



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 05:04 AM UTC

PDB ID : 6GKD / pdb_00006gkd
Title : human NBD1 of CFTR in complex with nanobodies D12 and G3a
Authors : Sigoillot, M.; Overtus, M.; Grodecka, M.; Scholl, D.; Garcia-Pino, A.; Laere-
mans, 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

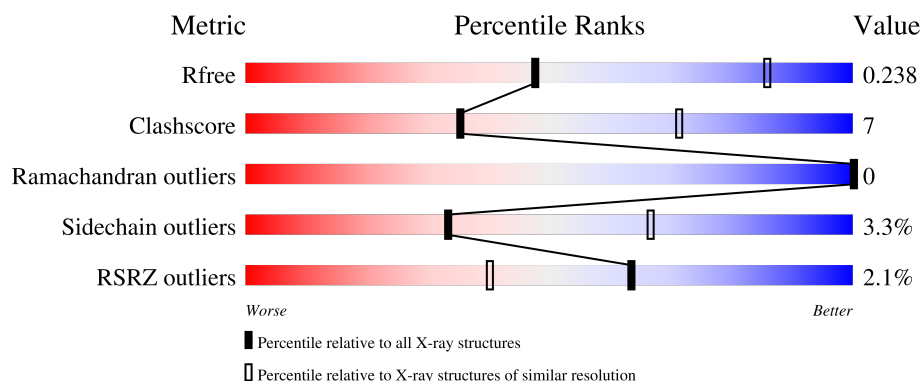
1 Overall quality at a glance

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	229	82% 12% 6%
1	F	229	7% 79% 10% 9%
1	I	229	2% 76% 16% 7%
1	L	229	2% 81% 12% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	O	229	
1	R	229	
2	B	149	
2	G	149	
2	J	149	
2	M	149	
2	P	149	
2	S	149	
3	C	149	
3	H	149	
3	K	149	
3	N	149	
3	Q	149	
3	T	149	
4	D	2	
4	E	2	
4	U	2	
4	V	2	
4	W	2	

2 Entry composition

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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
L	386	SER	ASN	expression tag	UNP Q20BJ8
L	?	-	PHE	deletion	UNP Q20BJ8

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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.

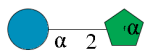
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	123	Total	C	N	O	S	0	0	0
			908	569	159	176	4			
3	H	123	Total	C	N	O	S	0	0	0
			944	591	162	187	4			
3	K	121	Total	C	N	O	S	0	0	0
			909	570	159	176	4			
3	N	124	Total	C	N	O	S	0	0	0
			947	594	165	184	4			
3	Q	123	Total	C	N	O	S	0	0	0
			909	569	156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

Continued on next page...

Continued from previous page...

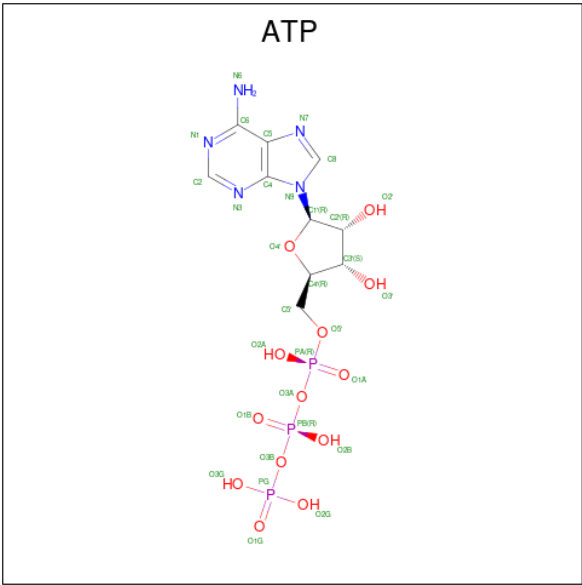
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	123	Total	C	N	O	S	0	0	0
			905	569	160	172	4			

- 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 (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 (CCD ID: 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 (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is water.

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

Continued on next page...

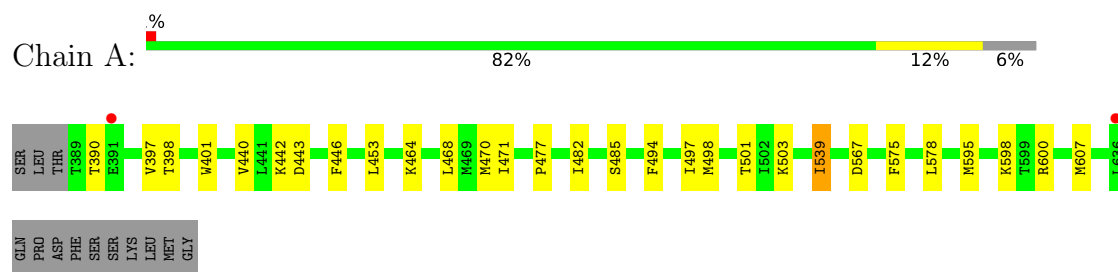
Continued from previous page...

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

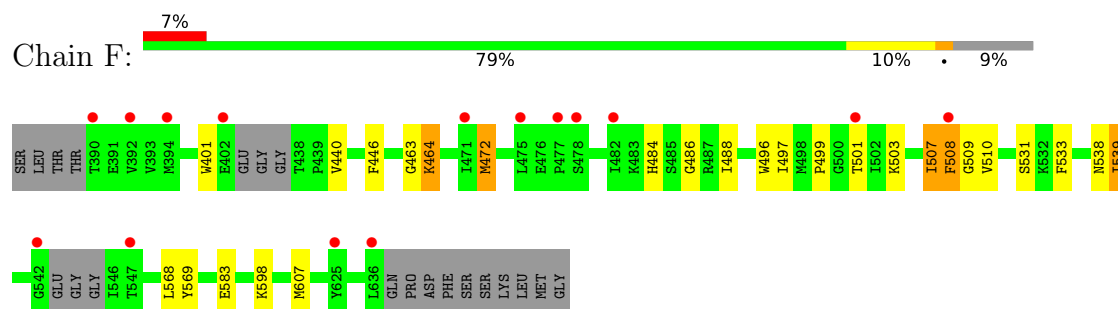
3 Residue-property plots [i](#)

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.

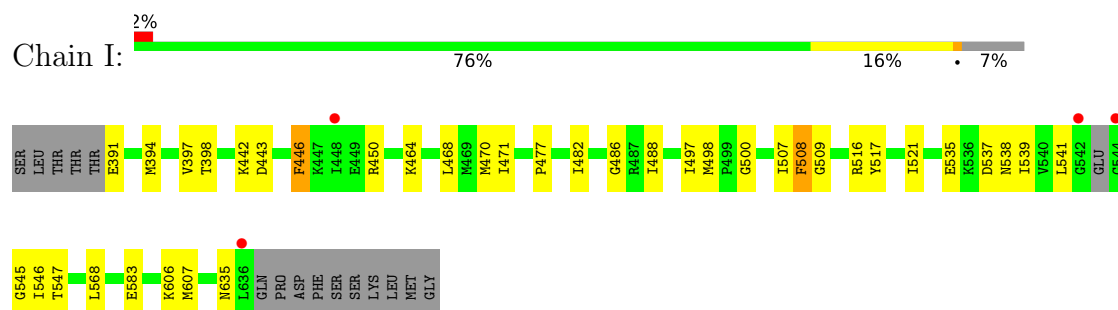
- Molecule 1: Cystic fibrosis transmembrane conductance regulator



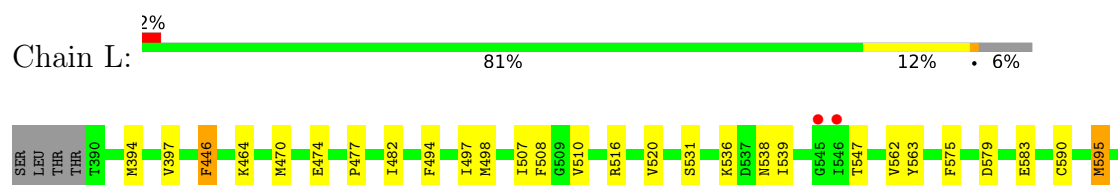
- Molecule 1: Cystic fibrosis transmembrane conductance regulator



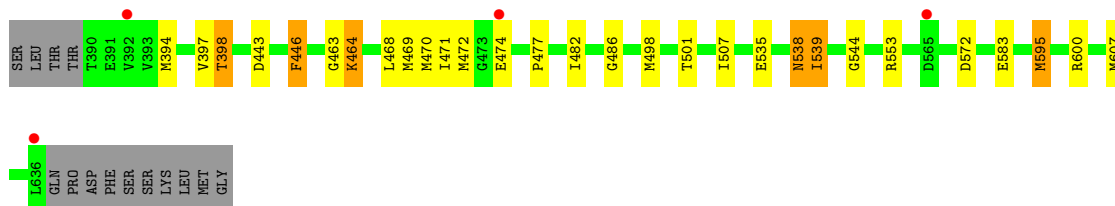
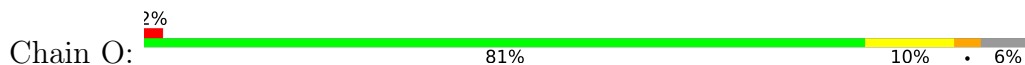
- Molecule 1: Cystic fibrosis transmembrane conductance regulator



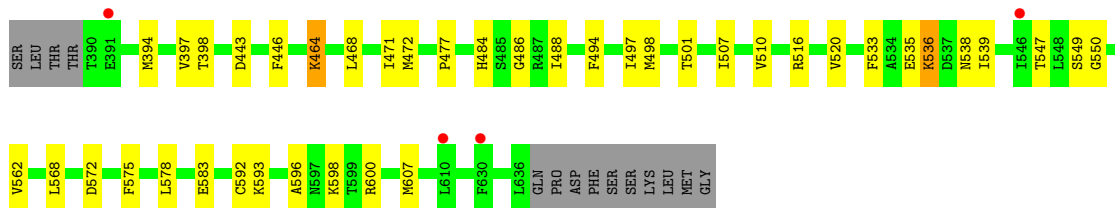
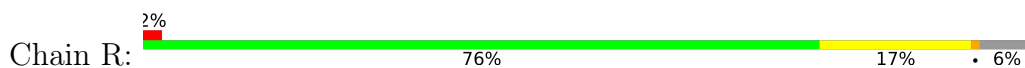
- Molecule 1: Cystic fibrosis transmembrane conductance regulator



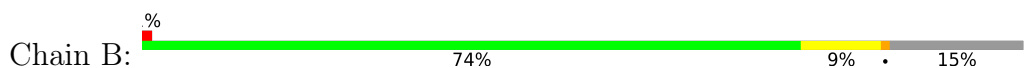
- Molecule 1: Cystic fibrosis transmembrane conductance regulator



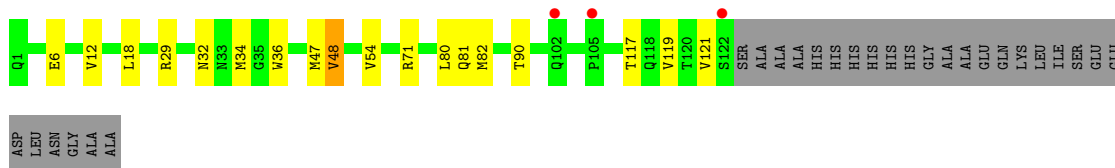
- Molecule 1: Cystic fibrosis transmembrane conductance regulator



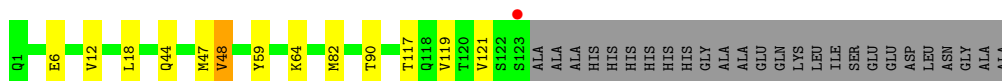
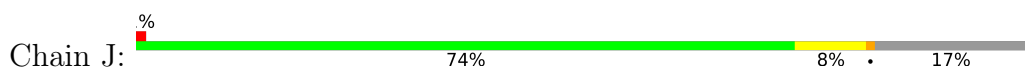
- Molecule 2: Nanobody D12



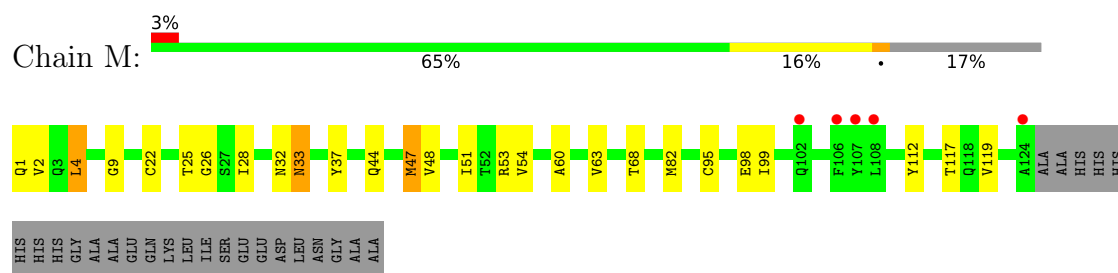
- Molecule 2: Nanobody D12



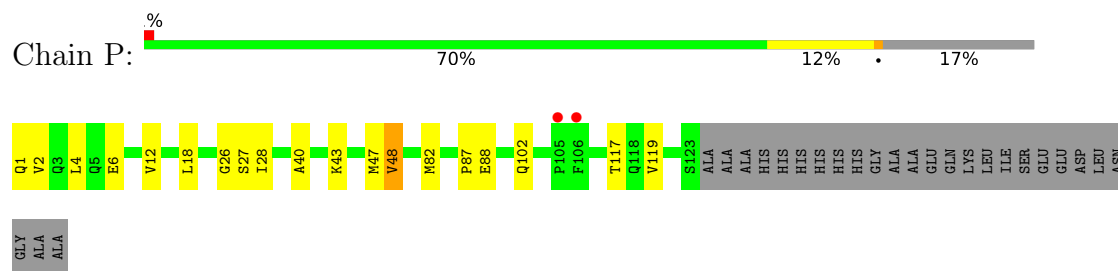
- Molecule 2: Nanobody D12



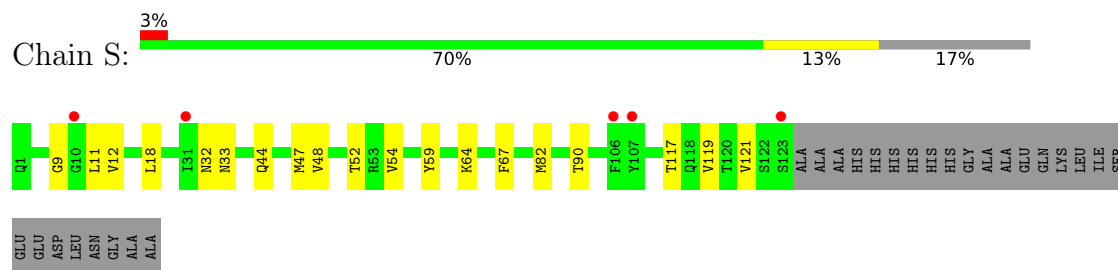
- Molecule 2: Nanobody D12



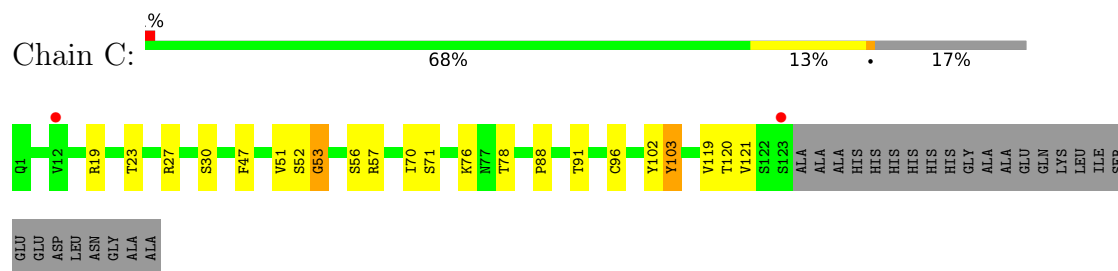
- Molecule 2: Nanobody D12



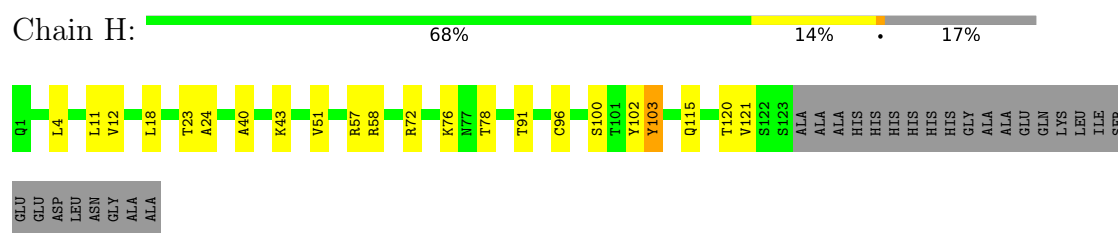
- Molecule 2: Nanobody D12



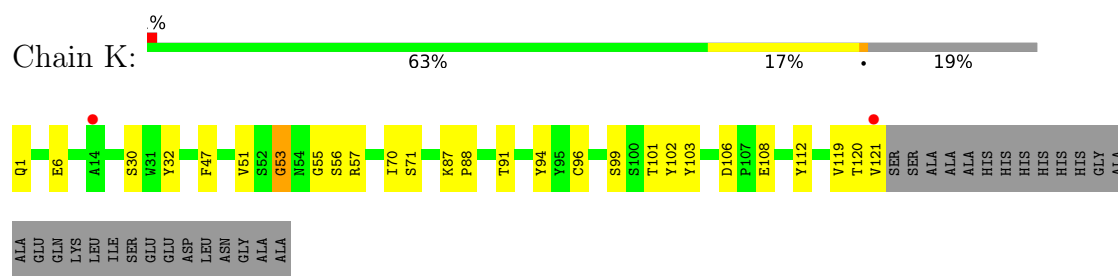
- Molecule 3: Nanobody G3a



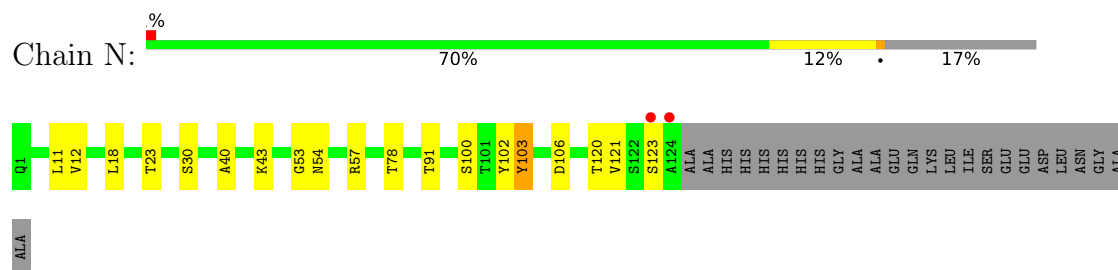
- Molecule 3: Nanobody G3a



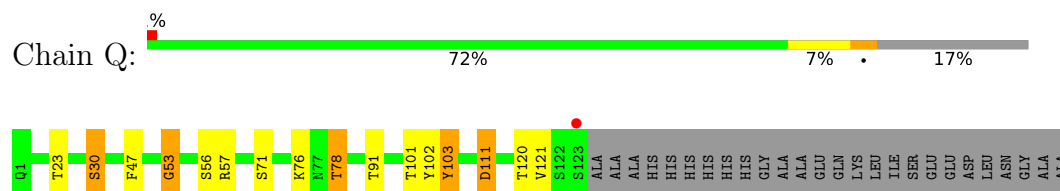
- Molecule 3: Nanobody G3a



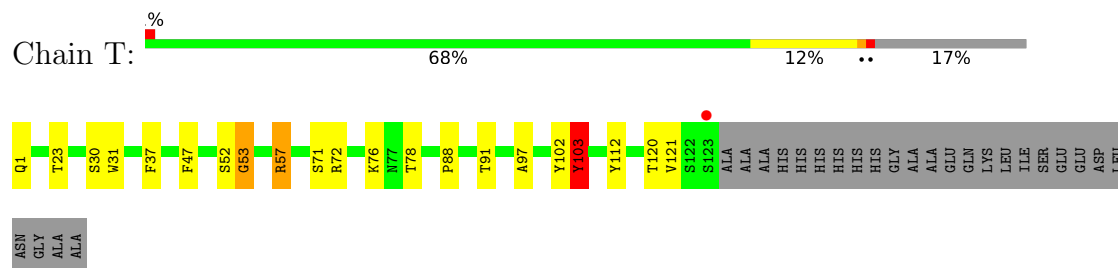
- Molecule 3: Nanobody G3a



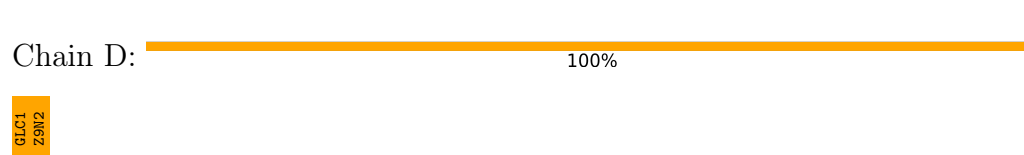
- Molecule 3: Nanobody G3a



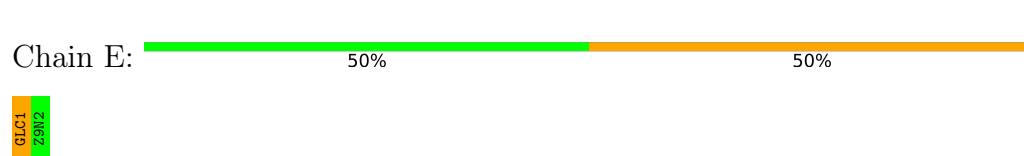
- Molecule 3: Nanobody G3a



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



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



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

Chain U:  50% 50%



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

Chain V:  50% 50%



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

Chain W:  50% 50%



4 Data and refinement statistics

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) 99.1 (34.43-2.99)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.36 , 93.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.74	1/1620 (0.1%)	1.27	3/2195 (0.1%)
1	F	0.75	0/1562	1.29	7/2115 (0.3%)
1	I	0.76	0/1618	1.29	8/2188 (0.4%)
1	L	0.75	1/1590 (0.1%)	1.28	5/2155 (0.2%)
1	O	0.74	0/1599	1.27	8/2167 (0.4%)
1	R	0.76	0/1574	1.28	8/2136 (0.4%)
2	B	0.74	0/947	1.12	2/1288 (0.2%)
2	G	0.72	0/909	1.09	2/1239 (0.2%)
2	J	0.68	0/951	1.06	1/1289 (0.1%)
2	M	0.71	0/919	1.03	1/1248 (0.1%)
2	P	0.70	0/922	1.09	4/1254 (0.3%)
2	S	0.69	0/863	1.12	3/1179 (0.3%)
3	C	0.77	1/930 (0.1%)	1.20	4/1263 (0.3%)
3	H	0.75	0/966	1.18	2/1310 (0.2%)
3	K	0.75	0/931	1.15	6/1266 (0.5%)
3	N	0.74	0/969	1.19	5/1314 (0.4%)
3	Q	0.72	0/931	1.20	4/1267 (0.3%)
3	T	0.74	0/927	1.16	4/1262 (0.3%)
All	All	0.74	3/20728 (0.0%)	1.20	77/28135 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	595	MET	SD-CE	-5.71	1.65	1.79
1	A	595	MET	SD-CE	-5.04	1.67	1.79
3	C	103	TYR	CA-C	-5.01	1.48	1.53

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	103	TYR	N-CA-C	16.11	131.16	111.02
3	H	103	TYR	N-CA-C	15.98	130.99	111.02
3	K	103	TYR	N-CA-C	13.35	129.66	111.24
3	Q	103	TYR	N-CA-C	13.08	129.28	111.24
3	T	103	TYR	N-CA-C	13.06	129.42	111.39
3	N	103	TYR	N-CA-C	12.62	128.65	111.24
3	Q	102	TYR	N-CA-C	7.85	121.73	109.96
2	G	48	VAL	N-CA-C	-7.76	104.18	111.48
3	N	102	TYR	N-CA-C	7.62	121.39	109.96
2	J	48	VAL	N-CA-C	-7.39	104.53	111.48
2	S	11	LEU	CD1-CG-CD2	-7.32	94.70	110.80
2	S	32	ASN	N-CA-C	7.07	118.78	111.14
2	P	48	VAL	N-CA-C	-7.06	104.84	111.48
1	I	635	ASN	CA-C-N	7.00	134.30	121.70
1	I	635	ASN	C-N-CA	7.00	134.30	121.70
3	C	53	GLY	CA-C-N	6.97	130.18	120.29
3	C	53	GLY	C-N-CA	6.97	130.18	120.29
3	N	123	SER	N-CA-C	-6.84	103.75	111.14
3	C	102	TYR	N-CA-C	6.28	119.74	109.76
3	N	106	ASP	CA-CB-CG	6.17	118.77	112.60
3	T	102	TYR	N-CA-C	6.10	119.46	109.76
3	Q	53	GLY	CA-C-N	6.09	128.94	120.29
3	Q	53	GLY	C-N-CA	6.09	128.94	120.29
1	F	463	GLY	CA-C-N	5.95	129.06	120.79
1	F	463	GLY	C-N-CA	5.95	129.06	120.79
1	I	546	ILE	N-CA-C	5.88	117.92	109.51
1	I	537	ASP	CA-CB-CG	5.85	118.45	112.60
3	T	53	GLY	CA-C-N	5.84	128.59	120.29
3	T	53	GLY	C-N-CA	5.84	128.59	120.29
1	O	607	MET	CA-C-N	5.75	127.98	120.28
1	O	607	MET	C-N-CA	5.75	127.98	120.28
3	N	54	ASN	CA-CB-CG	5.54	118.14	112.60
1	F	607	MET	CA-C-N	5.52	127.67	120.28
1	F	607	MET	C-N-CA	5.52	127.67	120.28
1	I	607	MET	CA-C-N	5.47	127.61	120.28
1	I	607	MET	C-N-CA	5.47	127.61	120.28
1	L	446	PHE	CA-CB-CG	5.45	119.25	113.80
2	P	88	GLU	CB-CG-CD	5.42	121.82	112.60
1	I	446	PHE	CA-CB-CG	5.40	119.20	113.80
2	B	31	ILE	CA-C-N	-5.38	113.64	122.79
2	B	31	ILE	C-N-CA	-5.38	113.64	122.79
1	O	446	PHE	CA-CB-CG	5.38	119.19	113.80
1	R	446	PHE	CA-CB-CG	5.38	119.18	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	486	GLY	N-CA-C	5.35	120.39	113.27
1	L	607	MET	CA-C-N	5.35	127.45	120.28
1	L	607	MET	C-N-CA	5.35	127.45	120.28
1	A	446	PHE	CA-CB-CG	5.34	119.14	113.80
1	F	446	PHE	CA-CB-CG	5.33	119.13	113.80
1	I	486	GLY	N-CA-C	5.33	120.35	113.27
1	R	549	SER	CA-C-N	5.32	125.89	119.98
1	R	549	SER	C-N-CA	5.32	125.89	119.98
2	P	87	PRO	CA-C-N	5.32	128.39	120.31
2	P	87	PRO	C-N-CA	5.32	128.39	120.31
2	G	29	ARG	N-CA-C	-5.30	104.93	111.40
3	H	102	TYR	N-CA-C	5.30	118.19	109.76
3	K	102	TYR	N-CA-C	5.23	117.80	109.96
1	R	607	MET	CA-C-N	5.22	127.27	120.28
1	R	607	MET	C-N-CA	5.22	127.27	120.28
3	K	102	TYR	CA-C-N	5.18	130.30	122.68
3	K	102	TYR	C-N-CA	5.18	130.30	122.68
2	M	33	ASN	N-CA-C	5.17	117.48	111.02
1	O	595	MET	CA-C-N	5.14	128.53	120.82
1	O	595	MET	C-N-CA	5.14	128.53	120.82
1	R	486	GLY	N-CA-C	5.13	120.09	113.27
1	O	486	GLY	N-CA-C	5.12	120.08	113.27
1	L	575	PHE	CA-C-N	5.12	125.77	119.99
1	L	575	PHE	C-N-CA	5.12	125.77	119.99
1	F	499	PRO	N-CA-C	5.08	120.45	113.84
2	S	67	PHE	CA-CB-CG	5.08	118.88	113.80
3	K	53	GLY	CA-C-N	5.08	127.50	120.29
3	K	53	GLY	C-N-CA	5.08	127.50	120.29
1	A	607	MET	CA-C-N	5.02	127.26	120.38
1	A	607	MET	C-N-CA	5.02	127.26	120.38
1	O	463	GLY	CA-C-N	5.00	127.25	120.65
1	O	463	GLY	C-N-CA	5.00	127.25	120.65
1	R	550	GLY	CA-C-N	5.00	125.39	119.94
1	R	550	GLY	C-N-CA	5.00	125.39	119.94

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	1592	0	1513	19	0
1	F	1537	0	1451	18	0
1	I	1591	0	1528	22	0
1	L	1563	0	1451	23	0
1	O	1571	0	1469	17	0
1	R	1547	0	1426	25	0
2	B	931	0	875	9	0
2	G	893	0	824	12	0
2	J	935	0	898	9	0
2	M	905	0	848	29	0
2	P	906	0	842	11	0
2	S	849	0	738	13	0
3	C	908	0	803	23	0
3	H	944	0	877	13	0
3	K	909	0	823	28	0
3	N	947	0	882	11	0
3	Q	909	0	807	11	0
3	T	905	0	810	25	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	293	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.

All (293) 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
3:T:53:GLY:HA2	3:T:72:ARG:HH22	1.20	1.05
3:K:88:PRO:HA	3:K:121:VAL:HG13	1.34	1.03
3:T:53:GLY:HA2	3:T:72:ARG:NH2	1.73	1.03
2:J:90:THR:HG22	2:J:121:VAL:H	1.24	1.02
3:T:53:GLY:CA	3:T:72:ARG:HH22	1.73	1.00
2:M:4:LEU:CD2	2:M:22:CYS:SG	2.50	1.00
1:A:390:THR:HG23	1:A:567:ASP:HB3	1.44	0.99
2:P:1:GLN:O	2:P:26:GLY:HA3	1.62	0.98
3:N:23:THR:HG22	3:N:78:THR:HG22	1.45	0.98
1:F:472:MET:HE3	1:F:472:MET:HA	1.46	0.97
2:G:90:THR:HG22	2:G:121:VAL:H	1.26	0.97
1:F:401:TRP:CD1	1:F:440:VAL:HG21	2.02	0.95
3:T:53:GLY:CA	3:T:72:ARG:NH2	2.30	0.94
3:T:23:THR:HG22	3:T:78:THR:HG22	1.47	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:23:THR:HG22	3:C:78:THR:HG22	1.52	0.91
1:A:390:THR:HG22	1:A:485:SER:HB2	1.54	0.89
3:C:71:SER:HB3	2:M:54:VAL:CG1	2.03	0.88
1:A:401:TRP:HD1	1:A:440:VAL:HG21	1.39	0.87
1:R:398:THR:HG22	1:R:443:ASP:H	1.40	0.85
3:K:91:THR:HG23	3:K:121:VAL:HG12	1.60	0.84
3:T:91:THR:HG22	3:T:121:VAL:H	1.41	0.83
1:F:401:TRP:HD1	1:F:440:VAL:HG21	1.45	0.82
2:B:31:ILE:HG12	2:B:99:ILE:HG12	1.62	0.81
1:L:516:ARG:HG2	1:L:563:TYR:CE1	2.16	0.81
1:R:516:ARG:O	1:R:520:VAL:HG23	1.80	0.81
3:T:23:THR:HG22	3:T:78:THR:CG2	2.12	0.80
1:A:398:THR:HG22	1:A:443:ASP:H	1.47	0.79
3:N:91:THR:HG22	3:N:121:VAL:H	1.47	0.78
3:H:91:THR:HG22	3:H:121:VAL:H	1.49	0.77
1:L:520:VAL:HG13	1:L:562:VAL:HG23	1.67	0.77
1:O:398:THR:HG22	1:O:443:ASP:H	1.48	0.76
1:F:464:LYS:N	5:F:701:ATP:O2B	2.19	0.76
1:I:398:THR:HG22	1:I:443:ASP:H	1.49	0.76
3:C:91:THR:HG22	3:C:121:VAL:H	1.50	0.75
2:M:2:VAL:HG21	2:M:112:TYR:CE2	2.22	0.75
1:O:469:MET:HG3	1:O:474:GLU:HB2	1.69	0.75
1:L:516:ARG:NH2	1:L:563:TYR:O	2.19	0.75
3:T:91:THR:CG2	3:T:121:VAL:H	2.01	0.74
2:M:1:GLN:O	2:M:26:GLY:HA3	1.87	0.74
3:Q:91:THR:HG22	3:Q:121:VAL:H	1.54	0.73
2:S:90:THR:CG2	2:S:121:VAL:H	1.98	0.72
1:R:520:VAL:HG13	1:R:562:VAL:HG23	1.71	0.71
3:N:23:THR:HG22	3:N:78:THR:CG2	2.19	0.71
3:T:53:GLY:N	3:T:72:ARG:HH22	1.88	0.70
2:S:90:THR:HG22	2:S:121:VAL:N	2.00	0.70
3:C:91:THR:CG2	3:C:121:VAL:H	2.04	0.69
3:K:99:SER:OG	3:K:101:THR:HG22	1.93	0.68
1:L:520:VAL:CG1	1:L:562:VAL:HG23	2.23	0.68
1:I:398:THR:CG2	1:I:443:ASP:H	2.07	0.68
2:M:2:VAL:HG21	2:M:112:TYR:CZ	2.29	0.68
2:M:2:VAL:CG2	2:M:112:TYR:CE2	2.77	0.68
1:I:539:ILE:HG13	1:I:539:ILE:O	1.94	0.67
2:M:4:LEU:CD2	2:M:95:CYS:SG	2.82	0.67
3:H:23:THR:HG22	3:H:78:THR:HG22	1.76	0.67
1:I:398:THR:HG22	1:I:442:LYS:HA	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:47:MET:HG2	2:M:48:VAL:N	2.08	0.66
2:S:47:MET:HG2	2:S:48:VAL:N	2.11	0.66
1:L:531:SER:HB3	3:N:100:SER:OG	1.96	0.65
2:P:1:GLN:O	2:P:26:GLY:CA	2.41	0.64
1:R:520:VAL:HG13	1:R:562:VAL:CG2	2.26	0.64
3:K:91:THR:HG22	3:K:121:VAL:H	1.63	0.64
1:A:398:THR:CG2	1:A:443:ASP:H	2.09	0.64
3:N:91:THR:CG2	3:N:121:VAL:H	2.09	0.64
3:H:91:THR:CG2	3:H:121:VAL:H	2.10	0.64
1:A:390:THR:HG23	1:A:567:ASP:CB	2.25	0.64
1:I:535:GLU:HG3	1:I:538:ASN:HB3	1.79	0.63
3:K:87:LYS:O	3:K:121:VAL:HG11	1.98	0.63
3:C:91:THR:HG22	3:C:120:THR:HA	1.80	0.63
5:A:701:ATP:H5'2	5:A:701:ATP:H8	1.63	0.63
2:P:2:VAL:HG22	2:P:28:ILE:HD13	1.79	0.62
3:Q:91:THR:CG2	3:Q:121:VAL:H	2.13	0.62
3:C:27:ARG:NH2	1:I:545:GLY:O	2.32	0.62
3:K:88:PRO:HA	3:K:121:VAL:CG1	2.21	0.62
3:K:71:SER:CB	2:S:54:VAL:CG1	2.77	0.61
3:K:94:TYR:CE1	3:K:119:VAL:CG2	2.83	0.61
1:L:520:VAL:HG13	1:L:562:VAL:CG2	2.30	0.61
3:C:56:SER:HA	1:L:494:PHE:CE2	2.37	0.60
1:A:398:THR:HG22	1:A:442:LYS:HA	1.83	0.59
3:T:52:SER:C	3:T:72:ARG:NH2	2.61	0.59
3:K:94:TYR:CE1	3:K:119:VAL:HG21	2.37	0.59
1:F:569:TYR:HE2	1:F:598:LYS:HD3	1.67	0.59
3:K:91:THR:HG23	3:K:121:VAL:CG1	2.31	0.59
3:H:51:VAL:HG12	3:H:58:ARG:HG2	1.84	0.59
3:Q:23:THR:HG22	3:Q:78:THR:HG22	1.84	0.59
2:J:90:THR:CG2	2:J:121:VAL:H	2.09	0.59
3:C:19:ARG:HG3	3:C:19:ARG:NH1	2.17	0.58
3:T:91:THR:HG22	3:T:120:THR:HA	1.85	0.58
3:K:71:SER:CB	2:S:54:VAL:HG11	2.33	0.58
2:G:90:THR:HG22	2:G:121:VAL:N	2.08	0.58
2:M:2:VAL:HA	2:M:25:THR:O	2.04	0.58
2:G:82:MET:HE1	2:G:119:VAL:HG11	1.85	0.58
1:R:394:MET:HE3	1:R:397:VAL:HG21	1.85	0.57
1:L:520:VAL:CG1	1:L:562:VAL:CG2	2.82	0.57
1:O:535:GLU:HG3	1:O:538:ASN:HB3	1.86	0.57
1:R:394:MET:CE	1:R:397:VAL:HG21	2.34	0.57
3:C:30:SER:O	3:C:53:GLY:HA3	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:507:ILE:HG13	1:O:507:ILE:O	2.03	0.57
1:R:598:LYS:O	1:R:600:ARG:HG3	2.04	0.57
3:T:37:PHE:HE2	3:T:97:ALA:HB3	1.70	0.56
1:R:592:CYS:O	1:R:596:ALA:HB2	2.05	0.56
2:M:4:LEU:HD22	2:M:95:CYS:SG	2.45	0.56
2:M:9:GLY:HA3	2:M:117:THR:HG22	1.86	0.56
1:I:516:ARG:HH21	4:U:1:GLC:H3	1.70	0.56
1:R:520:VAL:CG1	1:R:562:VAL:HG23	2.36	0.56
2:G:90:THR:CG2	2:G:121:VAL:H	2.09	0.56
1:R:488:ILE:HG12	1:R:568:LEU:HD23	1.87	0.55
1:F:533:PHE:CD1	1:F:539:ILE:HD13	2.41	0.55
3:C:71:SER:CB	2:M:54:VAL:CG1	2.81	0.55
1:F:488:ILE:HG12	1:F:568:LEU:HD23	1.87	0.55
3:K:71:SER:CB	2:S:54:VAL:HG12	2.37	0.55
2:M:2:VAL:O	2:M:2:VAL:HG23	2.05	0.55
3:Q:91:THR:HG22	3:Q:120:THR:HA	1.87	0.55
3:K:51:VAL:CG2	3:K:70:ILE:HG12	2.36	0.55
2:G:34:MET:HE2	2:G:71:ARG:CZ	2.37	0.55
2:J:90:THR:HG22	2:J:121:VAL:N	2.07	0.55
3:K:51:VAL:HG23	3:K:70:ILE:HG12	1.90	0.54
1:L:394:MET:HG3	1:L:446:PHE:CZ	2.43	0.54
3:K:91:THR:CG2	3:K:121:VAL:H	2.20	0.54
1:I:488:ILE:HG12	1:I:568:LEU:HD23	1.89	0.54
3:T:53:GLY:N	3:T:72:ARG:NH2	2.54	0.54
5:A:701:ATP:H5'2	5:A:701:ATP:C8	2.43	0.53
3:C:51:VAL:HG23	3:C:70:ILE:HG12	1.90	0.53
3:H:91:THR:HG22	3:H:120:THR:HA	1.90	0.53
2:M:28:ILE:HG23	2:M:99:ILE:HG23	1.89	0.53
3:C:19:ARG:HG3	3:C:19:ARG:HH11	1.73	0.53
1:F:472:MET:HA	1:F:472:MET:CE	2.28	0.53
2:P:6:GLU:HB3	2:P:117:THR:CG2	2.39	0.53
3:T:37:PHE:CD1	3:T:47:PHE:HA	2.43	0.53
2:S:33:ASN:OD1	2:S:52:THR:HA	2.09	0.53
3:H:12:VAL:HG21	3:H:18:LEU:HD13	1.91	0.52
3:H:115:GLN:HG3	2:M:68:THR:HG21	1.91	0.52
1:I:394:MET:HE2	1:I:446:PHE:CE2	2.44	0.52
2:B:47:MET:HG2	2:B:48:VAL:N	2.23	0.52
3:K:106:ASP:OD2	3:K:108:GLU:CB	2.57	0.52
3:N:12:VAL:HG21	3:N:18:LEU:HD13	1.91	0.52
4:D:1:GLC:O2	4:D:2:Z9N:O4	2.22	0.52
3:Q:111:ASP:N	3:Q:111:ASP:OD1	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:23:THR:HG22	3:H:78:THR:CG2	2.39	0.52
3:N:91:THR:HG22	3:N:120:THR:HA	1.91	0.51
1:L:531:SER:CB	3:N:100:SER:OG	2.57	0.51
3:K:101:THR:O	3:K:101:THR:HG23	2.08	0.51
3:T:52:SER:O	3:T:72:ARG:NH2	2.42	0.51
2:P:47:MET:HG2	2:P:48:VAL:N	2.25	0.51
3:C:23:THR:HG22	3:C:78:THR:CG2	2.33	0.51
1:F:531:SER:HB2	3:H:100:SER:OG	2.11	0.51
3:T:37:PHE:HD1	3:T:47:PHE:HA	1.75	0.51
3:H:76:LYS:O	3:H:78:THR:HG23	2.11	0.51
3:K:6:GLU:HG3	3:K:96:CYS:SG	2.50	0.50
3:K:94:TYR:CE1	3:K:119:VAL:HG22	2.45	0.50
2:M:32:ASN:O	2:M:98:GLU:HB2	2.11	0.50
3:K:91:THR:CG2	3:K:121:VAL:HG12	2.36	0.50
1:O:394:MET:HE2	1:O:446:PHE:CE2	2.47	0.50
3:C:88:PRO:HA	3:C:121:VAL:HB	1.93	0.49
3:C:51:VAL:CG2	3:C:70:ILE:HG12	2.42	0.49
2:J:47:MET:HG2	2:J:48:VAL:N	2.27	0.49
1:I:507:ILE:HD11	1:R:498:MET:SD	2.53	0.49
1:O:544:GLY:O	1:O:553:ARG:HD3	2.13	0.49
3:T:91:THR:HG22	3:T:121:VAL:N	2.21	0.49
3:C:91:THR:HG22	3:C:121:VAL:N	2.24	0.49
3:Q:23:THR:HG22	3:Q:78:THR:CG2	2.42	0.48
1:I:583:GLU:OE1	1:I:606:LYS:HE2	2.14	0.48
1:A:598:LYS:O	1:A:600:ARG:HG3	2.14	0.48
3:K:56:SER:HA	1:R:494:PHE:CE2	2.49	0.48
2:G:47:MET:HG2	2:G:48:VAL:N	2.28	0.48
2:M:82:MET:HE1	2:M:119:VAL:HG21	1.96	0.48
2:M:53:ARG:HG2	2:M:53:ARG:HH21	1.78	0.48
3:N:30:SER:O	3:N:53:GLY:HA3	2.13	0.48
3:T:37:PHE:CE2	3:T:97:ALA:HB3	2.49	0.47
2:B:2:VAL:HG11	2:B:99:ILE:HD13	1.96	0.47
3:K:30:SER:O	3:K:53:GLY:HA3	2.13	0.47
1:R:536:LYS:HD2	3:T:31:TRP:CD1	2.50	0.47
3:T:57:ARG:NH1	3:T:103:TYR:CD2	2.82	0.47
2:J:82:MET:HE1	2:J:119:VAL:HG21	1.97	0.47
2:S:9:GLY:HA3	2:S:117:THR:HG22	1.97	0.47
2:J:59:TYR:HB2	2:J:64:LYS:HE3	1.96	0.46
1:L:507:ILE:HD11	1:O:498:MET:SD	2.55	0.46
1:A:498:MET:SD	1:O:507:ILE:HD11	2.56	0.46
1:I:541:LEU:HD23	1:I:541:LEU:HA	1.74	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:94:TYR:HE1	3:K:119:VAL:CG2	2.28	0.46
2:P:6:GLU:CB	2:P:117:THR:CG2	2.93	0.46
1:R:507:ILE:CG2	1:R:510:VAL:O	2.63	0.46
1:R:397:VAL:HG13	1:R:477:PRO:HB3	1.97	0.46
3:C:51:VAL:HG12	3:C:52:SER:O	2.15	0.46
1:R:533:PHE:O	1:R:536:LYS:CE	2.64	0.46
1:R:533:PHE:O	1:R:536:LYS:HE3	2.15	0.46
2:G:6:GLU:HB2	2:G:117:THR:HG23	1.96	0.46
2:G:36:TRP:CD1	2:G:80:LEU:HB2	2.51	0.46
1:I:516:ARG:NH2	4:U:1:GLC:H3	2.31	0.46
1:F:508:PHE:HD1	1:F:508:PHE:HA	1.64	0.46
1:F:598:LYS:HD2	4:E:1:GLC:H5	1.98	0.46
3:K:91:THR:HG22	3:K:120:THR:HA	1.98	0.46
1:A:397:VAL:HG13	1:A:477:PRO:HB3	1.96	0.46
1:I:391:GLU:HG3	1:I:450:ARG:HA	1.96	0.46
1:I:397:VAL:HG13	1:I:477:PRO:HB3	1.98	0.46
2:S:59:TYR:HB2	2:S:64:LYS:HD3	1.97	0.46
3:Q:101:THR:O	3:Q:101:THR:HG23	2.15	0.46
1:L:474:GLU:O	4:D:2:Z9N:O3	2.34	0.45
3:C:19:ARG:NH2	2:M:54:VAL:O	2.45	0.45
3:K:1:GLN:CB	3:K:32:TYR:OH	2.63	0.45
2:S:82:MET:HE1	2:S:119:VAL:HG21	1.97	0.45
2:P:82:MET:HE1	2:P:119:VAL:HG21	1.99	0.45
3:Q:76:LYS:O	3:Q:78:THR:HG23	2.16	0.45
1:R:535:GLU:O	1:R:538:ASN:HB2	2.17	0.45
2:B:54:VAL:HG22	3:Q:71:SER:HB3	1.99	0.45
3:N:40:ALA:HB3	3:N:43:LYS:HB2	1.99	0.45
1:O:468:LEU:O	1:O:472:MET:HG2	2.17	0.45
3:T:88:PRO:HA	3:T:121:VAL:HB	1.98	0.45
2:J:6:GLU:HB2	2:J:117:THR:HG23	1.99	0.45
1:O:397:VAL:HG13	1:O:477:PRO:HB3	1.99	0.45
1:R:501:THR:HA	1:R:539:ILE:O	2.17	0.45
3:T:1:GLN:N	3:T:112:TYR:CE1	2.85	0.45
2:S:47:MET:CG	2:S:48:VAL:N	2.77	0.44
1:O:464:LYS:N	5:O:701:ATP:O1B	2.50	0.44
2:P:40:ALA:HB3	2:P:43:LYS:HD3	1.99	0.44
1:R:464:LYS:NZ	5:R:701:ATP:O3G	2.49	0.44
1:I:468:LEU:HA	1:I:471:ILE:HD12	2.00	0.44
1:I:470:MET:HG2	1:I:482:ILE:CD1	2.47	0.44
2:G:54:VAL:HG22	3:T:71:SER:HB3	2.00	0.44
2:M:53:ARG:HG2	2:M:53:ARG:NH2	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:MET:HE1	2:B:119:VAL:HG21	1.99	0.44
3:C:71:SER:CB	2:M:54:VAL:HG11	2.18	0.44
3:Q:30:SER:O	3:Q:53:GLY:HA3	2.17	0.44
3:T:76:LYS:O	3:T:78:THR:HG23	2.18	0.44
2:G:6:GLU:CB	2:G:117:THR:HG23	2.48	0.44
1:I:500:GLY:O	1:I:541:LEU:HB2	2.19	0.43
1:L:470:MET:HG2	1:L:482:ILE:CD1	2.48	0.43
2:G:32:ASN:O	2:G:71:ARG:NH1	2.48	0.43
1:A:470:MET:HG2	1:A:482:ILE:CD1	2.48	0.43
1:A:503:LYS:HE2	1:L:498:MET:HE1	1.99	0.43
1:L:397:VAL:HG13	1:L:477:PRO:HB3	2.00	0.43
3:C:27:ARG:HH22	1:I:545:GLY:C	2.23	0.43
2:M:53:ARG:HG2	2:M:53:ARG:H	1.58	0.43
1:F:496:TRP:HH2	1:F:508:PHE:CE2	2.37	0.43
1:F:569:TYR:CZ	4:E:1:GLC:O4	2.72	0.43
1:F:507:ILE:HG23	1:F:510:VAL:O	2.18	0.42
3:K:1:GLN:HG2	3:K:112:TYR:OH	2.18	0.42
1:R:520:VAL:CG1	1:R:562:VAL:CG2	2.94	0.42
1:I:508:PHE:HB3	1:I:509:GLY:H	1.65	0.42
1:L:394:MET:SD	1:L:482:ILE:HG12	2.59	0.42
1:O:468:LEU:HA	1:O:471:ILE:HD12	1.99	0.42
1:O:470:MET:HG2	1:O:482:ILE:CD1	2.49	0.42
1:F:508:PHE:HB3	1:F:509:GLY:H	1.67	0.42
1:L:590:CYS:O	1:L:595:MET:HG3	2.19	0.42
1:R:468:LEU:HA	1:R:471:ILE:HD12	2.02	0.42
2:B:9:GLY:HA3	2:B:117:THR:HG22	2.02	0.42
3:K:51:VAL:CG1	3:K:55:GLY:HA2	2.48	0.42
1:L:579:ASP:HB2	2:M:37:TYR:CE2	2.55	0.42
1:A:453:LEU:HB2	1:A:600:ARG:HH21	1.85	0.42
1:A:468:LEU:HA	1:A:471:ILE:HD12	2.00	0.42
3:C:91:THR:HA	3:C:119:VAL:O	2.19	0.42
3:H:51:VAL:HG23	3:H:72:ARG:HH11	1.84	0.42
2:P:12:VAL:HG11	2:P:18:LEU:HD13	2.01	0.42
1:O:595:MET:HE2	1:O:600:ARG:HG2	2.01	0.42
2:J:6:GLU:CB	2:J:117:THR:HG23	2.50	0.41
1:L:531:SER:HA	1:L:536:LYS:HD3	2.02	0.41
2:M:32:ASN:OD1	2:M:53:ARG:HD3	2.20	0.41
1:A:501:THR:HA	1:A:539:ILE:O	2.20	0.41
2:B:2:VAL:HB	2:B:112:TYR:CE2	2.56	0.41
2:B:27:SER:HB2	2:B:102:GLN:HB2	2.02	0.41
3:H:40:ALA:HB3	3:H:43:LYS:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:484:HIS:CD2	1:R:488:ILE:HD11	2.56	0.41
2:B:11:LEU:HG	2:B:125:ALA:HB2	2.02	0.41
1:R:468:LEU:HD12	1:R:572:ASP:HB2	2.00	0.41
1:A:503:LYS:HD3	1:L:498:MET:HE1	2.02	0.41
2:P:2:VAL:HG22	2:P:28:ILE:CD1	2.49	0.41
1:F:484:HIS:CD2	1:F:488:ILE:HD11	2.55	0.41
2:M:60:ALA:HB3	2:M:63:VAL:HG22	2.03	0.41
2:M:33:ASN:HA	2:M:51:ILE:O	2.21	0.41
1:A:494:PHE:CE2	3:Q:56:SER:HA	2.55	0.41
3:K:1:GLN:HB2	3:K:32:TYR:OH	2.21	0.41
1:I:517:TYR:CZ	1:I:521:ILE:HD11	2.56	0.41
2:M:47:MET:HE2	2:M:47:MET:HB3	1.77	0.41
2:S:12:VAL:HG11	2:S:18:LEU:HD13	2.03	0.41
3:T:53:GLY:C	3:T:72:ARG:NH2	2.77	0.41
2:G:12:VAL:HG11	2:G:18:LEU:HD13	2.03	0.40
3:H:4:LEU:HD23	3:H:24:ALA:HB2	2.03	0.40
2:J:12:VAL:HG11	2:J:18:LEU:HD13	2.03	0.40
1:L:394:MET:HG3	1:L:446:PHE:CE2	2.56	0.40
1:O:501:THR:HA	1:O:539:ILE:O	2.21	0.40
1:L:531:SER:HB3	3:N:100:SER:HG	1.84	0.40
1:O:468:LEU:HD12	1:O:572:ASP:HB2	2.04	0.40
1:R:575:PHE:HA	1:R:578:LEU:HD12	2.04	0.40
1:A:575:PHE:HA	1:A:578:LEU:HD12	2.04	0.40
3:C:76:LYS:O	3:C:78:THR:HG23	2.21	0.40
1:F:503:LYS:HD3	1:I:498:MET:HE1	2.04	0.40
1:O:469:MET:HG3	1:O:474:GLU:CB	2.46	0.40
2:P:27:SER:HB2	2:P:102:GLN:HB2	2.04	0.40
1:F:501:THR:HA	1:F:539:ILE:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 ⓘ

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%)	154 (98%)	3 (2%)	50	76
1	F	149/197 (76%)	141 (95%)	8 (5%)	20	53
1	I	162/197 (82%)	158 (98%)	4 (2%)	42	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	152/197 (77%)	144 (95%)	8 (5%)	20	54
1	O	153/197 (78%)	148 (97%)	5 (3%)	33	67
1	R	147/197 (75%)	140 (95%)	7 (5%)	23	57
2	B	93/118 (79%)	92 (99%)	1 (1%)	65	83
2	G	87/118 (74%)	86 (99%)	1 (1%)	65	83
2	J	97/118 (82%)	96 (99%)	1 (1%)	68	84
2	M	89/118 (75%)	86 (97%)	3 (3%)	32	66
2	P	90/118 (76%)	89 (99%)	1 (1%)	65	83
2	S	76/118 (64%)	75 (99%)	1 (1%)	61	81
3	C	82/117 (70%)	78 (95%)	4 (5%)	22	56
3	H	96/117 (82%)	92 (96%)	4 (4%)	26	61
3	K	87/117 (74%)	85 (98%)	2 (2%)	44	74
3	N	94/117 (80%)	91 (97%)	3 (3%)	34	67
3	Q	86/117 (74%)	80 (93%)	6 (7%)	14	44
3	T	83/117 (71%)	80 (96%)	3 (4%)	31	65
All	All	1980/2592 (76%)	1915 (97%)	65 (3%)	33	67

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	464	LYS
1	A	497	ILE
1	A	539	ILE
2	B	117	THR
3	C	47	PHE
3	C	57	ARG
3	C	96	CYS
3	C	103	TYR
1	F	464	LYS
1	F	472	MET
1	F	497	ILE
1	F	507	ILE
1	F	508	PHE
1	F	538	ASN
1	F	539	ILE
1	F	583	GLU
2	G	81	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	11	LEU
3	H	57	ARG
3	H	96	CYS
3	H	103	TYR
1	I	464	LYS
1	I	497	ILE
1	I	508	PHE
1	I	547	THR
2	J	44	GLN
3	K	47	PHE
3	K	57	ARG
1	L	464	LYS
1	L	497	ILE
1	L	508	PHE
1	L	510	VAL
1	L	538	ASN
1	L	539	ILE
1	L	547	THR
1	L	583	GLU
2	M	4	LEU
2	M	44	GLN
2	M	47	MET
3	N	11	LEU
3	N	57	ARG
3	N	103	TYR
1	O	398	THR
1	O	464	LYS
1	O	538	ASN
1	O	539	ILE
1	O	583	GLU
2	P	4	LEU
3	Q	30	SER
3	Q	47	PHE
3	Q	57	ARG
3	Q	78	THR
3	Q	103	TYR
3	Q	111	ASP
1	R	464	LYS
1	R	472	MET
1	R	497	ILE
1	R	536	LYS
1	R	547	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	583	GLU
1	R	593	LYS
2	S	44	GLN
3	T	30	SER
3	T	57	ARG
3	T	103	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	81	GLN
3	C	3	GLN
3	C	84	ASN
1	F	620	HIS
2	G	33	ASN
2	G	118	GLN
3	H	3	GLN
3	H	84	ASN
1	I	538	ASN
2	J	5	GLN
2	J	81	GLN
3	K	3	GLN
3	K	84	ASN
2	M	118	GLN
3	N	84	ASN
1	O	493	GLN
2	P	33	ASN
2	P	81	GLN
3	Q	3	GLN
3	Q	39	GLN
3	Q	84	ASN
3	Q	118	GLN
3	T	3	GLN
3	T	74	ASN
3	T	84	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

10 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	GLC	D	1	4	11,11,12	0.49	0	15,15,17	2.23	5 (33%)
4	Z9N	D	2	4	11,12,12	0.73	1 (9%)	10,18,18	1.10	1 (10%)
4	GLC	E	1	4	11,11,12	0.39	0	15,15,17	1.19	3 (20%)
4	Z9N	E	2	4	11,12,12	0.73	0	10,18,18	0.76	0
4	GLC	U	1	4	11,11,12	0.30	0	15,15,17	0.99	1 (6%)
4	Z9N	U	2	4	11,12,12	0.58	0	10,18,18	0.70	0
4	GLC	V	1	4	11,11,12	0.32	0	15,15,17	1.00	1 (6%)
4	Z9N	V	2	4	11,12,12	0.59	0	10,18,18	0.73	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	0.64	0	10,18,18	0.64	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	-	0/5/24/24	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	2.11	1.44	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	GLC	C1-O5-C5	5.12	119.04	112.19
4	D	1	GLC	C1-C2-C3	3.99	115.45	109.64
4	D	1	GLC	O5-C1-C2	3.26	118.56	110.79
4	V	1	GLC	C1-O5-C5	2.97	116.17	112.19
4	D	1	GLC	C3-C4-C5	-2.90	104.97	110.23
4	U	1	GLC	C1-O5-C5	2.80	115.94	112.19
4	D	1	GLC	O2-C2-C3	-2.54	104.89	110.15
4	E	1	GLC	O2-C2-C1	2.36	114.62	109.22
4	W	1	GLC	C1-O5-C5	2.25	115.21	112.19
4	E	1	GLC	O3-C3-C2	-2.17	105.63	110.05
4	E	1	GLC	O3-C3-C4	-2.11	105.39	110.38
4	D	2	Z9N	O3-C3-C4	-2.04	106.06	113.25

There are no chirality outliers.

All (8) torsion outliers are listed below:

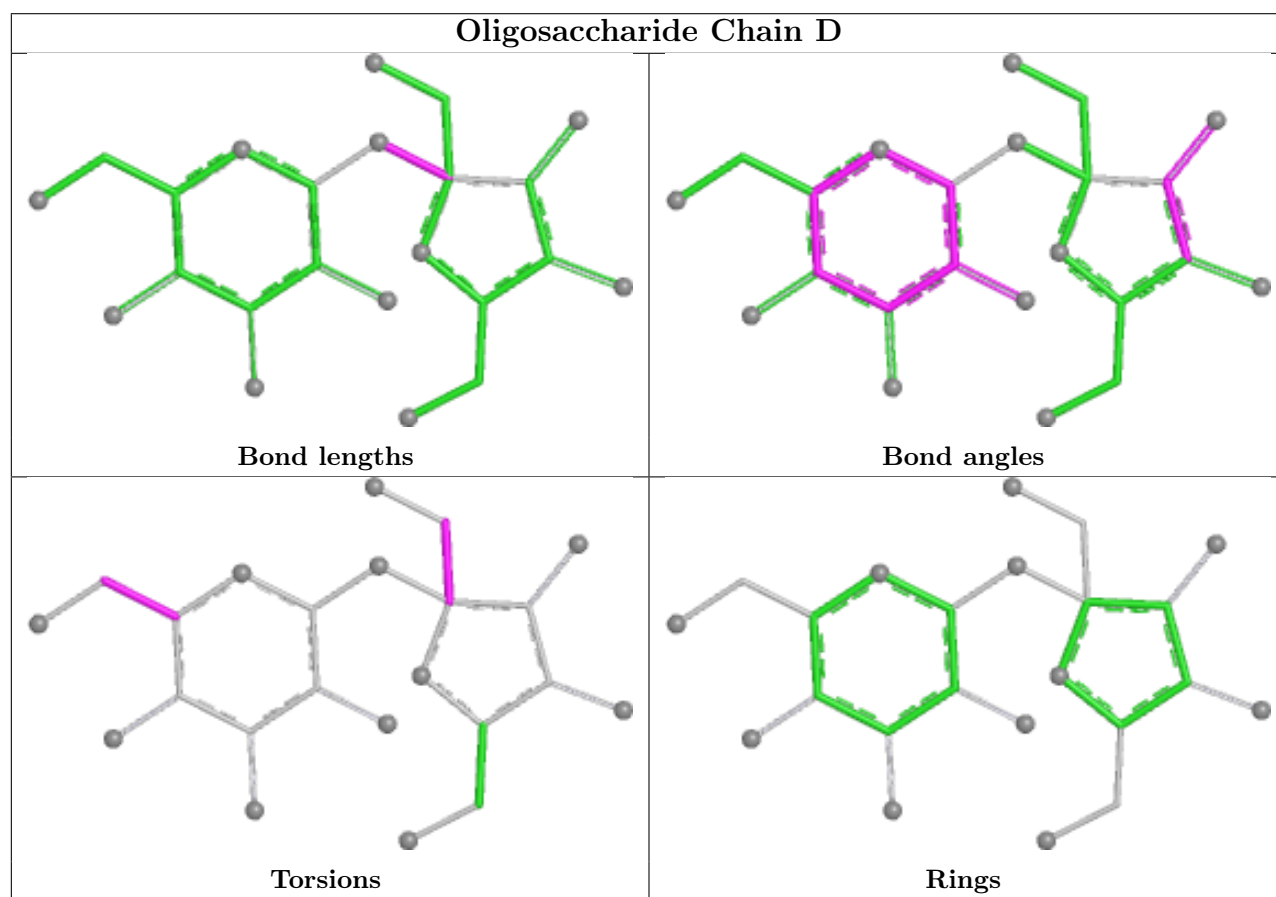
Mol	Chain	Res	Type	Atoms
4	D	2	Z9N	O1-C1-C2-O5
4	D	2	Z9N	O1-C1-C2-C3
4	V	1	GLC	C4-C5-C6-O6
4	W	1	GLC	O5-C5-C6-O6
4	U	1	GLC	O5-C5-C6-O6
4	V	1	GLC	O5-C5-C6-O6
4	D	2	Z9N	O1-C1-C2-O2
4	D	1	GLC	C4-C5-C6-O6

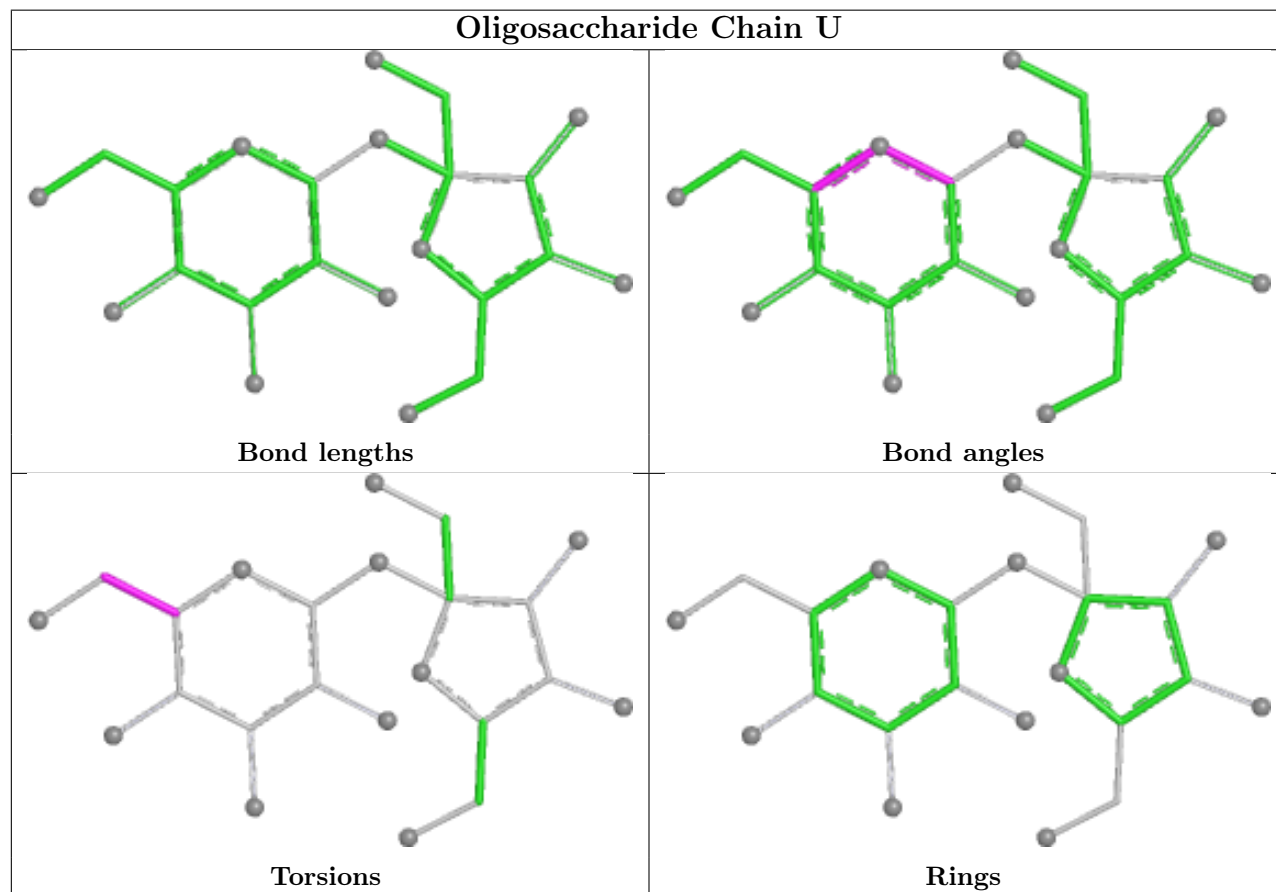
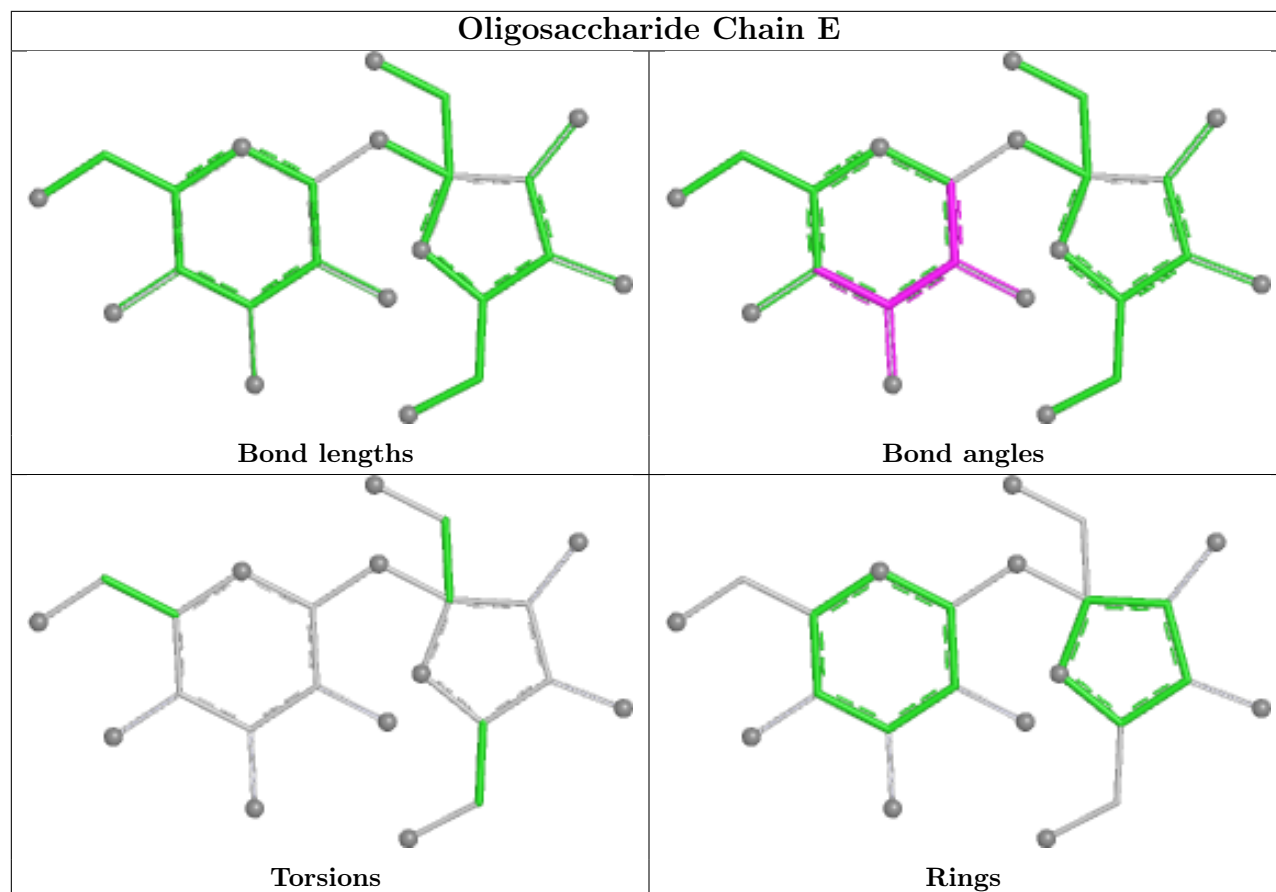
There are no ring outliers.

4 monomers are involved in 6 short contacts:

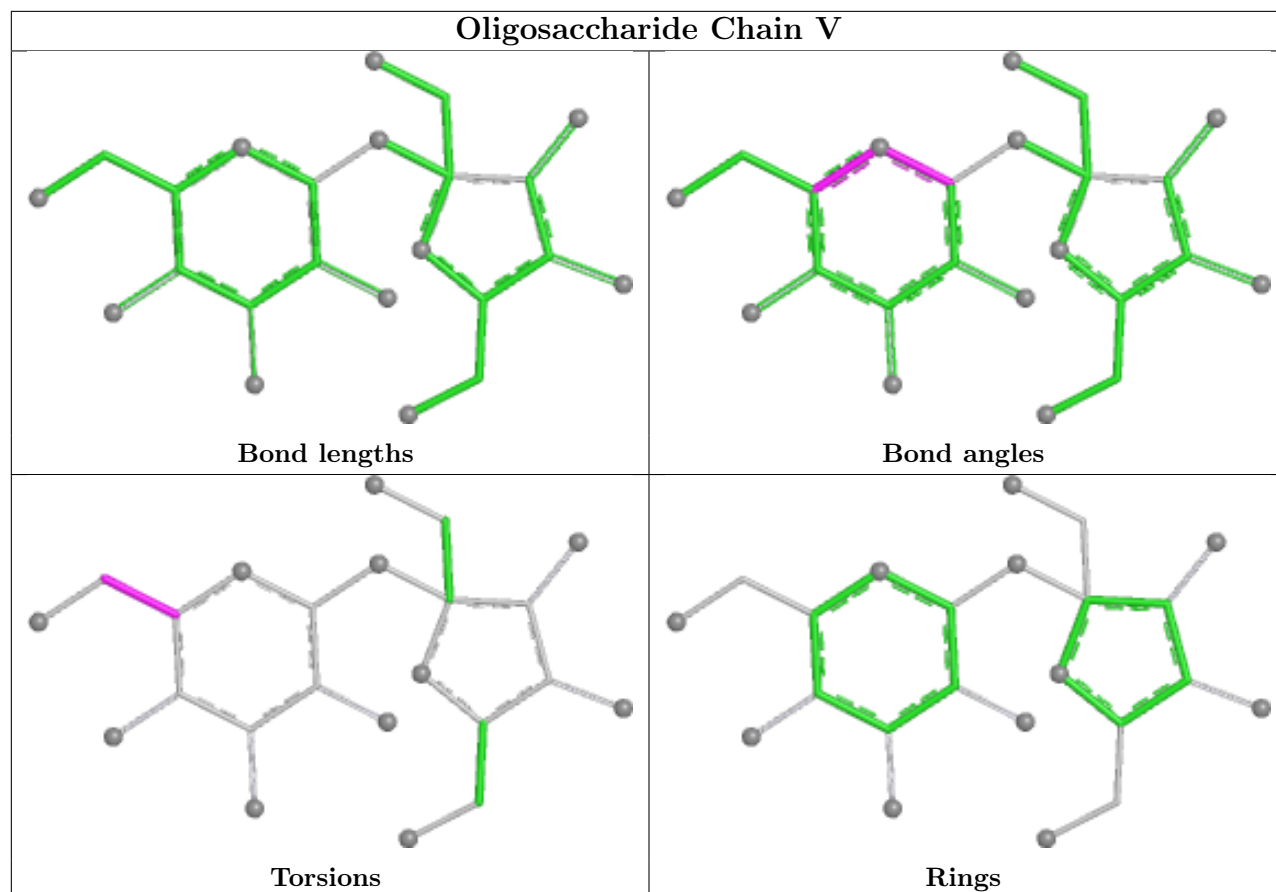
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	GLC	2	0
4	D	2	Z9N	2	0
4	U	1	GLC	2	0
4	D	1	GLC	1	0

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

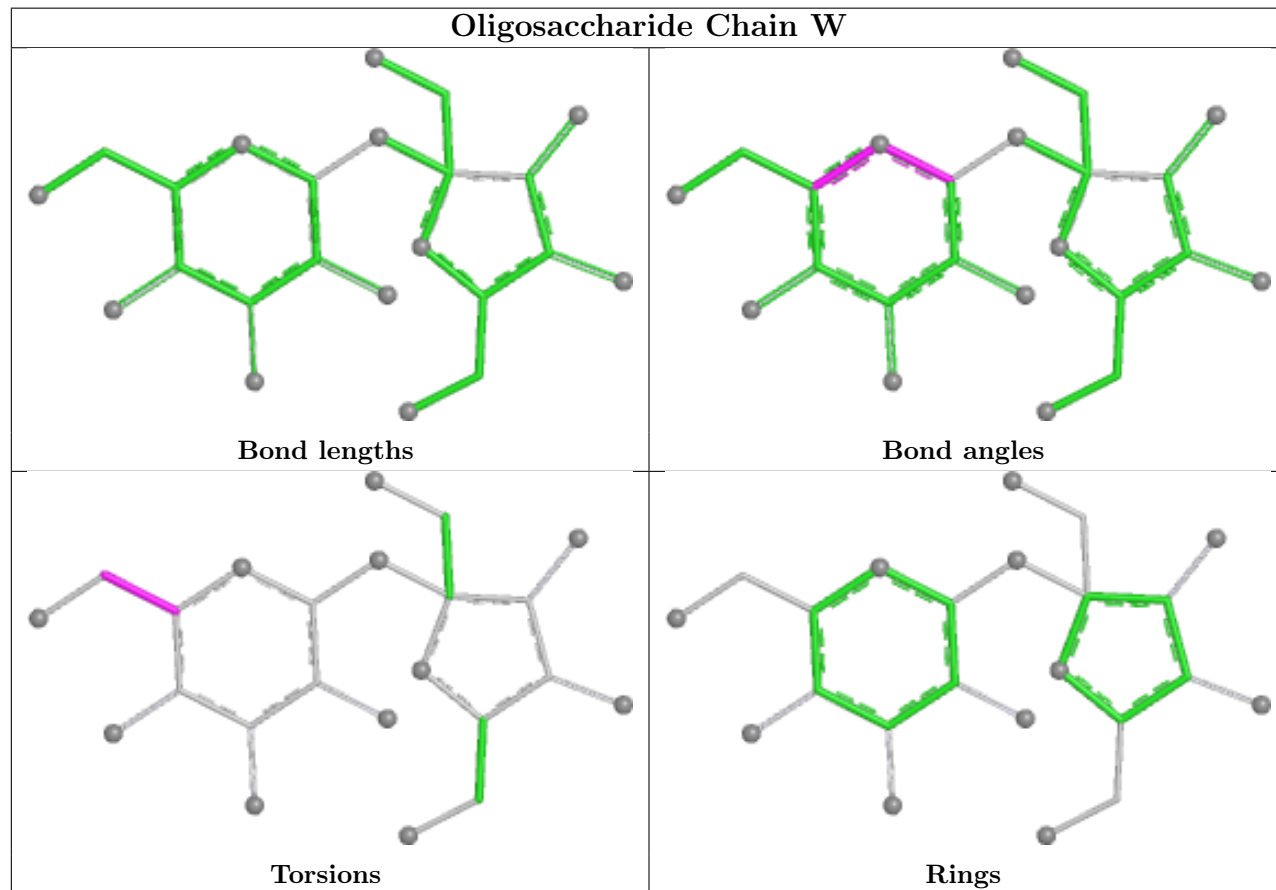




Oligosaccharide Chain V



Oligosaccharide Chain W



5.6 Ligand geometry

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	32,33,33	0.59	1 (3%)	48,52,52	0.77	0
5	ATP	F	701	6	32,33,33	0.81	2 (6%)	48,52,52	0.82	1 (2%)
5	ATP	O	701	6	32,33,33	0.81	1 (3%)	48,52,52	0.69	0
7	GOL	T	201	-	5,5,5	0.12	0	5,5,5	0.21	0
5	ATP	A	701	6	32,33,33	0.95	1 (3%)	48,52,52	0.80	1 (2%)
7	GOL	O	704	-	5,5,5	0.17	0	5,5,5	0.33	0
5	ATP	L	701	6	32,33,33	1.00	2 (6%)	48,52,52	0.82	1 (2%)
5	ATP	R	701	6	32,33,33	1.46	4 (12%)	48,52,52	1.31	5 (10%)

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	-	5/22/38/38	0/3/3/3
5	ATP	F	701	6	-	3/22/38/38	0/3/3/3
5	ATP	O	701	6	-	6/22/38/38	0/3/3/3
7	GOL	T	201	-	-	2/4/4/4	-
5	ATP	A	701	6	-	7/22/38/38	0/3/3/3
7	GOL	O	704	-	-	4/4/4/4	-
5	ATP	L	701	6	-	7/22/38/38	0/3/3/3
5	ATP	R	701	6	-	2/22/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	701	ATP	PG-O2G	-4.23	1.39	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	701	ATP	C5-N7	-3.87	1.32	1.39
5	A	701	ATP	PG-O3G	-3.71	1.41	1.54
5	L	701	ATP	PG-O1G	-3.24	1.40	1.50
5	R	701	ATP	C5-C4	3.14	1.44	1.39
5	F	701	ATP	PB-O2B	-2.42	1.44	1.55
5	R	701	ATP	C4-N3	-2.40	1.29	1.34
5	I	701	ATP	PG-O3G	-2.25	1.46	1.54
5	F	701	ATP	PG-O2G	-2.17	1.46	1.54
5	O	701	ATP	PG-O2G	-2.16	1.46	1.54
5	L	701	ATP	PA-O5'	-2.05	1.51	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	701	ATP	C5-C4-N9	-4.34	101.08	105.81
5	R	701	ATP	C4-N9-C8	2.89	108.78	105.74
5	R	701	ATP	C6-C5-C4	-2.78	113.38	117.18
5	L	701	ATP	C3'-C2'-C1'	2.39	105.98	101.46
5	A	701	ATP	PA-O5'-C5'	-2.34	107.96	121.35
5	R	701	ATP	N3-C4-N9	2.24	130.97	127.17
5	F	701	ATP	C3'-C2'-C1'	2.18	105.58	101.46
5	R	701	ATP	O3B-PB-O1B	-2.16	104.19	110.70

There are no chirality outliers.

All (36) 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	A	701	ATP	C5'-O5'-PA-O3A
5	I	701	ATP	C5'-O5'-PA-O1A
5	I	701	ATP	C5'-O5'-PA-O2A
5	I	701	ATP	C5'-O5'-PA-O3A
5	L	701	ATP	C5'-O5'-PA-O1A
5	L	701	ATP	C5'-O5'-PA-O2A
5	L	701	ATP	C5'-O5'-PA-O3A
5	O	701	ATP	C5'-O5'-PA-O1A
5	O	701	ATP	C5'-O5'-PA-O2A
5	O	701	ATP	C5'-O5'-PA-O3A
7	O	704	GOL	O1-C1-C2-C3
5	O	701	ATP	C3'-C4'-C5'-O5'
5	R	701	ATP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	L	701	ATP	O4'-C4'-C5'-O5'
5	L	701	ATP	C3'-C4'-C5'-O5'
5	O	701	ATP	O4'-C4'-C5'-O5'
5	R	701	ATP	C3'-C4'-C5'-O5'
7	O	704	GOL	C1-C2-C3-O3
7	T	201	GOL	C1-C2-C3-O3
7	T	201	GOL	O2-C2-C3-O3
5	A	701	ATP	C3'-C4'-C5'-O5'
5	F	701	ATP	O4'-C4'-C5'-O5'
5	A	701	ATP	O4'-C4'-C5'-O5'
5	I	701	ATP	O4'-C4'-C5'-O5'
5	F	701	ATP	C3'-C4'-C5'-O5'
5	A	701	ATP	PA-O3A-PB-O1B
5	L	701	ATP	PA-O3A-PB-O1B
7	O	704	GOL	O1-C1-C2-O2
5	I	701	ATP	C3'-C4'-C5'-O5'
5	O	701	ATP	PA-O3A-PB-O2B
7	O	704	GOL	O2-C2-C3-O3
5	A	701	ATP	PA-O3A-PB-O2B
5	L	701	ATP	PA-O3A-PB-O2B
5	F	701	ATP	PA-O3A-PB-O2B

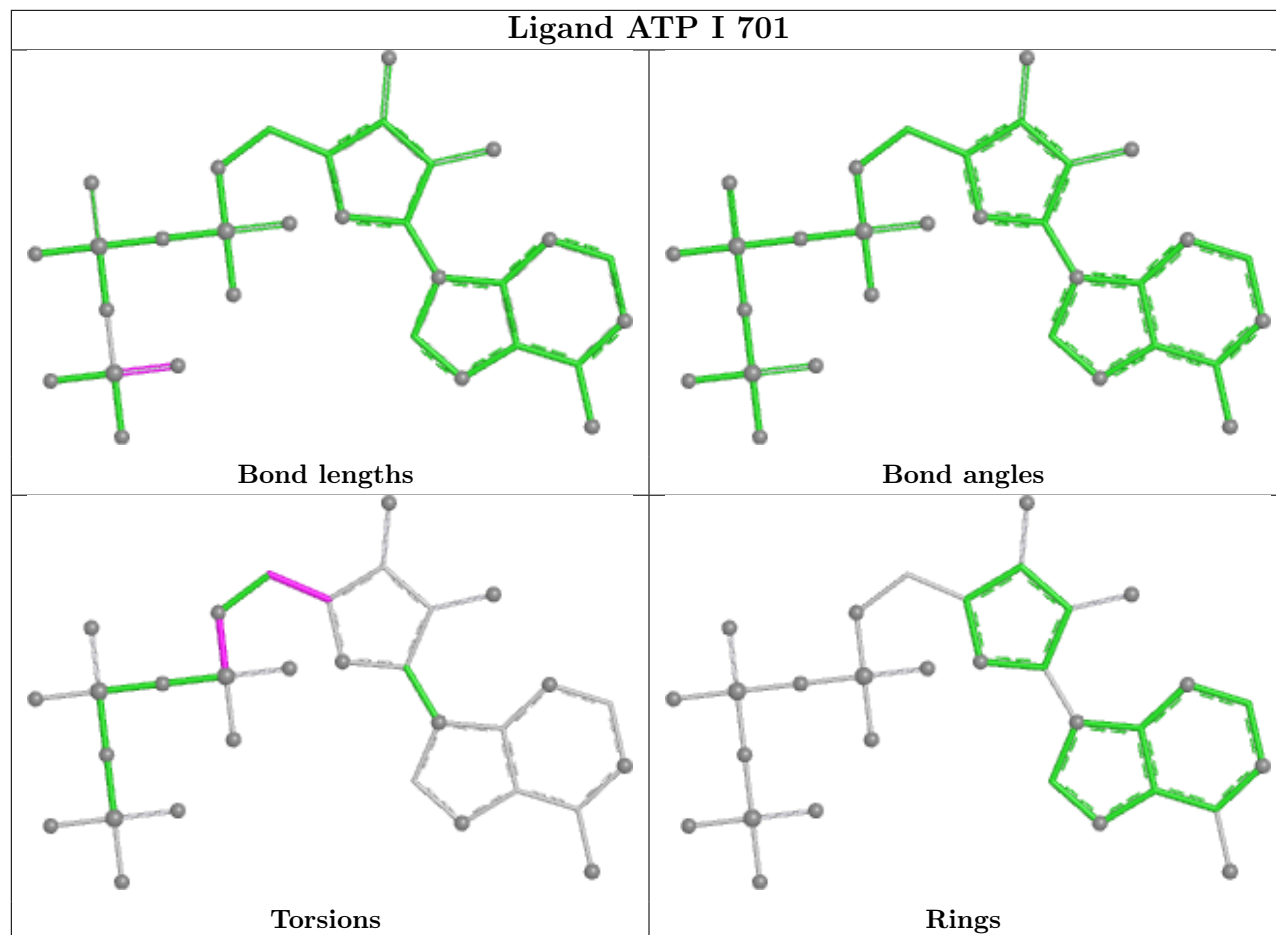
There are no ring outliers.

4 monomers are involved in 5 short contacts:

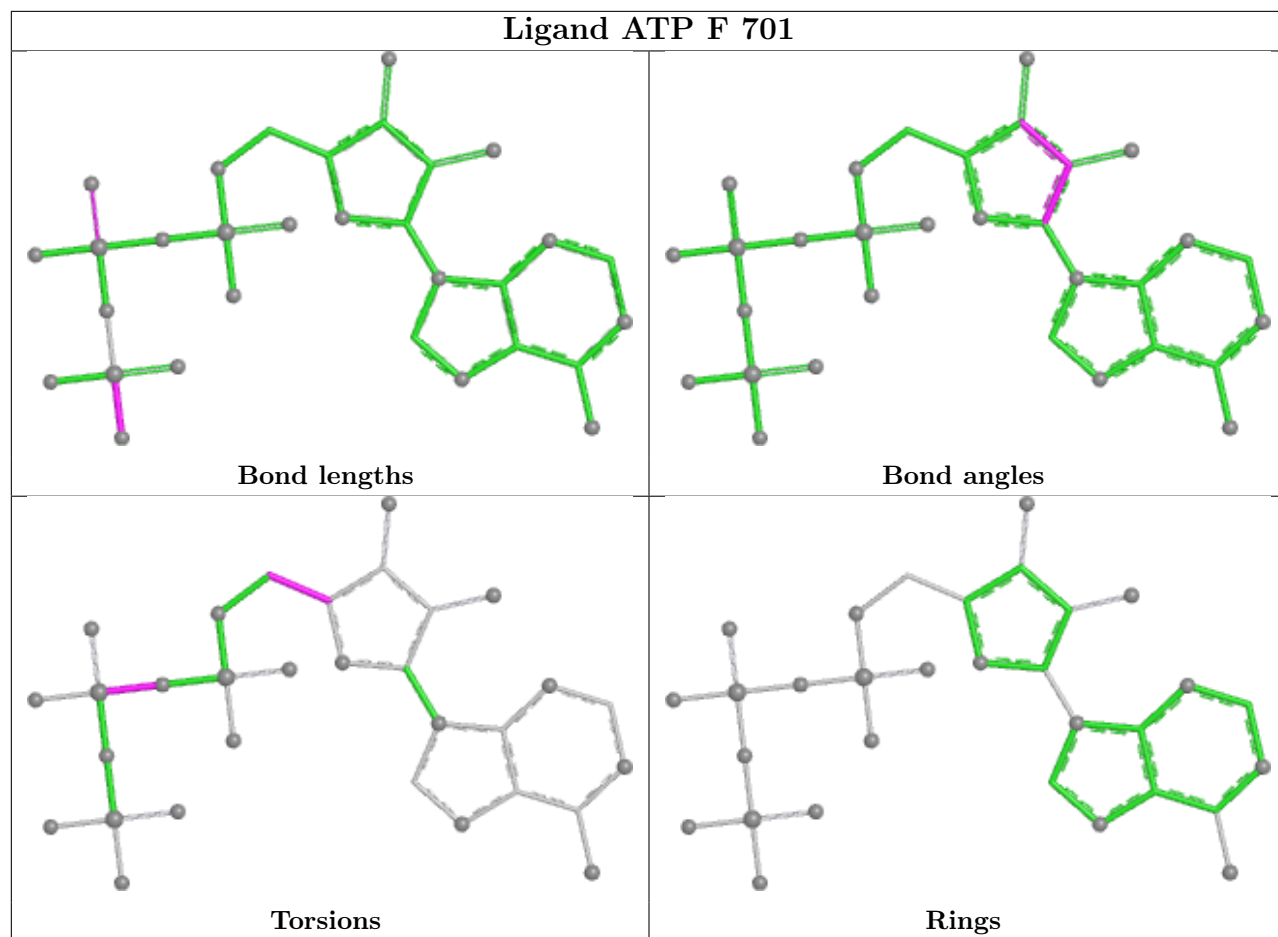
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	701	ATP	1	0
5	O	701	ATP	1	0
5	A	701	ATP	2	0
5	R	701	ATP	1	0

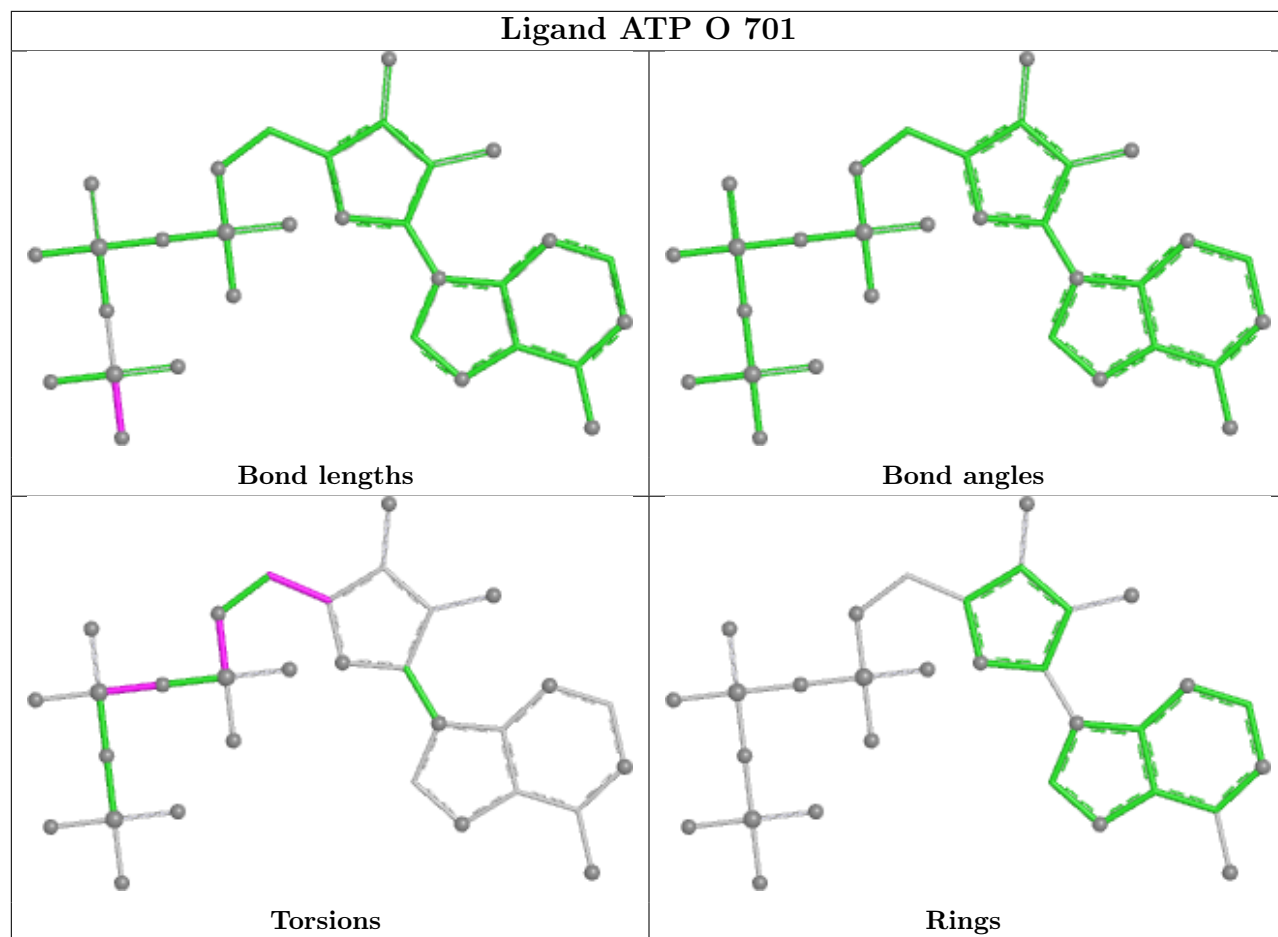
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

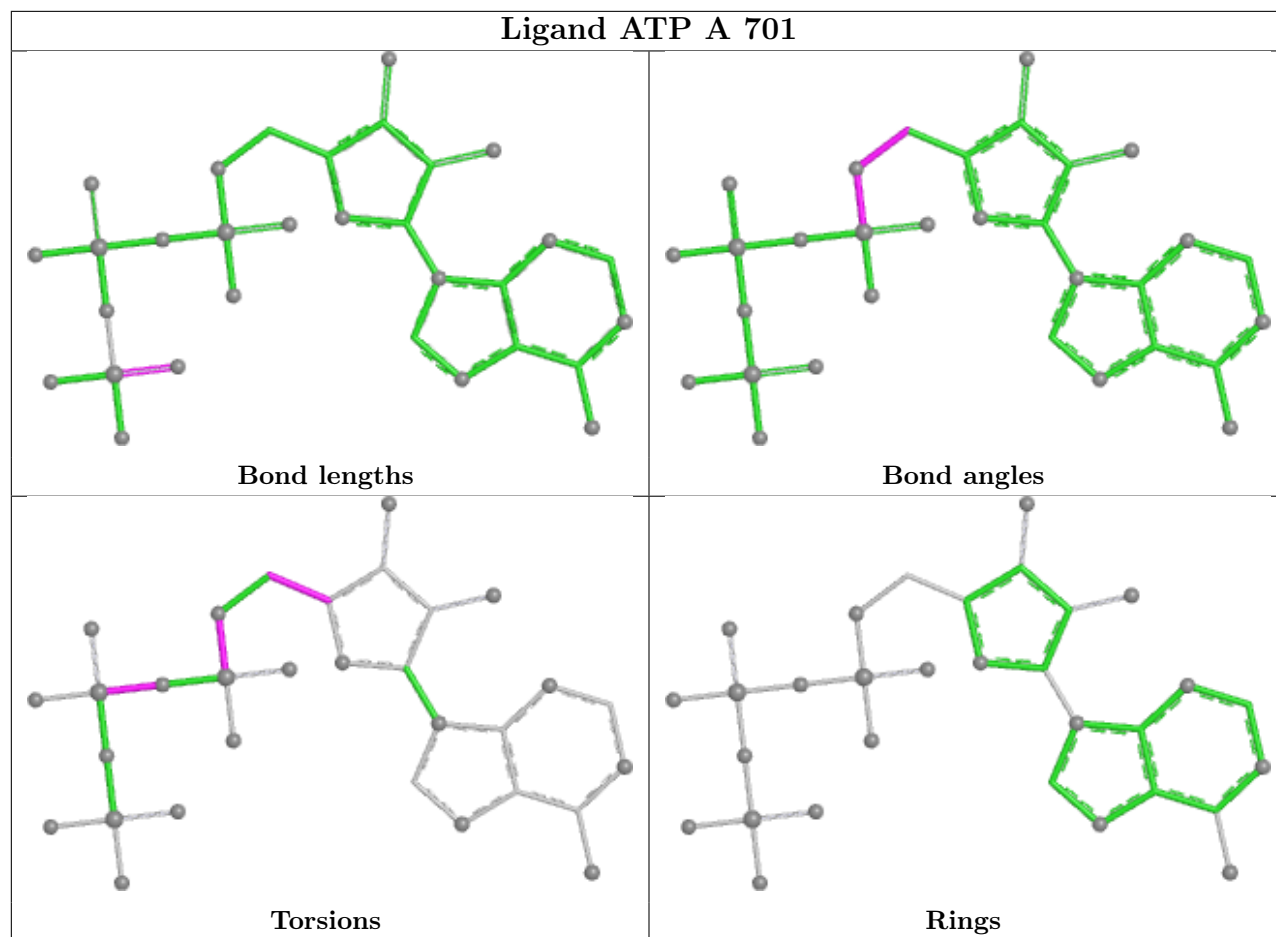
equivalents in the CSD to analyse the geometry.



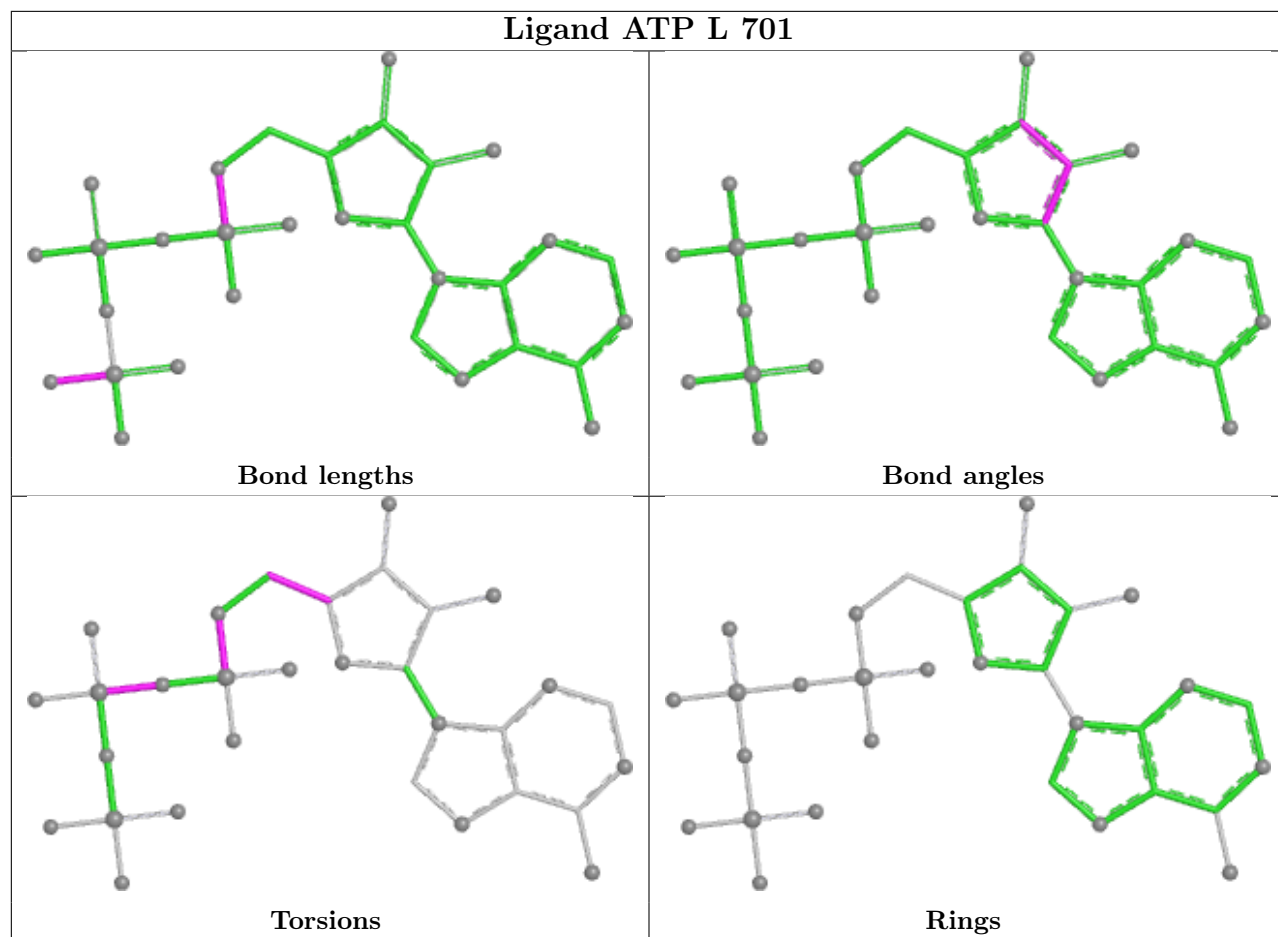
Ligand ATP F 701

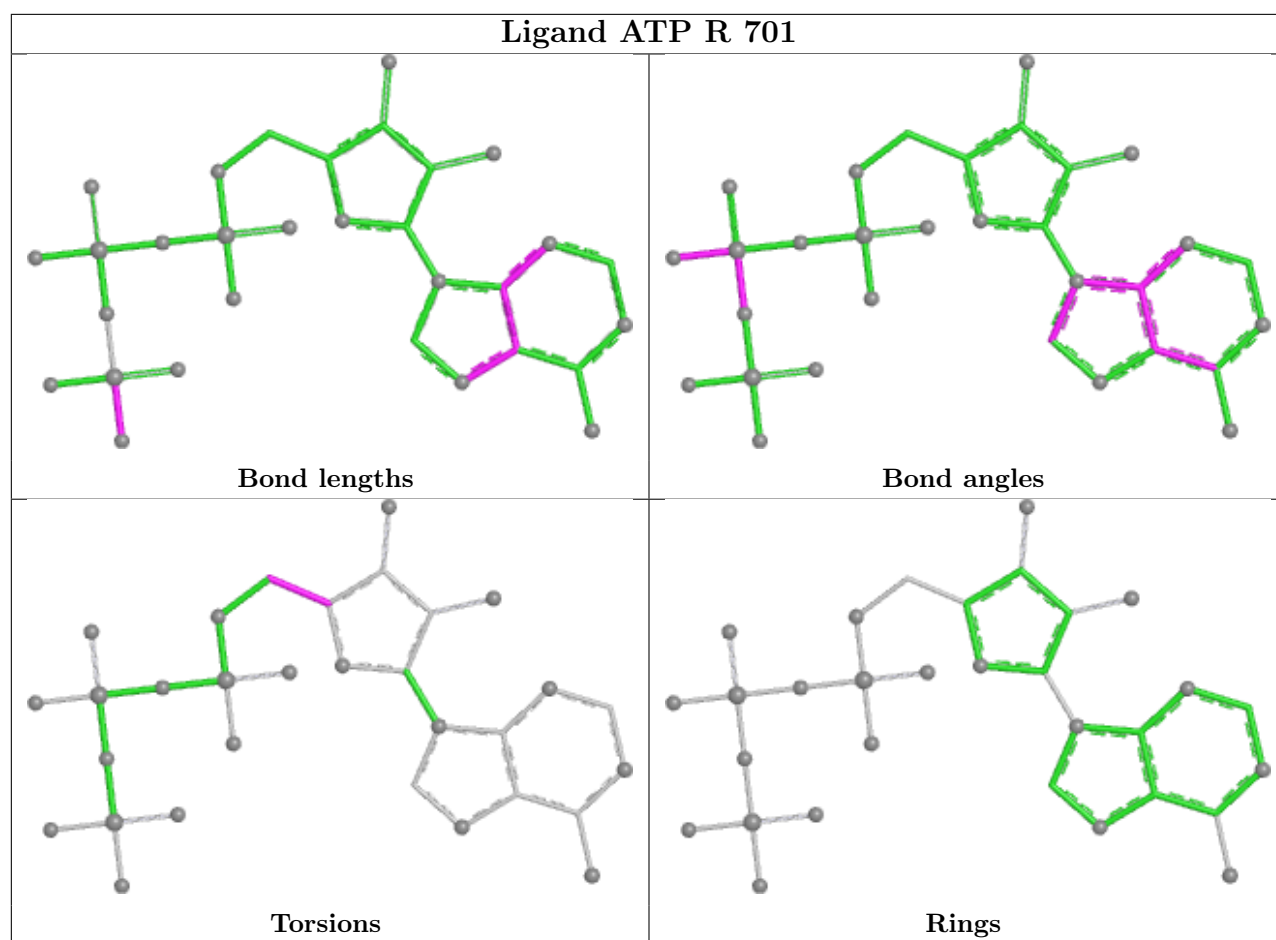






Ligand ATP L 701





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	216/229 (94%)	-0.05	2 (0%) 81 61	42, 70, 106, 115	0
1	F	209/229 (91%)	0.33	15 (7%) 21 11	14, 71, 136, 175	3 (1%)
1	I	213/229 (93%)	0.03	4 (1%) 66 43	37, 73, 110, 125	2 (0%)
1	L	215/229 (93%)	0.11	4 (1%) 66 43	43, 70, 111, 151	0
1	O	215/229 (93%)	-0.01	4 (1%) 66 43	49, 71, 99, 114	0
1	R	215/229 (93%)	0.16	4 (1%) 66 43	51, 85, 120, 153	0
2	B	126/149 (84%)	-0.18	2 (1%) 70 47	44, 63, 91, 108	0
2	G	122/149 (81%)	0.08	3 (2%) 58 35	55, 79, 110, 129	0
2	J	123/149 (82%)	0.02	1 (0%) 82 64	50, 68, 106, 121	0
2	M	124/149 (83%)	0.16	5 (4%) 42 23	46, 66, 136, 172	0
2	P	123/149 (82%)	0.09	2 (1%) 70 47	56, 82, 121, 144	0
2	S	123/149 (82%)	0.35	5 (4%) 41 23	63, 94, 126, 144	0
3	C	123/149 (82%)	0.15	2 (1%) 70 47	40, 69, 115, 158	0
3	H	123/149 (82%)	-0.03	0 100 100	43, 61, 90, 151	0
3	K	121/149 (81%)	0.14	2 (1%) 69 45	44, 72, 117, 133	0
3	N	124/149 (83%)	-0.04	2 (1%) 70 47	39, 67, 93, 113	0
3	Q	123/149 (82%)	0.13	1 (0%) 82 64	51, 79, 106, 121	0
3	T	123/149 (82%)	0.13	1 (0%) 82 64	47, 77, 112, 140	0
All	All	2761/3162 (87%)	0.09	59 (2%) 63 40	14, 73, 114, 175	5 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	542	GLY	7.2
1	F	547	THR	6.6
1	F	501	THR	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	G	122	SER	4.9
2	M	107	TYR	4.2
1	F	542	GLY	4.2
3	N	123	SER	4.1
3	C	123	SER	3.9
1	I	636	LEU	3.8
1	L	546	ILE	3.7
3	Q	123	SER	3.6
2	M	102	GLN	3.5
1	I	544	GLY	3.4
1	F	471	ILE	3.4
2	P	105	PRO	3.3
3	T	123	SER	3.1
2	S	123	SER	3.0
1	F	475	LEU	2.9
1	F	477	PRO	2.9
2	B	1	GLN	2.8
1	O	392	VAL	2.8
2	S	106	PHE	2.8
2	S	107	TYR	2.8
2	S	10	GLY	2.8
3	N	124	ALA	2.7
2	J	123	SER	2.7
2	M	106	PHE	2.7
1	F	394	MET	2.7
1	F	478	SER	2.7
3	K	121	VAL	2.6
1	A	391	GLU	2.6
1	F	402	GLU	2.5
1	A	636	LEU	2.5
1	R	391	GLU	2.4
2	S	31	ILE	2.4
1	R	610	LEU	2.4
1	F	482	ILE	2.4
2	B	126	ALA	2.3
1	R	546	ILE	2.3
2	G	105	PRO	2.3
3	C	12	VAL	2.3
1	F	636	LEU	2.2
2	P	106	PHE	2.2
1	O	636	LEU	2.2
2	M	108	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	390	THR	2.2
1	O	474	GLU	2.2
3	K	14	ALA	2.2
1	L	545	GLY	2.1
2	G	102	GLN	2.1
1	F	625	TYR	2.1
1	L	605	SER	2.1
1	O	565	ASP	2.1
1	F	392	VAL	2.0
1	L	633	LEU	2.0
1	I	448	ILE	2.0
1	F	508	PHE	2.0
1	R	630	PHE	2.0
2	M	124	ALA	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](#)

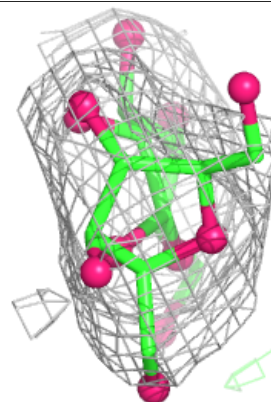
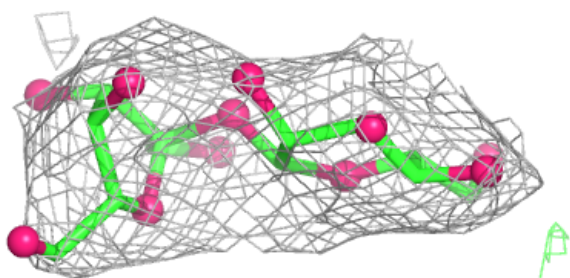
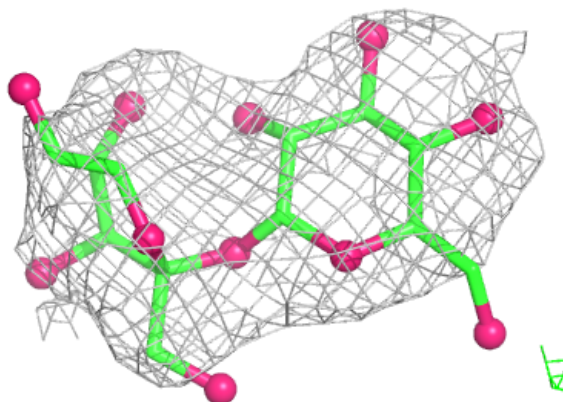
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GLC	D	1	11/12	-	-	111,113,114,114	0
4	Z9N	D	2	12/12	-	-	107,115,116,118	0
4	GLC	E	1	11/12	-	-	103,106,109,109	0
4	Z9N	E	2	12/12	-	-	106,108,110,110	0
4	Z9N	W	2	12/12	0.72	0.13	149,151,153,154	0
4	Z9N	U	2	12/12	0.76	0.15	123,130,133,135	0
4	GLC	W	1	11/12	0.79	0.19	152,154,158,159	0
4	Z9N	V	2	12/12	0.84	0.12	108,117,119,121	0
4	GLC	U	1	11/12	0.84	0.21	135,138,139,140	0
4	GLC	V	1	11/12	0.84	0.16	116,119,122,123	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.

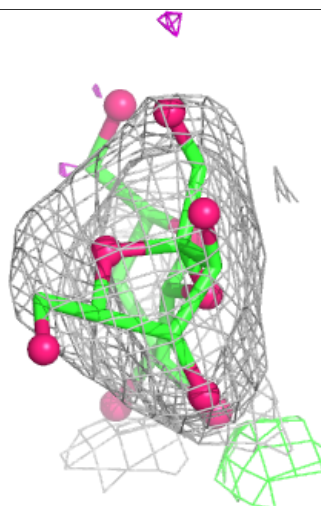
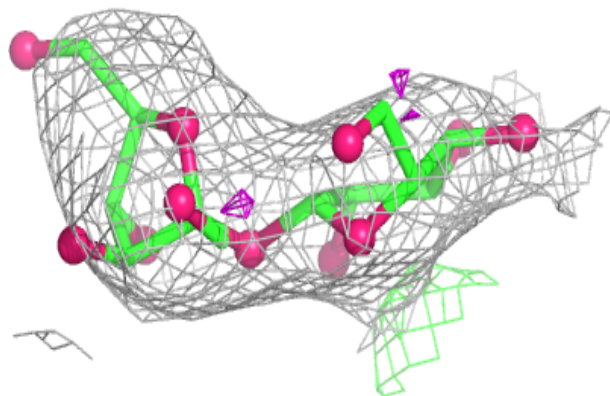
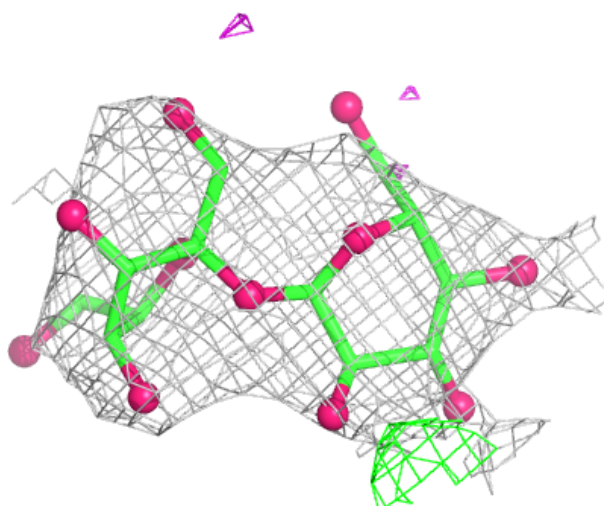
Electron density around Chain D:

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



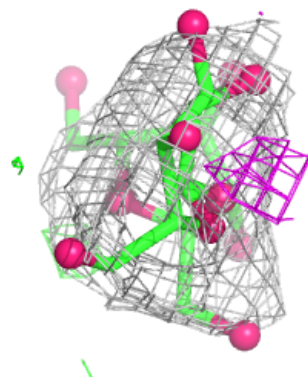
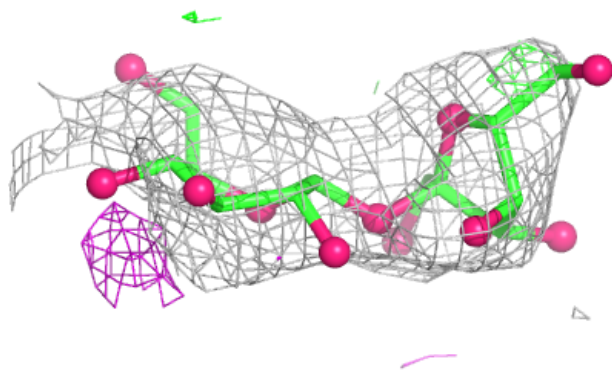
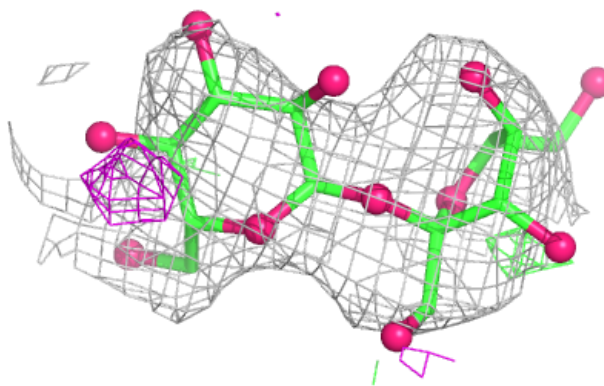
Electron density around Chain E:

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



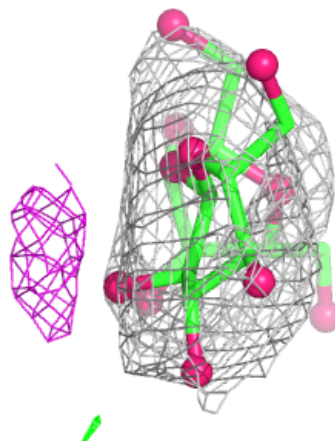
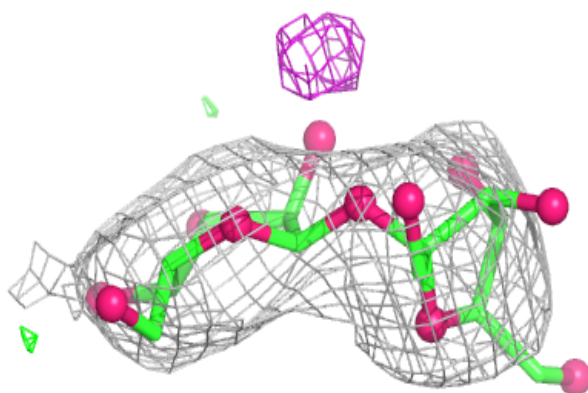
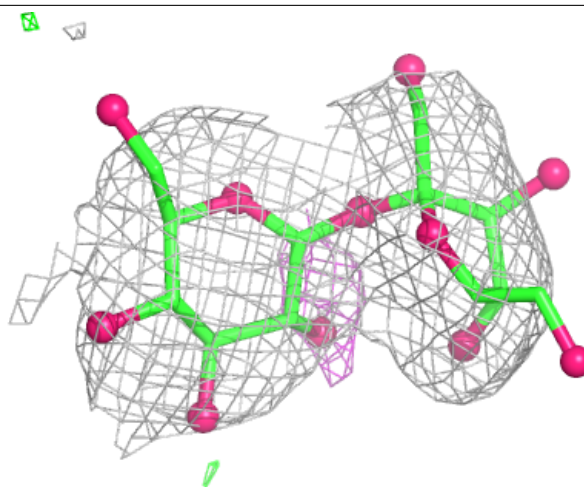
Electron density around Chain U:

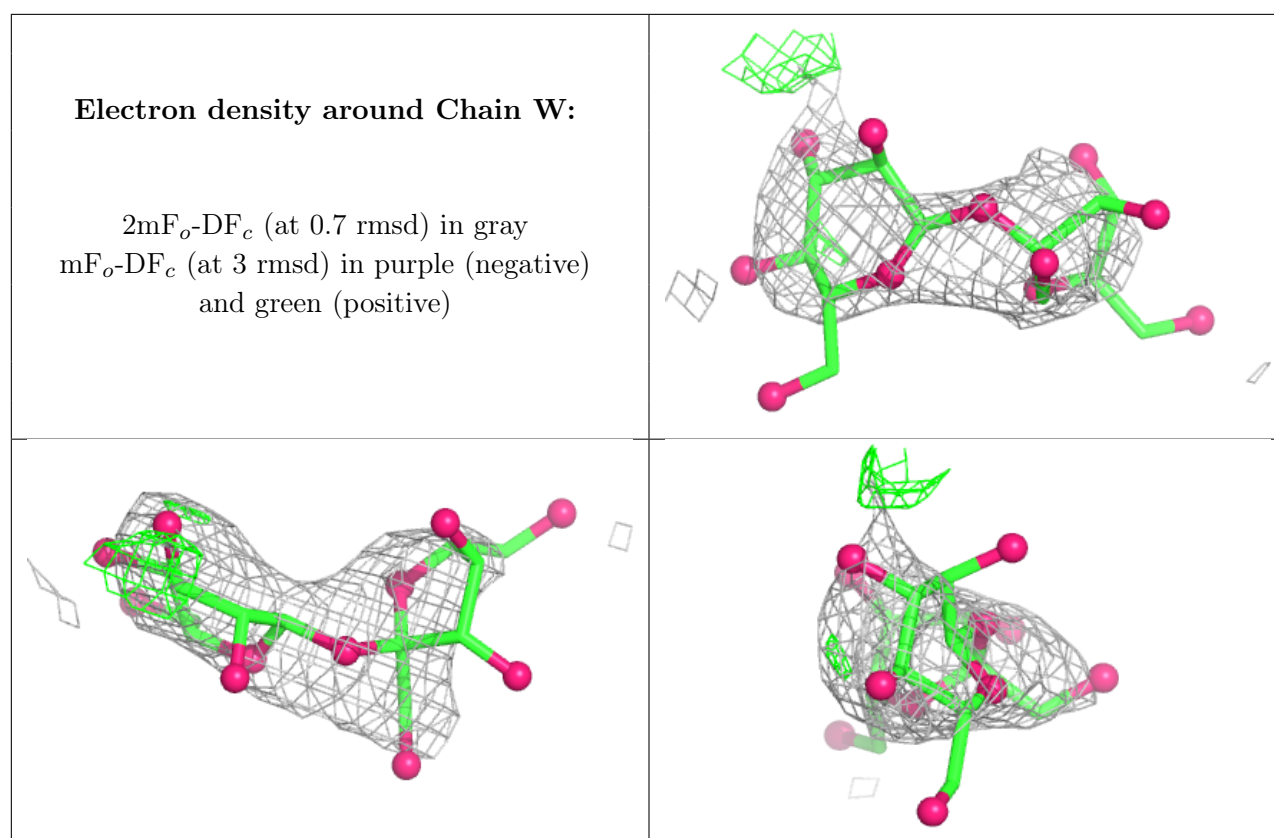
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	T	201	6/6	0.65	0.20	108,110,112,113	0
7	GOL	O	704	6/6	0.74	0.14	97,99,101,102	0
6	MG	F	703	1/1	0.81	0.15	66,66,66,66	0
5	ATP	F	701	31/31	0.92	0.07	92,100,104,105	0
5	ATP	R	701	31/31	0.94	0.08	76,92,99,100	0
6	MG	F	704	1/1	0.94	0.14	53,53,53,53	0
6	MG	A	703	1/1	0.95	0.14	67,67,67,67	0
5	ATP	I	701	31/31	0.95	0.06	49,65,75,75	0
5	ATP	L	701	31/31	0.95	0.07	62,73,83,84	0
6	MG	O	703	1/1	0.95	0.08	52,52,52,52	0
5	ATP	O	701	31/31	0.95	0.07	56,64,71,73	0
5	ATP	A	701	31/31	0.95	0.06	63,73,78,81	0
6	MG	I	702	1/1	0.96	0.09	55,55,55,55	0
6	MG	A	702	1/1	0.96	0.07	46,46,46,46	0

Continued on next page...

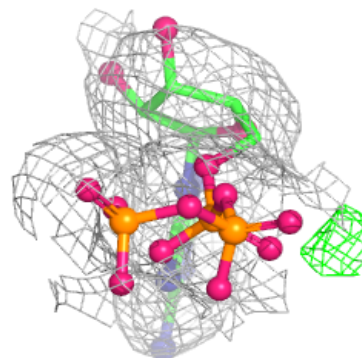
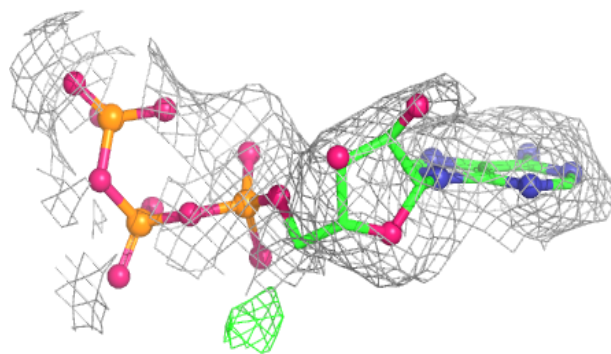
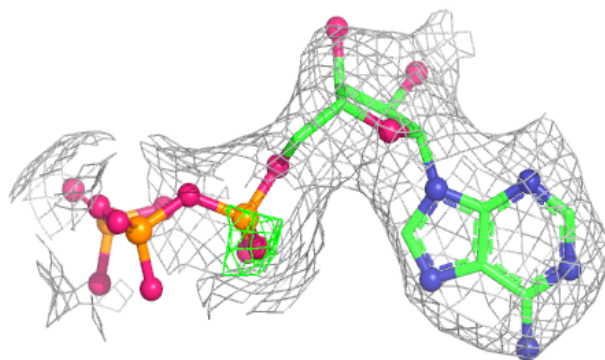
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	F	702	1/1	0.98	0.04	52,52,52,52	0
6	MG	R	702	1/1	0.98	0.07	88,88,88,88	0
6	MG	L	702	1/1	0.98	0.06	64,64,64,64	0
6	MG	O	702	1/1	0.98	0.06	53,53,53,53	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.

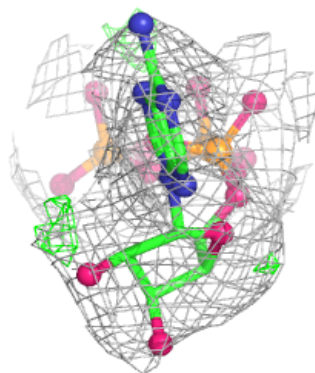
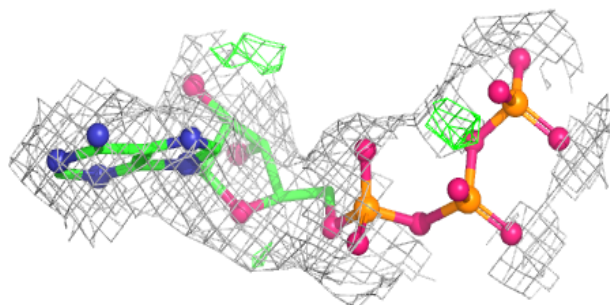
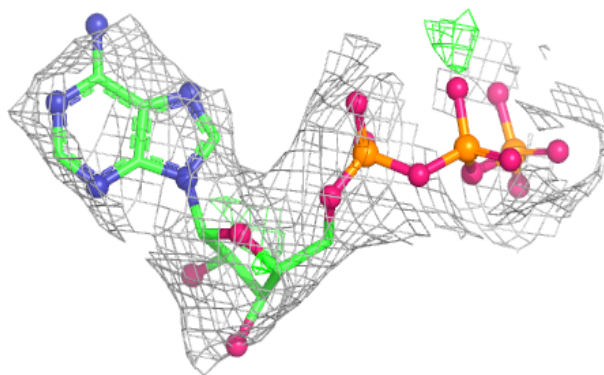
Electron density around ATP F 701:

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

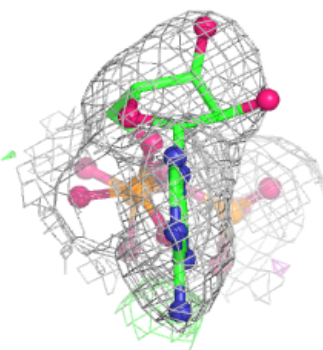
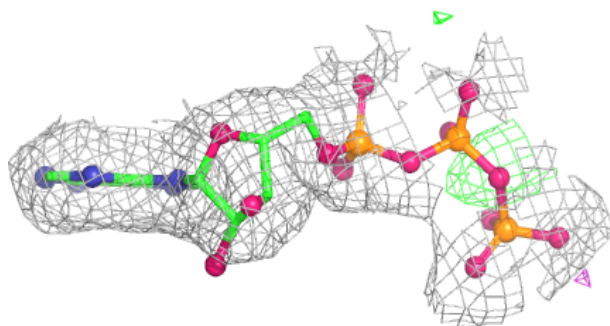
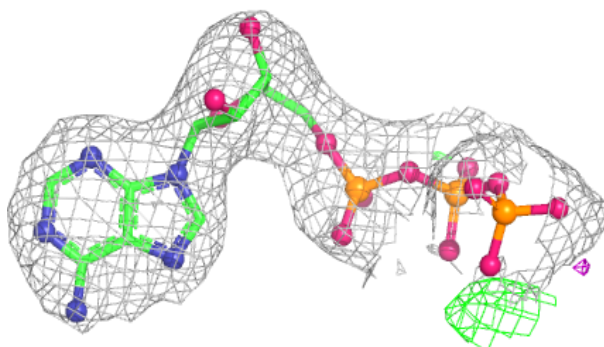


Electron density around ATP R 701:

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

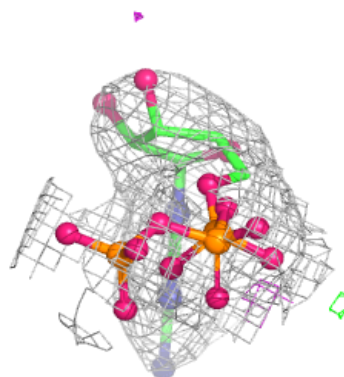
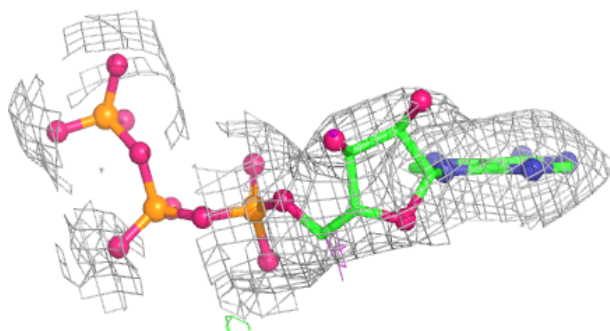
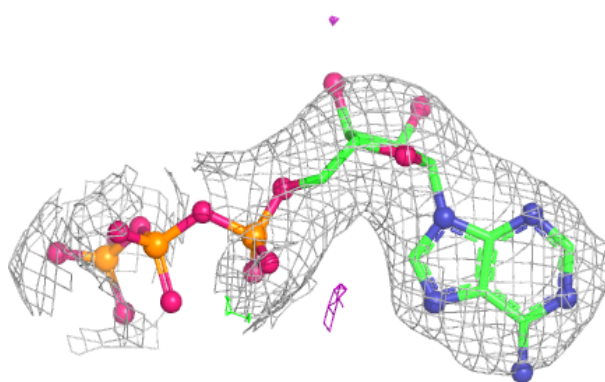
**Electron density around ATP I 701:**

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

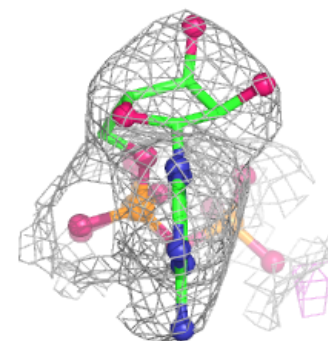
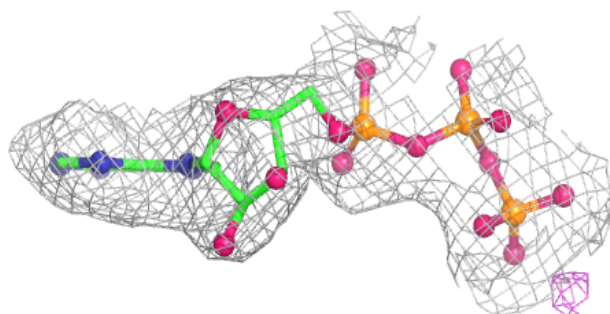
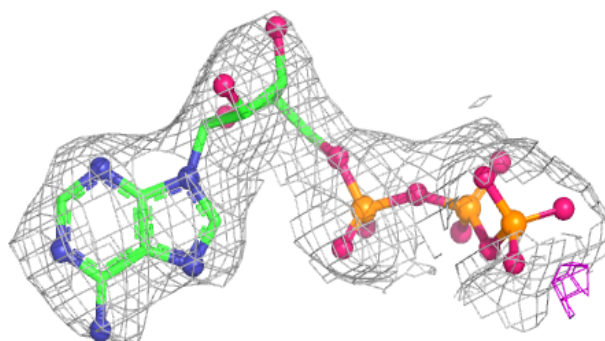


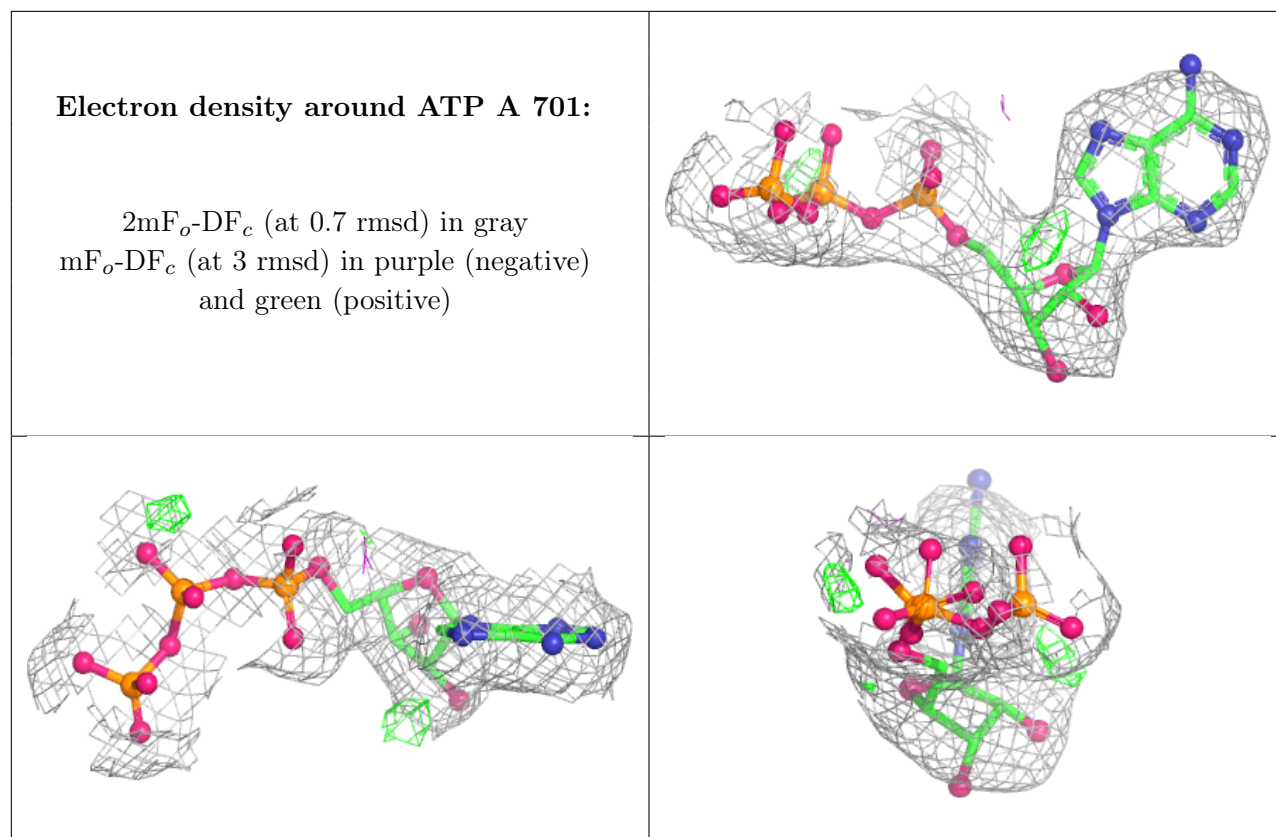
Electron density around ATP L 701:

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

**Electron density around ATP 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.