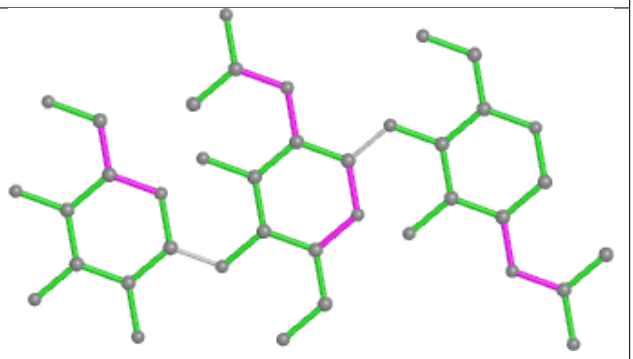
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	2	0
3	F	2	NAG	3	0
2	E	1	NAG	1	0

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

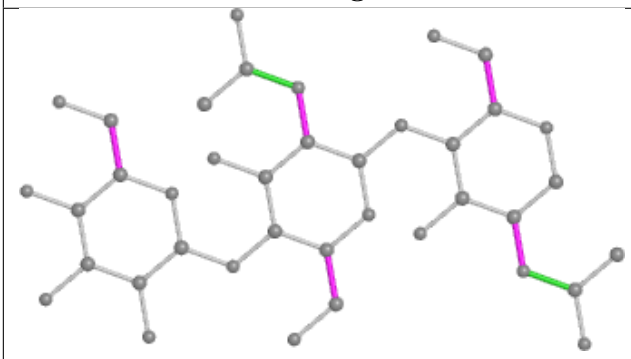
Oligosaccharide Chain E



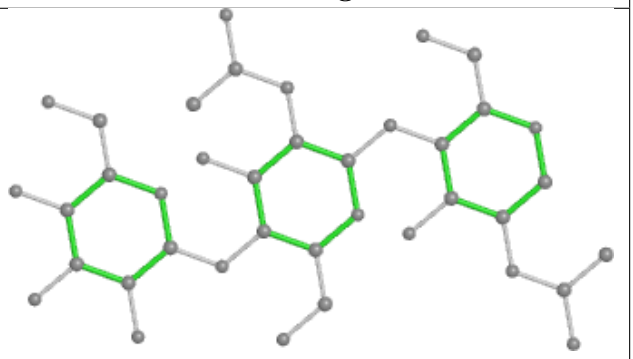
Bond lengths



Bond angles

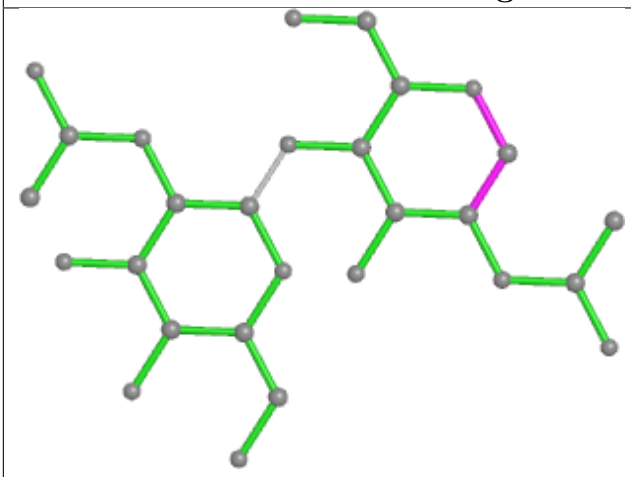


Torsions

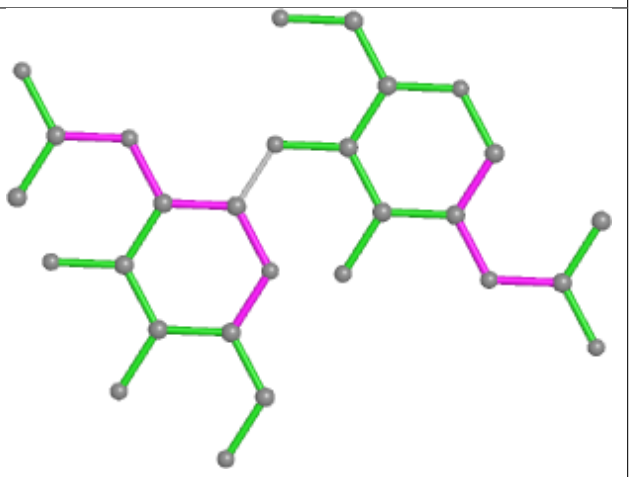


Rings

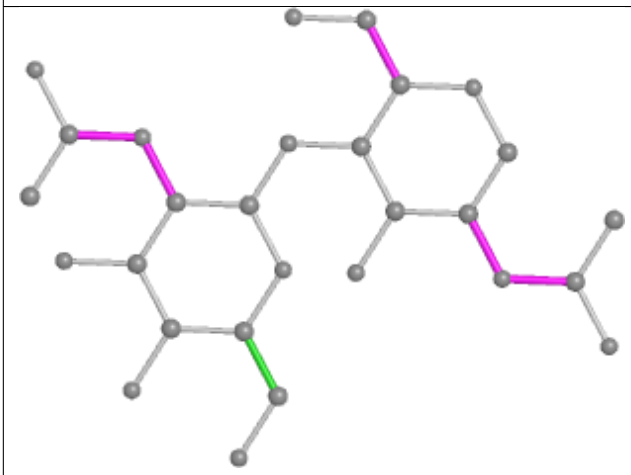
Oligosaccharide Chain F



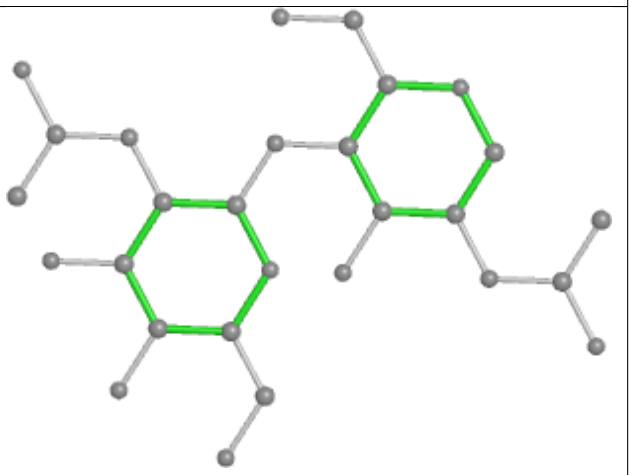
Bond lengths



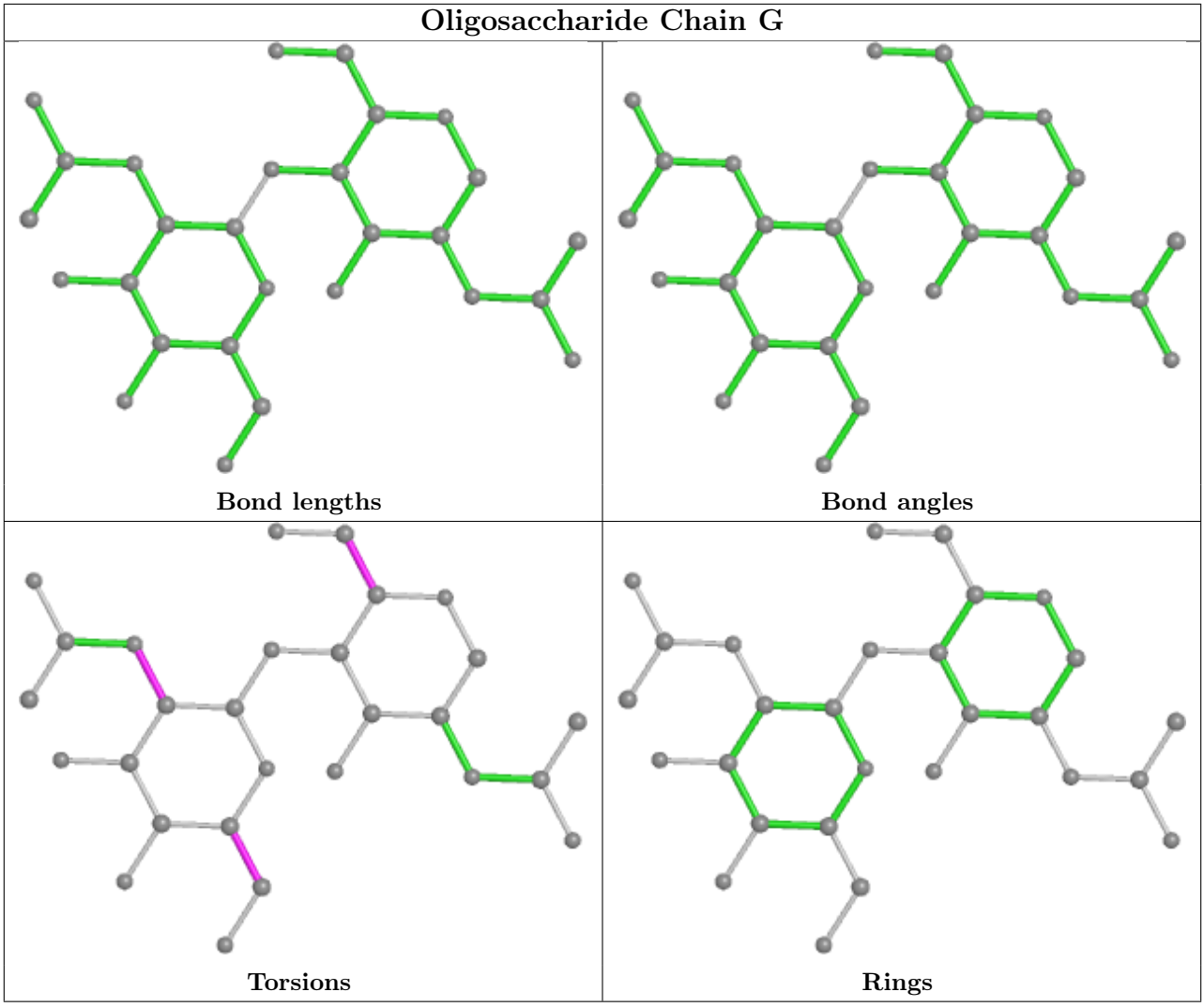
Bond angles



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	I0I	B	701	-	33,39,39	0.68	1 (3%)	43,56,56	1.28	2 (4%)
5	SO4	C	702	-	4,4,4	0.14	0	6,6,6	0.06	0
4	I0I	C	701	-	33,39,39	0.39	0	43,56,56	0.56	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	I0I	D	601	-	33,39,39	0.74	1 (3%)	43,56,56	0.51	1 (2%)
4	I0I	A	701	-	33,39,39	0.60	1 (3%)	43,56,56	1.50	3 (6%)

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	I0I	D	601	-	-	13/30/48/48	0/4/4/4
4	I0I	B	701	-	-	6/30/48/48	0/4/4/4
4	I0I	A	701	-	-	7/30/48/48	0/4/4/4
4	I0I	C	701	-	-	11/30/48/48	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	601	I0I	C02-N02	4.15	1.41	1.38
4	B	701	I0I	C02-N02	3.75	1.41	1.38
4	A	701	I0I	C02-N02	3.29	1.41	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	701	I0I	C29-C28-C01	-8.54	103.81	112.77
4	B	701	I0I	C29-C28-C01	-7.47	104.93	112.77
4	A	701	I0I	C30-C28-C01	-4.08	108.49	112.77
4	B	701	I0I	C04-C03-C19	2.53	118.96	112.33
4	C	701	I0I	C04-C03-C19	2.30	118.35	112.33
4	A	701	I0I	C03-N02-C25	2.09	120.75	117.44
4	D	601	I0I	C30-C28-C01	2.06	114.92	112.77

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	701	I0I	C26-C01-C28-C29
4	C	701	I0I	C26-C01-C28-C30
4	C	701	I0I	C27-C01-C28-C29
4	C	701	I0I	C27-C01-C28-C30

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Mol	Chain	Res	Type	Atoms
4	C	701	I0I	N01-C01-C28-C29
4	C	701	I0I	N01-C01-C28-C30
4	D	601	I0I	C26-C01-C28-C29
4	D	601	I0I	C26-C01-C28-C30
4	D	601	I0I	C27-C01-C28-C29
4	D	601	I0I	C27-C01-C28-C30
4	D	601	I0I	N01-C01-C28-C29
4	D	601	I0I	N01-C01-C28-C30
4	C	701	I0I	C06-C07-N03-C08
4	D	601	I0I	C16-C06-C07-N03
4	D	601	I0I	C16-C06-C07-O01
4	D	601	I0I	C05-C06-C07-N03
4	D	601	I0I	C05-C06-C07-O01
4	C	701	I0I	O01-C07-N03-C08
4	A	701	I0I	C16-C06-C07-N03
4	A	701	I0I	C16-C06-C07-O01
4	A	701	I0I	C05-C06-C07-N03
4	B	701	I0I	C04-C03-N02-C25
4	D	601	I0I	C19-C03-N02-C25
4	A	701	I0I	C05-C06-C07-O01
4	A	701	I0I	C15-C08-C09-C10
4	C	701	I0I	C15-C08-C09-C10
4	B	701	I0I	C15-C08-C09-C10
4	B	701	I0I	C16-C06-C07-O01
4	A	701	I0I	C15-C08-C09-C14
4	B	701	I0I	C15-C08-C09-C14
4	C	701	I0I	C15-C08-C09-C14
4	D	601	I0I	C15-C08-C09-C10
4	B	701	I0I	C16-C06-C07-N03
4	C	701	I0I	N02-C03-C04-C05
4	B	701	I0I	C05-C06-C07-O01
4	A	701	I0I	C19-C03-N02-C25
4	D	601	I0I	C04-C03-N02-C25

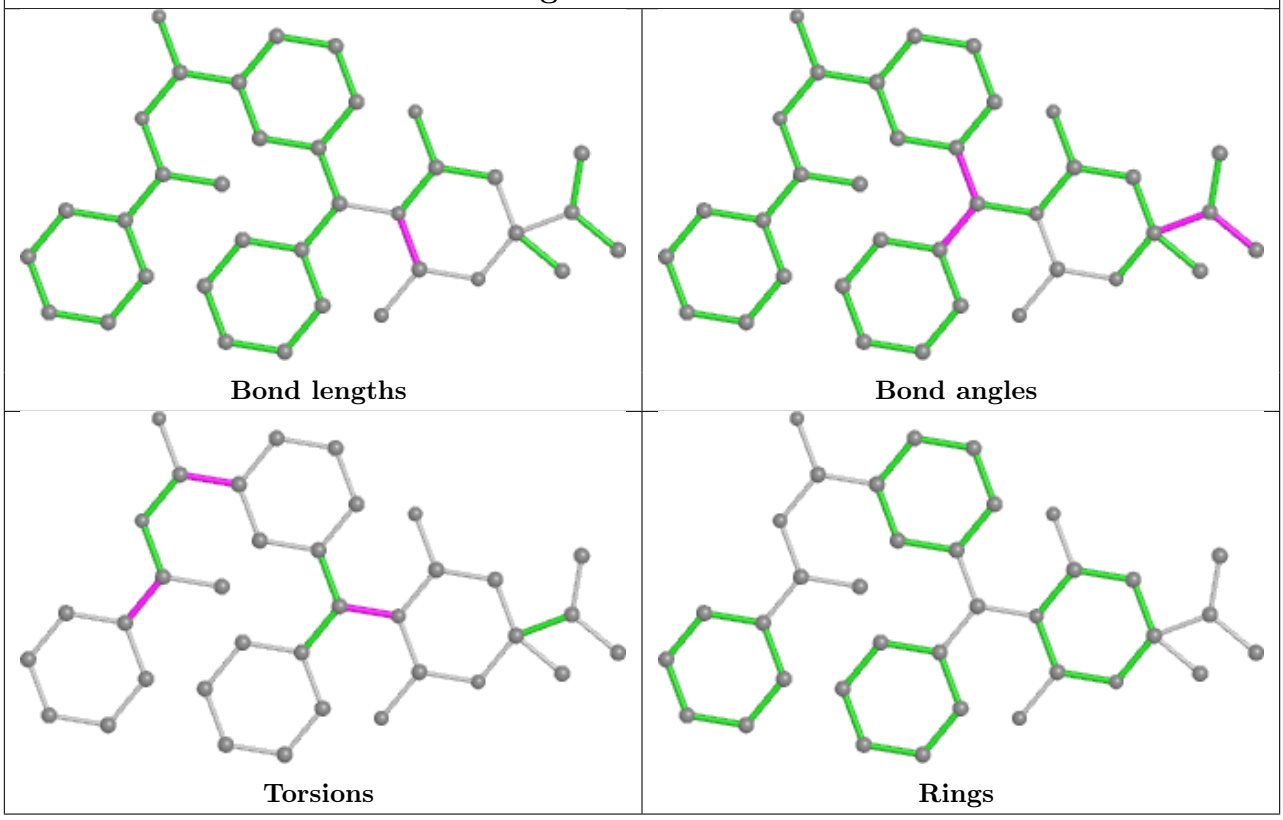
There are no ring outliers.

4 monomers are involved in 6 short contacts:

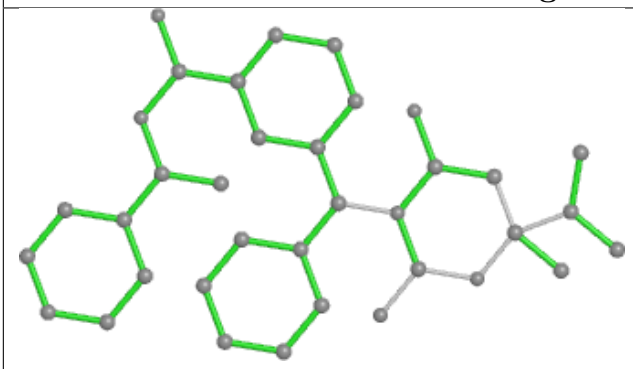
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	701	I0I	1	0
5	C	702	SO4	1	0
4	C	701	I0I	1	0
4	D	601	I0I	3	0

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.

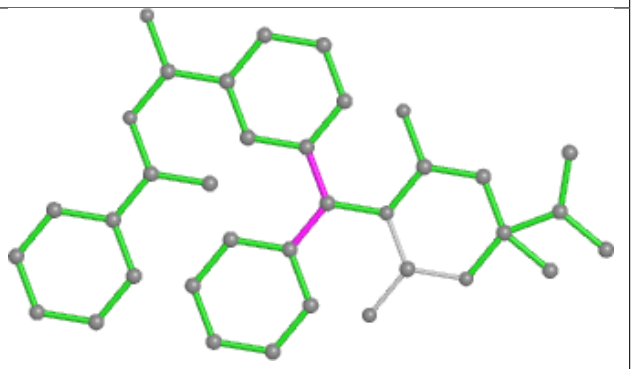
Ligand I0I B 701



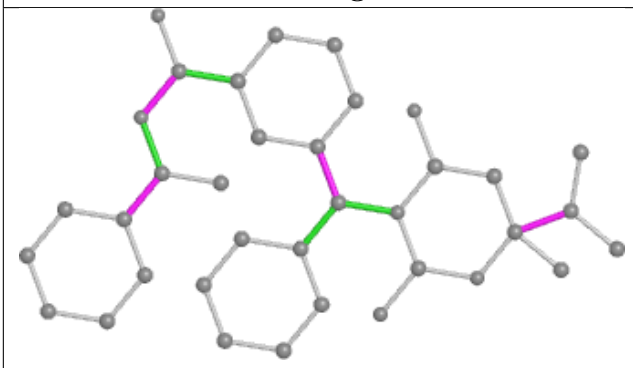
Ligand I0I C 701



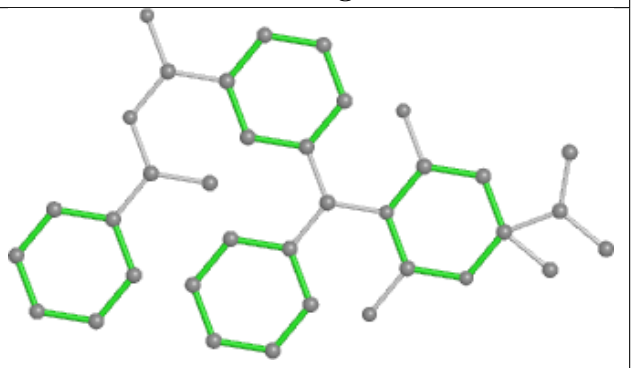
Bond lengths



Bond angles

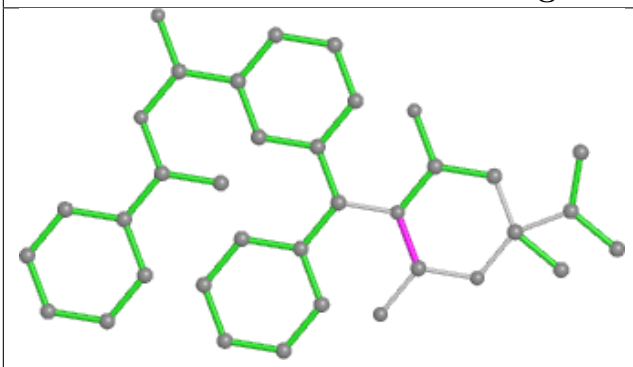


Torsions

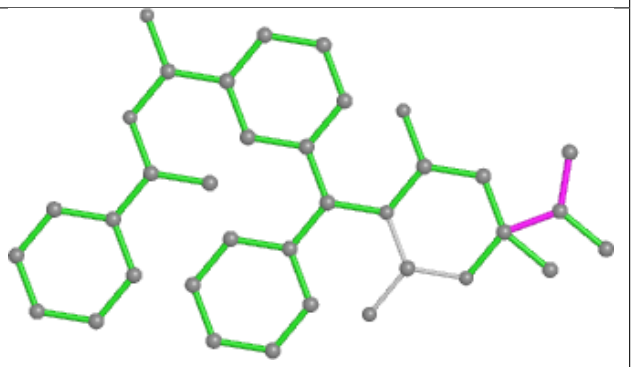


Rings

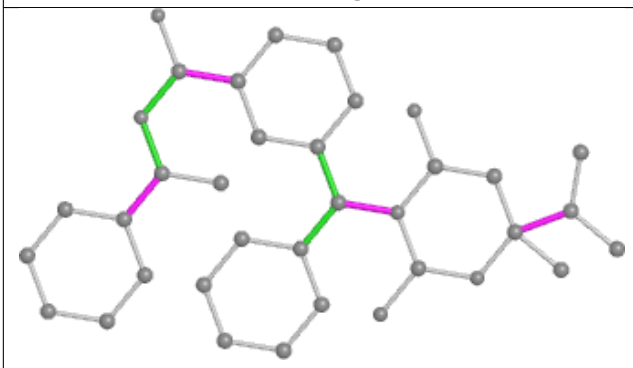
Ligand I0I D 601



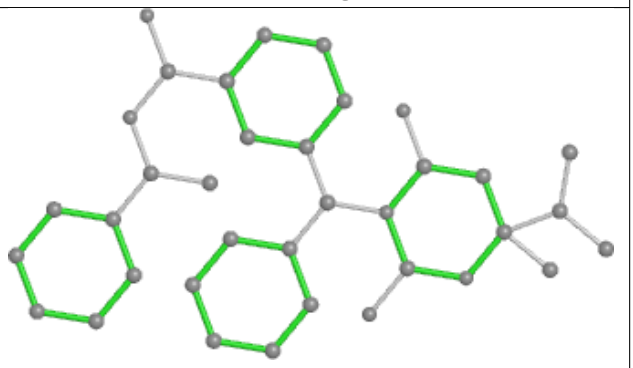
Bond lengths



Bond angles

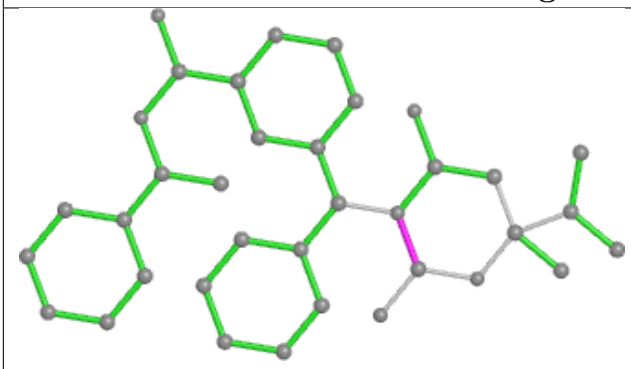


Torsions

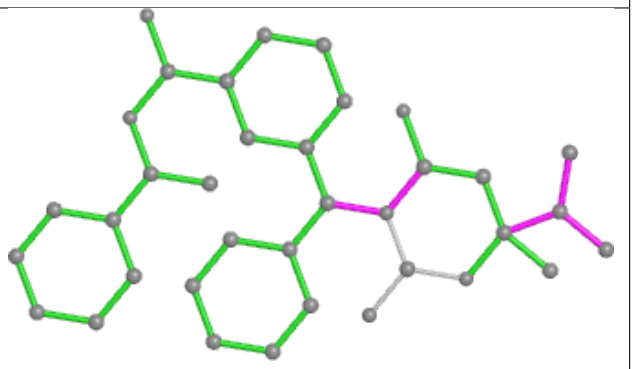


Rings

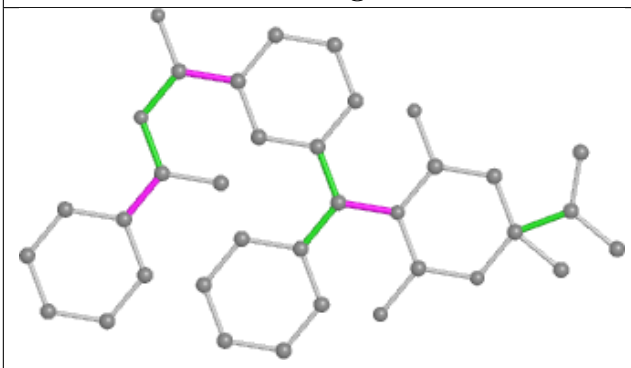
Ligand I0I A 701



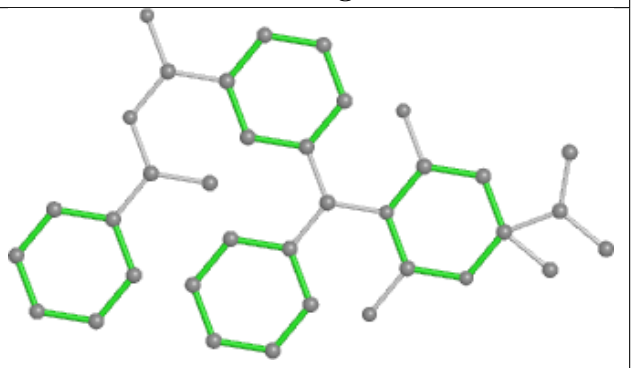
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	357/379 (94%)	0.09	10 (2%) 53 55	30, 47, 69, 82	0
1	B	357/379 (94%)	0.21	13 (3%) 42 45	29, 50, 82, 100	0
1	C	342/379 (90%)	0.12	11 (3%) 47 50	28, 48, 78, 92	0
1	D	340/379 (89%)	0.08	9 (2%) 56 58	31, 46, 76, 102	0
All	All	1396/1516 (92%)	0.13	43 (3%) 49 52	28, 48, 78, 102	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	443	SER	3.7
1	C	500	HIS	3.7
1	B	258	TYR	3.7
1	C	484	SER	3.7
1	B	317	ASN	3.6
1	B	310	ASN	3.5
1	D	451	TYR	3.4
1	B	458	TYR	3.3
1	A	322	ILE	3.2
1	D	447	THR	3.2
1	A	539	ALA	3.2
1	C	440	VAL	3.0
1	A	538	GLU	3.0
1	A	310	ASN	3.0
1	A	424	THR	3.0
1	A	320	ASP	2.9
1	D	440	VAL	2.9
1	D	450	ASN	2.8
1	C	320	ASP	2.7
1	D	446	CYS	2.6
1	B	440	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	431	SER	2.4
1	B	309	SER	2.4
1	C	250	LYS	2.4
1	D	410	ILE	2.3
1	B	439	ASP	2.3
1	C	452	GLN	2.3
1	C	454	VAL	2.3
1	D	295	HIS	2.3
1	D	401	ASP	2.2
1	B	441	VAL	2.2
1	C	497	GLU	2.2
1	B	344	PHE	2.2
1	A	541	GLN	2.2
1	A	323	ASP	2.2
1	A	321	TYR	2.2
1	B	477	TYR	2.1
1	B	252	VAL	2.1
1	B	541	GLN	2.1
1	C	246	GLU	2.1
1	D	500	HIS	2.1
1	A	348	LEU	2.0
1	B	278	SER	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	BMA	E	3	11/12	0.79	0.29	64,72,76,80	0
3	NAG	F	1	14/15	0.80	0.27	34,58,77,81	0
3	NAG	G	2	14/15	0.81	0.32	60,75,84,88	0
2	NAG	E	1	14/15	0.84	0.35	43,51,64,65	0
3	NAG	G	1	14/15	0.89	0.24	52,69,81,82	0
2	NAG	E	2	14/15	0.90	0.25	32,52,58,66	0

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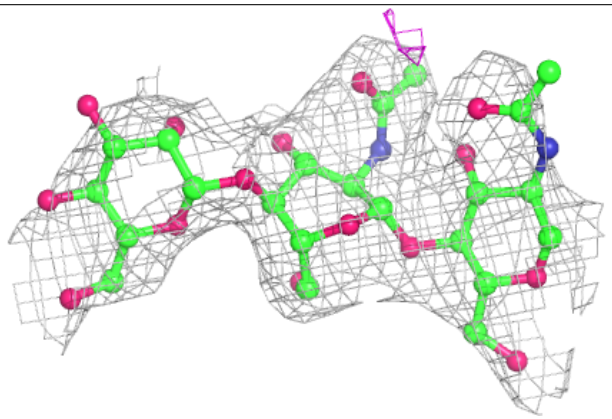
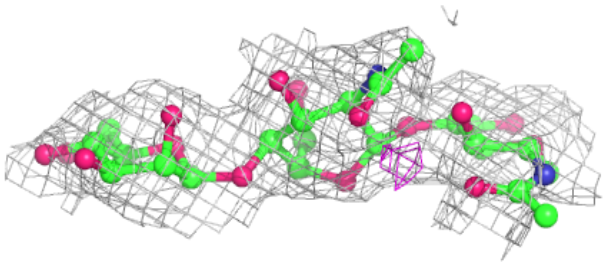
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	F	2	14/15	0.90	0.20	40,51,56,62	0

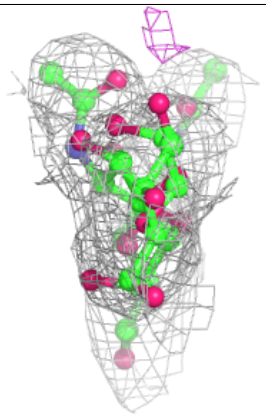
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

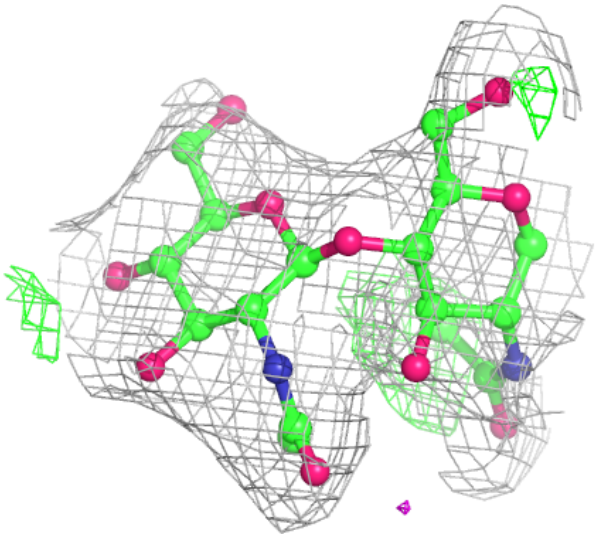


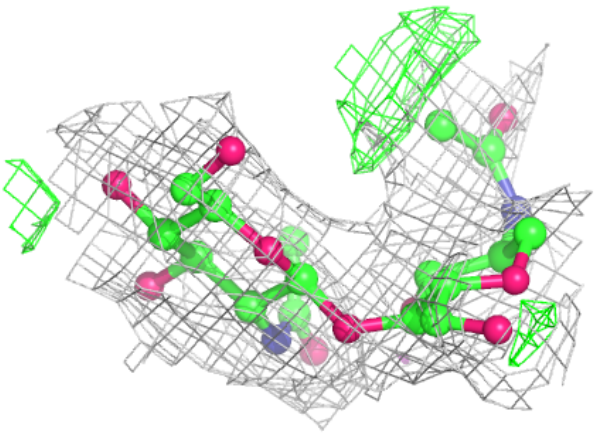


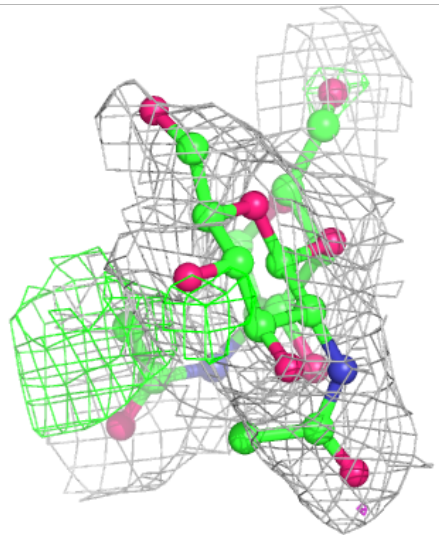


Electron density around Chain F:

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

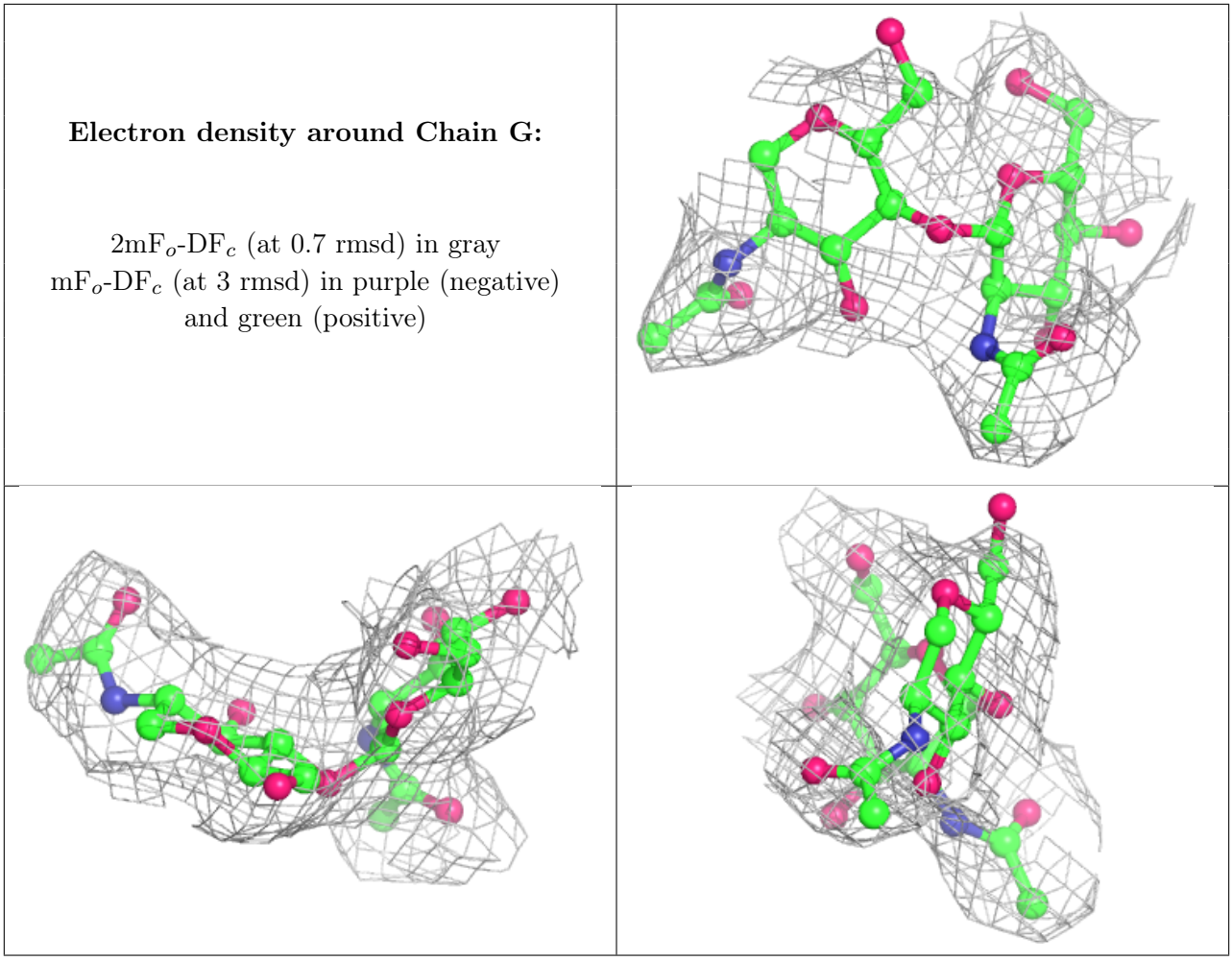






Electron density around Chain G:

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



6.4 Ligands

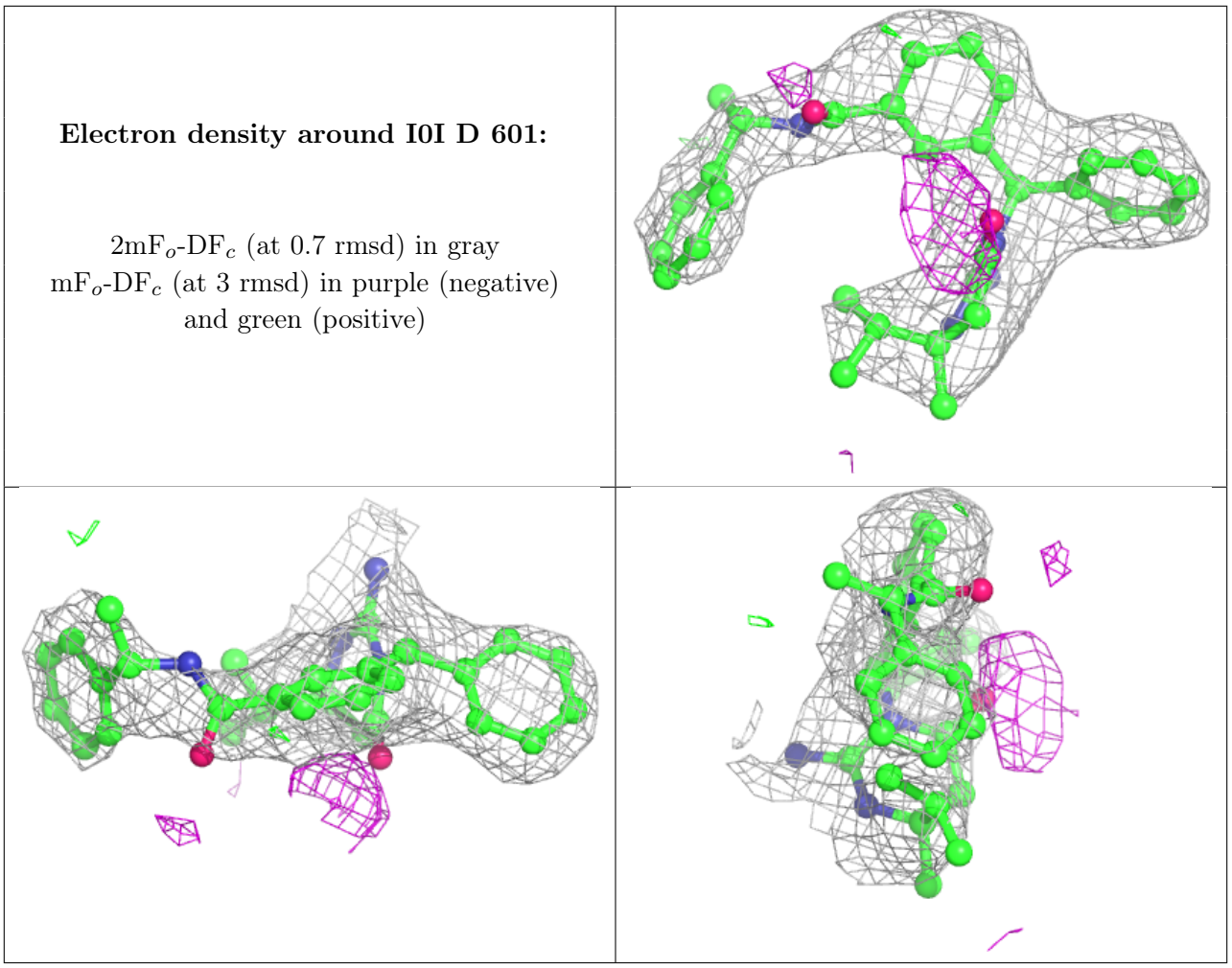
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	I0I	D	601	36/36	0.88	0.29	44,51,59,64	0
5	SO4	C	702	5/5	0.91	0.26	71,75,85,95	0
4	I0I	B	701	36/36	0.92	0.23	45,54,66,69	0
4	I0I	A	701	36/36	0.93	0.43	38,47,69,70	0
4	I0I	C	701	36/36	0.93	0.31	48,58,62,63	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.

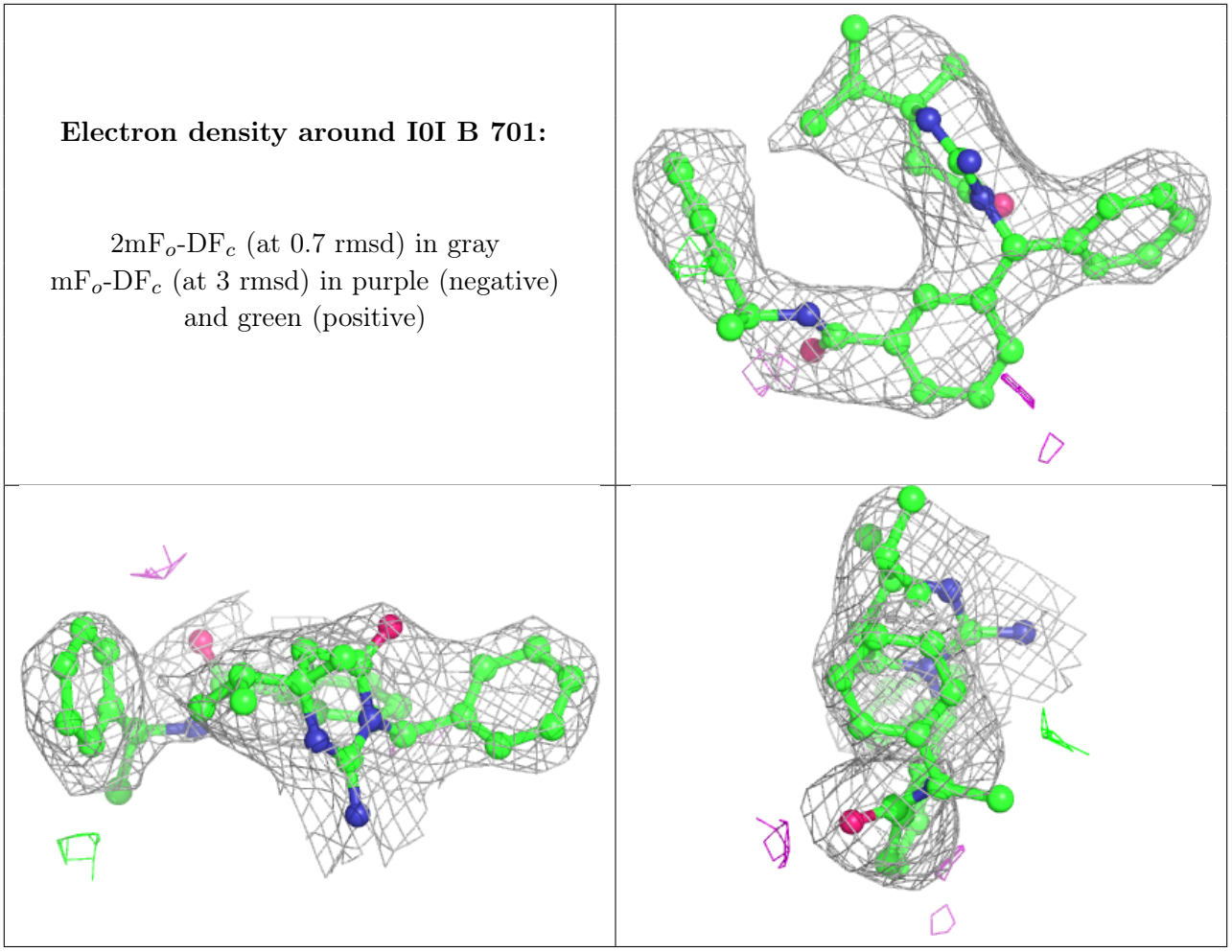
Electron density around I0I D 601:

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



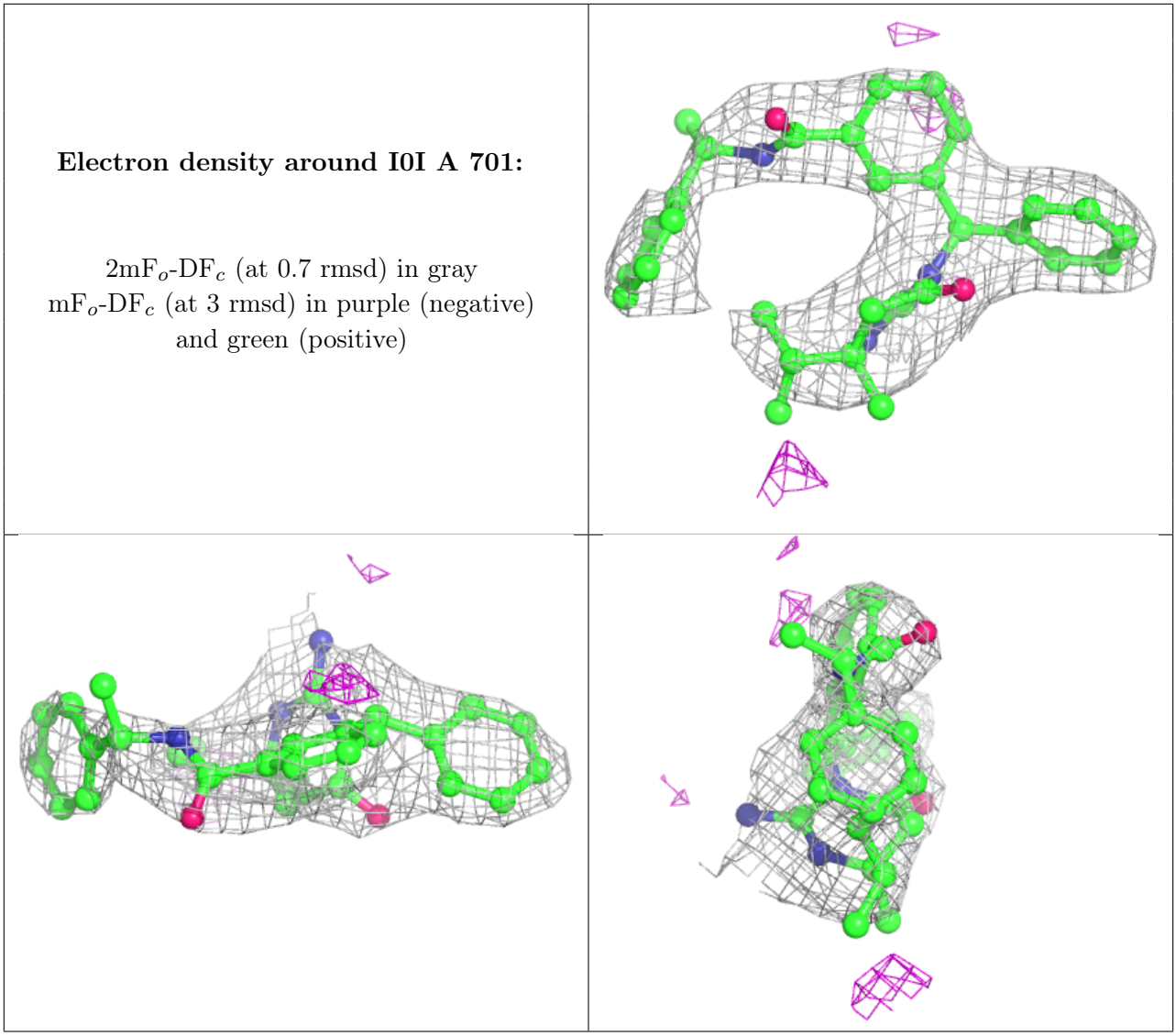
Electron density around I0I B 701:

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



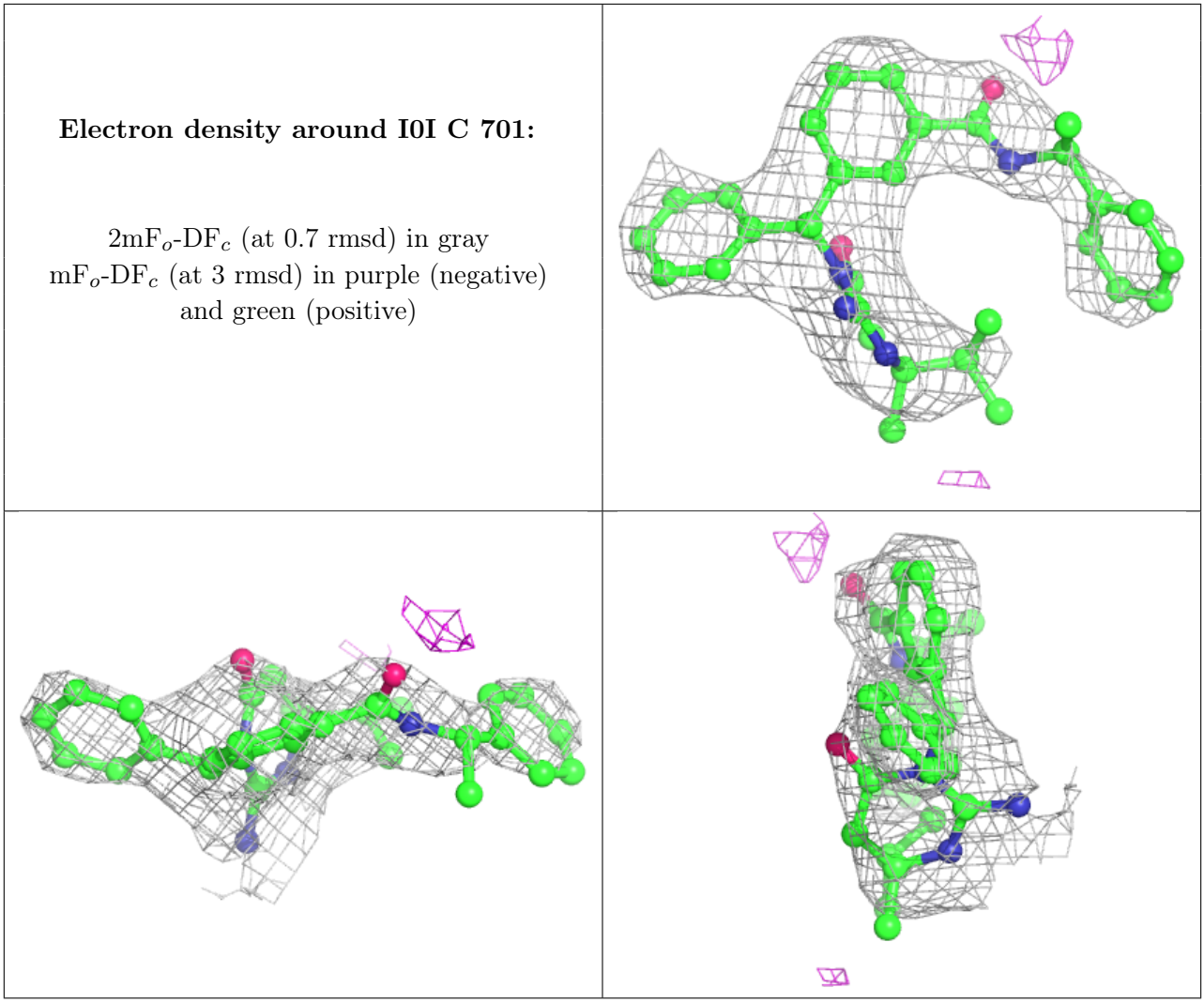
Electron density around I0I A 701:

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



Electron density around I0I C 701:

$2mF_o$-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.