wwPDB X-ray Structure Validation Summary Report (i)

Jun 24, 2024 – 06:07 PM EDT

PDB ID	:	6GKD
Title	:	human NBD1 of CFTR in complex with nanobodies D12 and G3a
Authors	:	Sigoillot, M.; Overtus, M.; Grodecka, M.; Scholl, D.; Garcia-Pino, A.; Laeremans, T.; He, L.; Pardon, E.; Hildebrandt, E.; Urbatsch, I.; Steyaert, J.; Riordan, J.R.; Govaerts, C.
Deposited on	:	2018-05-18
Resolution	:	2.99 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

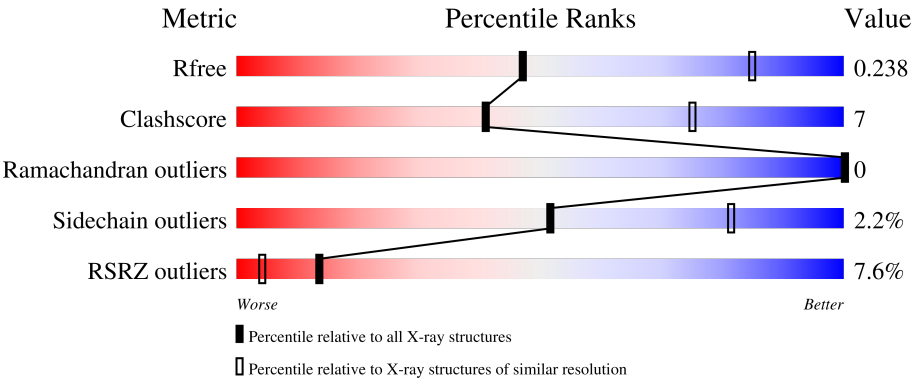
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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	229	5% 84% 10% 6%
1	F	229	10% 82% 9% 9%
1	I	229	4% 80% 13% 7%
1	L	229	4% 84% 10% 6%

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Mol	Chain	Length	Quality of chain
1	O	229	3% 85% 8% 6%
1	R	229	5% 79% 14% 6%
2	B	149	% 74% 9% 15%
2	G	149	9% 73% 9% 18%
2	J	149	8% 76% 7% 17%
2	M	149	6% 66% 15% 17%
2	P	149	9% 71% 11% 17%
2	S	149	17% 72% 11% 17%
3	C	149	13% 68% 13% 17%
3	H	149	2% 68% 13% 17%
3	K	149	7% 64% 16% 19%
3	N	149	3% 72% 10% 17%
3	Q	149	5% 73% 7% 17%
3	T	149	15% 68% 13% 17%
4	D	2	100%
4	E	2	50% 50%
4	U	2	50% 50%
4	V	2	50% 50%
4	W	2	50% 50%

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
4	GLC	W	1	-	-	-	X
4	Z9N	W	2	-	-	-	X
7	GOL	T	201	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 20891 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 Cystic fibrosis transmembrane conductance regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1592	1023	257	301	11			
1	F	209	Total	C	N	O	S	0	0	0
			1537	989	251	287	10			
1	I	213	Total	C	N	O	S	0	0	0
			1591	1018	260	303	10			
1	L	215	Total	C	N	O	S	0	0	0
			1563	995	256	301	11			
1	O	215	Total	C	N	O	S	0	0	0
			1571	1004	257	299	11			
1	R	215	Total	C	N	O	S	0	0	0
			1547	987	253	297	10			

There are 198 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	SER	ASN	expression tag	UNP Q20BJ8
A	?	-	PHE	deletion	UNP Q20BJ8
A	?	-	GLY	deletion	UNP Q20BJ8
A	?	-	GLU	deletion	UNP Q20BJ8
A	?	-	LEU	deletion	UNP Q20BJ8
A	?	-	PHE	deletion	UNP Q20BJ8
A	?	-	GLU	deletion	UNP Q20BJ8
A	?	-	LYS	deletion	UNP Q20BJ8
A	?	-	ALA	deletion	UNP Q20BJ8
A	?	-	LYS	deletion	UNP Q20BJ8
A	?	-	GLN	deletion	UNP Q20BJ8
A	?	-	ASN	deletion	UNP Q20BJ8
A	?	-	ASN	deletion	UNP Q20BJ8
A	?	-	ASN	deletion	UNP Q20BJ8
A	?	-	ASN	deletion	UNP Q20BJ8
A	?	-	ARG	deletion	UNP Q20BJ8
A	?	-	LYS	deletion	UNP Q20BJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP Q20BJ8
A	?	-	SER	deletion	UNP Q20BJ8
A	?	-	ASN	deletion	UNP Q20BJ8
A	?	-	GLY	deletion	UNP Q20BJ8
A	?	-	ASP	deletion	UNP Q20BJ8
A	?	-	ASP	deletion	UNP Q20BJ8
A	?	-	SER	deletion	UNP Q20BJ8
A	?	-	LEU	deletion	UNP Q20BJ8
A	?	-	PHE	deletion	UNP Q20BJ8
A	?	-	PHE	deletion	UNP Q20BJ8
A	?	-	SER	deletion	UNP Q20BJ8
A	?	-	ASN	deletion	UNP Q20BJ8
A	?	-	PHE	deletion	UNP Q20BJ8
A	?	-	SER	deletion	UNP Q20BJ8
A	?	-	LEU	deletion	UNP Q20BJ8
A	?	-	LEU	deletion	UNP Q20BJ8
F	386	SER	ASN	expression tag	UNP Q20BJ8
F	?	-	PHE	deletion	UNP Q20BJ8
F	?	-	GLY	deletion	UNP Q20BJ8
F	?	-	GLU	deletion	UNP Q20BJ8
F	?	-	LEU	deletion	UNP Q20BJ8
F	?	-	PHE	deletion	UNP Q20BJ8
F	?	-	GLU	deletion	UNP Q20BJ8
F	?	-	LYS	deletion	UNP Q20BJ8
F	?	-	ALA	deletion	UNP Q20BJ8
F	?	-	LYS	deletion	UNP Q20BJ8
F	?	-	GLN	deletion	UNP Q20BJ8
F	?	-	ASN	deletion	UNP Q20BJ8
F	?	-	ASN	deletion	UNP Q20BJ8
F	?	-	ASN	deletion	UNP Q20BJ8
F	?	-	ASN	deletion	UNP Q20BJ8
F	?	-	ARG	deletion	UNP Q20BJ8
F	?	-	LYS	deletion	UNP Q20BJ8
F	?	-	THR	deletion	UNP Q20BJ8
F	?	-	SER	deletion	UNP Q20BJ8
F	?	-	ASN	deletion	UNP Q20BJ8
F	?	-	GLY	deletion	UNP Q20BJ8
F	?	-	ASP	deletion	UNP Q20BJ8
F	?	-	ASP	deletion	UNP Q20BJ8
F	?	-	SER	deletion	UNP Q20BJ8
F	?	-	LEU	deletion	UNP Q20BJ8
F	?	-	PHE	deletion	UNP Q20BJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	PHE	deletion	UNP Q20BJ8
F	?	-	SER	deletion	UNP Q20BJ8
F	?	-	ASN	deletion	UNP Q20BJ8
F	?	-	PHE	deletion	UNP Q20BJ8
F	?	-	SER	deletion	UNP Q20BJ8
F	?	-	LEU	deletion	UNP Q20BJ8
F	?	-	LEU	deletion	UNP Q20BJ8
I	386	SER	ASN	expression tag	UNP Q20BJ8
I	?	-	PHE	deletion	UNP Q20BJ8
I	?	-	GLY	deletion	UNP Q20BJ8
I	?	-	GLU	deletion	UNP Q20BJ8
I	?	-	LEU	deletion	UNP Q20BJ8
I	?	-	PHE	deletion	UNP Q20BJ8
I	?	-	GLU	deletion	UNP Q20BJ8
I	?	-	LYS	deletion	UNP Q20BJ8
I	?	-	ALA	deletion	UNP Q20BJ8
I	?	-	LYS	deletion	UNP Q20BJ8
I	?	-	GLN	deletion	UNP Q20BJ8
I	?	-	ASN	deletion	UNP Q20BJ8
I	?	-	ASN	deletion	UNP Q20BJ8
I	?	-	ASN	deletion	UNP Q20BJ8
I	?	-	ASN	deletion	UNP Q20BJ8
I	?	-	ARG	deletion	UNP Q20BJ8
I	?	-	LYS	deletion	UNP Q20BJ8
I	?	-	THR	deletion	UNP Q20BJ8
I	?	-	SER	deletion	UNP Q20BJ8
I	?	-	ASN	deletion	UNP Q20BJ8
I	?	-	GLY	deletion	UNP Q20BJ8
I	?	-	ASP	deletion	UNP Q20BJ8
I	?	-	ASP	deletion	UNP Q20BJ8
I	?	-	SER	deletion	UNP Q20BJ8
I	?	-	LEU	deletion	UNP Q20BJ8
I	?	-	PHE	deletion	UNP Q20BJ8
I	?	-	PHE	deletion	UNP Q20BJ8
I	?	-	SER	deletion	UNP Q20BJ8
I	?	-	ASN	deletion	UNP Q20BJ8
I	?	-	PHE	deletion	UNP Q20BJ8
I	?	-	SER	deletion	UNP Q20BJ8
I	?	-	LEU	deletion	UNP Q20BJ8
I	?	-	LEU	deletion	UNP Q20BJ8
L	386	SER	ASN	expression tag	UNP Q20BJ8
L	?	-	PHE	deletion	UNP Q20BJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	GLY	deletion	UNP Q20BJ8
L	?	-	GLU	deletion	UNP Q20BJ8
L	?	-	LEU	deletion	UNP Q20BJ8
L	?	-	PHE	deletion	UNP Q20BJ8
L	?	-	GLU	deletion	UNP Q20BJ8
L	?	-	LYS	deletion	UNP Q20BJ8
L	?	-	ALA	deletion	UNP Q20BJ8
L	?	-	LYS	deletion	UNP Q20BJ8
L	?	-	GLN	deletion	UNP Q20BJ8
L	?	-	ASN	deletion	UNP Q20BJ8
L	?	-	ASN	deletion	UNP Q20BJ8
L	?	-	ASN	deletion	UNP Q20BJ8
L	?	-	ASN	deletion	UNP Q20BJ8
L	?	-	ARG	deletion	UNP Q20BJ8
L	?	-	LYS	deletion	UNP Q20BJ8
L	?	-	THR	deletion	UNP Q20BJ8
L	?	-	SER	deletion	UNP Q20BJ8
L	?	-	ASN	deletion	UNP Q20BJ8
L	?	-	GLY	deletion	UNP Q20BJ8
L	?	-	ASP	deletion	UNP Q20BJ8
L	?	-	ASP	deletion	UNP Q20BJ8
L	?	-	SER	deletion	UNP Q20BJ8
L	?	-	LEU	deletion	UNP Q20BJ8
L	?	-	PHE	deletion	UNP Q20BJ8
L	?	-	PHE	deletion	UNP Q20BJ8
L	?	-	SER	deletion	UNP Q20BJ8
L	?	-	ASN	deletion	UNP Q20BJ8
L	?	-	PHE	deletion	UNP Q20BJ8
L	?	-	SER	deletion	UNP Q20BJ8
L	?	-	LEU	deletion	UNP Q20BJ8
L	?	-	LEU	deletion	UNP Q20BJ8
O	386	SER	ASN	expression tag	UNP Q20BJ8
O	?	-	PHE	deletion	UNP Q20BJ8
O	?	-	GLY	deletion	UNP Q20BJ8
O	?	-	GLU	deletion	UNP Q20BJ8
O	?	-	LEU	deletion	UNP Q20BJ8
O	?	-	PHE	deletion	UNP Q20BJ8
O	?	-	GLU	deletion	UNP Q20BJ8
O	?	-	LYS	deletion	UNP Q20BJ8
O	?	-	ALA	deletion	UNP Q20BJ8
O	?	-	LYS	deletion	UNP Q20BJ8
O	?	-	GLN	deletion	UNP Q20BJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
O	?	-	ASN	deletion	UNP Q20BJ8
O	?	-	ASN	deletion	UNP Q20BJ8
O	?	-	ASN	deletion	UNP Q20BJ8
O	?	-	ASN	deletion	UNP Q20BJ8
O	?	-	ARG	deletion	UNP Q20BJ8
O	?	-	LYS	deletion	UNP Q20BJ8
O	?	-	THR	deletion	UNP Q20BJ8
O	?	-	SER	deletion	UNP Q20BJ8
O	?	-	ASN	deletion	UNP Q20BJ8
O	?	-	GLY	deletion	UNP Q20BJ8
O	?	-	ASP	deletion	UNP Q20BJ8
O	?	-	ASP	deletion	UNP Q20BJ8
O	?	-	SER	deletion	UNP Q20BJ8
O	?	-	LEU	deletion	UNP Q20BJ8
O	?	-	PHE	deletion	UNP Q20BJ8
O	?	-	PHE	deletion	UNP Q20BJ8
O	?	-	SER	deletion	UNP Q20BJ8
O	?	-	ASN	deletion	UNP Q20BJ8
O	?	-	PHE	deletion	UNP Q20BJ8
O	?	-	SER	deletion	UNP Q20BJ8
O	?	-	LEU	deletion	UNP Q20BJ8
O	?	-	LEU	deletion	UNP Q20BJ8
R	386	SER	ASN	expression tag	UNP Q20BJ8
R	?	-	PHE	deletion	UNP Q20BJ8
R	?	-	GLY	deletion	UNP Q20BJ8
R	?	-	GLU	deletion	UNP Q20BJ8
R	?	-	LEU	deletion	UNP Q20BJ8
R	?	-	PHE	deletion	UNP Q20BJ8
R	?	-	GLU	deletion	UNP Q20BJ8
R	?	-	LYS	deletion	UNP Q20BJ8
R	?	-	ALA	deletion	UNP Q20BJ8
R	?	-	LYS	deletion	UNP Q20BJ8
R	?	-	GLN	deletion	UNP Q20BJ8
R	?	-	ASN	deletion	UNP Q20BJ8
R	?	-	ASN	deletion	UNP Q20BJ8
R	?	-	ASN	deletion	UNP Q20BJ8
R	?	-	ASN	deletion	UNP Q20BJ8
R	?	-	ARG	deletion	UNP Q20BJ8
R	?	-	LYS	deletion	UNP Q20BJ8
R	?	-	THR	deletion	UNP Q20BJ8
R	?	-	SER	deletion	UNP Q20BJ8
R	?	-	ASN	deletion	UNP Q20BJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
R	?	-	GLY	deletion	UNP Q20BJ8
R	?	-	ASP	deletion	UNP Q20BJ8
R	?	-	ASP	deletion	UNP Q20BJ8
R	?	-	SER	deletion	UNP Q20BJ8
R	?	-	LEU	deletion	UNP Q20BJ8
R	?	-	PHE	deletion	UNP Q20BJ8
R	?	-	PHE	deletion	UNP Q20BJ8
R	?	-	SER	deletion	UNP Q20BJ8
R	?	-	ASN	deletion	UNP Q20BJ8
R	?	-	PHE	deletion	UNP Q20BJ8
R	?	-	SER	deletion	UNP Q20BJ8
R	?	-	LEU	deletion	UNP Q20BJ8
R	?	-	LEU	deletion	UNP Q20BJ8

- Molecule 2 is a protein called Nanobody D12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	126	Total	C	N	O	S	0	0	0
			931	576	164	186	5			
2	G	122	Total	C	N	O	S	0	0	0
			893	556	155	177	5			
2	J	123	Total	C	N	O	S	0	0	0
			935	578	168	184	5			
2	M	124	Total	C	N	O	S	0	0	0
			905	559	161	180	5			
2	P	123	Total	C	N	O	S	0	0	0
			906	562	158	181	5			
2	S	123	Total	C	N	O	S	0	0	0
			849	520	153	171	5			

- Molecule 3 is a protein called Nanobody G3a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	123	Total	C	N	O	S	0	0	0
			908	569	159	176	4			
3	H	123	Total	C	N	O	S	0	0	0
			944	591	162	187	4			
3	K	121	Total	C	N	O	S	0	0	0
			909	570	159	176	4			
3	N	124	Total	C	N	O	S	0	0	0
			947	594	165	184	4			
3	Q	123	Total	C	N	O	S	0	0	0
			909	569	156	180	4			

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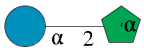
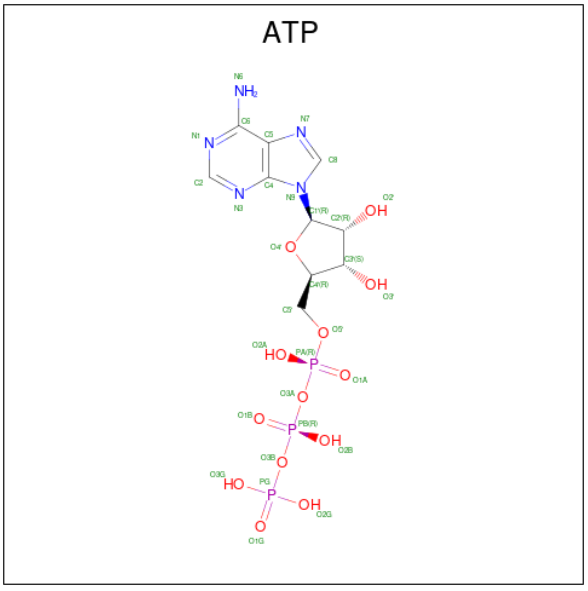
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	123	Total	C	N	O	S	0	0	0
			905	569	160	172	4			

- Molecule 4 is an oligosaccharide called alpha-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	D	2	Total	C	O	0	0	0
			23	12	11			
4	E	2	Total	C	O	0	0	0
			23	12	11			
4	U	2	Total	C	O	0	0	0
			23	12	11			
4	V	2	Total	C	O	0	0	0
			23	12	11			
4	W	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

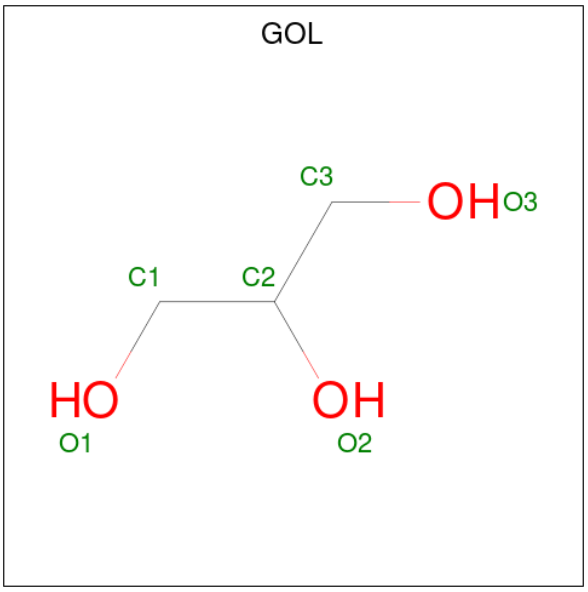


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	I	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	L	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	O	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	R	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		
6	F	3	Total	Mg	0	0
			3	3		
6	I	1	Total	Mg	0	0
			1	1		
6	L	1	Total	Mg	0	0
			1	1		
6	O	2	Total	Mg	0	0
			2	2		
6	R	1	Total	Mg	0	0
			1	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	O	1	Total C O 6 3 3	0	0
7	T	1	Total C O 6 3 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	17	Total O 17 17	0	0
8	B	12	Total O 12 12	0	0
8	C	12	Total O 12 12	0	0
8	F	10	Total O 10 10	0	0
8	G	7	Total O 7 7	0	0
8	H	18	Total O 18 18	0	0
8	I	23	Total O 23 23	0	0
8	J	14	Total O 14 14	0	0
8	K	9	Total O 9 9	0	0
8	L	21	Total O 21 21	0	0

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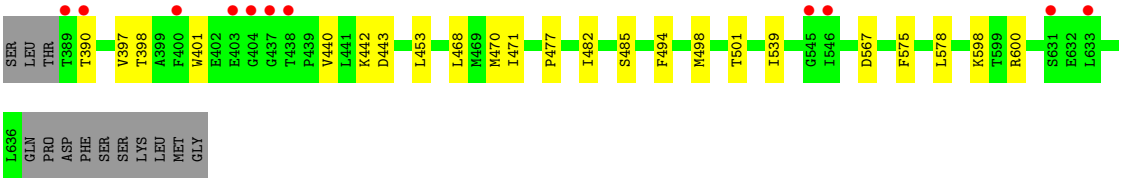
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	16	Total O 16 16	0	0
8	N	20	Total O 20 20	0	0
8	O	14	Total O 14 14	0	0
8	P	9	Total O 9 9	0	0
8	Q	9	Total O 9 9	0	0
8	R	4	Total O 4 4	0	0
8	S	2	Total O 2 2	0	0
8	T	9	Total O 9 9	0	0

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.

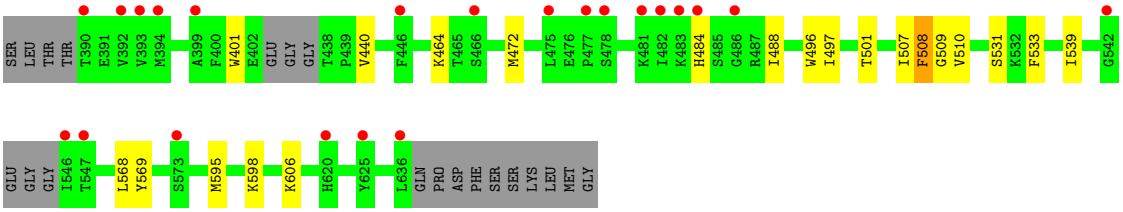
• Molecule 1: Cystic fibrosis transmembrane conductance regulator

Chain A:



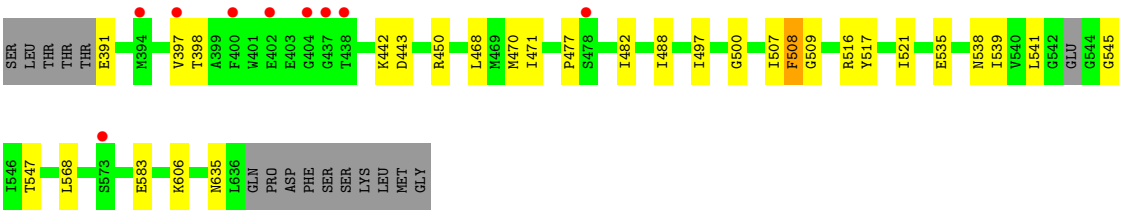
• Molecule 1: Cystic fibrosis transmembrane conductance regulator

Chain F:



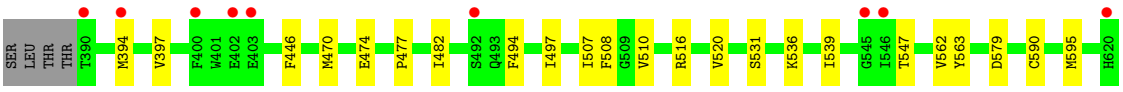
• Molecule 1: Cystic fibrosis transmembrane conductance regulator

Chain I:



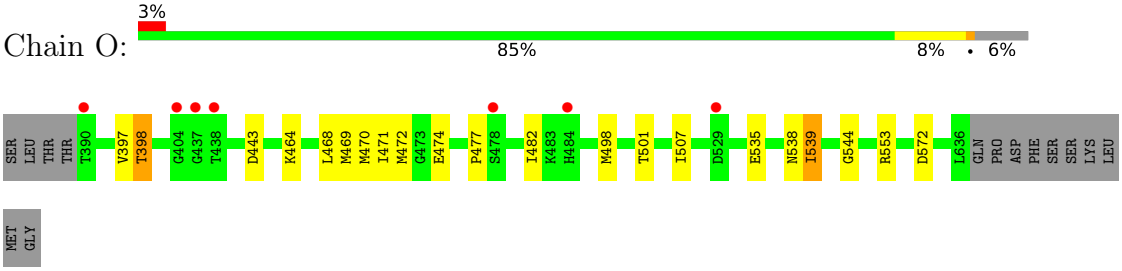
• Molecule 1: Cystic fibrosis transmembrane conductance regulator

Chain L:



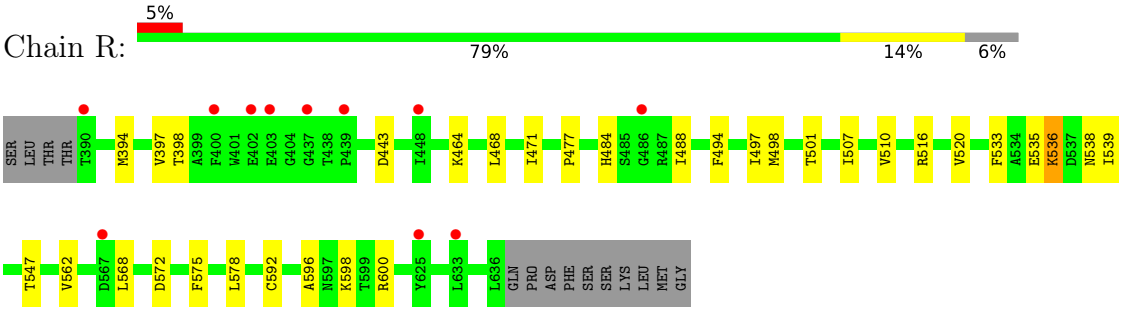
• Molecule 1: Cystic fibrosis transmembrane conductance regulator

Chain O:



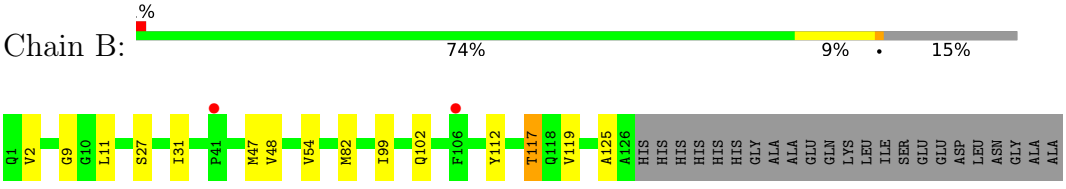
• Molecule 1: Cystic fibrosis transmembrane conductance regulator

Chain R:



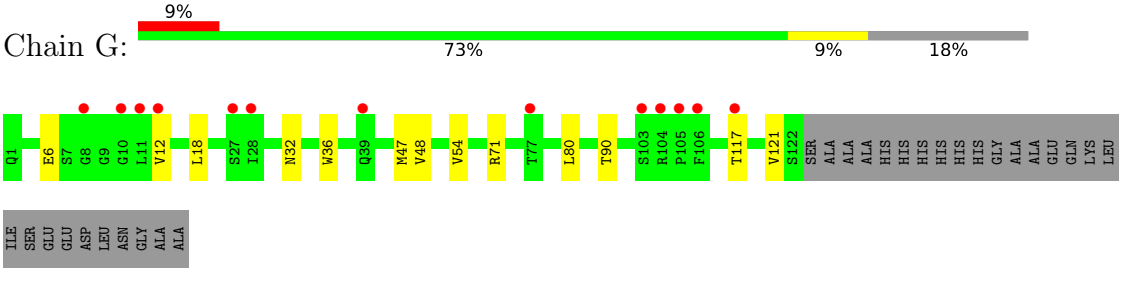
• Molecule 2: Nanobody D12

Chain B:



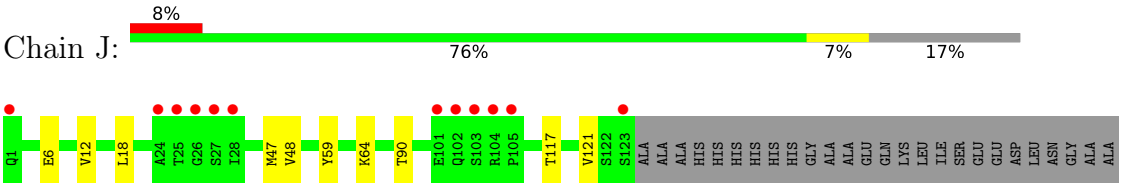
• Molecule 2: Nanobody D12

Chain G:



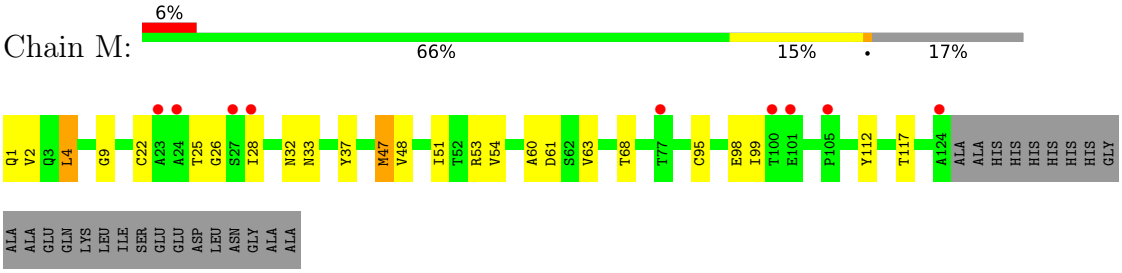
• Molecule 2: Nanobody D12

Chain J:



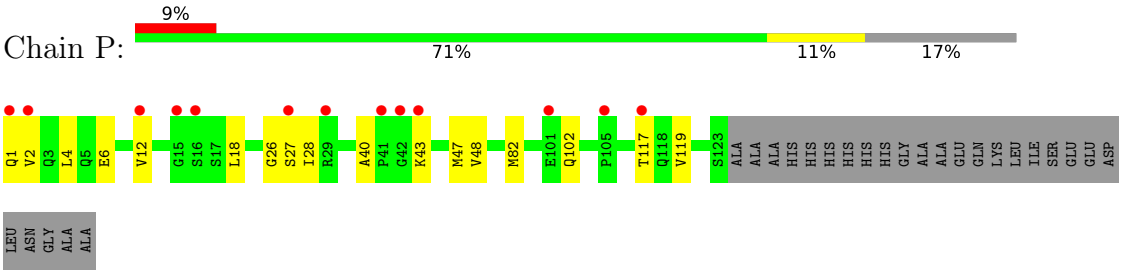
• Molecule 2: Nanobody D12

Chain M:



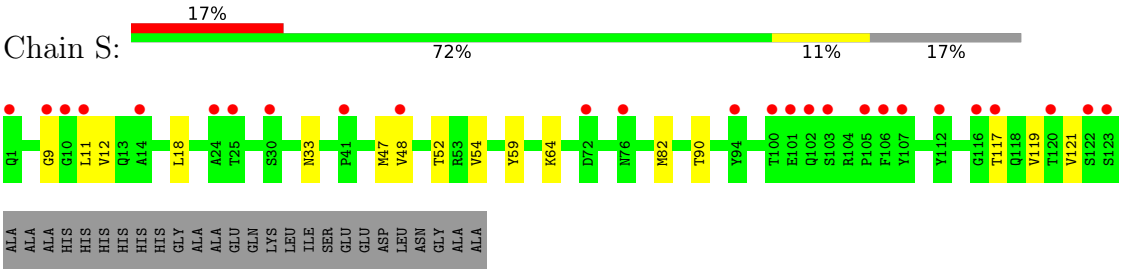
• Molecule 2: Nanobody D12

Chain P:



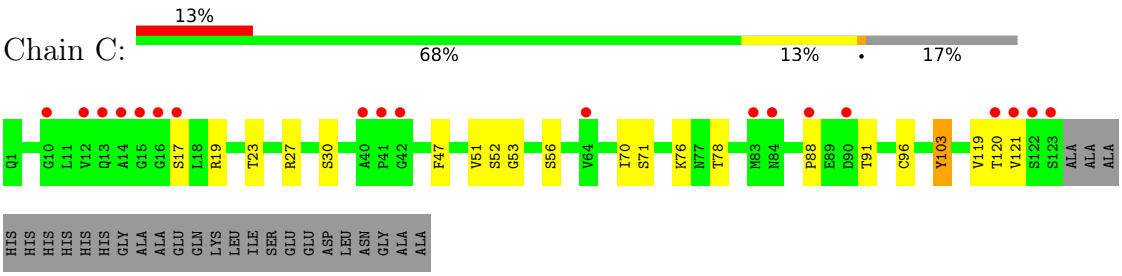
• Molecule 2: Nanobody D12

Chain S:



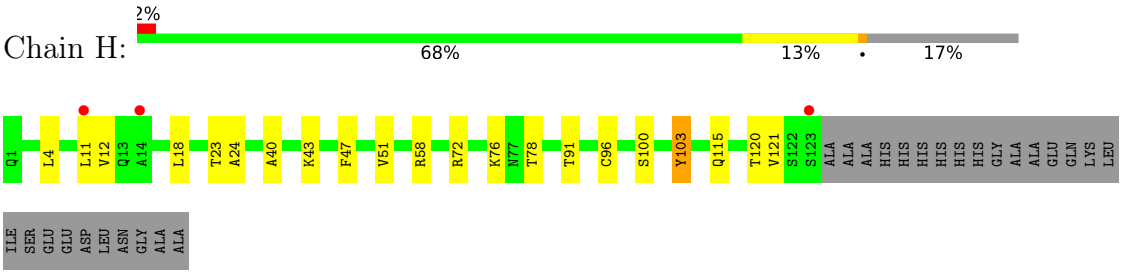
• Molecule 3: Nanobody G3a

Chain C:



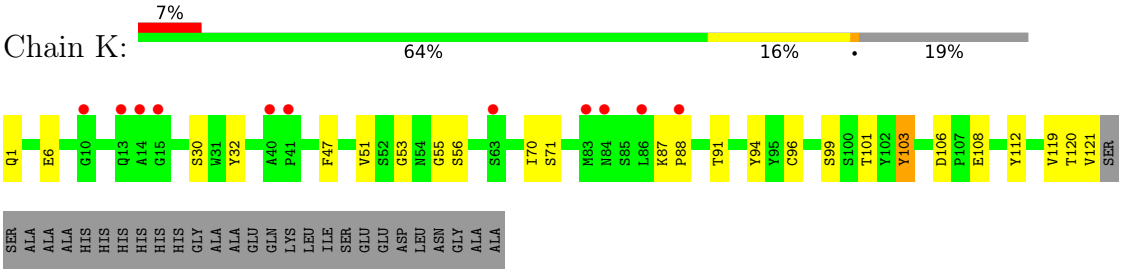
• Molecule 3: Nanobody G3a

Chain H:



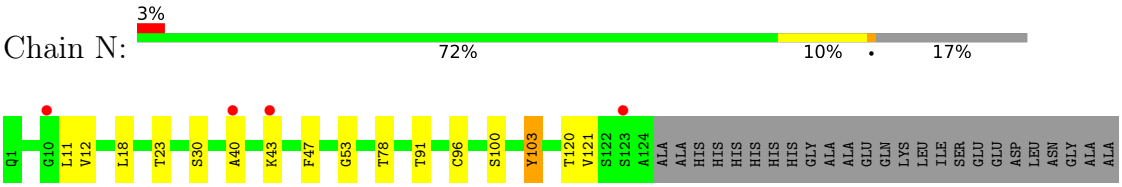
• Molecule 3: Nanobody G3a

Chain K:



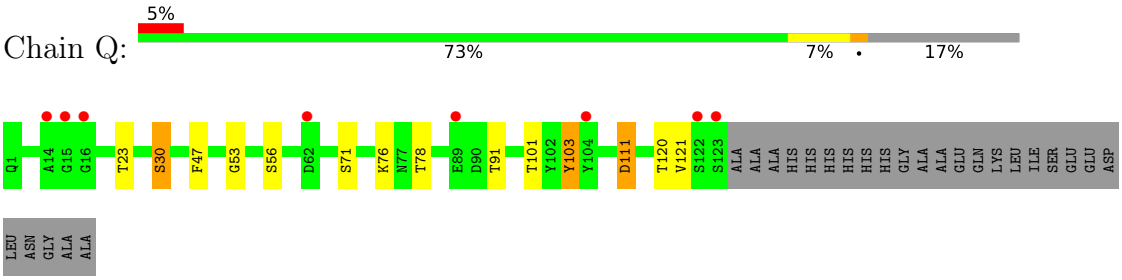
• Molecule 3: Nanobody G3a

Chain N:



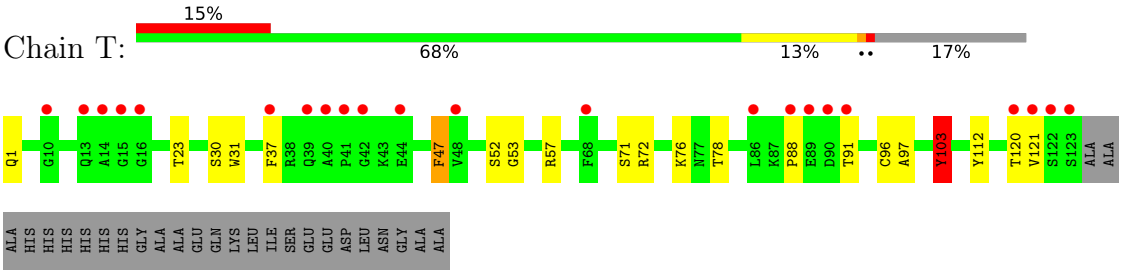
• Molecule 3: Nanobody G3a

Chain Q:



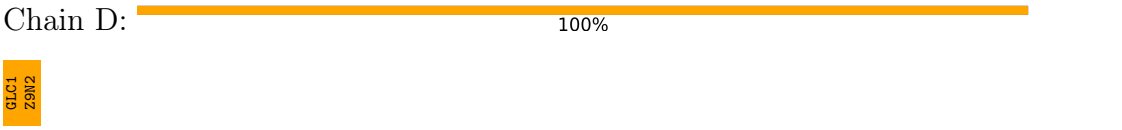
• Molecule 3: Nanobody G3a

Chain T:



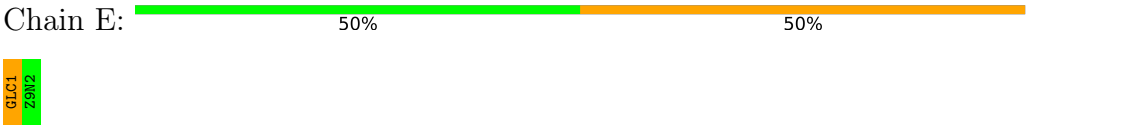
• Molecule 4: alpha-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain D:



• Molecule 4: alpha-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain E:



• Molecule 4: alpha-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain U:

• Molecule 4: alpha-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain V:

• Molecule 4: alpha-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain W:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.94Å 146.83Å 188.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.43 – 2.99 34.43 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.0 (34.43-2.99) 99.2 (34.43-2.99)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 3.00Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.204 , 0.235 0.208 , 0.238	Depositor DCC
R_{free} test set	3276 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	69.5	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 84.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	20891	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, GLC, GOL, Z9N, MG

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	0.42	0/1620	0.63	0/2195
1	F	0.43	0/1562	0.64	0/2115
1	I	0.44	0/1618	0.64	1/2188 (0.0%)
1	L	0.44	0/1590	0.63	0/2155
1	O	0.42	0/1599	0.62	0/2167
1	R	0.43	0/1574	0.62	0/2136
2	B	0.42	0/947	0.66	0/1288
2	G	0.41	0/909	0.65	0/1239
2	J	0.41	0/951	0.64	0/1289
2	M	0.43	0/919	0.64	0/1248
2	P	0.40	0/922	0.65	0/1254
2	S	0.40	0/863	0.67	1/1179 (0.1%)
3	C	0.55	0/930	0.70	1/1263 (0.1%)
3	H	0.54	0/966	0.70	1/1310 (0.1%)
3	K	0.55	0/931	0.69	1/1266 (0.1%)
3	N	0.55	0/969	0.70	1/1314 (0.1%)
3	Q	0.50	0/931	0.69	1/1267 (0.1%)
3	T	0.53	0/927	0.68	1/1262 (0.1%)
All	All	0.46	0/20728	0.65	8/28135 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	103	TYR	N-CA-C	7.47	131.16	111.00
3	H	103	TYR	N-CA-C	7.40	130.99	111.00
3	K	103	TYR	N-CA-C	6.91	129.66	111.00
3	T	103	TYR	N-CA-C	6.82	129.42	111.00
3	Q	103	TYR	N-CA-C	6.77	129.28	111.00

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	1592	0	1513	17	0
1	F	1537	0	1451	18	0
1	I	1591	0	1528	19	0
1	L	1563	0	1451	20	0
1	O	1571	0	1469	15	0
1	R	1547	0	1426	27	0
2	B	931	0	875	9	0
2	G	893	0	824	10	0
2	J	935	0	898	8	0
2	M	905	0	848	27	0
2	P	906	0	842	11	0
2	S	849	0	738	13	0
3	C	908	0	803	22	0
3	H	944	0	877	13	0
3	K	909	0	823	29	0
3	N	947	0	882	10	0
3	Q	909	0	807	11	0
3	T	905	0	810	24	0
4	D	23	0	10	2	0
4	E	23	0	10	2	0
4	U	23	0	10	2	0
4	V	23	0	10	0	0
4	W	23	0	10	0	0
5	A	31	0	12	2	0
5	F	31	0	12	1	0
5	I	31	0	12	0	0
5	L	31	0	12	0	0
5	O	31	0	12	1	0
5	R	31	0	12	1	0
6	A	2	0	0	0	0
6	F	3	0	0	0	0
6	I	1	0	0	0	0
6	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	O	2	0	0	0	0
6	R	1	0	0	0	0
7	O	6	0	8	0	0
7	T	6	0	8	0	0
8	A	17	0	0	0	0
8	B	12	0	0	0	0
8	C	12	0	0	0	0
8	F	10	0	0	0	0
8	G	7	0	0	0	0
8	H	18	0	0	0	0
8	I	23	0	0	0	0
8	J	14	0	0	0	0
8	K	9	0	0	0	0
8	L	21	0	0	0	0
8	M	16	0	0	0	0
8	N	20	0	0	0	0
8	O	14	0	0	0	0
8	P	9	0	0	0	0
8	Q	9	0	0	0	0
8	R	4	0	0	0	0
8	S	2	0	0	0	0
8	T	9	0	0	0	0
All	All	20891	0	19003	283	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 7.

The worst 5 of 283 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:4:LEU:HD23	2:M:22:CYS:SG	1.83	1.18
3:C:71:SER:HB3	2:M:54:VAL:HG11	1.26	1.16
1:L:516:ARG:O	1:L:520:VAL:HG23	1.48	1.13
2:S:90:THR:HG22	2:S:121:VAL:H	1.16	1.11
1:A:401:TRP:CD1	1:A:440:VAL:HG21	1.92	1.05

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	214/229 (93%)	206 (96%)	8 (4%)	0	100	100
1	F	203/229 (89%)	193 (95%)	10 (5%)	0	100	100
1	I	209/229 (91%)	200 (96%)	9 (4%)	0	100	100
1	L	213/229 (93%)	208 (98%)	5 (2%)	0	100	100
1	O	213/229 (93%)	205 (96%)	8 (4%)	0	100	100
1	R	213/229 (93%)	205 (96%)	8 (4%)	0	100	100
2	B	124/149 (83%)	123 (99%)	1 (1%)	0	100	100
2	G	120/149 (80%)	117 (98%)	3 (2%)	0	100	100
2	J	121/149 (81%)	118 (98%)	3 (2%)	0	100	100
2	M	122/149 (82%)	120 (98%)	2 (2%)	0	100	100
2	P	121/149 (81%)	118 (98%)	3 (2%)	0	100	100
2	S	121/149 (81%)	120 (99%)	1 (1%)	0	100	100
3	C	121/149 (81%)	119 (98%)	2 (2%)	0	100	100
3	H	121/149 (81%)	120 (99%)	1 (1%)	0	100	100
3	K	119/149 (80%)	119 (100%)	0	0	100	100
3	N	122/149 (82%)	122 (100%)	0	0	100	100
3	Q	121/149 (81%)	121 (100%)	0	0	100	100
3	T	121/149 (81%)	121 (100%)	0	0	100	100
All	All	2719/3162 (86%)	2655 (98%)	64 (2%)	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	157/197 (80%)	157 (100%)	0	100	100
1	F	149/197 (76%)	146 (98%)	3 (2%)	55	83
1	I	162/197 (82%)	159 (98%)	3 (2%)	57	84
1	L	152/197 (77%)	147 (97%)	5 (3%)	38	73
1	O	153/197 (78%)	151 (99%)	2 (1%)	69	89
1	R	147/197 (75%)	144 (98%)	3 (2%)	55	83
2	B	93/118 (79%)	92 (99%)	1 (1%)	73	90
2	G	87/118 (74%)	87 (100%)	0	100	100
2	J	97/118 (82%)	97 (100%)	0	100	100
2	M	89/118 (75%)	86 (97%)	3 (3%)	37	72
2	P	90/118 (76%)	89 (99%)	1 (1%)	73	90
2	S	76/118 (64%)	76 (100%)	0	100	100
3	C	82/117 (70%)	78 (95%)	4 (5%)	25	61
3	H	96/117 (82%)	92 (96%)	4 (4%)	30	66
3	K	87/117 (74%)	85 (98%)	2 (2%)	50	80
3	N	94/117 (80%)	90 (96%)	4 (4%)	29	66
3	Q	86/117 (74%)	82 (95%)	4 (5%)	26	63
3	T	83/117 (71%)	79 (95%)	4 (5%)	25	62
All	All	1980/2592 (76%)	1937 (98%)	43 (2%)	52	81

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	N	103	TYR
3	Q	111	ASP
1	O	398	THR
3	Q	30	SER
1	R	536	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	484	HIS

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Mol	Chain	Res	Type
1	I	538	ASN
1	O	493	GLN

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)

10 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GLC	D	1	4	11,11,12	0.51	0	15,15,17	2.54	5 (33%)
4	Z9N	D	2	4	11,12,12	0.77	1 (9%)	10,18,18	1.09	1 (10%)
4	GLC	E	1	4	11,11,12	0.41	0	15,15,17	1.27	3 (20%)
4	Z9N	E	2	4	11,12,12	0.85	0	10,18,18	0.74	0
4	GLC	U	1	4	11,11,12	0.31	0	15,15,17	1.02	1 (6%)
4	Z9N	U	2	4	11,12,12	0.62	0	10,18,18	0.68	0
4	GLC	V	1	4	11,11,12	0.32	0	15,15,17	1.04	1 (6%)
4	Z9N	V	2	4	11,12,12	0.61	0	10,18,18	0.71	0
4	GLC	W	1	4	11,11,12	0.37	0	15,15,17	0.64	1 (6%)
4	Z9N	W	2	4	11,12,12	0.70	0	10,18,18	0.62	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
4	GLC	D	1	4	-	1/2/19/22	0/1/1/1
4	Z9N	D	2	4	-	3/5/24/24	0/1/1/1
4	GLC	E	1	4	-	0/2/19/22	0/1/1/1
4	Z9N	E	2	4	-	0/5/24/24	0/1/1/1
4	GLC	U	1	4	-	1/2/19/22	0/1/1/1
4	Z9N	U	2	4	-	1/5/24/24	0/1/1/1
4	GLC	V	1	4	-	2/2/19/22	0/1/1/1
4	Z9N	V	2	4	-	0/5/24/24	0/1/1/1
4	GLC	W	1	4	-	1/2/19/22	0/1/1/1
4	Z9N	W	2	4	-	0/5/24/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	Z9N	O2-C2	2.12	1.44	1.40

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1	GLC	C1-O5-C5	5.06	119.04	112.19
4	D	1	GLC	O5-C1-C2	5.05	118.56	110.77
4	D	1	GLC	C1-C2-C3	4.71	115.45	109.67
4	D	1	GLC	C3-C4-C5	-2.95	104.97	110.24
4	V	1	GLC	C1-O5-C5	2.94	116.17	112.19

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	Z9N	O1-C1-C2-O5
4	D	2	Z9N	O1-C1-C2-C3
4	V	1	GLC	C4-C5-C6-O6
4	D	2	Z9N	O1-C1-C2-O2
4	W	1	GLC	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	Z9N	2	0
4	E	1	GLC	2	0

Continued on next page...

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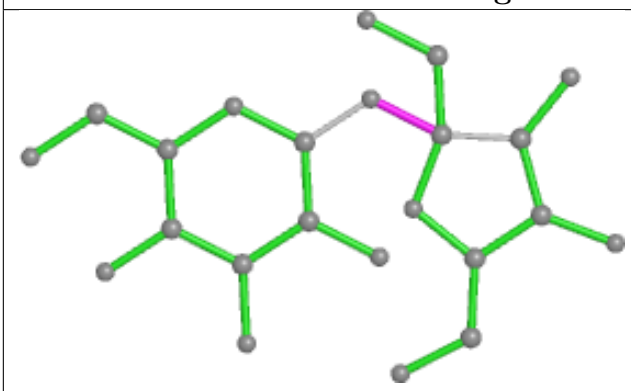
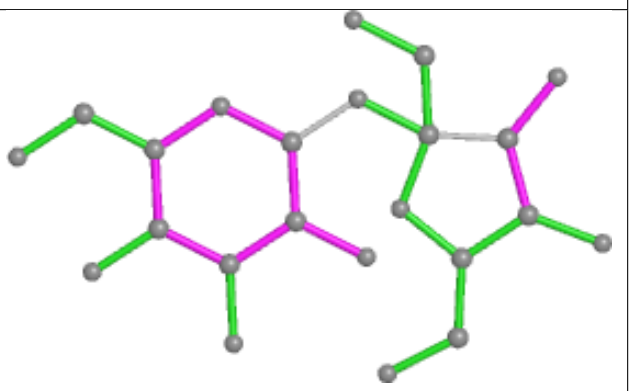
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	GLC	1	0
4	U	1	GLC	2	0

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

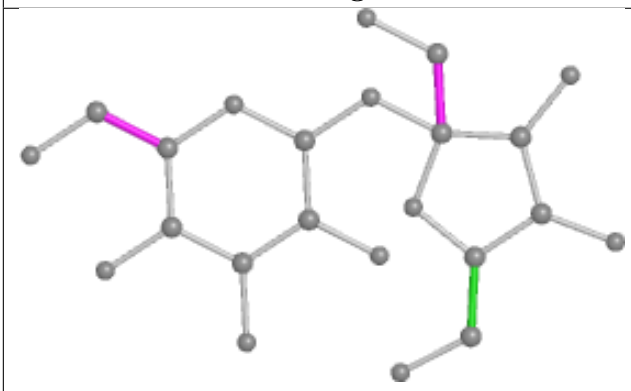
Oligosaccharide Chain D



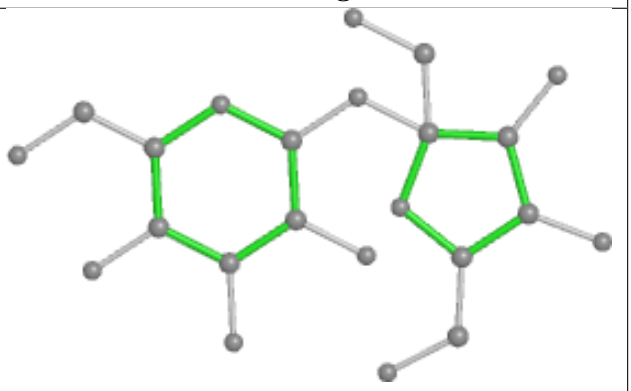
Bond lengths



Bond angles

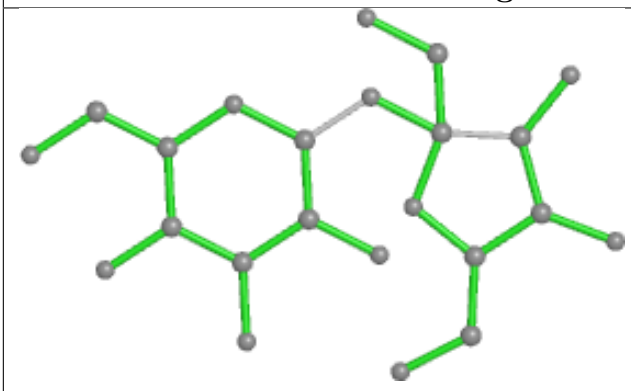


Torsions

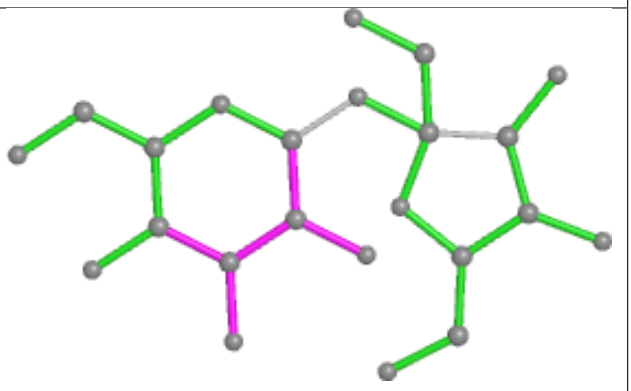


Rings

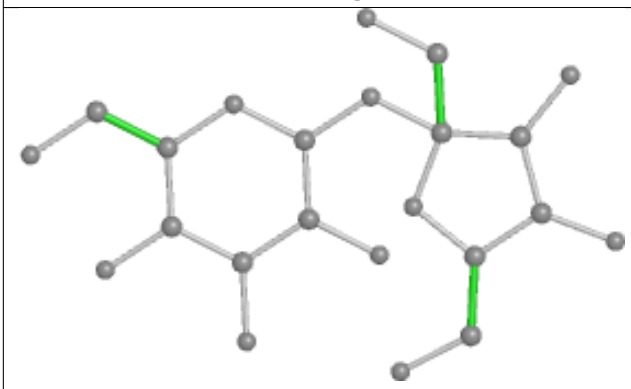
Oligosaccharide Chain E



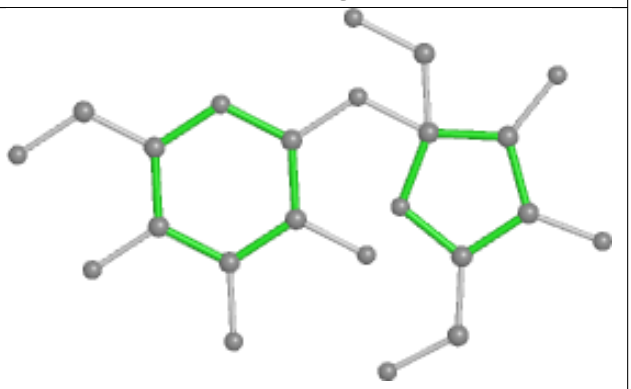
Bond lengths



Bond angles

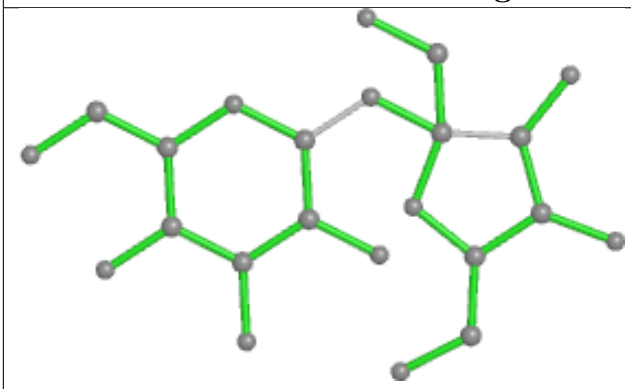


Torsions

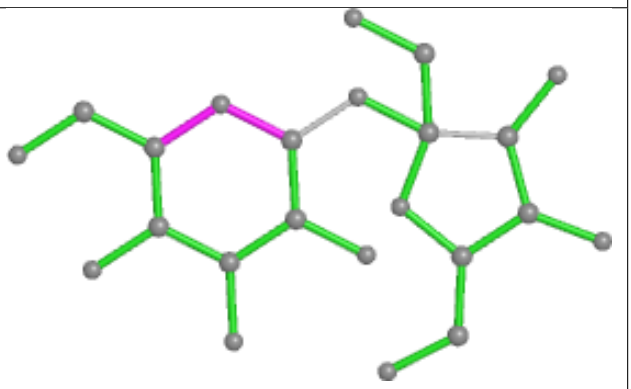


Rings

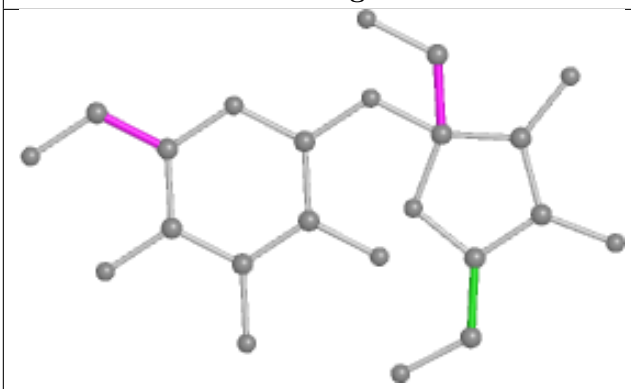
Oligosaccharide Chain U



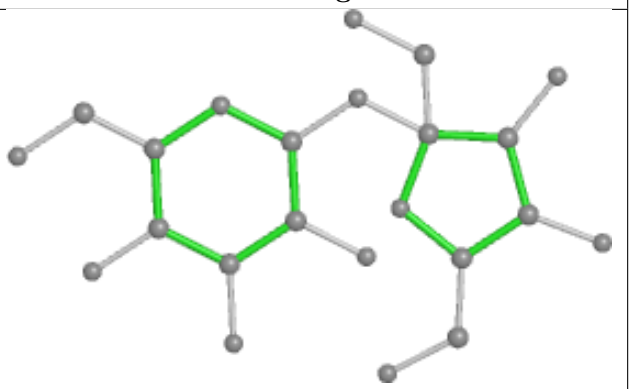
Bond lengths



Bond angles

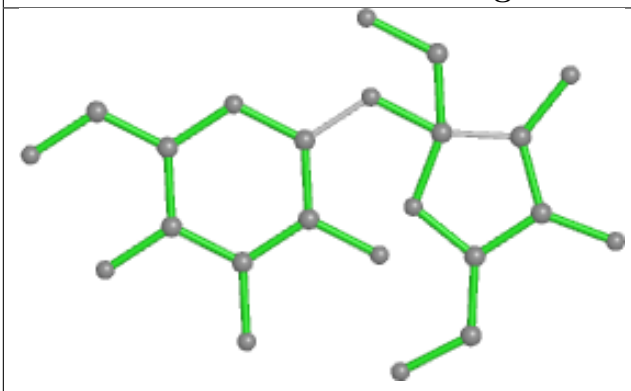


Torsions

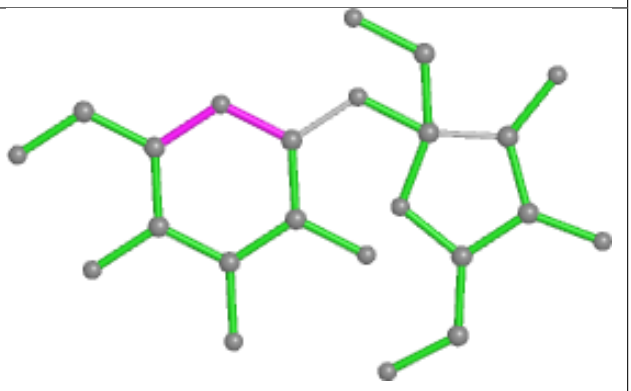


Rings

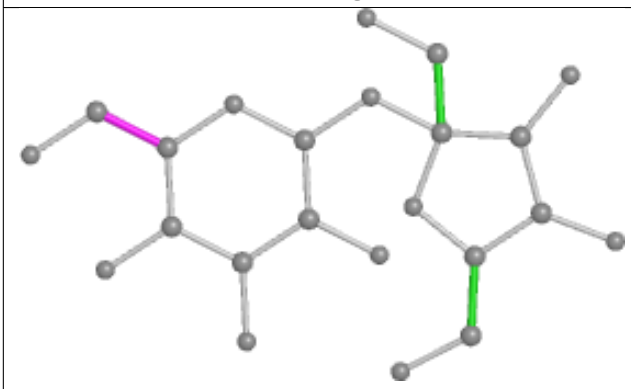
Oligosaccharide Chain V



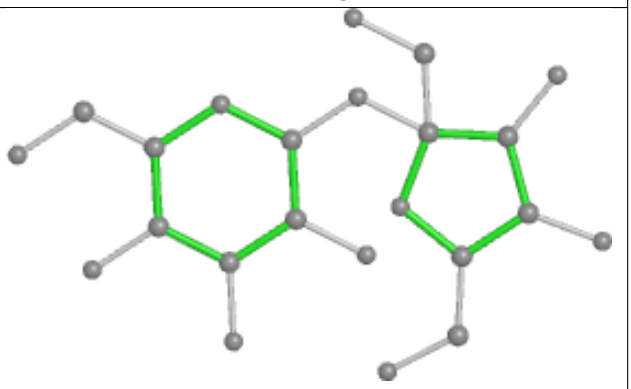
Bond lengths



Bond angles

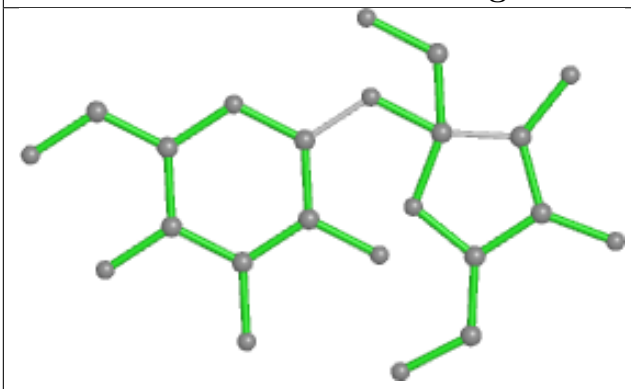


Torsions

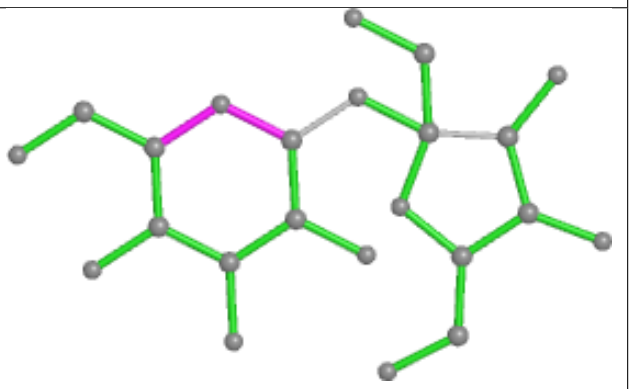


Rings

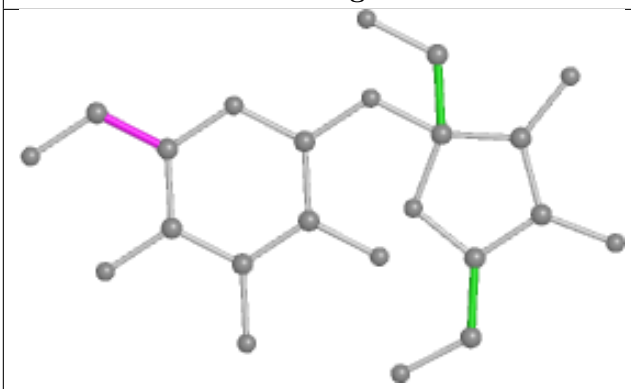
Oligosaccharide Chain W



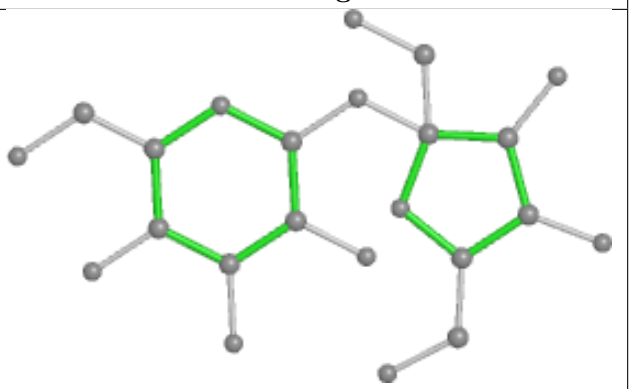
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ATP	I	701	6	26,33,33	0.76	2 (7%)	31,52,52	1.10	2 (6%)
5	ATP	A	701	6	26,33,33	1.09	1 (3%)	31,52,52	1.13	2 (6%)
5	ATP	R	701	6	26,33,33	1.49	3 (11%)	31,52,52	1.37	3 (9%)
5	ATP	L	701	6	26,33,33	1.10	1 (3%)	31,52,52	1.28	3 (9%)
5	ATP	F	701	6	26,33,33	0.93	2 (7%)	31,52,52	1.41	2 (6%)
7	GOL	O	704	-	5,5,5	0.16	0	5,5,5	0.31	0
7	GOL	T	201	-	5,5,5	0.11	0	5,5,5	0.22	0
5	ATP	O	701	6	26,33,33	0.95	1 (3%)	31,52,52	1.30	3 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	I	701	6	-	5/18/38/38	0/3/3/3
5	ATP	A	701	6	-	7/18/38/38	0/3/3/3
5	ATP	R	701	6	-	2/18/38/38	0/3/3/3
5	ATP	L	701	6	-	7/18/38/38	0/3/3/3
5	ATP	F	701	6	-	2/18/38/38	0/3/3/3
7	GOL	O	704	-	-	4/4/4/4	-
7	GOL	T	201	-	-	2/4/4/4	-
5	ATP	O	701	6	-	6/18/38/38	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	701	ATP	C4-N3	-4.15	1.29	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	701	ATP	PG-O2G	-4.09	1.39	1.54
5	A	701	ATP	PG-O3G	-3.59	1.41	1.54
5	L	701	ATP	PG-O1G	-3.15	1.40	1.50
5	F	701	ATP	PB-O2B	-2.38	1.44	1.55

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	O	701	ATP	PB-O3B-PG	-5.20	114.98	132.83
5	F	701	ATP	PB-O3B-PG	-5.13	115.21	132.83
5	L	701	ATP	PA-O3A-PB	-3.80	119.80	132.83
5	R	701	ATP	PB-O3B-PG	-3.74	120.01	132.83
5	R	701	ATP	PA-O3A-PB	-3.55	120.64	132.83

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	701	ATP	C5'-O5'-PA-O1A
5	A	701	ATP	C5'-O5'-PA-O2A
5	I	701	ATP	C5'-O5'-PA-O1A
5	I	701	ATP	C5'-O5'-PA-O2A
5	L	701	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

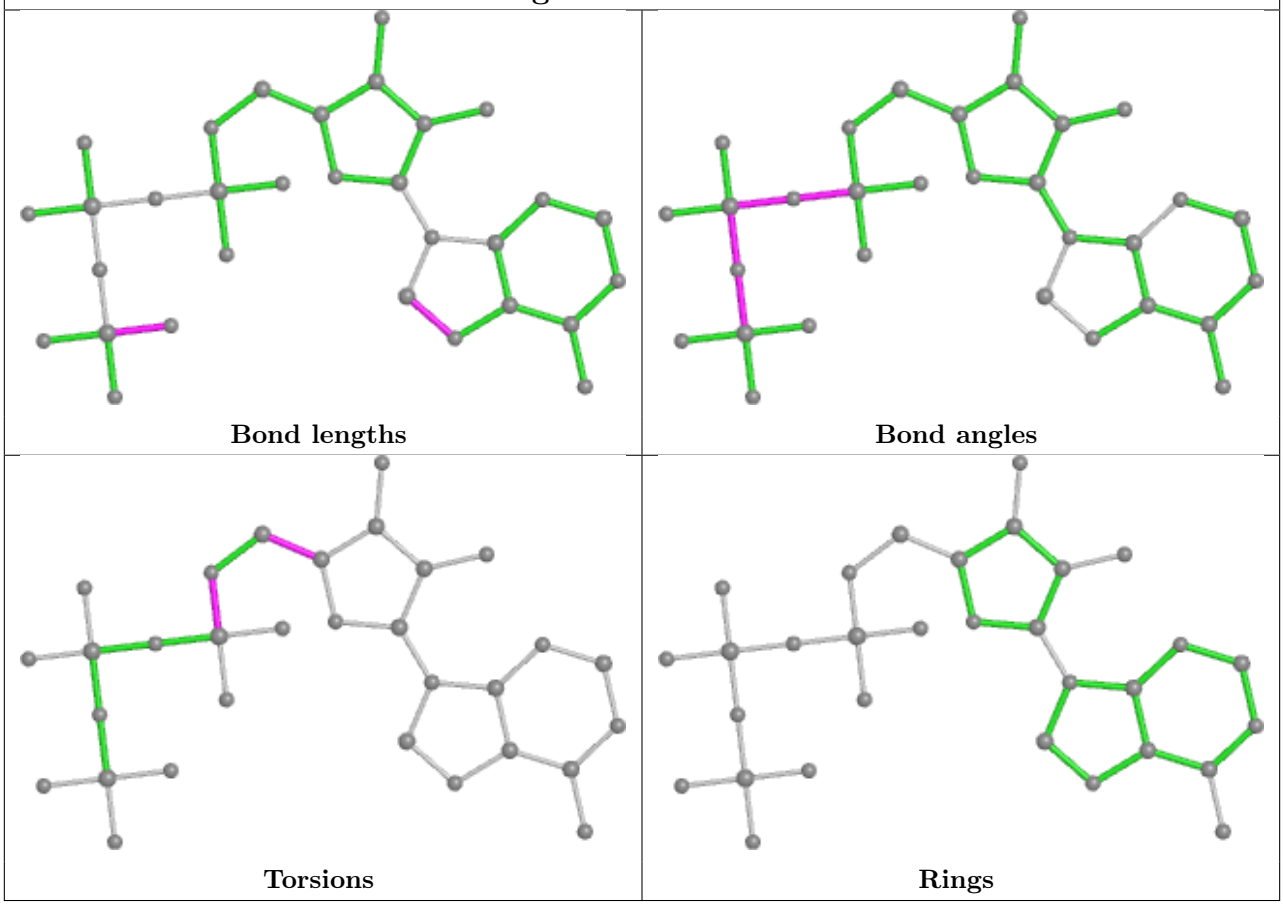
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	ATP	2	0
5	R	701	ATP	1	0
5	F	701	ATP	1	0
5	O	701	ATP	1	0

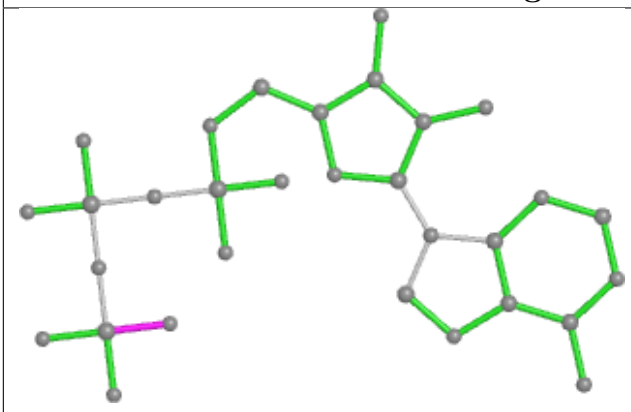
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

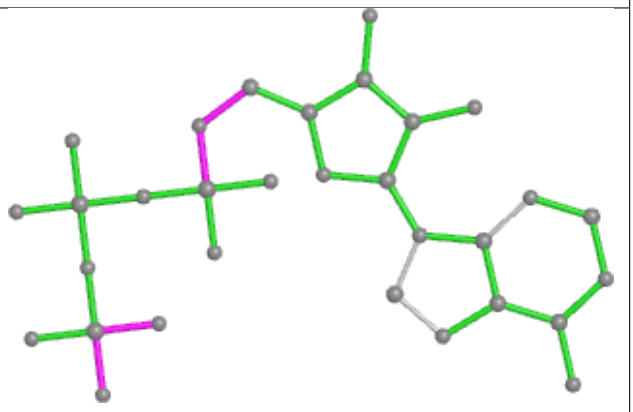
Ligand ATP I 701



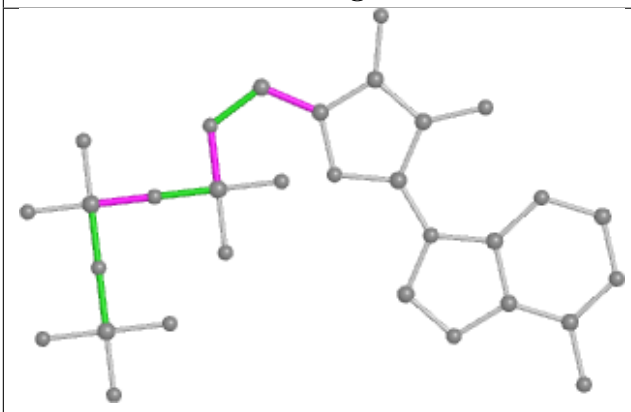
Ligand ATP A 701



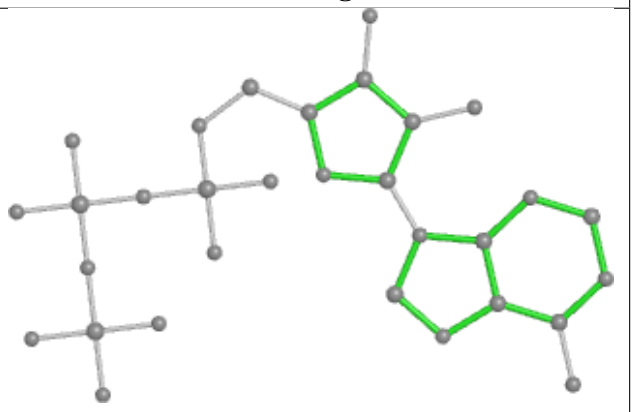
Bond lengths



Bond angles

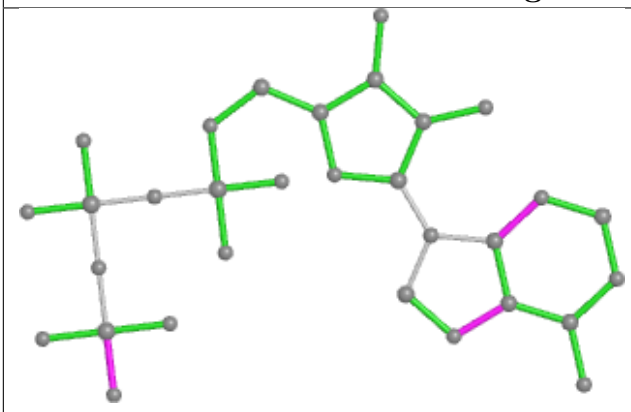


Torsions

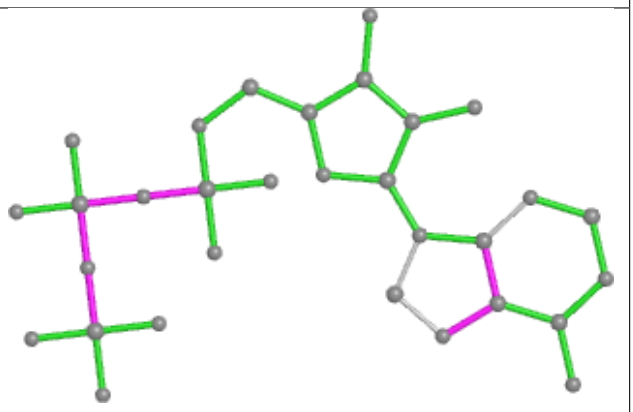


Rings

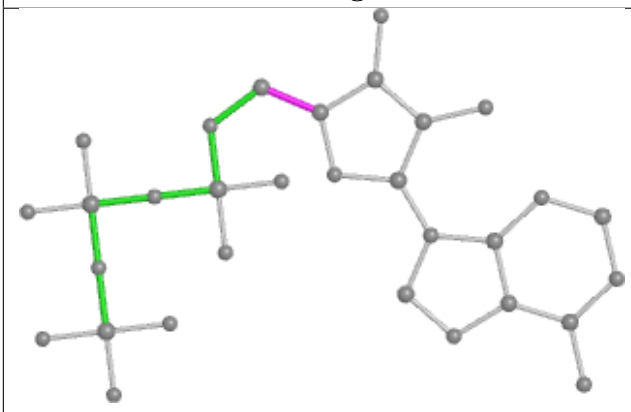
Ligand ATP R 701



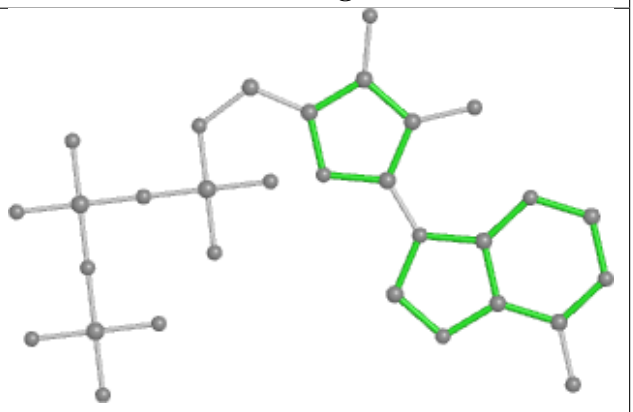
Bond lengths



Bond angles

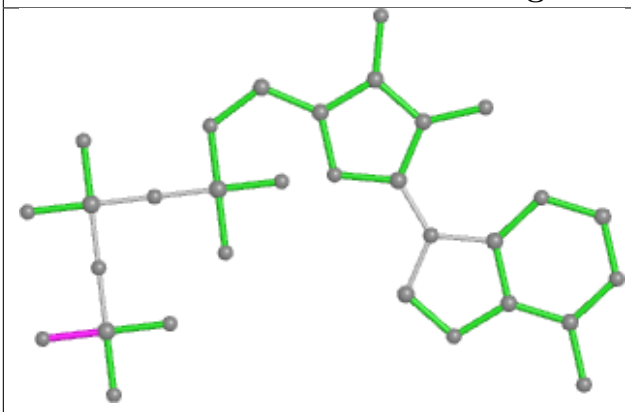


Torsions

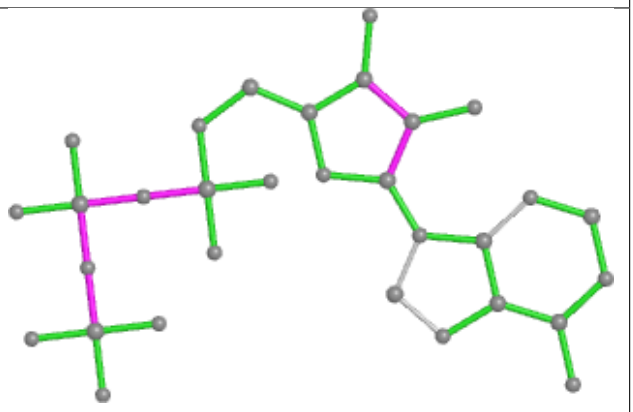


Rings

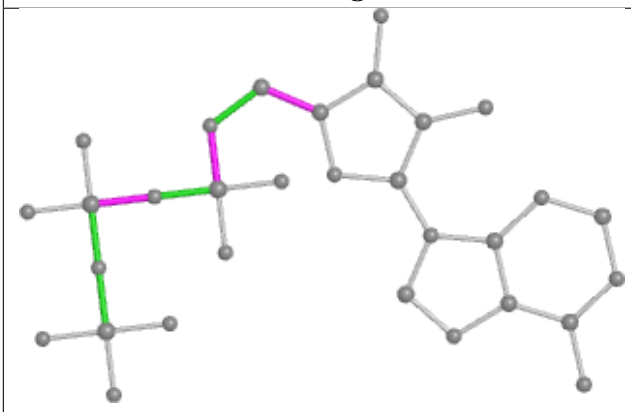
Ligand ATP L 701



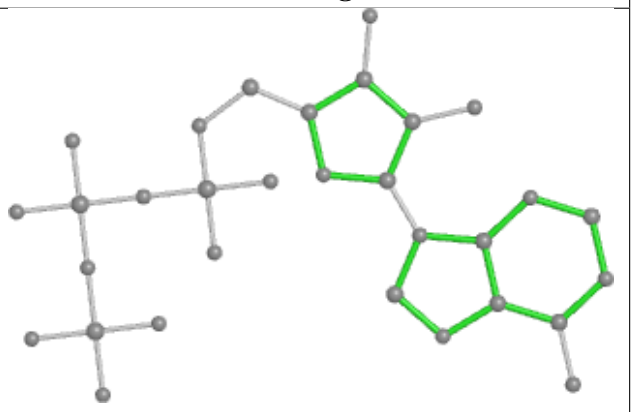
Bond lengths



Bond angles

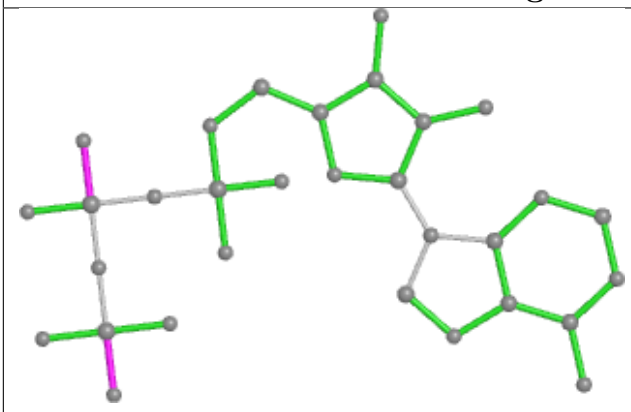


Torsions

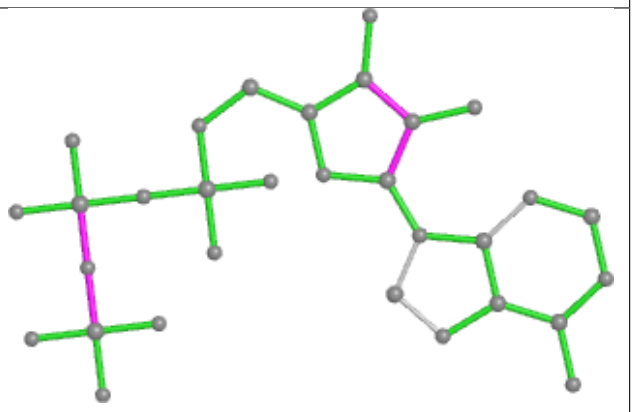


Rings

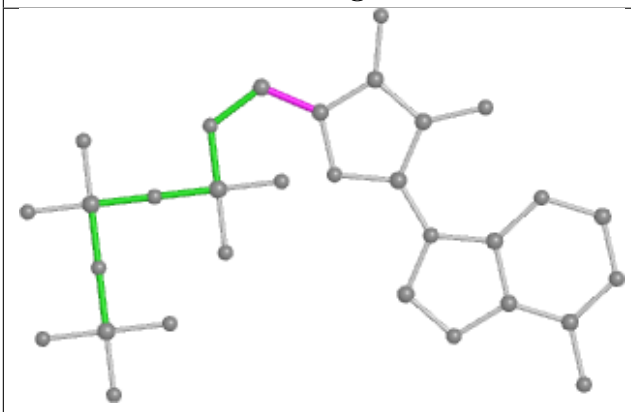
Ligand ATP F 701



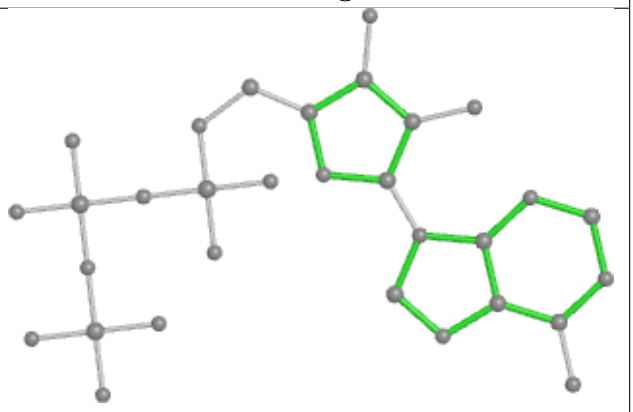
Bond lengths



Bond angles

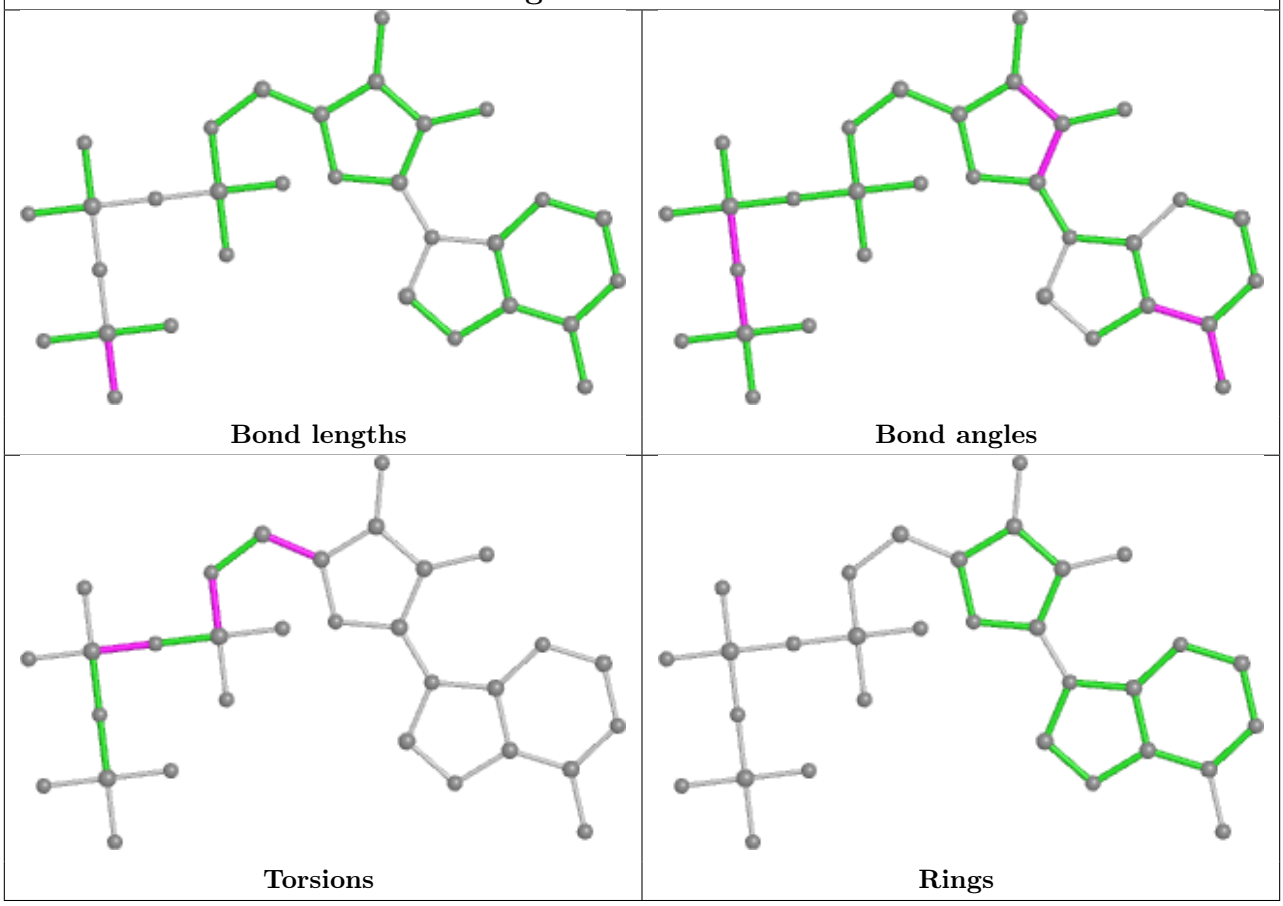


Torsions



Rings

Ligand ATP O 701



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	216/229 (94%)	0.22	11 (5%) 28 10	42, 70, 106, 115	0
1	F	209/229 (91%)	0.45	22 (10%) 6 2	28, 71, 136, 175	3 (1%)
1	I	213/229 (93%)	0.27	9 (4%) 36 14	40, 73, 110, 125	2 (0%)
1	L	215/229 (93%)	0.21	9 (4%) 36 14	43, 70, 111, 151	0
1	O	215/229 (93%)	0.20	7 (3%) 46 20	49, 71, 99, 114	0
1	R	215/229 (93%)	0.27	11 (5%) 28 10	51, 85, 120, 153	0
2	B	126/149 (84%)	-0.02	2 (1%) 72 44	44, 63, 91, 108	0
2	G	122/149 (81%)	0.66	13 (10%) 6 2	55, 79, 110, 129	0
2	J	123/149 (82%)	0.36	12 (9%) 7 2	50, 68, 106, 121	0
2	M	124/149 (83%)	0.35	9 (7%) 15 4	46, 66, 136, 172	0
2	P	123/149 (82%)	0.49	13 (10%) 6 2	56, 82, 121, 144	0
2	S	123/149 (82%)	1.06	26 (21%) 1 0	63, 94, 126, 144	0
3	C	123/149 (82%)	0.61	19 (15%) 2 1	40, 69, 115, 158	0
3	H	123/149 (82%)	0.22	3 (2%) 59 30	43, 61, 90, 151	0
3	K	121/149 (81%)	0.51	11 (9%) 9 3	44, 72, 117, 133	0
3	N	124/149 (83%)	0.20	4 (3%) 47 20	39, 67, 93, 113	0
3	Q	123/149 (82%)	0.42	8 (6%) 18 5	51, 79, 106, 121	0
3	T	123/149 (82%)	0.93	22 (17%) 1 0	47, 77, 112, 140	0
All	All	2761/3162 (87%)	0.38	211 (7%) 13 4	28, 73, 114, 175	5 (0%)

The worst 5 of 211 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	T	123	SER	8.6
1	L	390	THR	7.1
1	F	481	LYS	6.3

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Mol	Chain	Res	Type	RSRZ
1	F	478	SER	6.3
3	T	16	GLY	5.9

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)

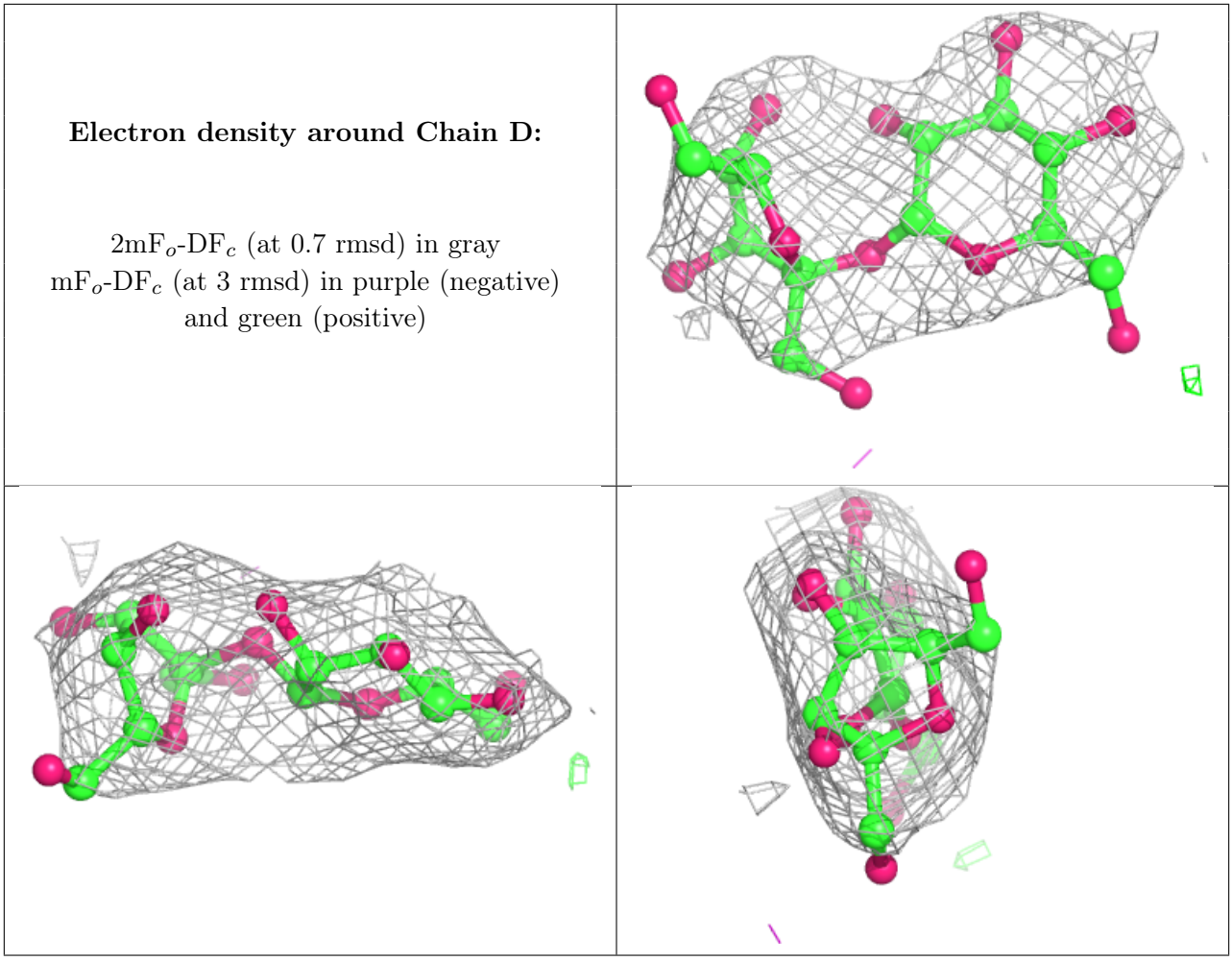
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	GLC	W	1	11/12	0.69	0.52	152,154,158,159	0
4	Z9N	W	2	12/12	0.78	0.42	149,151,153,154	0
4	GLC	U	1	11/12	0.81	0.32	135,138,139,140	0
4	GLC	V	1	11/12	0.85	0.29	116,119,122,123	0
4	Z9N	U	2	12/12	0.86	0.25	123,130,133,135	0
4	Z9N	V	2	12/12	0.86	0.28	108,117,119,121	0
4	GLC	E	1	11/12	0.89	0.26	103,106,109,109	0
4	GLC	D	1	11/12	0.90	0.16	111,113,114,114	0
4	Z9N	D	2	12/12	0.91	0.25	107,115,116,118	0
4	Z9N	E	2	12/12	0.92	0.19	106,108,110,110	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.

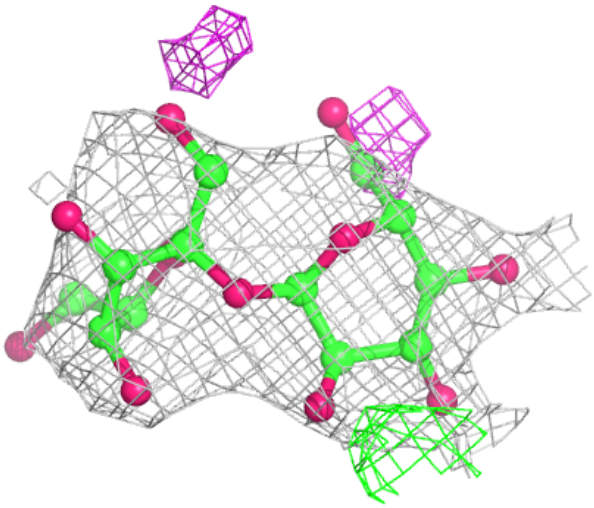
Electron density around Chain D:

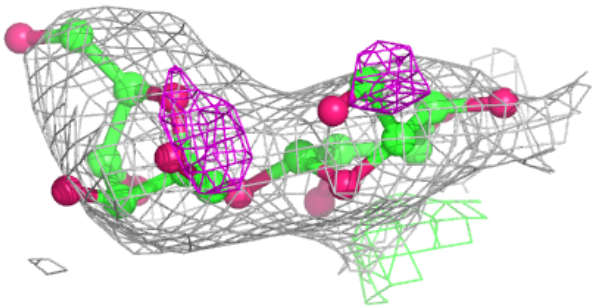
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

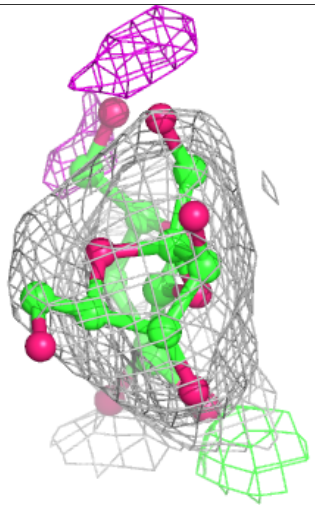


Electron density around Chain E:

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

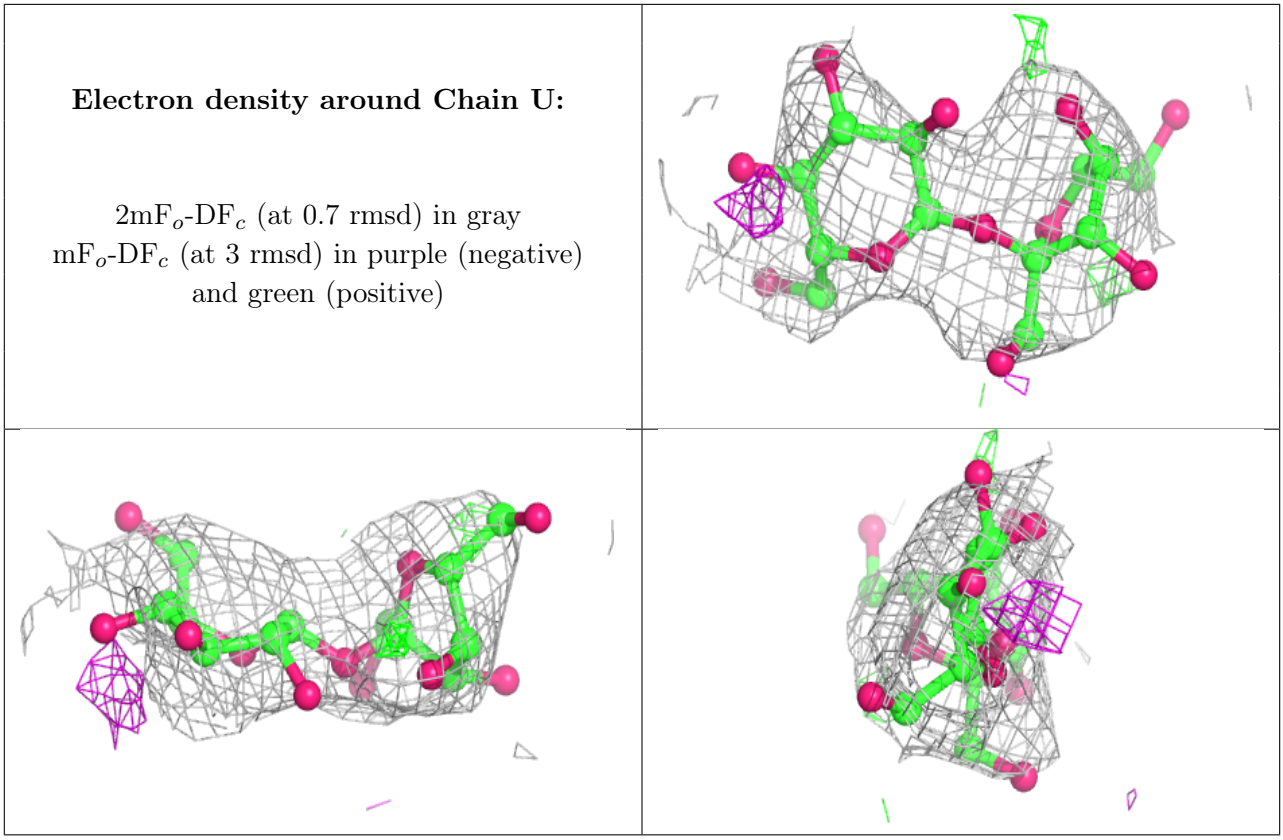






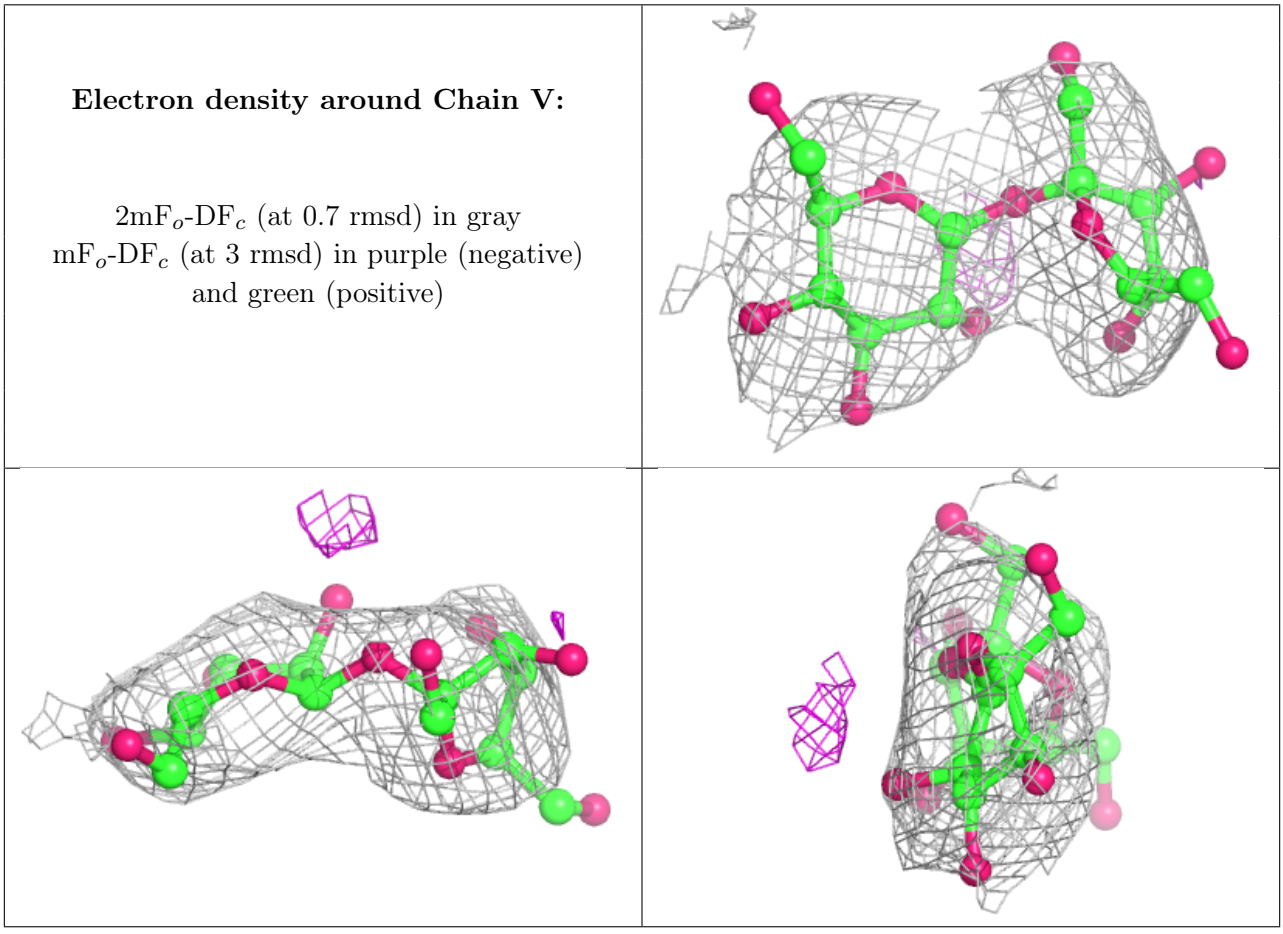
Electron density around Chain U:

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



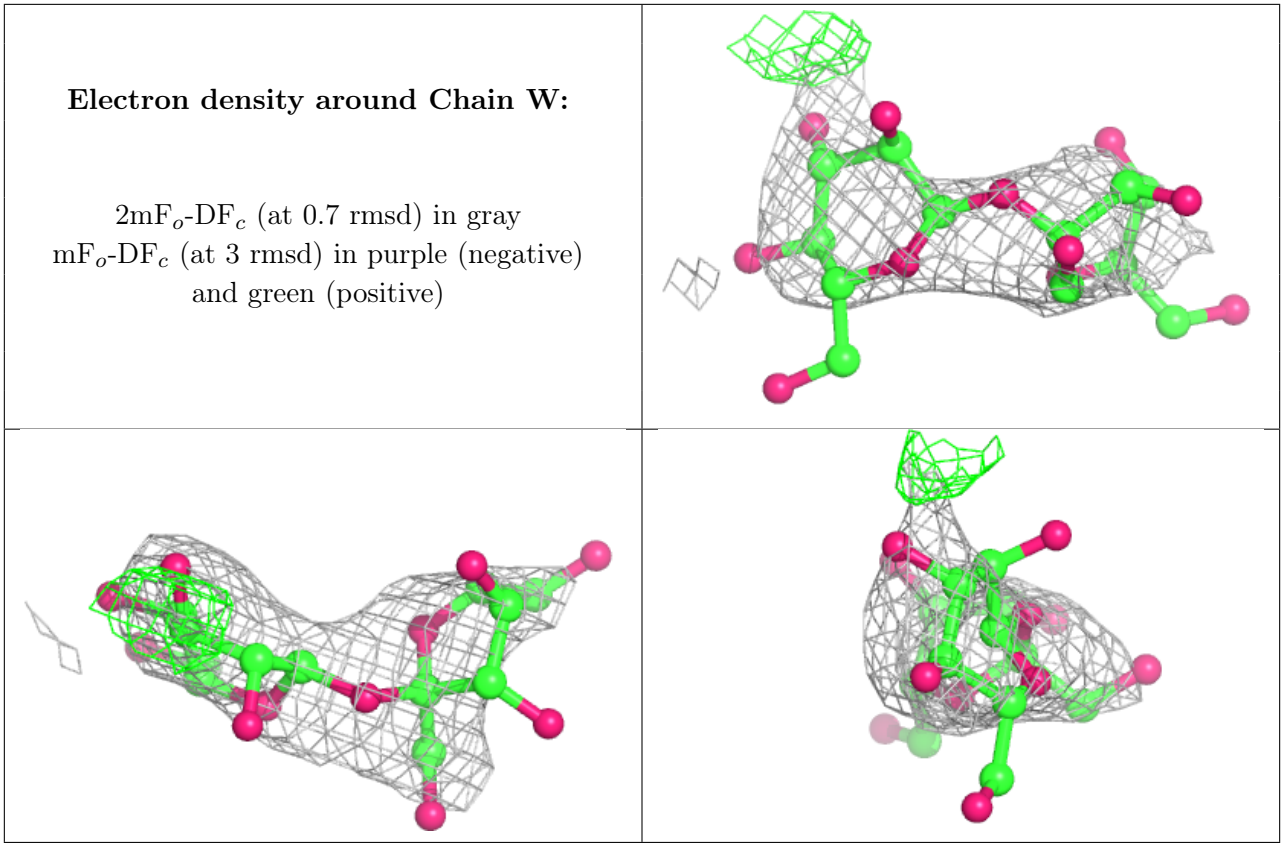
Electron density around Chain V:

$2mF_o$-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 W:

$2mF_o$-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
7	GOL	O	704	6/6	0.62	0.32	97,99,101,102	0
7	GOL	T	201	6/6	0.69	0.42	108,110,112,113	0
6	MG	F	703	1/1	0.84	0.19	66,66,66,66	0
5	ATP	F	701	31/31	0.90	0.17	92,100,104,105	0
6	MG	F	704	1/1	0.93	0.28	53,53,53,53	0
6	MG	L	702	1/1	0.93	0.18	64,64,64,64	0
5	ATP	L	701	31/31	0.93	0.17	62,73,83,84	0
5	ATP	I	701	31/31	0.93	0.18	49,65,75,75	0
5	ATP	O	701	31/31	0.94	0.18	56,64,71,73	0
5	ATP	R	701	31/31	0.94	0.17	76,92,99,100	0
6	MG	O	702	1/1	0.94	0.24	53,53,53,53	0
6	MG	O	703	1/1	0.94	0.21	52,52,52,52	0
6	MG	A	703	1/1	0.94	0.25	67,67,67,67	0
5	ATP	A	701	31/31	0.94	0.19	63,73,78,81	0

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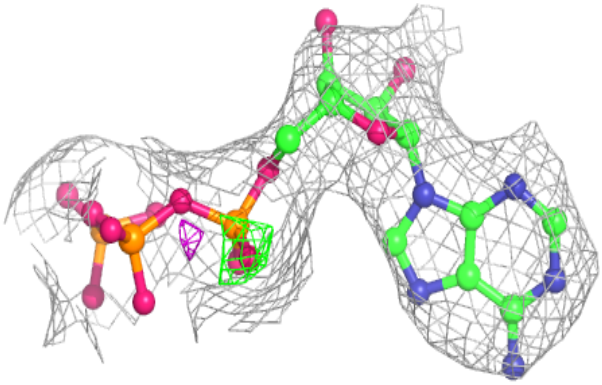
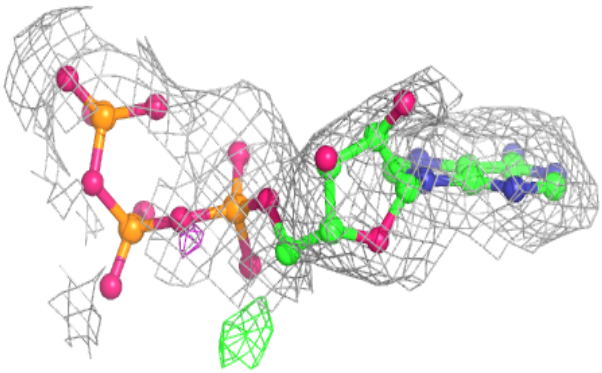
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	A	702	1/1	0.95	0.21	46,46,46,46	0
6	MG	I	702	1/1	0.96	0.34	55,55,55,55	0
6	MG	R	702	1/1	0.97	0.18	88,88,88,88	0
6	MG	F	702	1/1	0.98	0.11	52,52,52,52	0

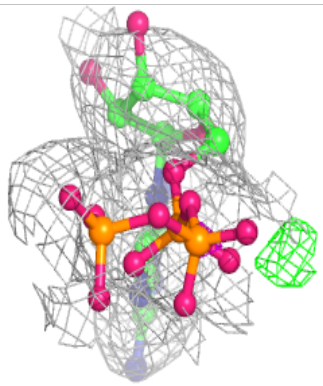
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP F 701:

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

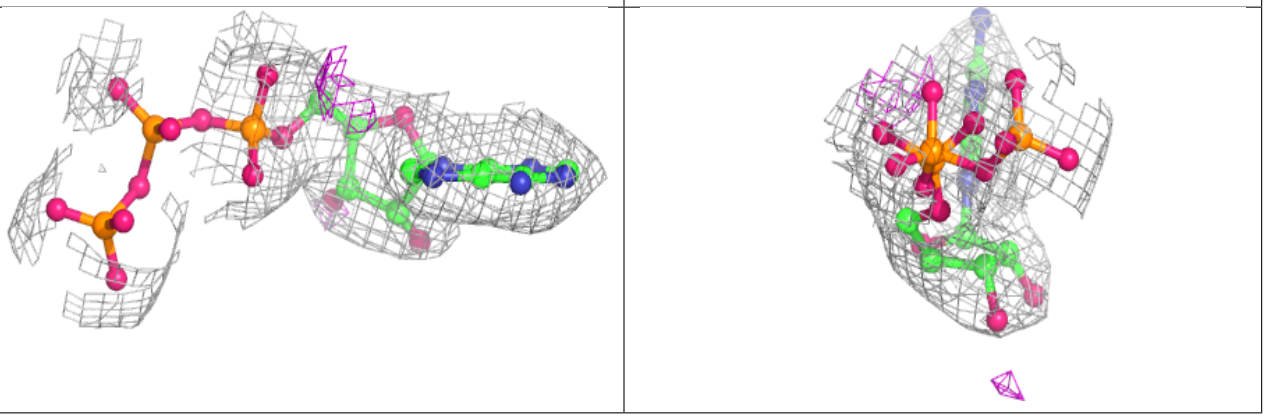






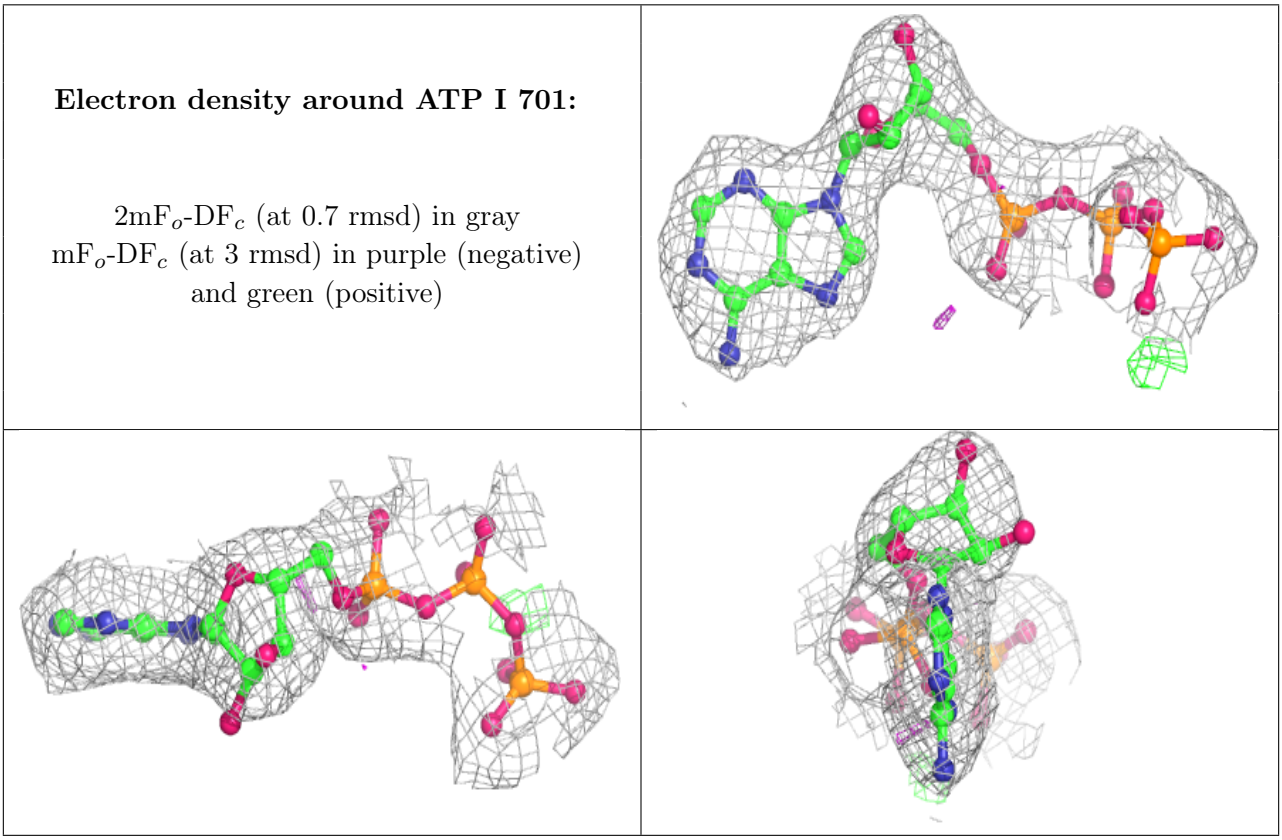
Electron density around ATP L 701:

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



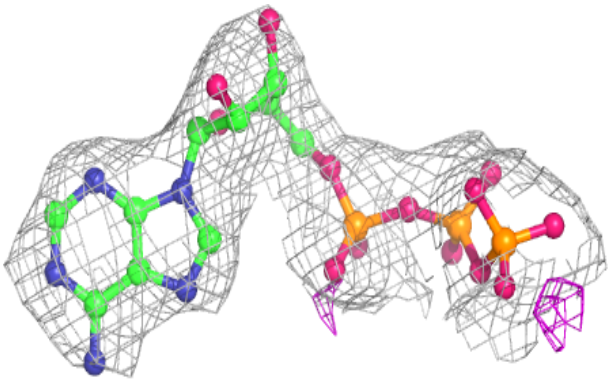
Electron density around ATP I 701:

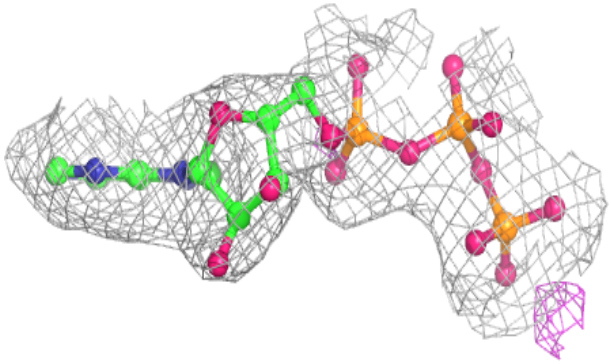
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

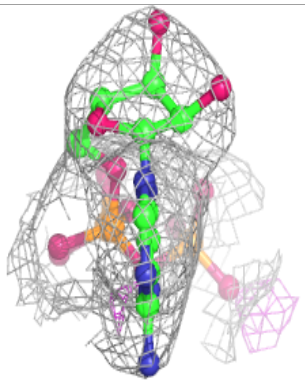


Electron density around ATP O 701:

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

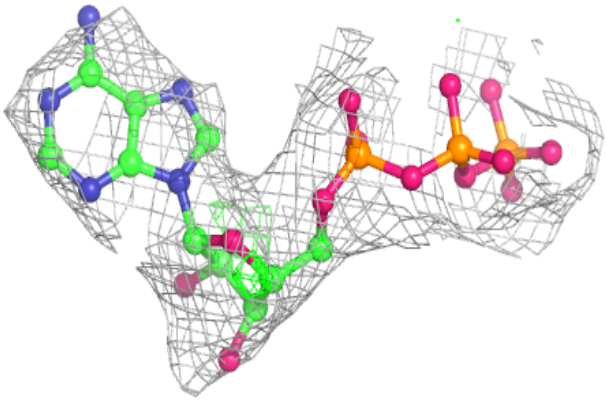


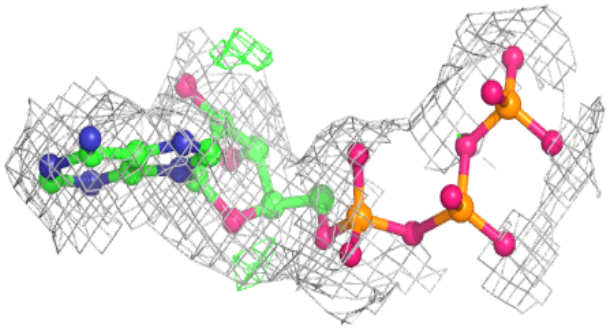


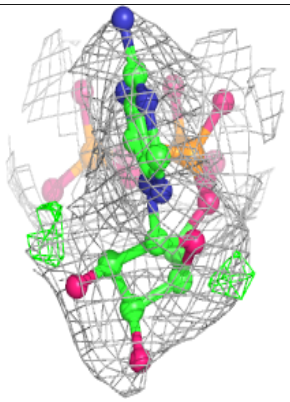


Electron density around ATP R 701:

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

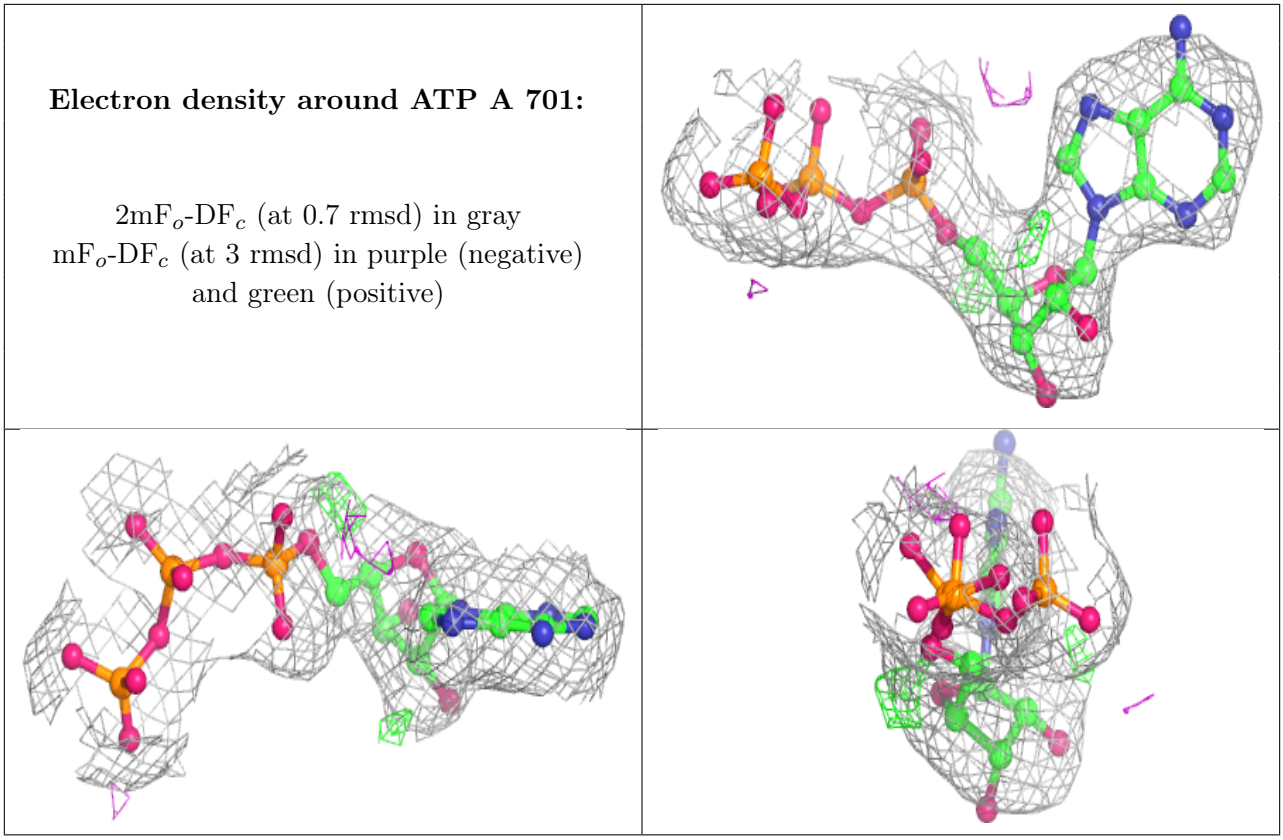






Electron density around ATP A 701:

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



6.5 Other polymers (i)

There are no such residues in this entry.