Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 01:31 pm GMT

PDB ID	:	6YSA
Title	:	Crystal structure of Arabidopsis thaliana legumain isoform beta in zymogen state
Authors	:	Dall, E.; Zauner, F.B.; Brandstetter, H.
Deposited on	:	2020-04-21
Resolution	:	2.01 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 (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:

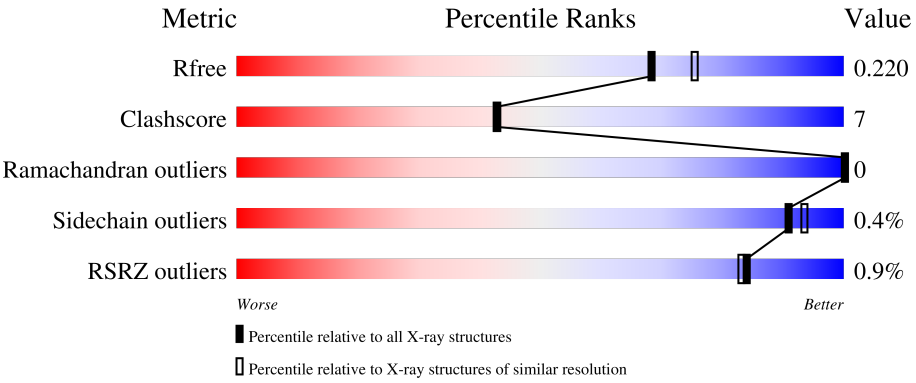
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.01 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	455	83% 9% 8%
1	B	455	83% 8% 8%
1	C	455	87% 6% 7%
1	D	455	% 85% 7% 7%
1	E	455	% 85% 8% 7%

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Mol	Chain	Length	Quality of chain
1	F	455	82% 11% 7%
1	G	455	81% 10% 8%
1	H	455	82% 10% 7%
1	I	455	82% 9% 8%
1	J	455	80% 12% 7%
1	K	455	82% 10% 7%
1	L	455	82% 11% 7%
2	M	2	100%
2	N	2	50% 50%
2	O	2	50% 50%
2	P	2	50% 50%
2	Q	2	50% 50%
2	R	2	100%
2	S	2	50% 50%
2	T	2	100%
2	U	2	50% 50%
2	V	2	100%
2	W	2	100%
2	X	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	C	503	-	-	X	-
3	SO4	D	503	-	-	X	-
3	SO4	F	503	-	-	X	-
3	SO4	G	505	-	-	X	-
3	SO4	J	507	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	L	505	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 80372 atoms, of which 38233 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 Vacuolar-processing enzyme beta-isozyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	418	Total	C	H	N	O	S	0	0	0
			6399	2050	3152	553	623	21			
1	B	417	Total	C	H	N	O	S	0	0	0
			6376	2044	3140	549	622	21			
1	C	424	Total	C	H	N	O	S	0	0	0
			6444	2076	3153	559	635	21			
1	D	423	Total	C	H	N	O	S	0	0	0
			6468	2073	3182	558	634	21			
1	E	422	Total	C	H	N	O	S	0	0	0
			6445	2064	3171	557	632	21			
1	F	422	Total	C	H	N	O	S	0	0	0
			6445	2064	3171	557	632	21			
1	G	419	Total	C	H	N	O	S	0	0	0
			6414	2055	3158	554	626	21			
1	H	422	Total	C	H	N	O	S	0	0	0
			6432	2064	3158	557	632	21			
1	I	417	Total	C	H	N	O	S	0	0	0
			6382	2044	3146	549	622	21			
1	J	422	Total	C	H	N	O	S	0	0	0
			6445	2064	3171	557	632	21			
1	K	422	Total	C	H	N	O	S	0	0	0
			6446	2064	3172	557	632	21			
1	L	423	Total	C	H	N	O	S	0	0	0
			6467	2073	3181	558	634	21			

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	SER	-	expression tag	UNP Q39044
A	33	LEU	-	expression tag	UNP Q39044
A	34	GLU	-	expression tag	UNP Q39044
A	35	HIS	-	expression tag	UNP Q39044
A	36	HIS	-	expression tag	UNP Q39044

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Chain	Residue	Modelled	Actual	Comment	Reference
A	37	HIS	-	expression tag	UNP Q39044
A	38	HIS	-	expression tag	UNP Q39044
A	39	HIS	-	expression tag	UNP Q39044
A	40	HIS	-	expression tag	UNP Q39044
A	41	GLU	-	expression tag	UNP Q39044
A	42	ASN	-	expression tag	UNP Q39044
A	43	LEU	-	expression tag	UNP Q39044
A	44	TYR	-	expression tag	UNP Q39044
A	45	PHE	-	expression tag	UNP Q39044
A	46	GLN	-	expression tag	UNP Q39044
A	168	SNN	ASP	modified residue	UNP Q39044
A	211	ALA	CYS	conflict	UNP Q39044
B	32	SER	-	expression tag	UNP Q39044
B	33	LEU	-	expression tag	UNP Q39044
B	34	GLU	-	expression tag	UNP Q39044
B	35	HIS	-	expression tag	UNP Q39044
B	36	HIS	-	expression tag	UNP Q39044
B	37	HIS	-	expression tag	UNP Q39044
B	38	HIS	-	expression tag	UNP Q39044
B	39	HIS	-	expression tag	UNP Q39044
B	40	HIS	-	expression tag	UNP Q39044
B	41	GLU	-	expression tag	UNP Q39044
B	42	ASN	-	expression tag	UNP Q39044
B	43	LEU	-	expression tag	UNP Q39044
B	44	TYR	-	expression tag	UNP Q39044
B	45	PHE	-	expression tag	UNP Q39044
B	46	GLN	-	expression tag	UNP Q39044
B	168	SNN	ASP	modified residue	UNP Q39044
B	211	ALA	CYS	conflict	UNP Q39044
C	32	SER	-	expression tag	UNP Q39044
C	33	LEU	-	expression tag	UNP Q39044
C	34	GLU	-	expression tag	UNP Q39044
C	35	HIS	-	expression tag	UNP Q39044
C	36	HIS	-	expression tag	UNP Q39044
C	37	HIS	-	expression tag	UNP Q39044
C	38	HIS	-	expression tag	UNP Q39044
C	39	HIS	-	expression tag	UNP Q39044
C	40	HIS	-	expression tag	UNP Q39044
C	41	GLU	-	expression tag	UNP Q39044
C	42	ASN	-	expression tag	UNP Q39044
C	43	LEU	-	expression tag	UNP Q39044
C	44	TYR	-	expression tag	UNP Q39044

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Chain	Residue	Modelled	Actual	Comment	Reference
C	45	PHE	-	expression tag	UNP Q39044
C	46	GLN	-	expression tag	UNP Q39044
C	168	SNN	ASP	modified residue	UNP Q39044
C	211	ALA	CYS	conflict	UNP Q39044
D	32	SER	-	expression tag	UNP Q39044
D	33	LEU	-	expression tag	UNP Q39044
D	34	GLU	-	expression tag	UNP Q39044
D	35	HIS	-	expression tag	UNP Q39044
D	36	HIS	-	expression tag	UNP Q39044
D	37	HIS	-	expression tag	UNP Q39044
D	38	HIS	-	expression tag	UNP Q39044
D	39	HIS	-	expression tag	UNP Q39044
D	40	HIS	-	expression tag	UNP Q39044
D	41	GLU	-	expression tag	UNP Q39044
D	42	ASN	-	expression tag	UNP Q39044
D	43	LEU	-	expression tag	UNP Q39044
D	44	TYR	-	expression tag	UNP Q39044
D	45	PHE	-	expression tag	UNP Q39044
D	46	GLN	-	expression tag	UNP Q39044
D	168	SNN	ASP	modified residue	UNP Q39044
D	211	ALA	CYS	conflict	UNP Q39044
E	32	SER	-	expression tag	UNP Q39044
E	33	LEU	-	expression tag	UNP Q39044
E	34	GLU	-	expression tag	UNP Q39044
E	35	HIS	-	expression tag	UNP Q39044
E	36	HIS	-	expression tag	UNP Q39044
E	37	HIS	-	expression tag	UNP Q39044
E	38	HIS	-	expression tag	UNP Q39044
E	39	HIS	-	expression tag	UNP Q39044
E	40	HIS	-	expression tag	UNP Q39044
E	41	GLU	-	expression tag	UNP Q39044
E	42	ASN	-	expression tag	UNP Q39044
E	43	LEU	-	expression tag	UNP Q39044
E	44	TYR	-	expression tag	UNP Q39044
E	45	PHE	-	expression tag	UNP Q39044
E	46	GLN	-	expression tag	UNP Q39044
E	168	SNN	ASP	modified residue	UNP Q39044
E	211	ALA	CYS	conflict	UNP Q39044
F	32	SER	-	expression tag	UNP Q39044
F	33	LEU	-	expression tag	UNP Q39044
F	34	GLU	-	expression tag	UNP Q39044
F	35	HIS	-	expression tag	UNP Q39044

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Chain	Residue	Modelled	Actual	Comment	Reference
F	36	HIS	-	expression tag	UNP Q39044
F	37	HIS	-	expression tag	UNP Q39044
F	38	HIS	-	expression tag	UNP Q39044
F	39	HIS	-	expression tag	UNP Q39044
F	40	HIS	-	expression tag	UNP Q39044
F	41	GLU	-	expression tag	UNP Q39044
F	42	ASN	-	expression tag	UNP Q39044
F	43	LEU	-	expression tag	UNP Q39044
F	44	TYR	-	expression tag	UNP Q39044
F	45	PHE	-	expression tag	UNP Q39044
F	46	GLN	-	expression tag	UNP Q39044
F	168	SNN	ASP	modified residue	UNP Q39044
F	211	ALA	CYS	conflict	UNP Q39044
G	32	SER	-	expression tag	UNP Q39044
G	33	LEU	-	expression tag	UNP Q39044
G	34	GLU	-	expression tag	UNP Q39044
G	35	HIS	-	expression tag	UNP Q39044
G	36	HIS	-	expression tag	UNP Q39044
G	37	HIS	-	expression tag	UNP Q39044
G	38	HIS	-	expression tag	UNP Q39044
G	39	HIS	-	expression tag	UNP Q39044
G	40	HIS	-	expression tag	UNP Q39044
G	41	GLU	-	expression tag	UNP Q39044
G	42	ASN	-	expression tag	UNP Q39044
G	43	LEU	-	expression tag	UNP Q39044
G	44	TYR	-	expression tag	UNP Q39044
G	45	PHE	-	expression tag	UNP Q39044
G	46	GLN	-	expression tag	UNP Q39044
G	168	SNN	ASP	modified residue	UNP Q39044
G	211	ALA	CYS	conflict	UNP Q39044
H	32	SER	-	expression tag	UNP Q39044
H	33	LEU	-	expression tag	UNP Q39044
H	34	GLU	-	expression tag	UNP Q39044
H	35	HIS	-	expression tag	UNP Q39044
H	36	HIS	-	expression tag	UNP Q39044
H	37	HIS	-	expression tag	UNP Q39044
H	38	HIS	-	expression tag	UNP Q39044
H	39	HIS	-	expression tag	UNP Q39044
H	40	HIS	-	expression tag	UNP Q39044
H	41	GLU	-	expression tag	UNP Q39044
H	42	ASN	-	expression tag	UNP Q39044
H	43	LEU	-	expression tag	UNP Q39044

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Chain	Residue	Modelled	Actual	Comment	Reference
H	44	TYR	-	expression tag	UNP Q39044
H	45	PHE	-	expression tag	UNP Q39044
H	46	GLN	-	expression tag	UNP Q39044
H	168	SNN	ASP	modified residue	UNP Q39044
H	211	ALA	CYS	conflict	UNP Q39044
I	32	SER	-	expression tag	UNP Q39044
I	33	LEU	-	expression tag	UNP Q39044
I	34	GLU	-	expression tag	UNP Q39044
I	35	HIS	-	expression tag	UNP Q39044
I	36	HIS	-	expression tag	UNP Q39044
I	37	HIS	-	expression tag	UNP Q39044
I	38	HIS	-	expression tag	UNP Q39044
I	39	HIS	-	expression tag	UNP Q39044
I	40	HIS	-	expression tag	UNP Q39044
I	41	GLU	-	expression tag	UNP Q39044
I	42	ASN	-	expression tag	UNP Q39044
I	43	LEU	-	expression tag	UNP Q39044
I	44	TYR	-	expression tag	UNP Q39044
I	45	PHE	-	expression tag	UNP Q39044
I	46	GLN	-	expression tag	UNP Q39044
I	168	SNN	ASP	modified residue	UNP Q39044
I	211	ALA	CYS	conflict	UNP Q39044
J	32	SER	-	expression tag	UNP Q39044
J	33	LEU	-	expression tag	UNP Q39044
J	34	GLU	-	expression tag	UNP Q39044
J	35	HIS	-	expression tag	UNP Q39044
J	36	HIS	-	expression tag	UNP Q39044
J	37	HIS	-	expression tag	UNP Q39044
J	38	HIS	-	expression tag	UNP Q39044
J	39	HIS	-	expression tag	UNP Q39044
J	40	HIS	-	expression tag	UNP Q39044
J	41	GLU	-	expression tag	UNP Q39044
J	42	ASN	-	expression tag	UNP Q39044
J	43	LEU	-	expression tag	UNP Q39044
J	44	TYR	-	expression tag	UNP Q39044
J	45	PHE	-	expression tag	UNP Q39044
J	46	GLN	-	expression tag	UNP Q39044
J	168	SNN	ASP	modified residue	UNP Q39044
J	211	ALA	CYS	conflict	UNP Q39044
K	32	SER	-	expression tag	UNP Q39044
K	33	LEU	-	expression tag	UNP Q39044
K	34	GLU	-	expression tag	UNP Q39044

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Chain	Residue	Modelled	Actual	Comment	Reference
K	35	HIS	-	expression tag	UNP Q39044
K	36	HIS	-	expression tag	UNP Q39044
K	37	HIS	-	expression tag	UNP Q39044
K	38	HIS	-	expression tag	UNP Q39044
K	39	HIS	-	expression tag	UNP Q39044
K	40	HIS	-	expression tag	UNP Q39044
K	41	GLU	-	expression tag	UNP Q39044
K	42	ASN	-	expression tag	UNP Q39044
K	43	LEU	-	expression tag	UNP Q39044
K	44	TYR	-	expression tag	UNP Q39044
K	45	PHE	-	expression tag	UNP Q39044
K	46	GLN	-	expression tag	UNP Q39044
K	168	SNN	ASP	modified residue	UNP Q39044
K	211	ALA	CYS	conflict	UNP Q39044
L	32	SER	-	expression tag	UNP Q39044
L	33	LEU	-	expression tag	UNP Q39044
L	34	GLU	-	expression tag	UNP Q39044
L	35	HIS	-	expression tag	UNP Q39044
L	36	HIS	-	expression tag	UNP Q39044
L	37	HIS	-	expression tag	UNP Q39044
L	38	HIS	-	expression tag	UNP Q39044
L	39	HIS	-	expression tag	UNP Q39044
L	40	HIS	-	expression tag	UNP Q39044
L	41	GLU	-	expression tag	UNP Q39044
L	42	ASN	-	expression tag	UNP Q39044
L	43	LEU	-	expression tag	UNP Q39044
L	44	TYR	-	expression tag	UNP Q39044
L	45	PHE	-	expression tag	UNP Q39044
L	46	GLN	-	expression tag	UNP Q39044
L	168	SNN	ASP	modified residue	UNP Q39044
L	211	ALA	CYS	conflict	UNP Q39044

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	2	Total	C	H	N	O	0	0	0
			51	16	23	2	10			

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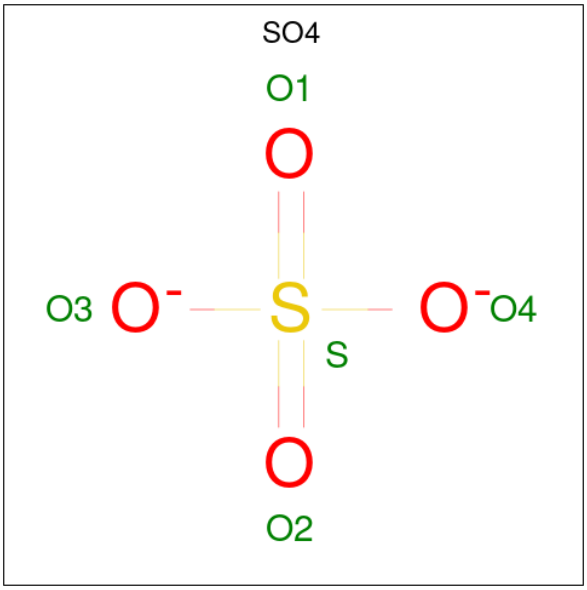
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	2	Total	C	H	N	O	0	0	0
			51	16	23	2	10			
2	O	2	Total	C	H	N	O	0	0	0
			51	16	23	2	10			
2	P	2	Total	C	H	N	O	0	0	0
			51	16	23	2	10			
2	Q	2	Total	C	H	N	O	0	0	0
			51	16	23	2	10			
2	R	2	Total	C	H	N	O	0	0	0
			51	16	23	2	10			
2	S	2	Total	C	H	N	O	0	0	0
			50	16	22	2	10			
2	T	2	Total	C	H	N	O	0	0	0
			51	16	23	2	10			
2	U	2	Total	C	H	N	O	0	0	0
			51	16	23	2	10			
2	V	2	Total	C	H	N	O	0	0	0
			51	16	23	2	10			
2	W	2	Total	C	H	N	O	0	0	0
			51	16	23	2	10			
2	X	2	Total	C	H	N	O	0	0	0
			51	16	23	2	10			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0

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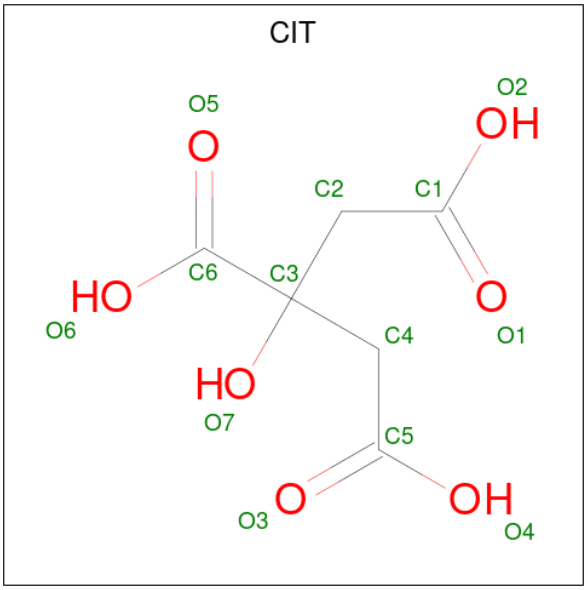
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C H O 16 6 3 7	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	216	Total O 216 216	0	0
5	B	202	Total O 202 202	0	0
5	C	183	Total O 183 183	0	0
5	D	193	Total O 193 193	0	0
5	E	180	Total O 180 180	0	0
5	F	184	Total O 184 184	0	0

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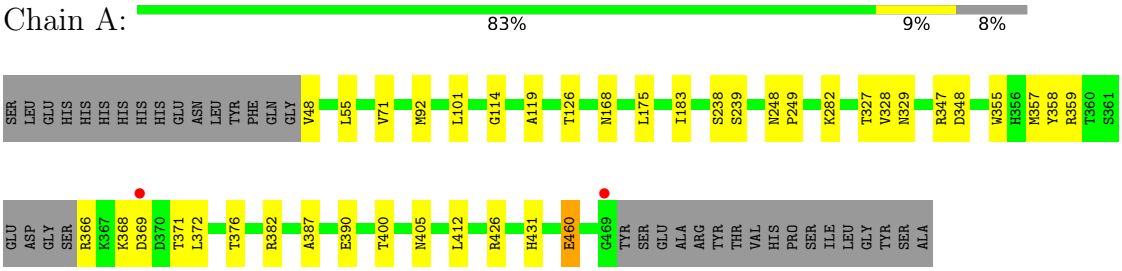
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	175	Total O 175 175	0	0
5	H	191	Total O 191 191	0	0
5	I	188	Total O 188 188	0	0
5	J	197	Total O 197 197	0	0
5	K	171	Total O 171 171	0	0
5	L	172	Total O 172 172	0	0

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.

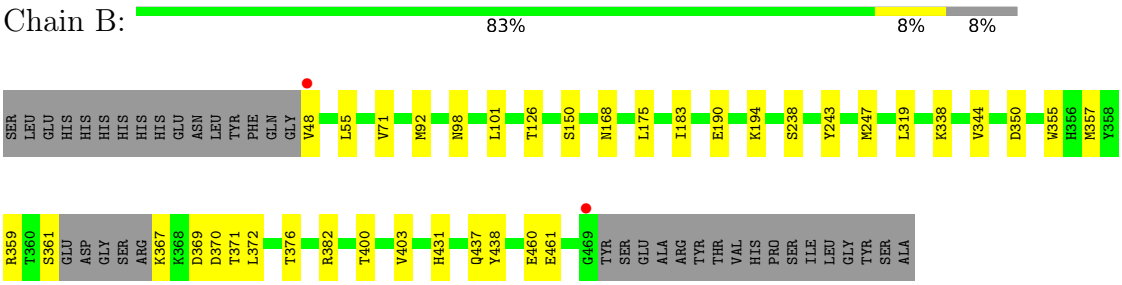
• Molecule 1: Vacuolar-processing enzyme beta-isozyme

Chain A:



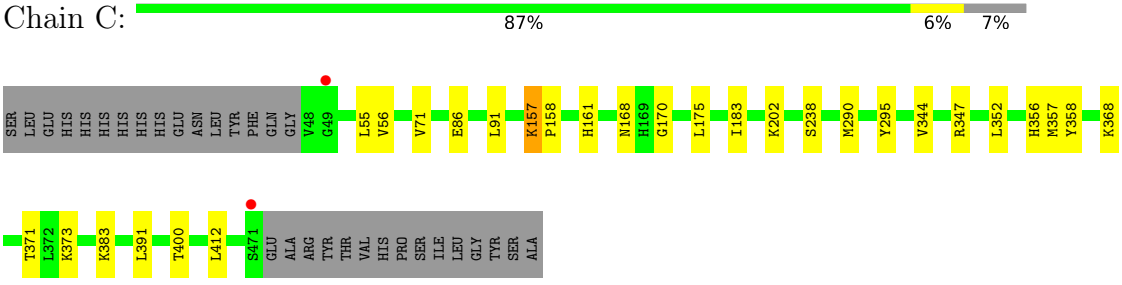
• Molecule 1: Vacuolar-processing enzyme beta-isozyme

Chain B:



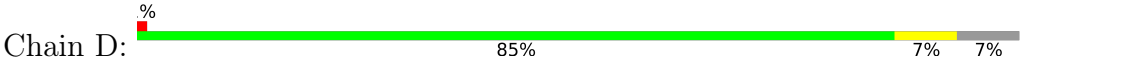
• Molecule 1: Vacuolar-processing enzyme beta-isozyme

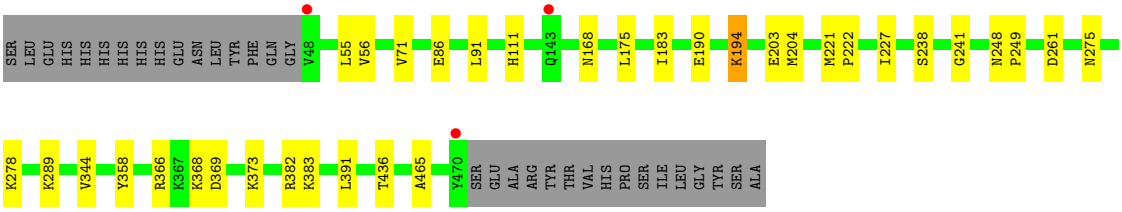
Chain C:



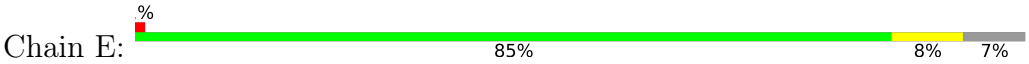
• Molecule 1: Vacuolar-processing enzyme beta-isozyme

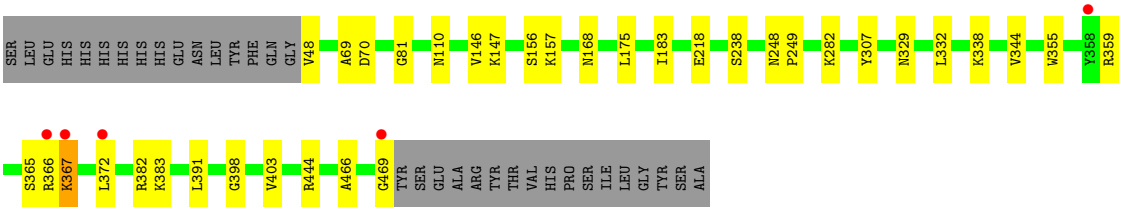
Chain D:



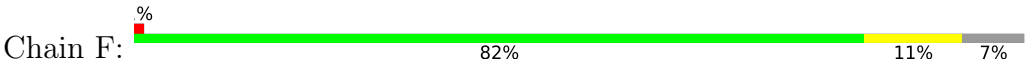


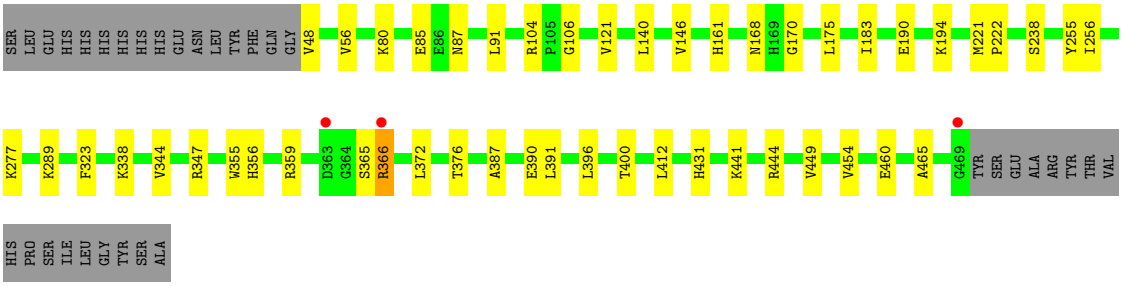
• Molecule 1: Vacuolar-processing enzyme beta-isozyme



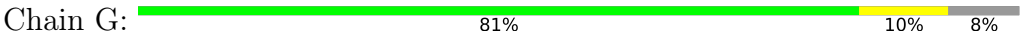


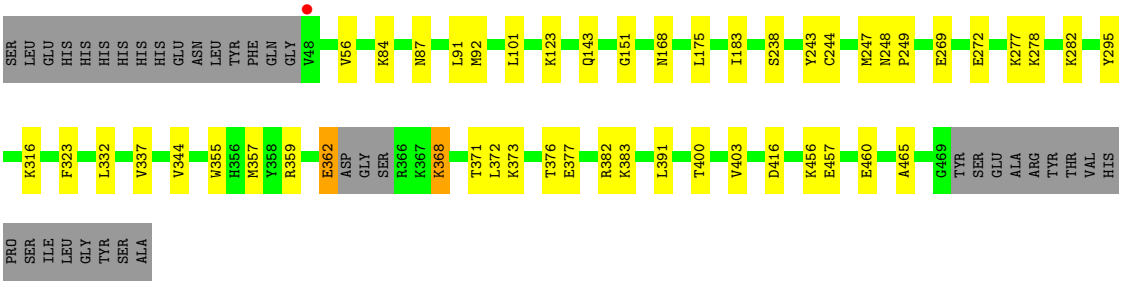
• Molecule 1: Vacuolar-processing enzyme beta-isozyme





• Molecule 1: Vacuolar-processing enzyme beta-isozyme

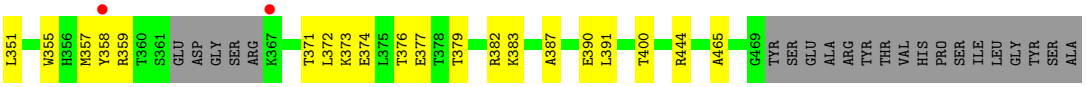




• Molecule 1: Vacuolar-processing enzyme beta-isozyme

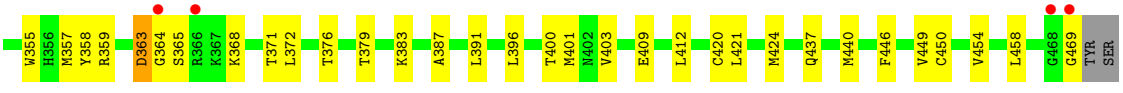
• Molecule 1: Vacuolar-processing enzyme beta-isozyme

Chain I:



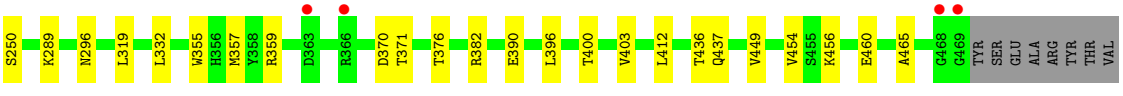
• Molecule 1: Vacuolar-processing enzyme beta-isozyme

Chain J:



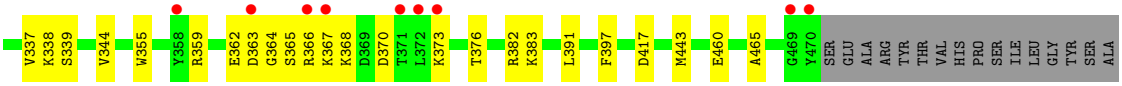
• Molecule 1: Vacuolar-processing enzyme beta-isozyme

Chain K:



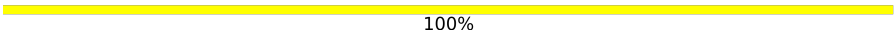
• Molecule 1: Vacuolar-processing enzyme beta-isozyme

Chain L:



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

Chain M:



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

Chain N:

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

Chain O:

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

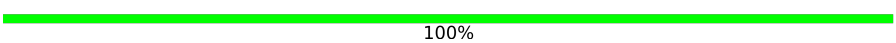
Chain P:

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

Chain Q:

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

Chain R:

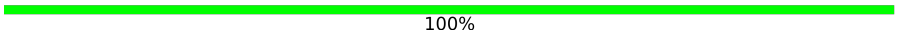


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

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

Chain T:

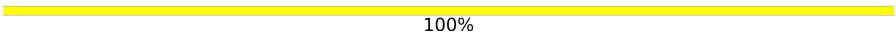


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

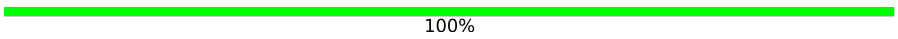
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



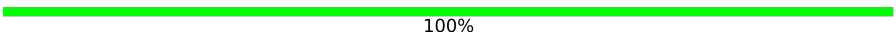
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



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

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	170.47Å 170.47Å 196.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.68 – 2.01 49.68 – 2.01	Depositor EDS
% Data completeness (in resolution range)	90.1 (49.68-2.01) 90.3 (49.68-2.01)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.209 , 0.219 0.210 , 0.220	Depositor DCC
R_{free} test set	17065 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 33.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.480 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	80372	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SNN, NAG, SO4, CIT

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	0.25	0/3315	0.43	0/4494
1	B	0.24	0/3304	0.44	0/4480
1	C	0.30	0/3361	0.45	0/4558
1	D	0.26	0/3356	0.42	0/4551
1	E	0.25	0/3343	0.44	0/4533
1	F	0.27	0/3343	0.45	0/4533
1	G	0.28	0/3324	0.45	0/4506
1	H	0.27	0/3343	0.45	0/4533
1	I	0.26	0/3304	0.44	0/4480
1	J	0.27	0/3343	0.47	0/4533
1	K	0.26	0/3343	0.45	0/4533
1	L	0.28	0/3356	0.47	0/4551
All	All	0.27	0/40035	0.45	0/54285

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3247	3152	3154	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3236	3140	3141	40	0
1	C	3291	3153	3184	27	1
1	D	3286	3182	3182	27	0
1	E	3274	3171	3173	45	0
1	F	3274	3171	3173	53	0
1	G	3256	3158	3160	43	0
1	H	3274	3158	3173	50	0
1	I	3236	3146	3141	39	0
1	J	3274	3171	3173	68	0
1	K	3274	3172	3173	60	0
1	L	3286	3181	3182	63	0
2	M	28	23	25	0	0
2	N	28	23	25	0	0
2	O	28	23	25	0	0
2	P	28	23	25	0	0
2	Q	28	23	25	0	0
2	R	28	23	25	0	0
2	S	28	22	25	1	0
2	T	28	23	25	0	0
2	U	28	23	25	0	0
2	V	28	23	25	0	0
2	W	28	23	25	0	0
2	X	28	23	25	0	0
3	A	25	0	0	2	0
3	B	30	0	0	0	0
3	C	30	0	0	4	0
3	D	20	0	0	4	0
3	E	25	0	0	1	0
3	F	35	0	0	5	0
3	G	20	0	0	2	0
3	H	35	0	0	2	0
3	I	40	0	0	0	0
3	J	25	0	0	2	0
3	K	25	0	0	3	0
3	L	20	0	0	3	0
4	E	13	3	5	0	0
5	A	216	0	0	26	0
5	B	202	0	0	19	1
5	C	183	0	0	11	0
5	D	193	0	0	16	0
5	E	180	0	0	24	1
5	F	184	0	0	24	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	175	0	0	19	0
5	H	191	0	0	22	0
5	I	188	0	0	18	0
5	J	197	0	0	45	0
5	K	171	0	0	35	0
5	L	172	0	0	33	0
All	All	42139	38233	38314	532	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (532) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:450:CYS:SG	5:J:608:HOH:O	1.90	1.29
1:I:92:MET:SD	5:I:773:HOH:O	2.04	1.16
1:G:92:MET:SD	5:G:771:HOH:O	2.04	1.15
1:A:366:ARG:HA	5:B:605:HOH:O	1.46	1.13
1:K:64:ASN:CB	5:K:606:HOH:O	1.95	1.13
1:B:48:VAL:CG2	1:B:319:LEU:HD22	1.79	1.12
1:D:369:ASP:N	5:D:601:HOH:O	1.82	1.10
1:L:362:GLU:HB3	5:L:605:HOH:O	1.54	1.07
1:J:365:SER:N	5:J:603:HOH:O	1.87	1.06
1:K:48:VAL:HG22	1:K:319:LEU:HD22	1.09	1.06
1:K:48:VAL:HG22	1:K:319:LEU:CD2	1.85	1.05
1:E:444:ARG:NH1	5:E:603:HOH:O	1.91	1.04
1:F:161:HIS:CG	5:F:604:HOH:O	2.09	1.04
1:A:239:SER:HB2	5:A:606:HOH:O	1.58	1.04
1:B:48:VAL:HG21	1:B:319:LEU:CD2	1.87	1.04
1:E:366:ARG:C	5:E:601:HOH:O	1.96	1.03
1:J:143:GLN:HG3	5:J:609:HOH:O	1.58	1.03
1:E:70:ASP:N	5:E:602:HOH:O	1.89	1.03
1:L:86:GLU:CD	5:L:601:HOH:O	1.97	1.01
1:K:71:VAL:HG23	5:K:603:HOH:O	1.61	1.01
1:B:247:MET:SD	5:B:790:HOH:O	2.18	1.01
1:K:48:VAL:CG2	1:K:319:LEU:HD22	1.90	1.01
1:F:161:HIS:CE1	5:F:604:HOH:O	2.11	1.01
1:E:382:ARG:NH2	5:E:604:HOH:O	1.92	1.00
1:K:71:VAL:CB	5:K:603:HOH:O	2.08	1.00
1:K:71:VAL:CG2	5:K:603:HOH:O	2.07	0.99
1:K:48:VAL:CG2	1:K:319:LEU:CD2	2.40	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:VAL:HG21	1:B:319:LEU:HD22	1.42	0.99
1:B:361:SER:O	5:B:601:HOH:O	1.80	0.99
1:J:143:GLN:CG	5:J:609:HOH:O	2.10	0.98
1:E:365:SER:O	5:E:601:HOH:O	1.81	0.98
1:F:390:GLU:OE1	5:F:601:HOH:O	1.81	0.98
1:A:348:ASP:OD1	5:A:601:HOH:O	1.80	0.97
1:K:71:VAL:HB	5:K:603:HOH:O	1.65	0.97
1:K:87:ASN:CG	5:K:601:HOH:O	2.02	0.97
1:F:161:HIS:CD2	5:F:604:HOH:O	2.17	0.96
1:J:401:MET:O	5:J:601:HOH:O	1.82	0.96
1:K:87:ASN:OD1	5:K:601:HOH:O	1.82	0.96
1:F:161:HIS:ND1	5:F:604:HOH:O	1.94	0.96
1:E:367:LYS:N	5:E:601:HOH:O	1.97	0.95
1:H:409:GLU:OE1	5:H:601:HOH:O	1.84	0.95
1:J:350:ASP:OD1	5:J:602:HOH:O	1.85	0.95
1:C:347:ARG:NH2	5:C:603:HOH:O	2.01	0.94
1:I:465:ALA:O	5:I:601:HOH:O	1.86	0.94
5:G:623:HOH:O	2:S:1:NAG:H83	1.68	0.94
1:K:64:ASN:HB3	5:K:606:HOH:O	1.62	0.93
1:A:348:ASP:OD2	5:A:602:HOH:O	1.84	0.93
3:G:505:SO4:O2	5:G:601:HOH:O	1.87	0.92
1:H:367:LYS:HA	5:H:602:HOH:O	1.68	0.92
1:I:374:GLU:OE2	5:I:602:HOH:O	1.88	0.92
1:A:239:SER:CB	5:A:606:HOH:O	2.14	0.92
1:K:106:GLY:O	5:K:604:HOH:O	1.88	0.92
1:I:444:ARG:NH1	5:I:604:HOH:O	2.01	0.91
1:K:403:VAL:O	5:K:602:HOH:O	1.87	0.91
1:L:86:GLU:OE2	5:L:601:HOH:O	1.83	0.91
1:J:421:LEU:HA	5:J:606:HOH:O	1.68	0.91
1:B:190:GLU:OE1	5:B:602:HOH:O	1.87	0.90
1:C:412:LEU:O	5:C:601:HOH:O	1.87	0.90
1:F:146:VAL:O	5:F:602:HOH:O	1.89	0.90
1:B:150:SER:O	5:B:604:HOH:O	1.88	0.89
1:K:67:HIS:O	5:K:603:HOH:O	1.88	0.89
1:H:366:ARG:O	5:H:602:HOH:O	1.89	0.89
1:L:417:ASP:OD1	5:L:602:HOH:O	1.91	0.89
1:L:460:GLU:OE2	5:L:603:HOH:O	1.91	0.89
1:K:437:GLN:OE1	5:K:605:HOH:O	1.91	0.89
1:G:403:VAL:O	5:G:602:HOH:O	1.89	0.88
3:A:503:SO4:O2	5:A:603:HOH:O	1.90	0.88
1:F:460:GLU:OE1	5:F:603:HOH:O	1.90	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:59:SER:OG	5:K:606:HOH:O	1.91	0.87
1:J:421:LEU:CA	5:J:606:HOH:O	2.20	0.87
1:H:383:LYS:HD2	1:I:387:ALA:HB2	1.54	0.87
1:J:437:GLN:HA	5:J:605:HOH:O	1.74	0.87
1:L:363:ASP:N	5:L:605:HOH:O	2.07	0.87
1:B:370:ASP:CG	5:B:606:HOH:O	2.12	0.86
1:J:363:ASP:O	5:J:603:HOH:O	1.93	0.86
3:J:507:SO4:O2	5:J:604:HOH:O	1.91	0.86
1:J:437:GLN:O	5:J:605:HOH:O	1.91	0.86
1:C:347:ARG:NE	5:C:603:HOH:O	2.09	0.86
1:G:295:TYR:O	5:G:603:HOH:O	1.92	0.86
1:J:421:LEU:O	5:J:606:HOH:O	1.92	0.85
1:B:48:VAL:HG22	1:B:319:LEU:HD22	1.58	0.85
1:F:460:GLU:CD	5:F:603:HOH:O	2.15	0.85
1:K:370:ASP:HB3	5:K:613:HOH:O	1.75	0.85
1:L:196:HIS:CD2	1:L:225:LEU:HA	2.12	0.85
1:H:390:GLU:CD	5:H:606:HOH:O	2.15	0.85
1:I:64:ASN:OD1	5:I:603:HOH:O	1.94	0.85
1:L:367:LYS:CB	5:L:613:HOH:O	2.26	0.84
1:G:143:GLN:NE2	1:G:151:GLY:O	2.09	0.84
1:J:334:GLU:OE1	5:J:607:HOH:O	1.94	0.84
1:B:369:ASP:OD1	5:B:605:HOH:O	1.94	0.84
1:F:359:ARG:NH2	5:F:607:HOH:O	2.11	0.84
1:K:59:SER:CB	5:K:606:HOH:O	2.25	0.83
1:E:110:ASN:OD1	5:E:602:HOH:O	1.96	0.83
1:C:347:ARG:CZ	5:C:603:HOH:O	2.27	0.83
1:J:144:LYS:N	5:J:609:HOH:O	2.03	0.82
1:A:114:GLY:O	5:A:604:HOH:O	1.97	0.82
1:L:460:GLU:HG3	5:L:603:HOH:O	1.78	0.82
1:B:367:LYS:N	5:B:608:HOH:O	2.11	0.82
3:C:503:SO4:O1	5:C:602:HOH:O	1.96	0.82
1:J:446:PHE:O	5:J:608:HOH:O	1.97	0.82
1:J:350:ASP:N	5:J:612:HOH:O	2.12	0.82
1:L:460:GLU:CD	5:L:603:HOH:O	2.18	0.81
1:H:59:SER:O	5:H:603:HOH:O	1.98	0.81
1:J:421:LEU:C	5:J:606:HOH:O	2.17	0.81
1:L:364:GLY:O	1:L:366:ARG:NH1	2.14	0.81
1:A:390:GLU:OE1	5:A:605:HOH:O	1.99	0.81
1:L:460:GLU:CG	5:L:603:HOH:O	2.29	0.81
1:B:338:LYS:CE	5:B:603:HOH:O	2.22	0.80
1:B:338:LYS:NZ	5:B:603:HOH:O	1.87	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:460:GLU:OE2	5:F:603:HOH:O	1.98	0.80
1:L:367:LYS:HB2	5:L:613:HOH:O	1.78	0.80
1:B:370:ASP:OD1	5:B:606:HOH:O	2.01	0.78
3:D:503:SO4:O3	5:D:602:HOH:O	2.01	0.78
1:K:454:VAL:O	5:K:608:HOH:O	2.00	0.78
1:K:412:LEU:O	5:K:609:HOH:O	2.00	0.78
5:A:612:HOH:O	1:H:332:LEU:HG	1.83	0.78
1:B:48:VAL:CG2	1:B:319:LEU:CD2	2.54	0.78
1:C:371:THR:O	5:C:604:HOH:O	2.02	0.78
1:G:416:ASP:OD1	5:G:606:HOH:O	2.01	0.78
1:F:85:GLU:OE1	5:F:605:HOH:O	2.01	0.77
1:E:403:VAL:O	5:E:605:HOH:O	2.02	0.77
1:B:101:LEU:O	5:B:607:HOH:O	2.02	0.77
1:I:382:ARG:NH2	5:I:607:HOH:O	2.18	0.77
1:J:424:MET:HB2	5:J:606:HOH:O	1.84	0.77
1:F:87:ASN:ND2	5:F:609:HOH:O	2.14	0.76
1:I:104:ARG:NH2	1:I:254:GLU:OE2	2.18	0.76
1:J:48:VAL:HG22	1:J:319:LEU:CD2	2.16	0.76
1:J:469:GLY:HA3	5:J:625:HOH:O	1.84	0.76
1:G:457:GLU:OE1	5:G:607:HOH:O	2.04	0.76
1:A:390:GLU:HB2	5:A:605:HOH:O	1.85	0.76
3:K:505:SO4:O3	5:K:610:HOH:O	2.04	0.75
1:E:466:ALA:O	5:E:606:HOH:O	2.03	0.75
1:J:420:CYS:O	5:J:606:HOH:O	2.06	0.74
1:J:440:MET:HE2	5:J:605:HOH:O	1.88	0.74
1:L:382:ARG:NH1	5:L:604:HOH:O	2.07	0.74
1:E:382:ARG:CZ	5:E:604:HOH:O	2.34	0.73
1:E:81:GLY:O	5:E:607:HOH:O	2.06	0.73
1:F:347:ARG:NH2	3:F:503:SO4:O4	2.21	0.73
1:C:347:ARG:NH1	3:C:503:SO4:O3	2.22	0.72
1:I:133:ALA:O	5:I:605:HOH:O	2.07	0.72
1:K:59:SER:HB2	5:K:606:HOH:O	1.86	0.72
1:J:350:ASP:CG	5:J:602:HOH:O	2.25	0.72
1:L:367:LYS:CA	5:L:613:HOH:O	2.37	0.72
3:F:507:SO4:O3	5:F:606:HOH:O	2.08	0.71
1:I:373:LYS:O	1:I:377:GLU:HG3	1.91	0.71
1:A:101:LEU:O	5:A:607:HOH:O	2.09	0.71
1:D:86:GLU:HG2	5:D:768:HOH:O	1.89	0.71
1:E:382:ARG:NE	5:E:604:HOH:O	2.22	0.71
1:H:203:GLU:OE1	5:H:604:HOH:O	2.07	0.71
1:J:338:LYS:CE	5:J:611:HOH:O	2.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:88:ILE:O	5:H:605:HOH:O	2.08	0.70
1:E:69:ALA:C	5:E:602:HOH:O	2.24	0.70
1:C:347:ARG:NH1	3:C:503:SO4:S	2.64	0.70
3:G:505:SO4:O1	5:G:608:HOH:O	2.10	0.69
1:F:347:ARG:NH2	3:F:503:SO4:S	2.66	0.69
3:D:503:SO4:S	5:D:602:HOH:O	2.51	0.69
1:A:48:VAL:HG12	1:A:48:VAL:O	1.91	0.69
1:K:382:ARG:NH1	5:K:611:HOH:O	2.10	0.68
1:K:101:LEU:HB3	5:K:614:HOH:O	1.92	0.68
1:L:196:HIS:HD2	1:L:225:LEU:HA	1.58	0.68
1:F:106:GLY:O	5:F:608:HOH:O	2.11	0.68
1:J:454:VAL:O	5:J:613:HOH:O	2.12	0.68
1:K:296:ASN:OD1	5:K:612:HOH:O	2.11	0.68
1:A:358:TYR:CE2	5:A:612:HOH:O	2.47	0.67
1:J:450:CYS:CB	5:J:608:HOH:O	2.31	0.67
1:H:90:VAL:HG23	5:H:605:HOH:O	1.94	0.67
1:H:390:GLU:OE2	5:H:606:HOH:O	2.10	0.67
1:H:48:VAL:O	5:H:607:HOH:O	2.11	0.67
1:H:361:SER:OG	1:H:367:LYS:NZ	2.28	0.67
1:L:339:SER:HB2	5:L:609:HOH:O	1.93	0.67
1:L:417:ASP:CG	5:L:602:HOH:O	2.32	0.66
3:D:503:SO4:O4	5:D:602:HOH:O	2.13	0.66
1:B:338:LYS:HE2	5:B:603:HOH:O	1.88	0.66
1:C:352:LEU:HD11	5:C:611:HOH:O	1.96	0.66
1:A:358:TYR:HE2	5:A:612:HOH:O	1.78	0.66
1:D:203:GLU:OE1	5:D:603:HOH:O	2.13	0.65
1:H:146:VAL:O	5:H:608:HOH:O	2.13	0.65
1:I:390:GLU:HB2	5:I:615:HOH:O	1.95	0.65
1:L:366:ARG:O	1:L:370:ASP:N	2.29	0.65
1:J:338:LYS:HE2	5:J:611:HOH:O	1.96	0.65
1:J:437:GLN:CA	5:J:605:HOH:O	2.39	0.65
1:D:190:GLU:OE1	5:D:604:HOH:O	2.14	0.64
1:J:48:VAL:HG22	1:J:319:LEU:HD22	1.78	0.64
1:L:365:SER:HB2	5:L:613:HOH:O	1.95	0.64
1:L:367:LYS:N	5:L:613:HOH:O	2.29	0.64
1:J:363:ASP:C	5:J:603:HOH:O	2.35	0.64
1:H:190:GLU:O	1:H:194:LYS:HG3	1.98	0.64
1:H:390:GLU:OE1	1:I:383:LYS:NZ	2.23	0.63
1:L:359:ARG:NH2	5:L:616:HOH:O	2.32	0.63
1:J:278:LYS:NZ	3:J:507:SO4:O4	2.25	0.63
1:A:400:THR:HG21	1:D:344:VAL:HG23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:506:SO4:O2	5:A:608:HOH:O	2.16	0.63
1:K:48:VAL:HG21	1:K:319:LEU:CD2	2.28	0.62
1:J:364:GLY:C	5:J:603:HOH:O	2.30	0.62
1:J:358:TYR:CE1	1:J:368:LYS:HE2	2.34	0.62
1:L:338:LYS:NZ	3:L:506:SO4:O1	2.31	0.62
1:D:369:ASP:CA	5:D:601:HOH:O	2.37	0.62
1:G:316:LYS:NZ	5:G:605:HOH:O	1.99	0.62
1:K:64:ASN:HB2	5:K:606:HOH:O	1.75	0.62
1:D:190:GLU:O	1:D:194:LYS:HG3	2.00	0.62
1:L:99:HIS:NE2	3:L:505:SO4:O2	2.33	0.62
1:L:86:GLU:CG	5:L:601:HOH:O	2.37	0.62
1:E:469:GLY:O	5:E:608:HOH:O	2.16	0.61
3:L:505:SO4:O4	5:L:607:HOH:O	2.11	0.61
1:L:365:SER:CB	5:L:613:HOH:O	2.49	0.61
1:C:170:GLY:O	1:C:347:ARG:NH2	2.34	0.60
1:J:403:VAL:O	5:J:614:HOH:O	2.16	0.60
1:J:440:MET:CE	5:J:605:HOH:O	2.45	0.60
1:D:368:LYS:C	5:D:601:HOH:O	2.27	0.60
1:L:368:LYS:N	5:L:613:HOH:O	2.34	0.60
1:I:104:ARG:HG2	1:I:104:ARG:HH11	1.66	0.60
1:G:362:GLU:C	1:G:368:LYS:HD3	2.21	0.60
1:K:370:ASP:OD1	5:K:613:HOH:O	2.15	0.60
1:G:243:TYR:N	5:G:612:HOH:O	2.25	0.59
1:D:369:ASP:OD1	5:D:601:HOH:O	2.16	0.59
1:E:366:ARG:CA	5:E:601:HOH:O	2.46	0.59
1:F:48:VAL:HG12	1:F:48:VAL:O	2.02	0.59
1:J:143:GLN:HG2	5:J:609:HOH:O	1.89	0.59
1:J:350:ASP:CB	5:J:602:HOH:O	2.50	0.59
1:A:358:TYR:O	1:A:368:LYS:NZ	2.35	0.59
1:K:244:CYS:HB2	1:K:247:MET:HE2	1.83	0.59
1:B:190:GLU:HG3	1:B:194:LYS:NZ	2.17	0.59
1:E:355:TRP:CZ2	1:E:359:ARG:HD2	2.38	0.58
1:E:366:ARG:HD2	1:E:366:ARG:O	2.03	0.58
1:H:362:GLU:O	1:H:365:SER:OG	2.20	0.58
1:I:382:ARG:NE	5:I:607:HOH:O	2.36	0.58
1:H:56:VAL:HG22	1:H:91:LEU:HD13	1.85	0.58
1:A:382:ARG:NE	5:A:610:HOH:O	2.17	0.58
1:L:48:VAL:O	5:L:608:HOH:O	2.17	0.58
1:D:358:TYR:OH	1:J:332:LEU:HD12	2.04	0.58
1:F:80:LYS:HD3	5:F:626:HOH:O	2.03	0.58
1:K:238:SER:OG	3:K:504:SO4:O4	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:ARG:NH1	3:C:503:SO4:O1	2.35	0.58
1:F:365:SER:O	1:F:366:ARG:HB3	2.04	0.58
1:B:400:THR:HG21	1:C:344:VAL:HG23	1.86	0.57
1:I:147:LYS:NZ	5:I:617:HOH:O	2.37	0.57
1:E:366:ARG:CB	5:E:601:HOH:O	2.53	0.57
1:J:387:ALA:HB2	1:L:383:LYS:HG2	1.85	0.57
1:G:373:LYS:O	1:G:377:GLU:HG3	2.04	0.57
1:H:355:TRP:CZ2	1:H:359:ARG:HD2	2.39	0.57
1:L:355:TRP:CZ2	1:L:359:ARG:HD2	2.40	0.57
1:B:431:HIS:NE2	1:B:460:GLU:OE1	2.36	0.57
1:F:355:TRP:CZ2	1:F:359:ARG:HD2	2.40	0.57
1:G:357:MET:HG2	1:G:371:THR:HG21	1.87	0.57
1:F:400:THR:HG21	1:G:344:VAL:HG23	1.86	0.57
1:H:367:LYS:CA	5:H:602:HOH:O	2.41	0.57
1:B:461:GLU:OE2	1:C:368:LYS:NZ	2.31	0.57
1:G:238:SER:HB3	5:G:690:HOH:O	2.04	0.57
1:K:370:ASP:CB	5:K:613:HOH:O	2.39	0.57
1:F:238:SER:OG	3:F:503:SO4:O2	2.23	0.57
1:G:457:GLU:N	5:G:604:HOH:O	1.95	0.56
1:L:365:SER:O	1:L:368:LYS:HB3	2.04	0.56
1:J:350:ASP:HB2	5:J:612:HOH:O	2.04	0.56
1:J:379:THR:O	1:J:383:LYS:HG2	2.05	0.56
1:K:86:GLU:HG3	1:K:87:ASN:OD1	2.05	0.56
1:K:355:TRP:CZ2	1:K:359:ARG:HD2	2.41	0.56
1:K:436:THR:HB	3:K:506:SO4:O4	2.04	0.56
1:F:444:ARG:HB3	5:F:659:HOH:O	2.04	0.56
1:G:123:LYS:NZ	5:G:610:HOH:O	2.23	0.56
1:F:140:LEU:HD21	1:F:194:LYS:HG3	1.87	0.56
1:A:405:ASN:OD1	5:A:609:HOH:O	2.17	0.55
1:E:383:LYS:NZ	1:K:390:GLU:OE1	2.34	0.55
1:G:382:ARG:NH1	5:G:614:HOH:O	2.26	0.55
1:C:356:HIS:HE1	5:C:611:HOH:O	1.89	0.55
1:J:244:CYS:HB2	1:J:247:MET:HE2	1.88	0.55
1:K:359:ARG:NH1	5:K:621:HOH:O	2.38	0.55
1:L:196:HIS:HD2	1:L:225:LEU:CD2	2.20	0.55
1:I:355:TRP:CZ2	1:I:359:ARG:HD2	2.42	0.54
1:G:316:LYS:CE	5:G:605:HOH:O	2.50	0.54
1:K:101:LEU:O	5:K:614:HOH:O	2.18	0.54
1:I:348:ASP:OD2	5:I:608:HOH:O	2.19	0.54
1:L:238:SER:HB3	5:L:623:HOH:O	2.08	0.54
1:E:365:SER:C	1:E:367:LYS:H	2.10	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:THR:O	5:A:611:HOH:O	2.18	0.53
1:B:243:TYR:N	5:B:619:HOH:O	2.35	0.53
1:E:344:VAL:HG23	1:K:400:THR:HG21	1.89	0.53
1:I:337:VAL:HG21	1:L:355:TRP:HH2	1.73	0.53
1:F:80:LYS:CD	5:F:626:HOH:O	2.57	0.53
1:B:98:ASN:ND2	5:B:623:HOH:O	2.40	0.53
1:G:456:LYS:HE2	1:G:460:GLU:OE2	2.09	0.53
1:F:277:LYS:HE2	1:F:323:PHE:CZ	2.44	0.53
1:J:98:ASN:ND2	5:J:618:HOH:O	2.28	0.53
1:J:409:GLU:OE2	5:J:615:HOH:O	2.19	0.53
1:A:355:TRP:HH2	1:H:337:VAL:HG21	1.74	0.53
1:H:370:ASP:HB2	5:H:602:HOH:O	2.09	0.53
1:F:256:ILE:HG23	1:F:356:HIS:HB3	1.90	0.52
1:F:56:VAL:HG22	1:F:91:LEU:HD13	1.90	0.52
1:F:465:ALA:HB1	1:G:372:LEU:HD21	1.91	0.52
1:E:355:TRP:HH2	1:G:337:VAL:HG21	1.75	0.52
1:J:383:LYS:HE3	5:J:623:HOH:O	2.09	0.52
1:A:347:ARG:O	1:A:382:ARG:NH2	2.31	0.52
1:G:355:TRP:CZ2	1:G:359:ARG:HD2	2.44	0.52
3:D:504:SO4:O1	5:D:605:HOH:O	2.18	0.52
1:F:170:GLY:O	1:F:347:ARG:NH1	2.43	0.52
1:I:351:LEU:HD11	5:I:607:HOH:O	2.10	0.52
1:A:355:TRP:CZ2	1:A:359:ARG:HD2	2.45	0.51
1:L:362:GLU:CA	5:L:605:HOH:O	2.57	0.51
1:F:121:VAL:O	5:F:610:HOH:O	2.19	0.51
1:J:101:LEU:HD13	1:J:357:MET:HE1	1.91	0.51
1:I:382:ARG:CZ	5:I:607:HOH:O	2.54	0.51
1:L:330:LEU:HD12	1:L:331:PRO:HD2	1.92	0.51
1:B:355:TRP:CH2	1:B:359:ARG:HD2	2.46	0.51
1:H:362:GLU:HB2	1:H:365:SER:OG	2.11	0.51
1:I:289:LYS:NZ	5:I:606:HOH:O	2.15	0.51
1:L:244:CYS:HB2	1:L:247:MET:HE2	1.92	0.51
1:J:316:LYS:HG2	5:J:697:HOH:O	2.10	0.51
1:K:456:LYS:O	1:K:460:GLU:HG3	2.11	0.51
1:G:175:LEU:HB2	1:G:183:ILE:HB	1.93	0.50
1:H:396:LEU:HD23	1:L:332:LEU:HD11	1.94	0.50
1:J:363:ASP:OD1	1:J:363:ASP:N	2.44	0.50
1:J:355:TRP:CZ2	1:J:359:ARG:HD2	2.46	0.50
1:B:376:THR:HG22	1:C:391:LEU:HD21	1.93	0.50
1:L:362:GLU:CB	5:L:605:HOH:O	2.34	0.50
1:J:104:ARG:NH1	5:J:627:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:TRP:CZ2	1:B:359:ARG:HD2	2.47	0.50
1:E:70:ASP:CA	5:E:602:HOH:O	2.52	0.50
1:E:338:LYS:CE	5:E:615:HOH:O	2.59	0.50
1:H:344:VAL:HG23	1:I:400:THR:HG21	1.94	0.50
1:C:161:HIS:HD2	5:C:762:HOH:O	1.94	0.49
1:K:56:VAL:HG22	1:K:91:LEU:HD13	1.94	0.49
1:J:338:LYS:NZ	5:J:611:HOH:O	2.11	0.49
1:A:431:HIS:HE2	1:A:460:GLU:CD	2.15	0.49
1:E:391:LEU:HD21	1:K:376:THR:HG22	1.94	0.49
1:B:55:LEU:HB3	1:B:71:VAL:HG13	1.94	0.49
1:C:157:LYS:HG3	1:C:158:PRO:HD2	1.93	0.49
1:B:92:MET:O	1:B:126:THR:HA	2.12	0.49
1:G:244:CYS:HB2	1:G:247:MET:HE2	1.93	0.49
1:F:161:HIS:NE2	5:F:604:HOH:O	2.21	0.49
1:H:121:VAL:O	5:H:609:HOH:O	2.20	0.49
1:I:357:MET:HG2	1:I:371:THR:HG21	1.95	0.49
1:H:362:GLU:C	1:H:365:SER:HG	2.16	0.49
1:A:119:ALA:HB2	5:A:666:HOH:O	2.13	0.49
1:H:370:ASP:CG	5:H:602:HOH:O	2.51	0.48
1:I:104:ARG:HH11	1:I:104:ARG:CG	2.26	0.48
1:A:347:ARG:C	5:A:601:HOH:O	2.50	0.48
1:A:376:THR:HG22	1:D:391:LEU:HD21	1.94	0.48
1:F:431:HIS:NE2	5:F:603:HOH:O	2.33	0.48
1:G:316:LYS:HE2	5:G:605:HOH:O	2.13	0.48
1:H:289:LYS:HE3	5:H:700:HOH:O	2.13	0.48
1:E:338:LYS:NZ	5:E:615:HOH:O	2.36	0.48
1:I:175:LEU:HB2	1:I:183:ILE:HB	1.95	0.48
1:A:357:MET:HG2	1:A:371:THR:HG21	1.96	0.48
5:A:623:HOH:O	1:D:373:LYS:HE2	2.14	0.48
1:B:437:GLN:OE1	5:B:609:HOH:O	2.20	0.48
1:F:344:VAL:HG23	1:G:400:THR:HG21	1.95	0.48
1:I:355:TRP:HH2	1:L:337:VAL:HG21	1.78	0.48
5:B:622:HOH:O	1:C:383:LYS:HD3	2.12	0.48
1:F:387:ALA:HB2	1:G:383:LYS:HG2	1.94	0.48
1:L:365:SER:N	5:L:605:HOH:O	2.37	0.48
1:A:382:ARG:NH2	5:A:610:HOH:O	2.45	0.48
1:F:391:LEU:HD21	1:G:376:THR:HG22	1.96	0.48
1:G:278:LYS:O	1:G:316:LYS:NZ	2.46	0.48
1:G:362:GLU:O	1:G:368:LYS:HD3	2.14	0.48
1:K:86:GLU:HG2	5:K:617:HOH:O	2.13	0.47
1:L:196:HIS:HD2	1:L:225:LEU:HD23	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:SER:HB3	5:C:698:HOH:O	2.15	0.47
1:J:357:MET:HG2	1:J:371:THR:HG21	1.96	0.47
1:E:366:ARG:HG3	1:E:366:ARG:HH11	1.78	0.47
1:F:104:ARG:HD2	1:F:255:TYR:OH	2.14	0.47
1:F:347:ARG:HD2	3:F:503:SO4:O1	2.15	0.47
1:H:338:LYS:NZ	3:H:509:SO4:O1	2.45	0.47
1:K:357:MET:HG2	1:K:371:THR:HG21	1.96	0.47
1:H:204:MET:HB3	1:H:227:ILE:HG12	1.97	0.47
1:J:56:VAL:HG22	1:J:91:LEU:HD13	1.96	0.47
1:F:390:GLU:HB3	5:F:601:HOH:O	2.14	0.47
1:H:376:THR:HG22	1:I:391:LEU:HD21	1.96	0.47
1:I:332:LEU:HD11	1:J:396:LEU:HD23	1.95	0.47
1:K:157:LYS:HB3	1:K:157:LYS:HE2	1.58	0.47
1:E:156:SER:C	1:E:157:LYS:HD2	2.35	0.47
1:K:249:PRO:O	1:K:250:SER:OG	2.31	0.47
1:L:383:LYS:HD2	1:L:383:LYS:HA	1.64	0.47
1:B:190:GLU:HG3	1:B:194:LYS:HZ1	1.79	0.46
1:D:382:ARG:NH1	5:D:606:HOH:O	2.20	0.46
1:G:101:LEU:HD22	1:G:357:MET:HE2	1.96	0.46
1:A:412:LEU:HD22	1:J:282:LYS:HD3	1.96	0.46
1:F:347:ARG:HD3	1:F:441:LYS:HD2	1.97	0.46
1:L:328:VAL:O	1:L:329:ASN:OD1	2.34	0.46
5:A:621:HOH:O	1:H:359:ARG:NH2	2.49	0.46
1:I:358:TYR:CD1	1:I:372:LEU:HG	2.51	0.46
1:G:282:LYS:HB2	1:G:282:LYS:HE3	1.81	0.46
1:F:289:LYS:HE3	5:F:694:HOH:O	2.16	0.46
1:I:248:ASN:HA	1:I:249:PRO:HA	1.79	0.46
1:L:175:LEU:HB2	1:L:183:ILE:HB	1.98	0.46
1:A:55:LEU:HB3	1:A:71:VAL:HG13	1.97	0.46
1:J:55:LEU:HB3	1:J:71:VAL:HG13	1.97	0.46
1:D:111:HIS:CE1	5:D:610:HOH:O	2.67	0.46
1:A:369:ASP:HB2	1:B:369:ASP:OD1	2.16	0.45
1:G:295:TYR:CB	5:G:603:HOH:O	2.64	0.45
1:J:316:LYS:HE2	5:J:631:HOH:O	2.17	0.45
1:J:412:LEU:HD23	5:J:702:HOH:O	2.16	0.45
1:K:86:GLU:CG	5:K:617:HOH:O	2.64	0.45
1:K:370:ASP:CG	5:K:613:HOH:O	2.52	0.45
1:G:56:VAL:HG22	1:G:91:LEU:HD13	1.98	0.45
1:E:332:LEU:HD11	1:F:396:LEU:HD23	1.97	0.45
1:B:367:LYS:O	1:B:371:THR:HG23	2.17	0.45
1:A:369:ASP:HA	1:A:372:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:LEU:HB2	1:D:183:ILE:HB	1.98	0.45
1:G:332:LEU:HD11	1:K:396:LEU:HD23	1.99	0.45
1:H:383:LYS:HE2	1:H:383:LYS:HB2	1.73	0.45
1:A:426:ARG:NH1	5:A:632:HOH:O	2.49	0.45
1:B:403:VAL:O	5:B:610:HOH:O	2.20	0.45
1:E:175:LEU:HB2	1:E:183:ILE:HB	1.99	0.45
1:L:362:GLU:HB3	1:L:365:SER:H	1.82	0.44
1:H:372:LEU:HD21	1:I:465:ALA:HB1	1.99	0.44
1:H:444:ARG:HB3	5:H:674:HOH:O	2.17	0.44
1:L:417:ASP:OD2	5:L:610:HOH:O	2.21	0.44
1:D:275:ASN:HB3	1:D:278:LYS:HE2	1.98	0.44
1:I:119:ALA:HB2	5:I:659:HOH:O	2.17	0.44
1:B:357:MET:HG2	1:B:371:THR:HG21	2.00	0.44
1:E:366:ARG:HB3	5:E:601:HOH:O	2.14	0.44
1:E:398:GLY:HA3	5:E:643:HOH:O	2.17	0.44
1:F:256:ILE:HG22	1:F:256:ILE:O	2.17	0.44
1:L:367:LYS:C	5:L:613:HOH:O	2.55	0.44
1:H:238:SER:OG	3:H:504:SO4:O4	2.34	0.44
1:H:383:LYS:NZ	5:H:623:HOH:O	2.39	0.44
1:I:274:HIS:O	5:I:609:HOH:O	2.21	0.44
1:D:241:GLY:HA2	1:D:261:ASP:HA	2.00	0.44
1:I:238:SER:HB3	5:I:712:HOH:O	2.18	0.44
1:J:376:THR:HG22	1:L:391:LEU:HD21	2.00	0.44
1:C:55:LEU:HB3	1:C:71:VAL:HG13	1.99	0.43
1:E:282:LYS:HB2	1:E:282:LYS:HE3	1.79	0.43
1:A:347:ARG:O	5:A:601:HOH:O	2.20	0.43
1:G:295:TYR:HB2	5:G:603:HOH:O	2.17	0.43
1:H:391:LEU:HD21	1:I:376:THR:HG22	2.00	0.43
1:J:372:LEU:HD21	1:L:465:ALA:HB1	2.00	0.43
1:J:437:GLN:C	5:J:605:HOH:O	2.41	0.43
1:D:289:LYS:HE3	5:D:649:HOH:O	2.18	0.43
1:F:194:LYS:HB3	1:F:194:LYS:HE2	1.62	0.43
1:B:344:VAL:HG23	1:C:400:THR:HG21	2.01	0.43
1:E:282:LYS:HD3	1:F:412:LEU:HD22	2.00	0.43
1:I:101:LEU:HD13	1:I:357:MET:HE1	2.00	0.43
1:D:56:VAL:HG22	1:D:91:LEU:HD13	2.01	0.43
1:D:238:SER:HB3	5:D:680:HOH:O	2.18	0.43
1:L:330:LEU:CD1	1:L:331:PRO:HD2	2.48	0.43
1:F:338:LYS:HE2	5:F:634:HOH:O	2.19	0.43
1:H:449:VAL:HG13	1:H:454:VAL:HB	2.00	0.43
1:A:366:ARG:N	5:A:636:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:LEU:HB3	1:D:71:VAL:HG13	2.01	0.43
1:E:146:VAL:C	1:E:147:LYS:HD2	2.39	0.43
1:F:449:VAL:HG13	1:F:454:VAL:HB	2.01	0.43
1:A:372:LEU:HD21	1:D:465:ALA:HB1	2.01	0.43
1:B:238:SER:HB3	5:B:716:HOH:O	2.18	0.43
1:E:338:LYS:HE2	5:E:615:HOH:O	2.17	0.43
1:K:104:ARG:NH1	5:K:632:HOH:O	2.50	0.43
1:A:48:VAL:O	1:A:48:VAL:CG1	2.62	0.43
1:C:175:LEU:HB2	1:C:183:ILE:HB	2.00	0.43
1:A:282:LYS:HB2	1:A:282:LYS:HE3	1.79	0.42
1:C:86:GLU:H	1:C:86:GLU:HG2	1.60	0.42
1:C:357:MET:HG2	1:C:371:THR:HG21	2.01	0.42
1:H:175:LEU:HB2	1:H:183:ILE:HB	2.01	0.42
1:J:391:LEU:HD21	1:L:376:THR:HG22	2.01	0.42
1:L:48:VAL:N	5:L:608:HOH:O	2.51	0.42
1:L:55:LEU:HB3	1:L:71:VAL:HG13	2.00	0.42
1:E:329:ASN:N	5:E:627:HOH:O	2.52	0.42
1:F:190:GLU:HG3	1:F:194:LYS:HE3	2.01	0.42
1:K:449:VAL:HG13	1:K:454:VAL:HB	2.01	0.42
1:D:204:MET:HB3	1:D:227:ILE:HG12	2.02	0.42
1:D:221:MET:HA	1:D:222:PRO:HD3	1.89	0.42
1:F:376:THR:HG22	1:G:391:LEU:HD21	2.00	0.42
1:H:362:GLU:N	1:H:365:SER:OG	2.52	0.42
1:H:370:ASP:CB	5:H:602:HOH:O	2.67	0.42
1:J:458:LEU:HD12	5:J:676:HOH:O	2.19	0.42
1:K:289:LYS:HE2	5:K:713:HOH:O	2.20	0.42
1:A:238:SER:HB3	5:A:720:HOH:O	2.19	0.42
1:D:248:ASN:HA	1:D:249:PRO:HA	1.79	0.42
1:L:397:PHE:HB3	5:L:739:HOH:O	2.19	0.42
1:G:101:LEU:HD13	1:G:357:MET:HE1	2.00	0.42
5:H:606:HOH:O	1:I:379:THR:HG23	2.18	0.42
1:K:68:GLN:HA	5:K:603:HOH:O	2.19	0.42
1:L:282:LYS:HB2	1:L:282:LYS:HE3	1.83	0.42
1:A:368:LYS:O	1:A:371:THR:OG1	2.34	0.42
1:B:175:LEU:HB2	1:B:183:ILE:HB	2.01	0.42
1:F:277:LYS:HE2	1:F:323:PHE:CE1	2.55	0.42
1:I:123:LYS:NZ	5:I:612:HOH:O	2.33	0.42
1:J:400:THR:HG21	1:L:344:VAL:HG23	2.02	0.42
1:K:64:ASN:ND2	5:K:606:HOH:O	2.52	0.42
1:A:328:VAL:HG12	1:A:329:ASN:OD1	2.20	0.42
1:J:358:TYR:CE1	1:J:372:LEU:HD13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:175:LEU:HB2	1:K:183:ILE:HB	2.02	0.41
1:L:56:VAL:HG22	1:L:91:LEU:HD13	2.02	0.41
1:C:56:VAL:HG22	1:C:91:LEU:HD13	2.02	0.41
1:C:290:MET:HE2	1:C:295:TYR:HD1	1.85	0.41
1:C:373:LYS:HA	1:C:373:LYS:HD2	1.80	0.41
1:E:248:ASN:HA	1:E:249:PRO:HA	1.82	0.41
1:E:146:VAL:O	1:E:147:LYS:HD2	2.19	0.41
1:F:175:LEU:HB2	1:F:183:ILE:HB	2.03	0.41
1:L:362:GLU:C	5:L:605:HOH:O	2.47	0.41
1:C:202:LYS:NZ	5:C:606:HOH:O	2.27	0.41
1:E:365:SER:C	1:E:367:LYS:N	2.73	0.41
1:G:248:ASN:HA	1:G:249:PRO:HA	1.87	0.41
1:H:48:VAL:HG22	1:H:319:LEU:HD22	2.02	0.41
1:J:48:VAL:O	1:J:161:HIS:HD2	2.02	0.41
1:K:146:VAL:O	5:K:615:HOH:O	2.21	0.41
1:A:175:LEU:HB2	1:A:183:ILE:HB	2.02	0.41
1:I:221:MET:HA	1:I:222:PRO:HD3	1.93	0.41
1:L:248:ASN:HA	1:L:249:PRO:HA	1.84	0.41
1:F:454:VAL:O	5:F:612:HOH:O	2.22	0.41
1:A:387:ALA:HB2	1:D:383:LYS:HG3	2.02	0.41
1:B:190:GLU:HG3	1:B:194:LYS:HZ3	1.83	0.41
1:H:221:MET:HA	1:H:222:PRO:HD3	1.90	0.41
1:H:412:LEU:HD11	5:H:601:HOH:O	2.20	0.41
1:J:277:LYS:HE2	1:J:323:PHE:CZ	2.56	0.41
1:J:449:VAL:HG13	1:J:454:VAL:HB	2.03	0.41
1:L:174:VAL:HG21	1:L:443:MET:HE2	2.03	0.41
1:B:382:ARG:NH1	1:B:438:TYR:CD1	2.89	0.41
1:K:48:VAL:CG2	1:K:319:LEU:HD21	2.44	0.41
1:K:144:LYS:O	1:K:144:LYS:HG3	2.18	0.41
1:A:372:LEU:O	1:A:376:THR:HG23	2.21	0.41
1:D:436:THR:N	5:D:627:HOH:O	2.54	0.41
1:K:55:LEU:HB3	1:K:71:VAL:HG13	2.02	0.41
1:E:238:SER:HB3	5:E:662:HOH:O	2.20	0.40
1:F:221:MET:HA	1:F:222:PRO:HD3	1.89	0.40
1:F:372:LEU:HD21	1:G:465:ALA:HB1	2.02	0.40
1:G:277:LYS:HE2	1:G:323:PHE:CE1	2.55	0.40
1:H:113:ASP:OD1	5:H:611:HOH:O	2.21	0.40
1:L:289:LYS:HE3	5:L:704:HOH:O	2.21	0.40
1:E:218:GLU:HG3	1:E:307:TYR:CE1	2.56	0.40
1:G:84:LYS:HE2	1:G:87:ASN:ND2	2.37	0.40
1:G:269:GLU:HA	1:G:272:GLU:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:358:TYR:CE1	1:H:372:LEU:HD13	2.56	0.40
1:K:247:MET:O	1:K:250:SER:HB3	2.20	0.40
1:A:390:GLU:CD	5:A:605:HOH:O	2.54	0.40
1:E:238:SER:OG	3:E:503:SO4:O2	2.37	0.40
1:E:372:LEU:HD21	1:K:465:ALA:HB1	2.03	0.40
1:L:92:MET:O	1:L:126:THR:HA	2.21	0.40
1:A:92:MET:O	1:A:126:THR:HA	2.22	0.40
1:G:243:TYR:CA	5:G:612:HOH:O	2.68	0.40
1:H:194:LYS:HG3	1:H:194:LYS:H	1.69	0.40
1:A:248:ASN:HA	1:A:249:PRO:HA	1.75	0.40
1:B:372:LEU:O	1:B:376:THR:HG23	2.21	0.40
1:E:366:ARG:HG3	1:E:366:ARG:NH1	2.36	0.40
1:H:157:LYS:N	1:H:160:ASP:OD2	2.46	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:MET:SD	5:E:776:HOH:O[3_455]	1.86	0.34
5:B:789:HOH:O	5:F:774:HOH:O[3_455]	2.13	0.07

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	413/455 (91%)	405 (98%)	8 (2%)	0	100	100
1	B	412/455 (90%)	405 (98%)	7 (2%)	0	100	100
1	C	421/455 (92%)	412 (98%)	9 (2%)	0	100	100
1	D	420/455 (92%)	412 (98%)	8 (2%)	0	100	100
1	E	419/455 (92%)	409 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	419/455 (92%)	410 (98%)	9 (2%)	0	100	100
1	G	414/455 (91%)	407 (98%)	7 (2%)	0	100	100
1	H	419/455 (92%)	411 (98%)	8 (2%)	0	100	100
1	I	412/455 (90%)	404 (98%)	8 (2%)	0	100	100
1	J	419/455 (92%)	411 (98%)	8 (2%)	0	100	100
1	K	419/455 (92%)	407 (97%)	12 (3%)	0	100	100
1	L	420/455 (92%)	410 (98%)	10 (2%)	0	100	100
All	All	5007/5460 (92%)	4903 (98%)	104 (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	352/384 (92%)	351 (100%)	1 (0%)	92	95
1	B	351/384 (91%)	350 (100%)	1 (0%)	92	95
1	C	356/384 (93%)	354 (99%)	2 (1%)	86	90
1	D	356/384 (93%)	354 (99%)	2 (1%)	86	90
1	E	355/384 (92%)	353 (99%)	2 (1%)	86	90
1	F	355/384 (92%)	354 (100%)	1 (0%)	92	95
1	G	353/384 (92%)	351 (99%)	2 (1%)	86	90
1	H	355/384 (92%)	354 (100%)	1 (0%)	92	95
1	I	351/384 (91%)	351 (100%)	0	100	100
1	J	355/384 (92%)	353 (99%)	2 (1%)	86	90
1	K	355/384 (92%)	353 (99%)	2 (1%)	86	90
1	L	356/384 (93%)	354 (99%)	2 (1%)	86	90
All	All	4250/4608 (92%)	4232 (100%)	18 (0%)	91	93

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	460	GLU
1	B	350	ASP
1	C	157	LYS
1	C	358	TYR
1	D	194	LYS
1	D	366	ARG
1	E	48	VAL
1	E	367	LYS
1	F	366	ARG
1	G	362	GLU
1	G	368	LYS
1	H	332	LEU
1	J	332	LEU
1	J	363	ASP
1	K	144	LYS
1	K	332	LEU
1	L	196	HIS
1	L	373	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	98	ASN
1	C	161	HIS
1	C	356	HIS
1	G	384	HIS
1	J	161	HIS
1	L	196	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	SNN	E	168	1	5,6,8	0.51	0	3,6,11	1.98	1 (33%)
1	SNN	K	168	1	5,6,8	0.57	0	3,6,11	2.10	2 (66%)
1	SNN	L	168	1	5,6,8	0.53	0	3,6,11	2.09	2 (66%)
1	SNN	A	168	1	5,6,8	0.52	0	3,6,11	2.00	2 (66%)
1	SNN	F	168	1	5,6,8	0.57	0	3,6,11	2.06	2 (66%)
1	SNN	H	168	1	5,6,8	0.49	0	3,6,11	1.98	2 (66%)
1	SNN	J	168	1	5,6,8	0.58	0	3,6,11	2.14	2 (66%)
1	SNN	B	168	1	5,6,8	0.58	0	3,6,11	1.99	2 (66%)
1	SNN	D	168	1	5,6,8	0.52	0	3,6,11	1.92	2 (66%)
1	SNN	G	168	1	5,6,8	0.58	0	3,6,11	1.89	2 (66%)
1	SNN	C	168	1	5,6,8	0.57	0	3,6,11	1.92	2 (66%)
1	SNN	I	168	1	5,6,8	0.57	0	3,6,11	2.06	2 (66%)

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
1	SNN	E	168	1	-	3/3/5/12	-
1	SNN	K	168	1	-	3/3/5/12	-
1	SNN	L	168	1	-	3/3/5/12	-
1	SNN	A	168	1	-	3/3/5/12	-
1	SNN	F	168	1	-	3/3/5/12	-
1	SNN	H	168	1	-	3/3/5/12	-
1	SNN	J	168	1	-	3/3/5/12	-
1	SNN	B	168	1	-	3/3/5/12	-
1	SNN	D	168	1	-	3/3/5/12	-
1	SNN	G	168	1	-	3/3/5/12	-
1	SNN	C	168	1	-	3/3/5/12	-
1	SNN	I	168	1	-	3/3/5/12	-

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	168	SNN	CA-C4-C5	-2.52	104.91	114.44
1	I	168	SNN	O5-C5-C4	-2.40	118.43	125.43
1	K	168	SNN	CA-C4-C5	-2.37	105.46	114.44
1	J	168	SNN	CA-C4-C5	-2.35	105.54	114.44
1	J	168	SNN	O5-C5-C4	-2.35	118.59	125.43
1	K	168	SNN	O5-C5-C4	-2.33	118.64	125.43
1	L	168	SNN	O5-C5-C4	-2.33	118.64	125.43
1	H	168	SNN	CA-C4-C5	-2.32	105.64	114.44
1	E	168	SNN	CA-C4-C5	-2.26	105.88	114.44
1	C	168	SNN	O5-C5-C4	-2.24	118.91	125.43
1	B	168	SNN	CA-C4-C5	-2.22	106.03	114.44
1	A	168	SNN	CA-C4-C5	-2.22	106.04	114.44
1	G	168	SNN	O5-C5-C4	-2.21	118.98	125.43
1	L	168	SNN	CA-C4-C5	-2.21	106.06	114.44
1	H	168	SNN	O5-C5-C4	-2.21	118.99	125.43
1	I	168	SNN	CA-C4-C5	-2.20	106.10	114.44
1	A	168	SNN	O5-C5-C4	-2.20	119.03	125.43
1	F	168	SNN	O5-C5-C4	-2.18	119.06	125.43
1	B	168	SNN	O5-C5-C4	-2.17	119.09	125.43
1	D	168	SNN	CA-C4-C5	-2.13	106.38	114.44
1	G	168	SNN	CA-C4-C5	-2.12	106.41	114.44
1	D	168	SNN	O5-C5-C4	-2.12	119.26	125.43
1	C	168	SNN	CA-C4-C5	-2.11	106.46	114.44

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	168	SNN	O-C-CA-C4
1	A	168	SNN	C5-C4-CA-N
1	A	168	SNN	CA-C4-C5-O5
1	B	168	SNN	O-C-CA-C4
1	B	168	SNN	C5-C4-CA-N
1	B	168	SNN	CA-C4-C5-O5
1	C	168	SNN	O-C-CA-C4
1	C	168	SNN	C5-C4-CA-N
1	C	168	SNN	CA-C4-C5-O5
1	D	168	SNN	O-C-CA-C4
1	D	168	SNN	C5-C4-CA-N
1	D	168	SNN	CA-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
1	E	168	SNN	O-C-CA-C4
1	E	168	SNN	C5-C4-CA-N
1	E	168	SNN	CA-C4-C5-O5
1	F	168	SNN	O-C-CA-C4
1	F	168	SNN	C5-C4-CA-N
1	F	168	SNN	CA-C4-C5-O5
1	G	168	SNN	O-C-CA-C4
1	G	168	SNN	C5-C4-CA-N
1	G	168	SNN	CA-C4-C5-O5
1	H	168	SNN	O-C-CA-C4
1	H	168	SNN	C5-C4-CA-N
1	H	168	SNN	CA-C4-C5-O5
1	I	168	SNN	O-C-CA-C4
1	I	168	SNN	C5-C4-CA-N
1	I	168	SNN	CA-C4-C5-O5
1	J	168	SNN	O-C-CA-C4
1	J	168	SNN	C5-C4-CA-N
1	J	168	SNN	CA-C4-C5-O5
1	K	168	SNN	O-C-CA-C4
1	K	168	SNN	C5-C4-CA-N
1	K	168	SNN	CA-C4-C5-O5
1	L	168	SNN	O-C-CA-C4
1	L	168	SNN	C5-C4-CA-N
1	L	168	SNN	CA-C4-C5-O5

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

24 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	$\#\|Z\|>2$

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	M	1	1,2	14,14,15	0.33	0	17,19,21	0.97	2 (11%)
2	NAG	M	2	2	14,14,15	0.34	0	17,19,21	1.22	2 (11%)
2	NAG	N	1	1,2	14,14,15	0.56	0	17,19,21	1.05	1 (5%)
2	NAG	N	2	2	14,14,15	0.27	0	17,19,21	0.63	0
2	NAG	O	1	1,2	14,14,15	0.26	0	17,19,21	0.68	0
2	NAG	O	2	2	14,14,15	0.26	0	17,19,21	1.00	1 (5%)
2	NAG	P	1	1,2	14,14,15	0.25	0	17,19,21	0.67	0
2	NAG	P	2	2	14,14,15	0.26	0	17,19,21	0.87	1 (5%)
2	NAG	Q	1	1,2	14,14,15	0.28	0	17,19,21	0.60	1 (5%)
2	NAG	Q	2	2	14,14,15	0.31	0	17,19,21	0.56	0
2	NAG	R	1	1,2	14,14,15	0.24	0	17,19,21	0.75	0
2	NAG	R	2	2	14,14,15	0.30	0	17,19,21	0.57	0
2	NAG	S	1	1,2	14,14,15	0.24	0	17,19,21	0.69	1 (5%)
2	NAG	S	2	2	14,14,15	0.39	0	17,19,21	1.35	3 (17%)
2	NAG	T	1	1,2	14,14,15	0.27	0	17,19,21	0.80	0
2	NAG	T	2	2	14,14,15	0.30	0	17,19,21	0.51	0
2	NAG	U	1	1,2	14,14,15	0.26	0	17,19,21	0.82	1 (5%)
2	NAG	U	2	2	14,14,15	0.26	0	17,19,21	0.75	0
2	NAG	V	1	1,2	14,14,15	0.26	0	17,19,21	0.78	1 (5%)
2	NAG	V	2	2	14,14,15	0.33	0	17,19,21	0.72	1 (5%)
2	NAG	W	1	1,2	14,14,15	0.39	0	17,19,21	0.92	0
2	NAG	W	2	2	14,14,15	0.30	0	17,19,21	0.69	0
2	NAG	X	1	1,2	14,14,15	0.26	0	17,19,21	0.61	0
2	NAG	X	2	2	14,14,15	0.29	0	17,19,21	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	1/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	P	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	P	2	2	-	1/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
2	NAG	S	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	S	2	2	-	3/6/23/26	0/1/1/1
2	NAG	T	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	2/6/23/26	0/1/1/1
2	NAG	U	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	U	2	2	-	0/6/23/26	0/1/1/1
2	NAG	V	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	V	2	2	-	2/6/23/26	0/1/1/1
2	NAG	W	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	W	2	2	-	0/6/23/26	0/1/1/1
2	NAG	X	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	X	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	2	NAG	C1-O5-C5	3.63	117.11	112.19
2	S	2	NAG	C3-C4-C5	2.76	115.16	110.24
2	S	2	NAG	O5-C1-C2	-2.68	107.06	111.29
2	M	2	NAG	O5-C1-C2	2.63	115.44	111.29
2	N	1	NAG	C4-C3-C2	-2.46	107.42	111.02
2	V	2	NAG	O5-C5-C6	2.32	110.84	107.20
2	O	2	NAG	O5-C1-C2	-2.21	107.80	111.29
2	S	2	NAG	C4-C3-C2	2.18	114.21	111.02
2	U	1	NAG	O5-C5-C6	2.14	110.57	107.20
2	S	1	NAG	O5-C5-C6	2.13	110.54	107.20
2	P	2	NAG	O5-C1-C2	-2.08	108.00	111.29
2	M	1	NAG	C1-O5-C5	2.08	115.01	112.19
2	M	1	NAG	O5-C5-C6	2.03	110.39	107.20
2	V	1	NAG	O5-C5-C6	2.02	110.37	107.20
2	Q	1	NAG	O5-C5-C6	2.01	110.35	107.20

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	R	2	NAG	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
2	S	2	NAG	C8-C7-N2-C2
2	V	2	NAG	C4-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
2	S	1	NAG	C8-C7-N2-C2
2	S	1	NAG	O7-C7-N2-C2
2	S	2	NAG	O7-C7-N2-C2
2	V	2	NAG	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
2	S	2	NAG	O5-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6

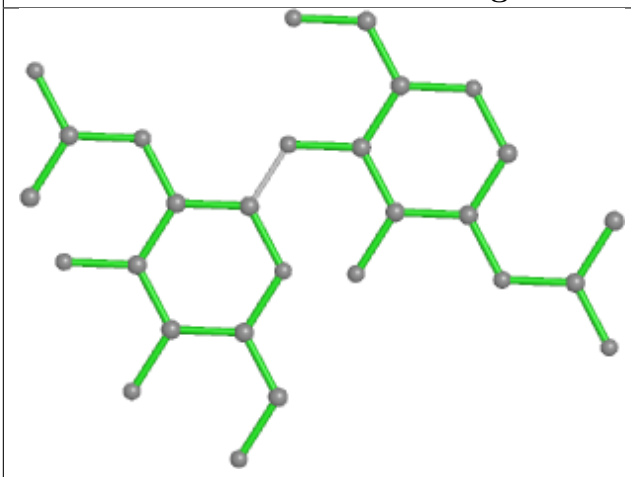
There are no ring outliers.

1 monomer is involved in 1 short contact:

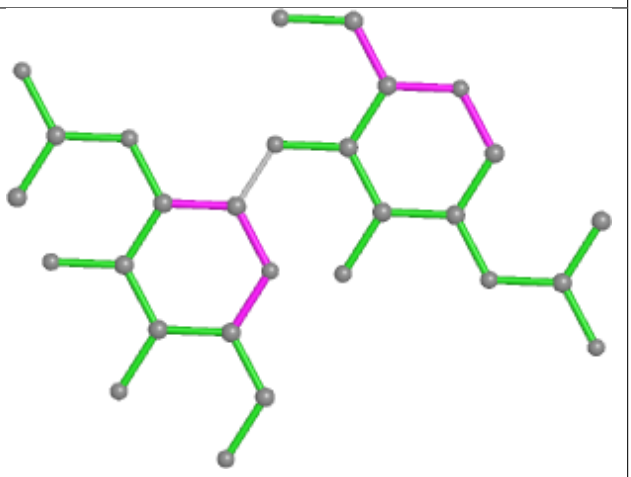
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	S	1	NAG	1	0

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

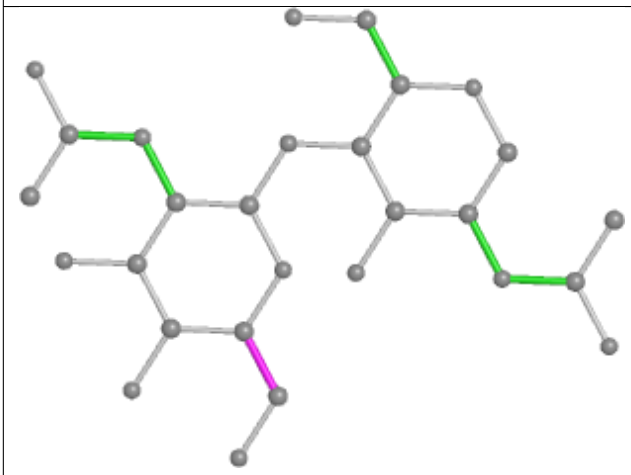
Oligosaccharide Chain M



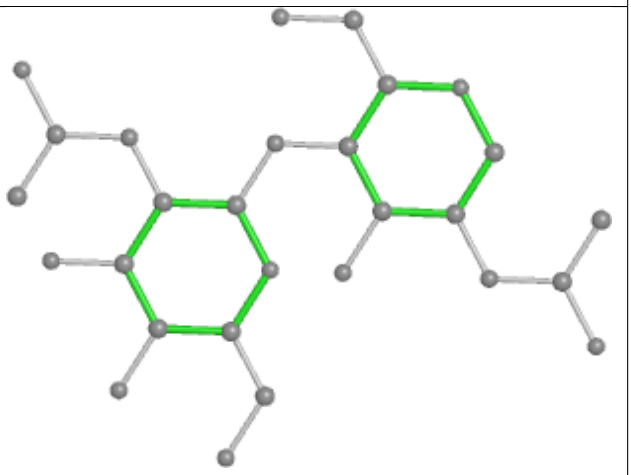
Bond lengths



Bond angles

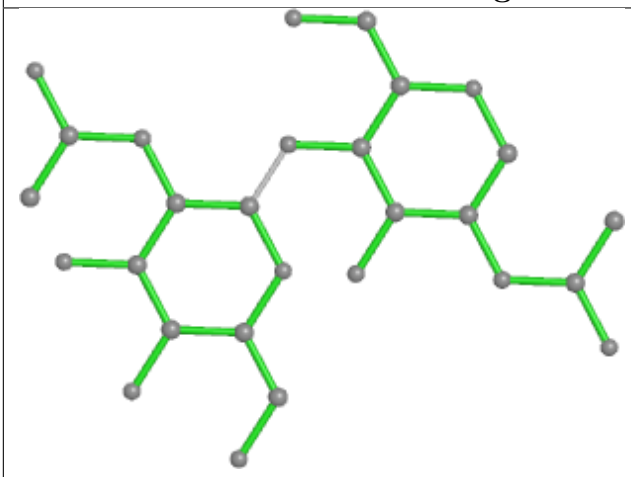


Torsions

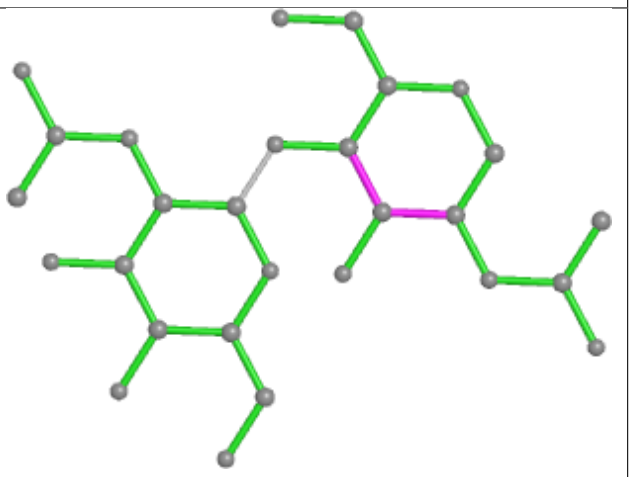


Rings

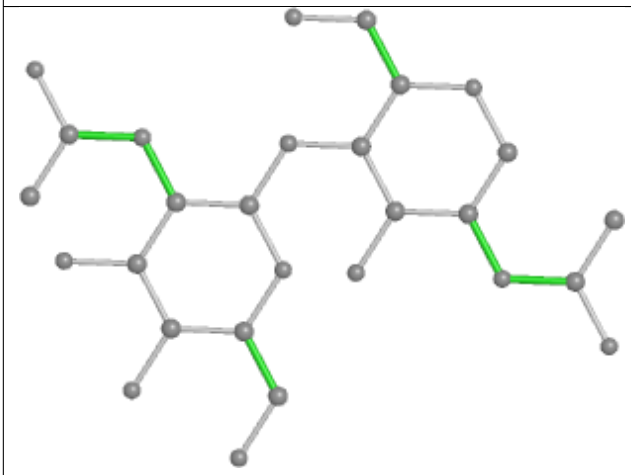
Oligosaccharide Chain N



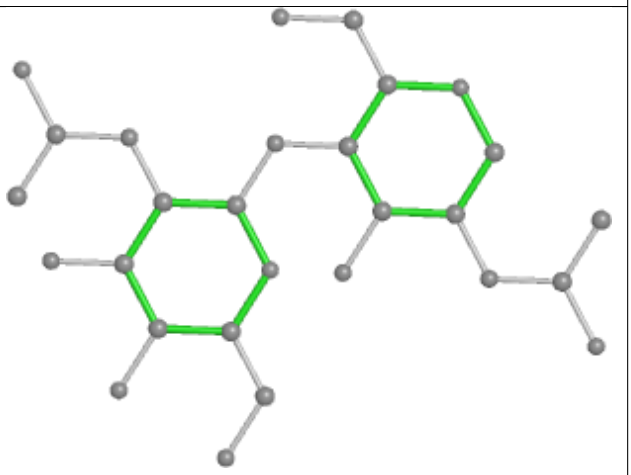
Bond lengths



Bond angles

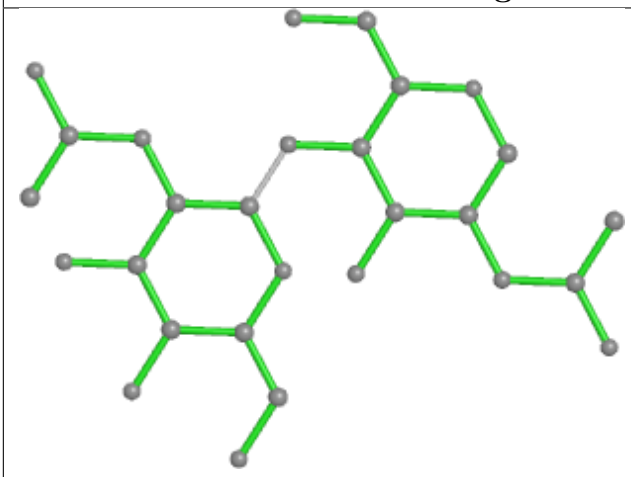


Torsions

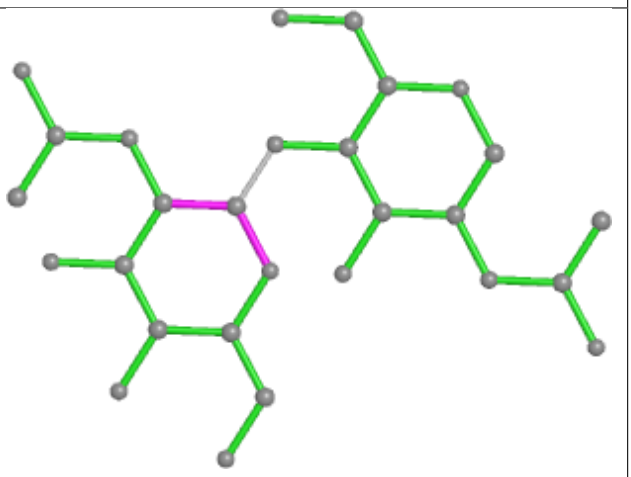


Rings

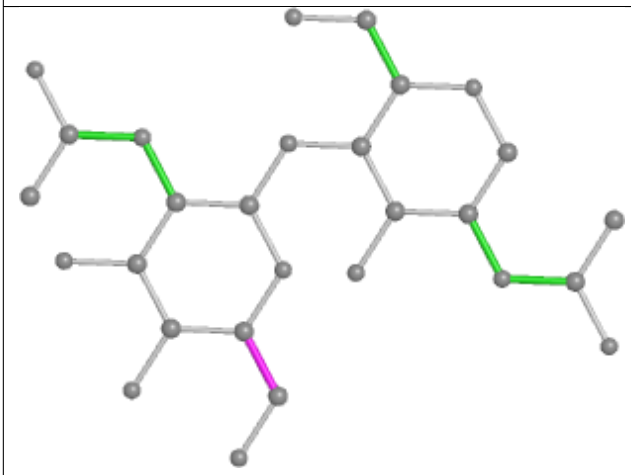
Oligosaccharide Chain O



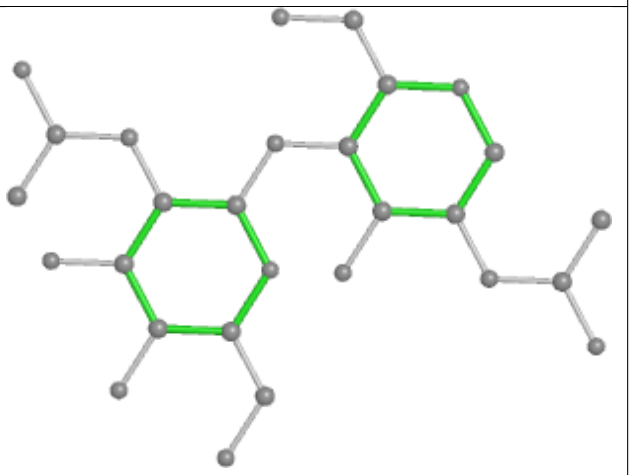
Bond lengths



Bond angles

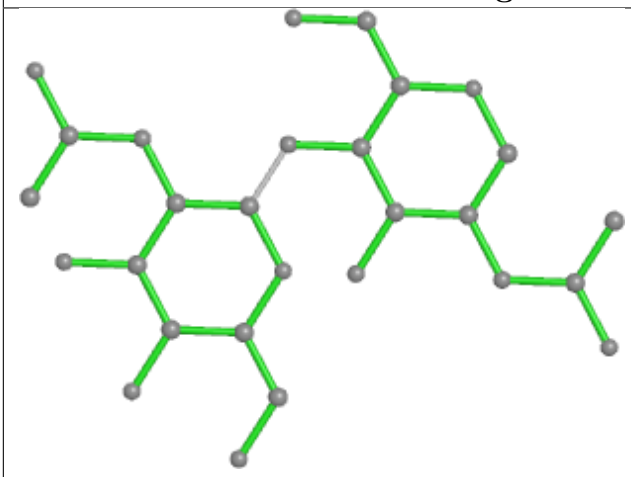


Torsions

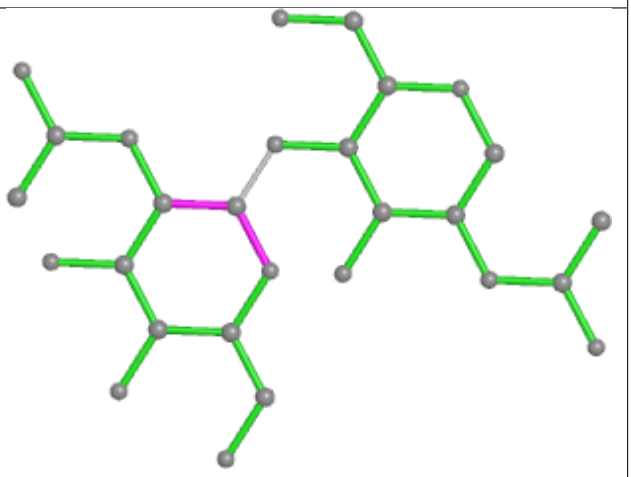


Rings

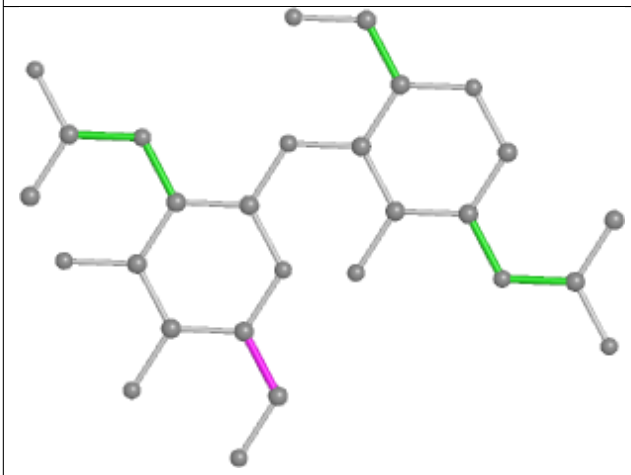
Oligosaccharide Chain P



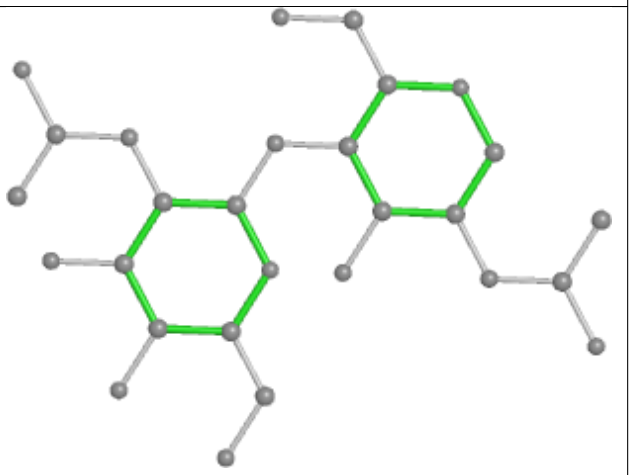
Bond lengths



Bond angles

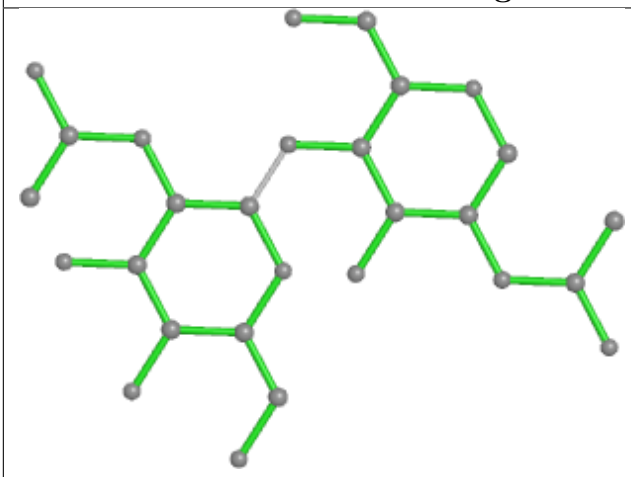


Torsions

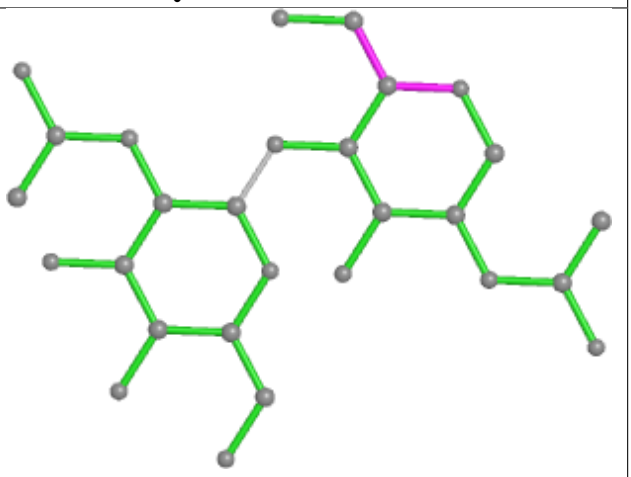


Rings

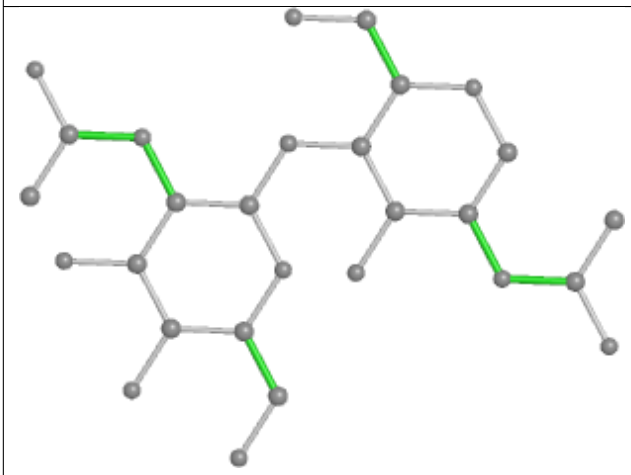
Oligosaccharide Chain Q



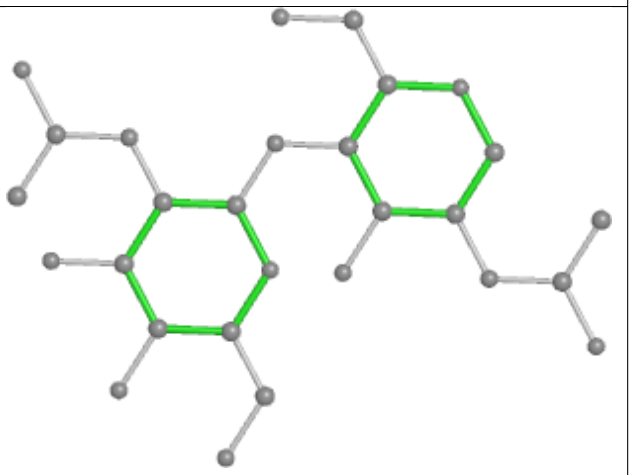
Bond lengths



Bond angles

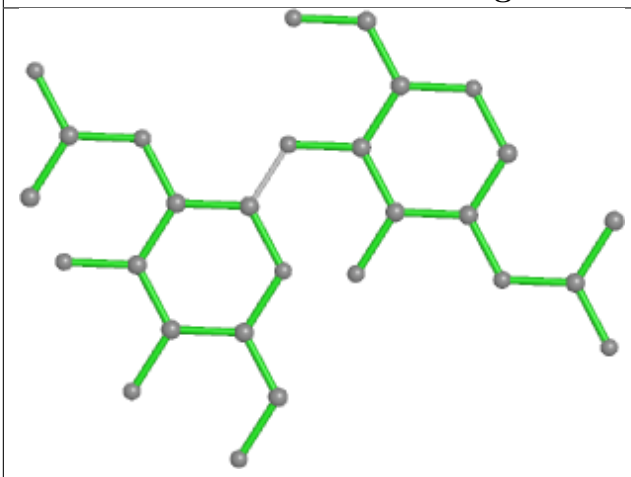


Torsions

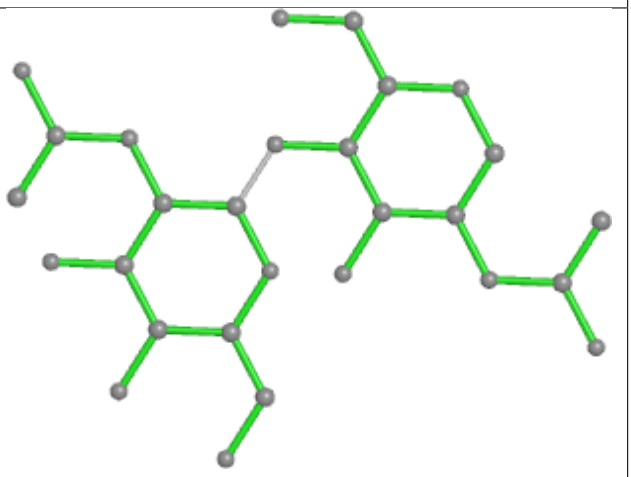


Rings

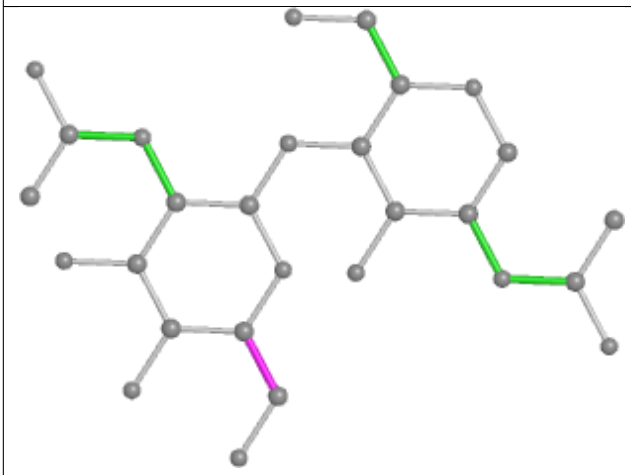
Oligosaccharide Chain R



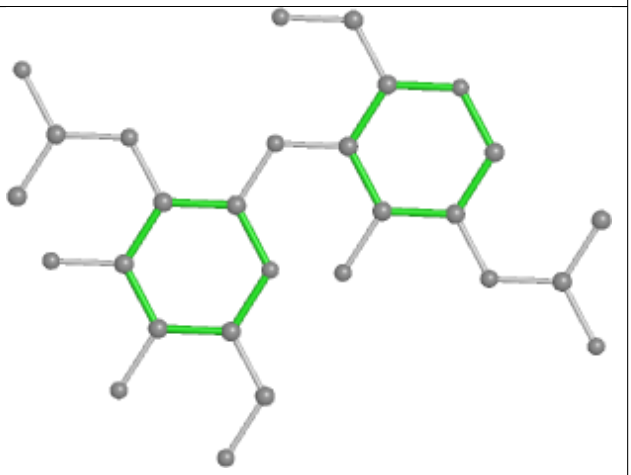
Bond lengths



Bond angles

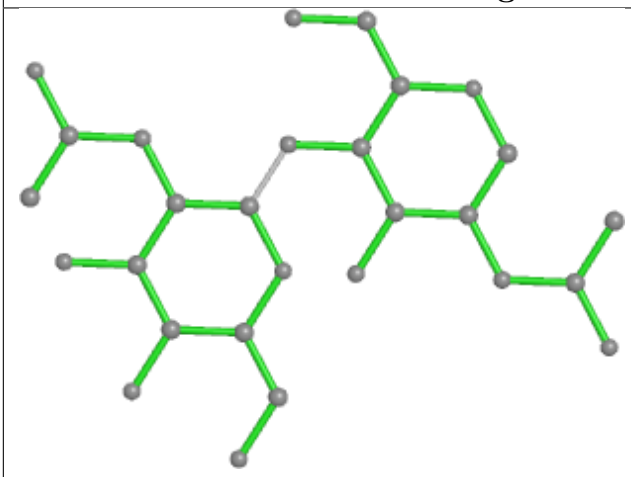


Torsions

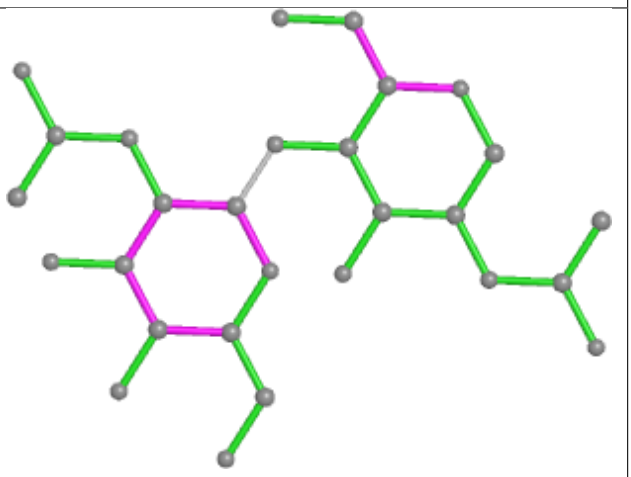


Rings

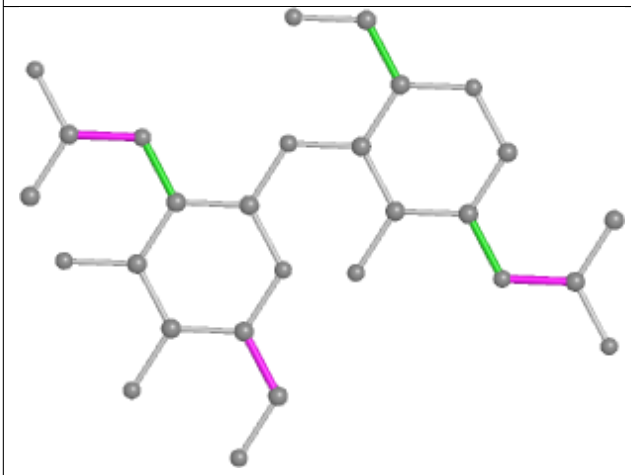
Oligosaccharide Chain S



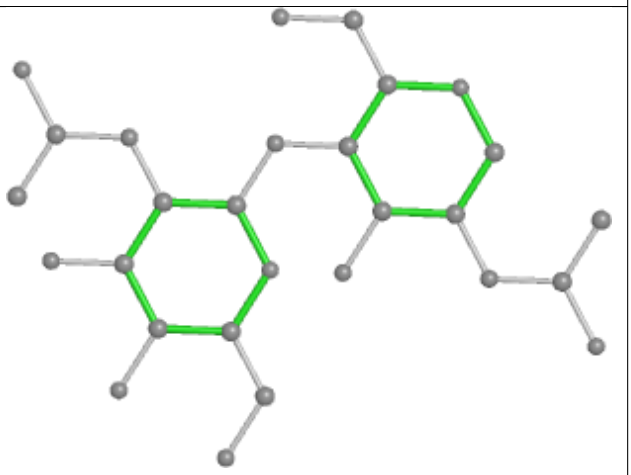
Bond lengths



Bond angles

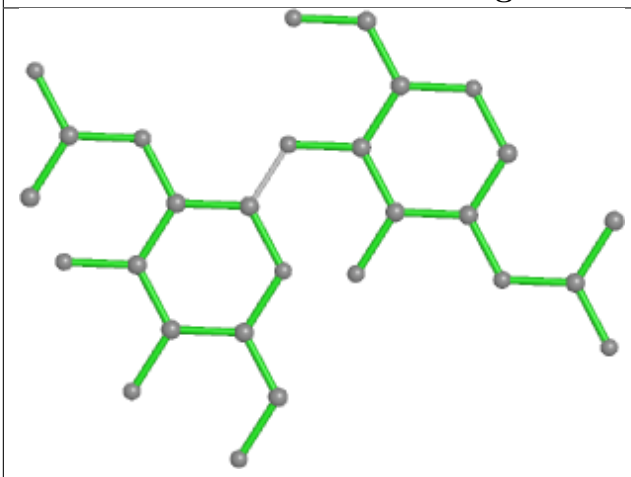


Torsions

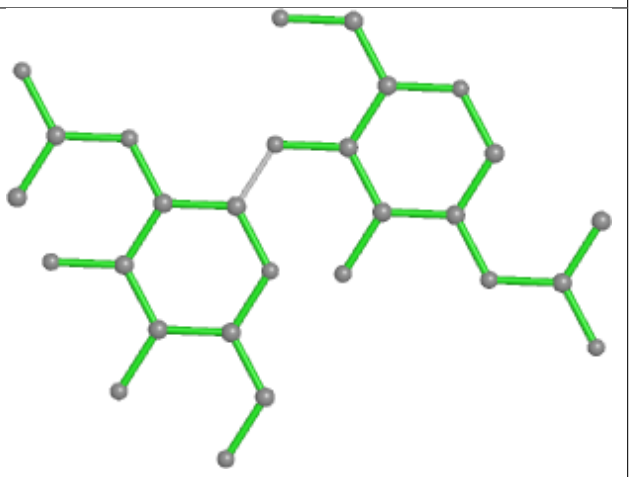


Rings

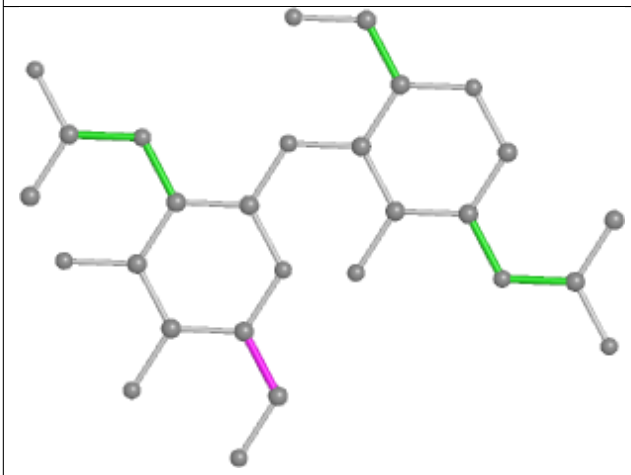
Oligosaccharide Chain T



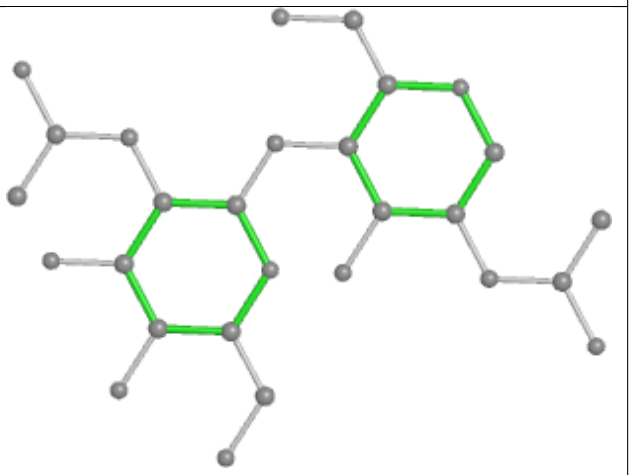
Bond lengths



Bond angles

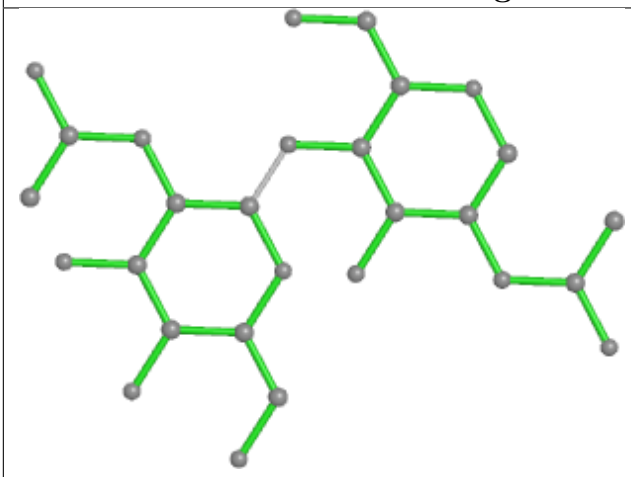


Torsions

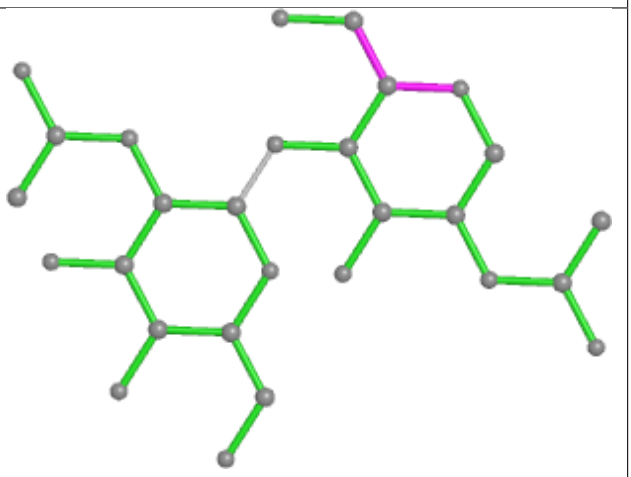


Rings

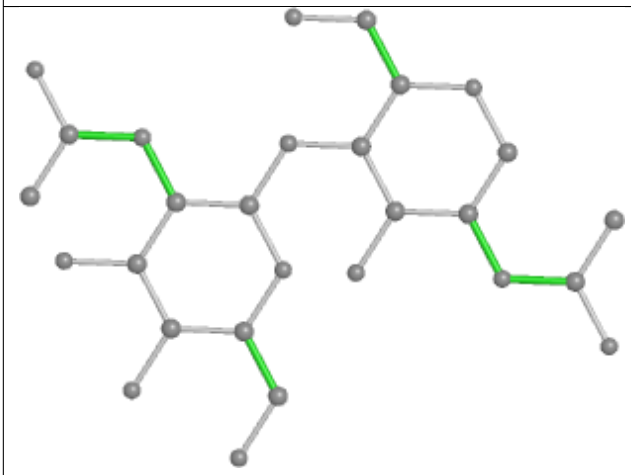
Oligosaccharide Chain U



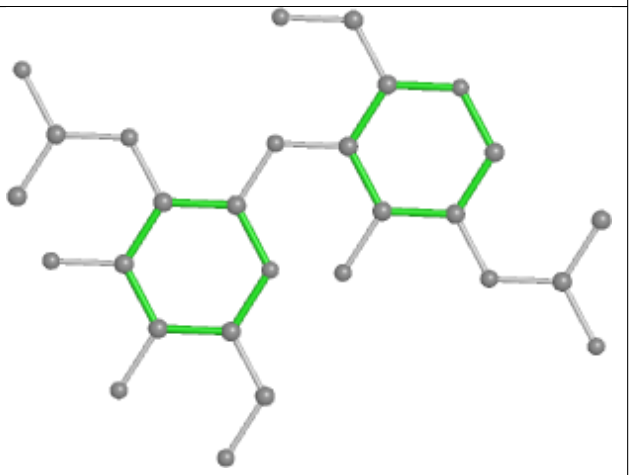
Bond lengths



Bond angles

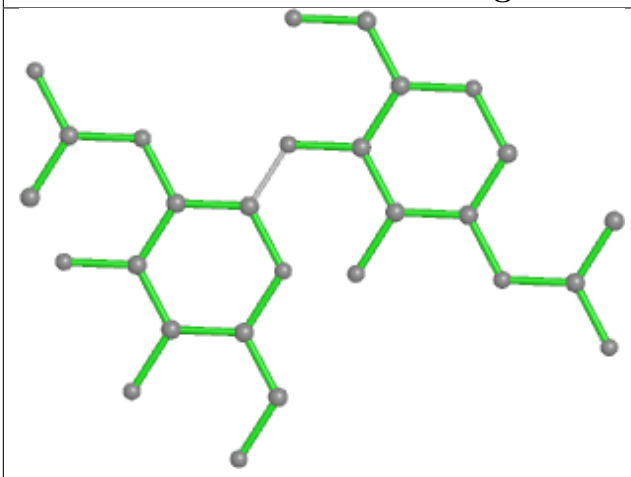


Torsions

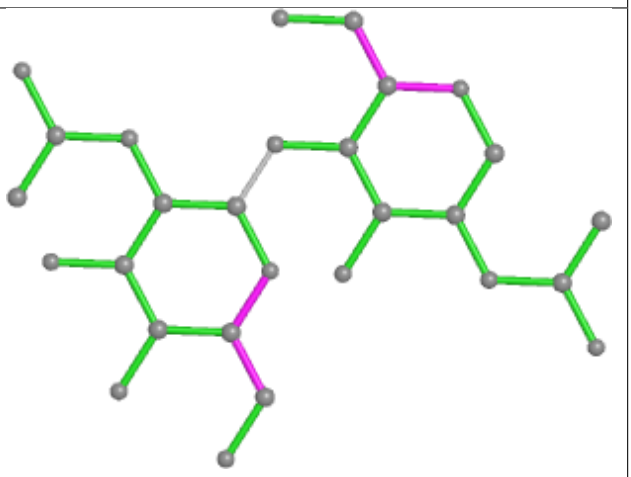


Rings

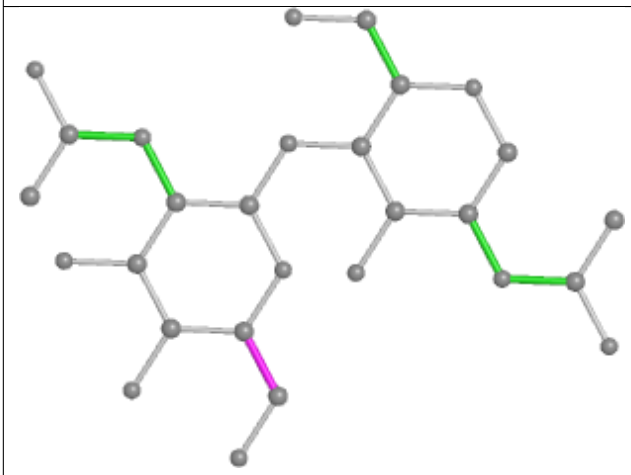
Oligosaccharide Chain V



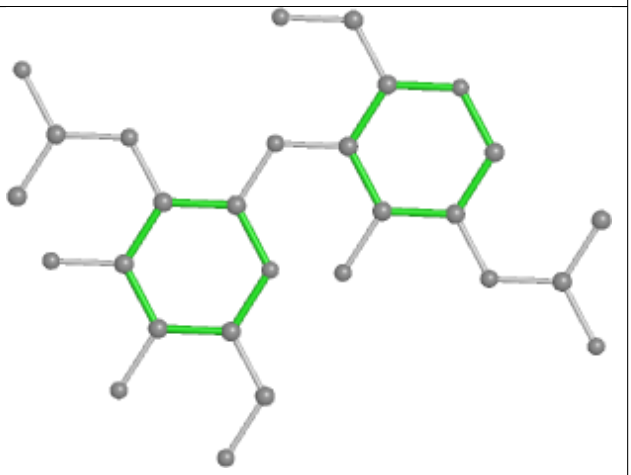
Bond lengths



Bond angles

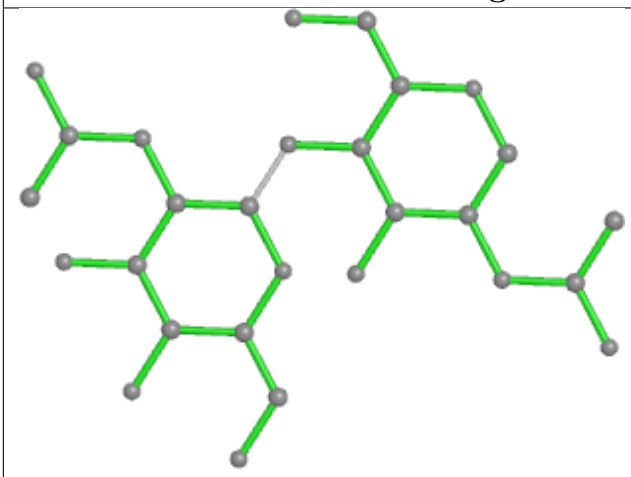


Torsions

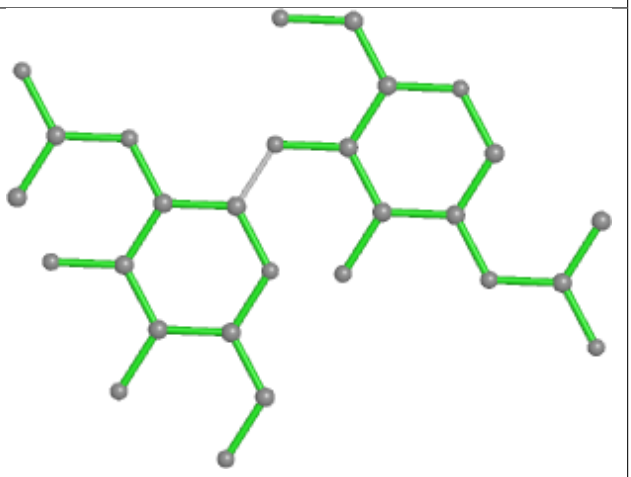


Rings

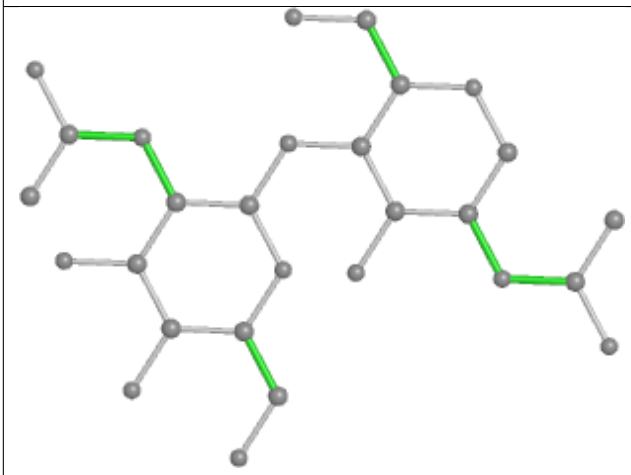
Oligosaccharide Chain W



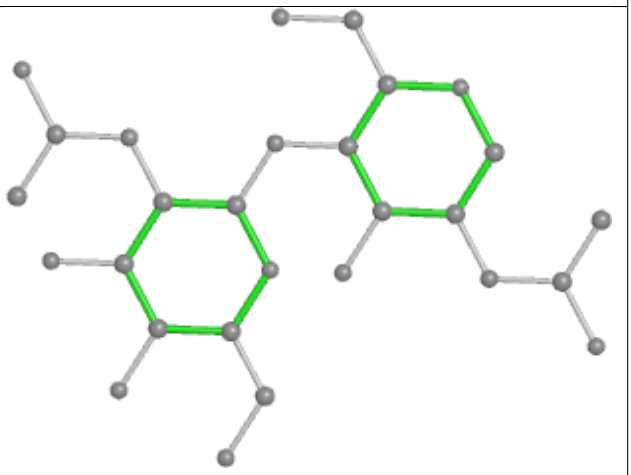
Bond lengths



Bond angles

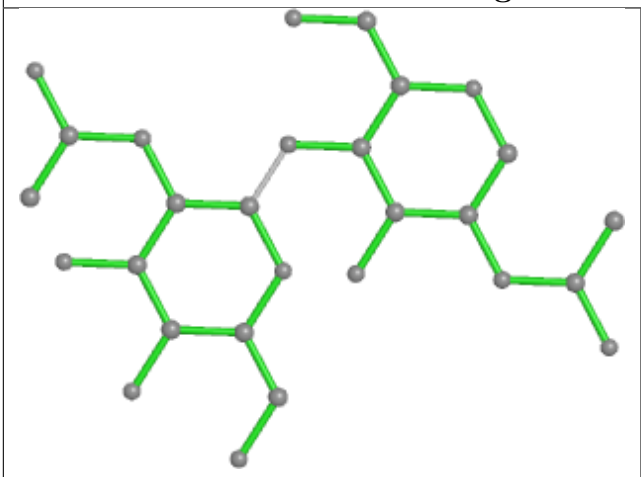


Torsions

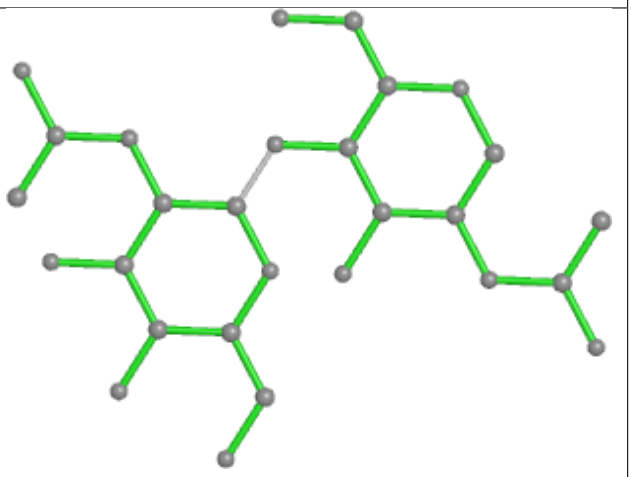


Rings

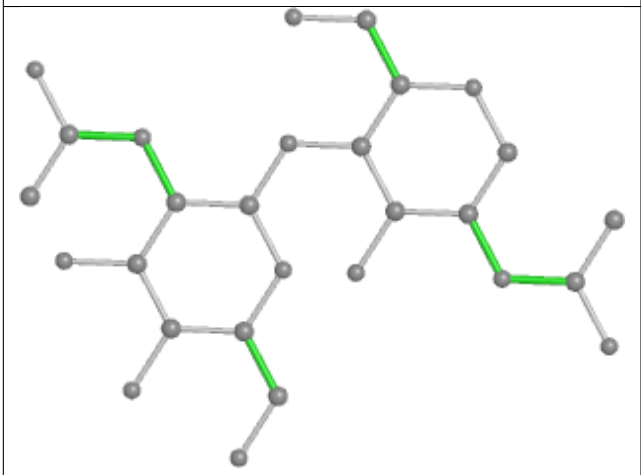
Oligosaccharide Chain X



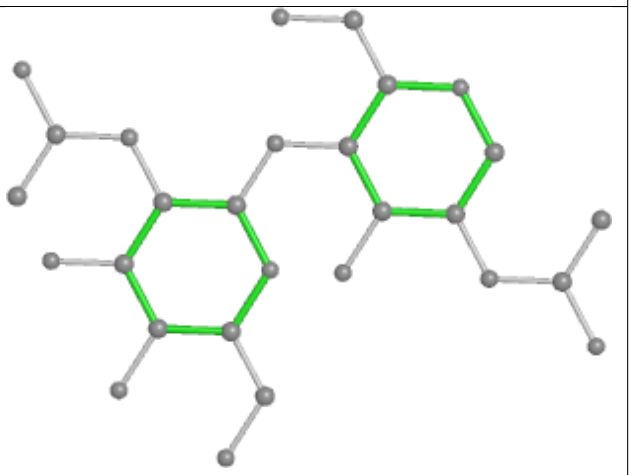
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

67 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	H	506	-	4,4,4	0.32	0	6,6,6	0.05	0
3	SO4	I	505	-	4,4,4	0.32	0	6,6,6	0.06	0
3	SO4	B	504	-	4,4,4	0.31	0	6,6,6	0.07	0
3	SO4	H	508	-	4,4,4	0.33	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	L	501	-	4,4,4	0.32	0	6,6,6	0.05	0
3	SO4	L	505	-	4,4,4	0.33	0	6,6,6	0.06	0
3	SO4	J	503	-	4,4,4	0.30	0	6,6,6	0.08	0
3	SO4	E	506	-	4,4,4	0.31	0	6,6,6	0.07	0
3	SO4	C	504	-	4,4,4	0.34	0	6,6,6	0.05	0
3	SO4	G	504	-	4,4,4	0.31	0	6,6,6	0.06	0
3	SO4	K	504	-	4,4,4	0.33	0	6,6,6	0.07	0
3	SO4	F	505	-	4,4,4	0.32	0	6,6,6	0.07	0
3	SO4	H	509	-	4,4,4	0.31	0	6,6,6	0.06	0
3	SO4	I	510	-	4,4,4	0.33	0	6,6,6	0.05	0
3	SO4	F	503	-	4,4,4	0.36	0	6,6,6	0.24	0
3	SO4	D	503	-	4,4,4	0.32	0	6,6,6	0.05	0
3	SO4	E	504	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	J	506	-	4,4,4	0.39	0	6,6,6	0.28	0
3	SO4	K	506	-	4,4,4	0.24	0	6,6,6	0.22	0
3	SO4	B	506	-	4,4,4	0.21	0	6,6,6	0.14	0
3	SO4	L	504	-	4,4,4	0.32	0	6,6,6	0.07	0
3	SO4	D	506	-	4,4,4	0.32	0	6,6,6	0.07	0
3	SO4	I	501	-	4,4,4	0.31	0	6,6,6	0.07	0
3	SO4	E	508	-	4,4,4	0.32	0	6,6,6	0.12	0
3	SO4	A	505	-	4,4,4	0.22	0	6,6,6	0.08	0
3	SO4	F	507	-	4,4,4	0.33	0	6,6,6	0.06	0
3	SO4	K	505	-	4,4,4	0.31	0	6,6,6	0.10	0
3	SO4	A	503	-	4,4,4	0.33	0	6,6,6	0.07	0
3	SO4	C	506	-	4,4,4	0.34	0	6,6,6	0.06	0
3	SO4	J	504	-	4,4,4	0.32	0	6,6,6	0.07	0
3	SO4	I	508	-	4,4,4	0.35	0	6,6,6	0.04	0
3	SO4	A	507	-	4,4,4	0.32	0	6,6,6	0.05	0
3	SO4	F	508	-	4,4,4	0.32	0	6,6,6	0.06	0
3	SO4	L	506	-	4,4,4	0.31	0	6,6,6	0.10	0
3	SO4	G	505	-	4,4,4	0.33	0	6,6,6	0.07	0
3	SO4	C	505	-	4,4,4	0.32	0	6,6,6	0.09	0
3	SO4	F	504	-	4,4,4	0.33	0	6,6,6	0.06	0
3	SO4	D	504	-	4,4,4	0.32	0	6,6,6	0.08	0
3	SO4	A	504	-	4,4,4	0.34	0	6,6,6	0.06	0
3	SO4	I	507	-	4,4,4	0.33	0	6,6,6	0.05	0
3	SO4	F	506	-	4,4,4	0.34	0	6,6,6	0.05	0
3	SO4	H	507	-	4,4,4	0.32	0	6,6,6	0.05	0
3	SO4	I	509	-	4,4,4	0.32	0	6,6,6	0.09	0
3	SO4	E	503	-	4,4,4	0.32	0	6,6,6	0.06	0
4	CIT	E	507	-	12,12,12	1.11	0	17,17,17	1.34	2 (11%)
3	SO4	H	501	-	4,4,4	0.32	0	6,6,6	0.06	0
3	SO4	H	505	-	4,4,4	0.32	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	G	506	-	4,4,4	0.31	0	6,6,6	0.09	0
3	SO4	J	505	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	C	507	-	4,4,4	0.33	0	6,6,6	0.06	0
3	SO4	B	505	-	4,4,4	0.31	0	6,6,6	0.06	0
3	SO4	A	506	-	4,4,4	0.34	0	6,6,6	0.06	0
3	SO4	D	505	-	4,4,4	0.33	0	6,6,6	0.08	0
3	SO4	B	503	-	4,4,4	0.31	0	6,6,6	0.06	0
3	SO4	E	505	-	4,4,4	0.37	0	6,6,6	0.17	0
3	SO4	G	503	-	4,4,4	0.28	0	6,6,6	0.40	0
3	SO4	I	504	-	4,4,4	0.31	0	6,6,6	0.21	0
3	SO4	F	509	-	4,4,4	0.33	0	6,6,6	0.06	0
3	SO4	H	504	-	4,4,4	0.31	0	6,6,6	0.08	0
3	SO4	I	506	-	4,4,4	0.33	0	6,6,6	0.06	0
3	SO4	B	507	-	4,4,4	0.32	0	6,6,6	0.04	0
3	SO4	C	503	-	4,4,4	0.31	0	6,6,6	0.09	0
3	SO4	B	508	-	4,4,4	0.50	0	6,6,6	0.46	0
3	SO4	K	507	-	4,4,4	0.34	0	6,6,6	0.04	0
3	SO4	C	508	-	4,4,4	0.29	0	6,6,6	0.06	0
3	SO4	J	507	-	4,4,4	0.38	0	6,6,6	0.22	0
3	SO4	K	501	-	4,4,4	0.34	0	6,6,6	0.06	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	CIT	E	507	-	-	0/16/16/16	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	507	CIT	O6-C6-C3	3.49	119.11	113.05
4	E	507	CIT	O5-C6-C3	-2.60	118.58	122.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	505	SO4	2	0
3	K	504	SO4	1	0
3	H	509	SO4	1	0
3	F	503	SO4	4	0
3	D	503	SO4	3	0
3	K	506	SO4	1	0
3	F	507	SO4	1	0
3	K	505	SO4	1	0
3	A	503	SO4	1	0
3	L	506	SO4	1	0
3	G	505	SO4	2	0
3	D	504	SO4	1	0
3	E	503	SO4	1	0
3	A	506	SO4	1	0
3	H	504	SO4	1	0
3	C	503	SO4	4	0
3	J	507	SO4	2	0

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	417/455 (91%)	-0.15	2 (0%)	91	90	23, 32, 50, 71	0
1	B	416/455 (91%)	-0.14	2 (0%)	91	90	23, 32, 50, 73	0
1	C	423/455 (92%)	-0.11	2 (0%)	91	90	23, 34, 51, 77	0
1	D	422/455 (92%)	-0.10	3 (0%)	87	87	24, 34, 51, 62	0
1	E	421/455 (92%)	-0.07	5 (1%)	79	78	22, 33, 52, 84	0
1	F	421/455 (92%)	-0.05	3 (0%)	87	87	22, 34, 52, 89	0
1	G	418/455 (91%)	-0.12	1 (0%)	95	94	24, 33, 51, 79	0
1	H	421/455 (92%)	-0.09	5 (1%)	79	78	23, 34, 52, 84	0
1	I	416/455 (91%)	-0.10	3 (0%)	87	87	23, 33, 51, 73	0
1	J	421/455 (92%)	-0.09	5 (1%)	79	78	24, 35, 52, 88	0
1	K	421/455 (92%)	-0.08	5 (1%)	79	78	24, 34, 53, 88	0
1	L	422/455 (92%)	-0.03	9 (2%)	63	62	23, 33, 54, 86	0
All	All	5039/5460 (92%)	-0.09	45 (0%)	84	83	22, 33, 52, 89	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	469	GLY	10.2
1	K	469	GLY	8.7
1	B	48	VAL	7.7
1	L	470	TYR	7.3
1	A	469	GLY	6.2
1	K	48	VAL	5.6
1	L	469	GLY	5.2
1	I	48	VAL	4.4
1	L	366	ARG	4.2
1	H	469	GLY	3.8
1	G	48	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	469	GLY	3.8
1	F	366	ARG	3.7
1	J	366	ARG	3.6
1	K	468	GLY	3.5
1	F	469	GLY	3.5
1	I	367	LYS	3.3
1	K	363	ASP	3.3
1	L	372	LEU	3.1
1	D	470	TYR	2.9
1	E	358	TYR	2.9
1	D	48	VAL	2.8
1	H	366	ARG	2.7
1	J	468	GLY	2.6
1	I	358	TYR	2.5
1	J	364	GLY	2.5
1	B	469	GLY	2.5
1	K	366	ARG	2.5
1	E	367	LYS	2.5
1	E	366	ARG	2.4
1	C	49	GLY	2.4
1	D	143	GLN	2.3
1	J	48	VAL	2.3
1	A	369	ASP	2.3
1	L	358	TYR	2.3
1	F	363	ASP	2.3
1	E	372	LEU	2.2
1	C	471	SER	2.2
1	L	373	LYS	2.2
1	L	363	ASP	2.1
1	L	367	LYS	2.1
1	H	372	LEU	2.1
1	H	363	ASP	2.1
1	H	367	LYS	2.0
1	L	371	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	SNN	I	168	7/8	0.94	0.13	26,30,36,36	0
1	SNN	G	168	7/8	0.95	0.11	24,29,39,39	0
1	SNN	E	168	7/8	0.96	0.12	25,29,31,31	0
1	SNN	H	168	7/8	0.96	0.10	26,33,37,40	0
1	SNN	F	168	7/8	0.96	0.09	27,33,38,40	0
1	SNN	J	168	7/8	0.96	0.10	30,33,36,37	0
1	SNN	L	168	7/8	0.96	0.15	24,29,35,35	0
1	SNN	D	168	7/8	0.97	0.12	24,29,36,36	0
1	SNN	A	168	7/8	0.97	0.12	24,28,31,34	0
1	SNN	B	168	7/8	0.97	0.12	23,29,31,34	0
1	SNN	K	168	7/8	0.97	0.12	27,32,35,36	0
1	SNN	C	168	7/8	0.97	0.10	27,32,38,38	0

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	N	2	14/15	0.67	0.20	65,80,99,100	0
2	NAG	O	2	14/15	0.68	0.25	68,87,103,109	0
2	NAG	S	2	14/15	0.73	0.16	63,79,100,106	0
2	NAG	U	2	14/15	0.73	0.24	67,85,102,106	0
2	NAG	W	2	14/15	0.75	0.23	71,86,107,111	0
2	NAG	P	2	14/15	0.76	0.20	67,82,99,107	0
2	NAG	M	2	14/15	0.76	0.25	71,83,96,99	0
2	NAG	V	2	14/15	0.81	0.23	61,88,102,111	0
2	NAG	R	2	14/15	0.81	0.24	67,85,104,111	0
2	NAG	T	2	14/15	0.82	0.23	68,81,100,101	0
2	NAG	N	1	14/15	0.86	0.17	47,58,74,84	0
2	NAG	Q	2	14/15	0.87	0.25	65,78,89,98	0
2	NAG	R	1	14/15	0.87	0.17	45,62,77,83	0
2	NAG	U	1	14/15	0.88	0.14	47,61,74,77	0
2	NAG	W	1	14/15	0.88	0.14	45,57,73,76	0
2	NAG	P	1	14/15	0.88	0.14	50,60,72,84	0
2	NAG	X	2	14/15	0.89	0.26	64,78,92,95	0
2	NAG	S	1	14/15	0.91	0.13	44,59,71,75	0
2	NAG	V	1	14/15	0.91	0.11	36,59,73,85	0
2	NAG	O	1	14/15	0.91	0.10	49,63,72,81	0
2	NAG	M	1	14/15	0.92	0.14	45,61,73,88	0
2	NAG	Q	1	14/15	0.93	0.12	38,52,65,75	0

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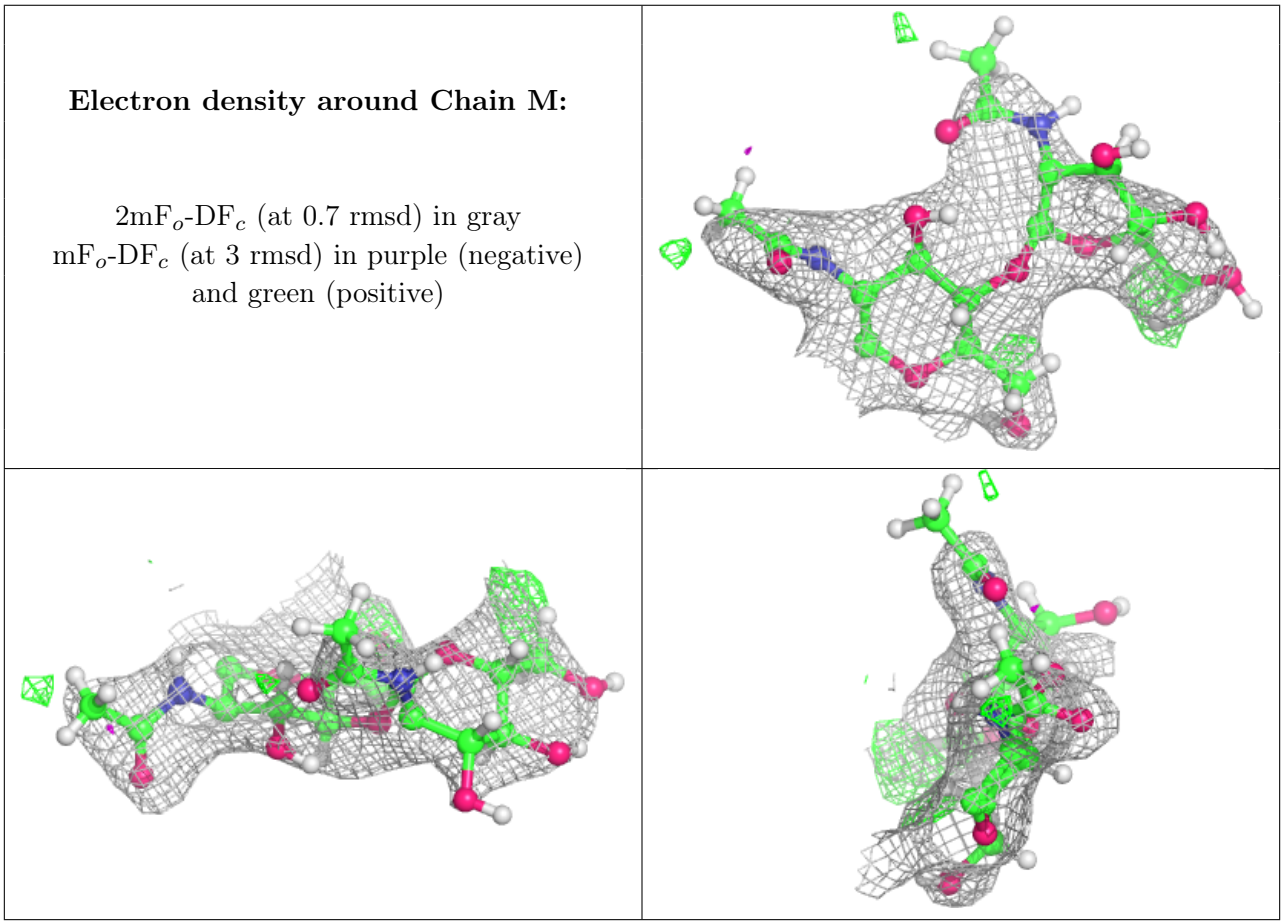
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	T	1	14/15	0.93	0.14	43,60,72,77	0
2	NAG	X	1	14/15	0.94	0.13	41,55,67,77	0

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.

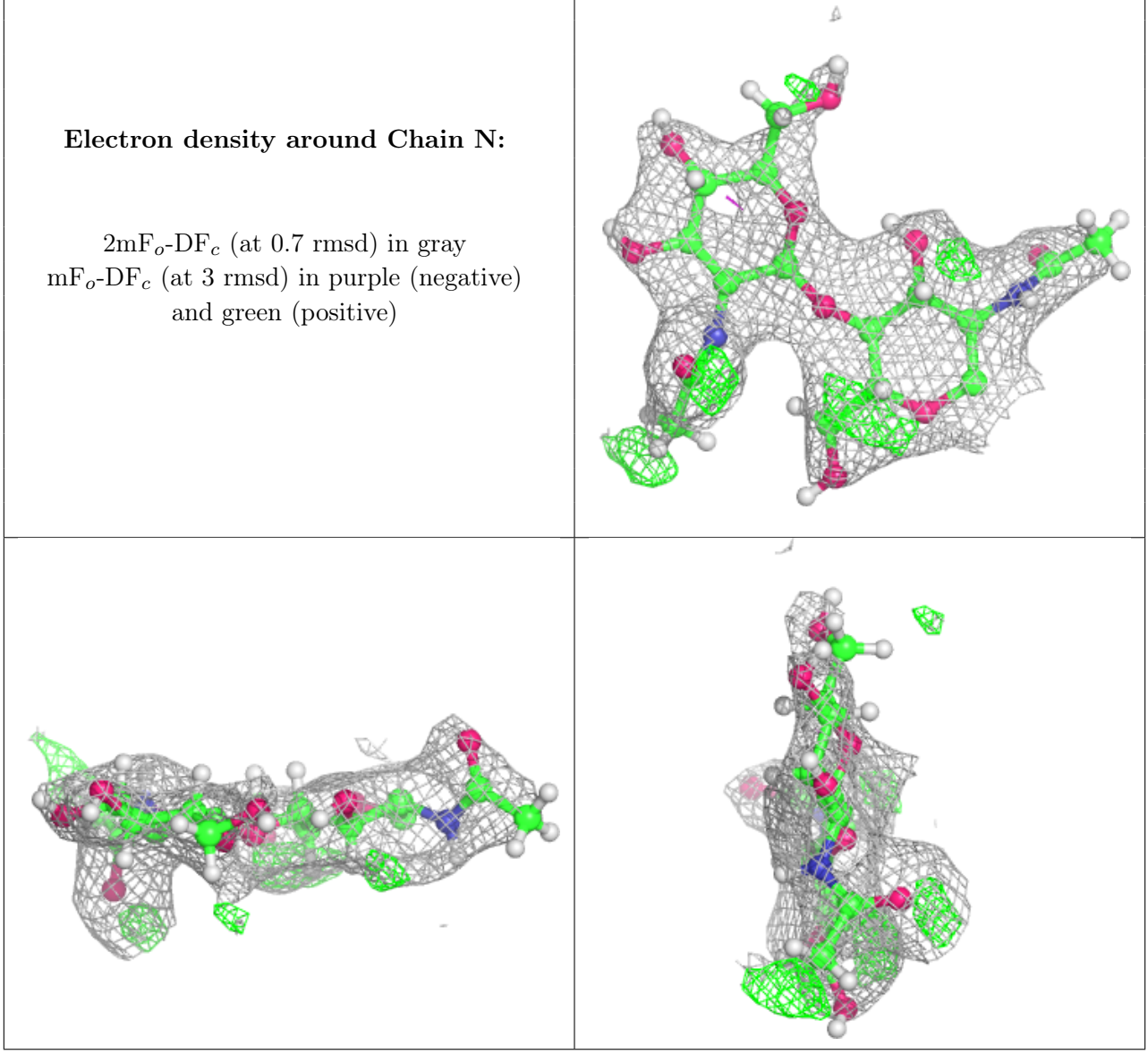
Electron density around Chain M:

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



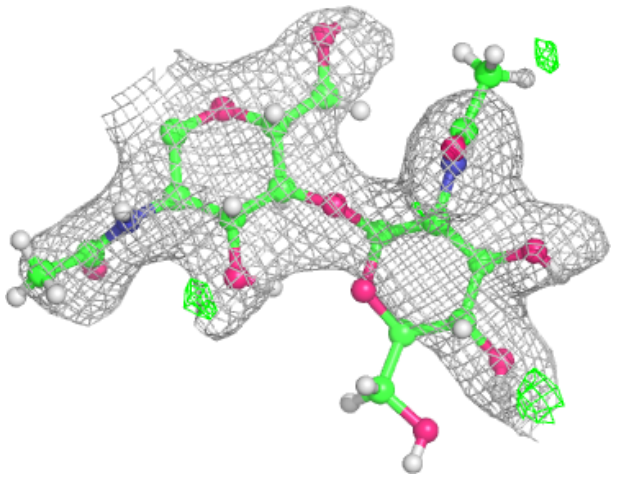
Electron density around Chain N:

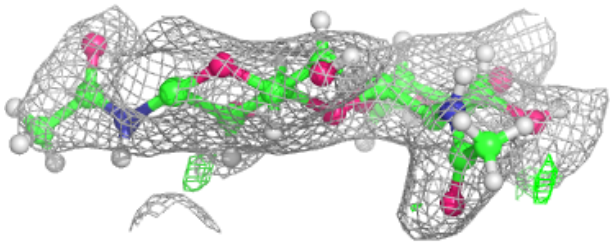
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

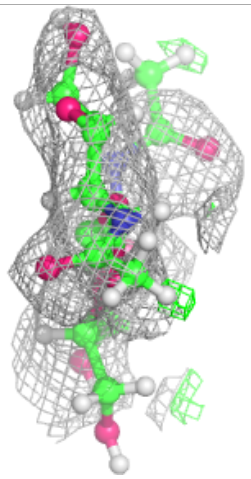


Electron density around Chain O:

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

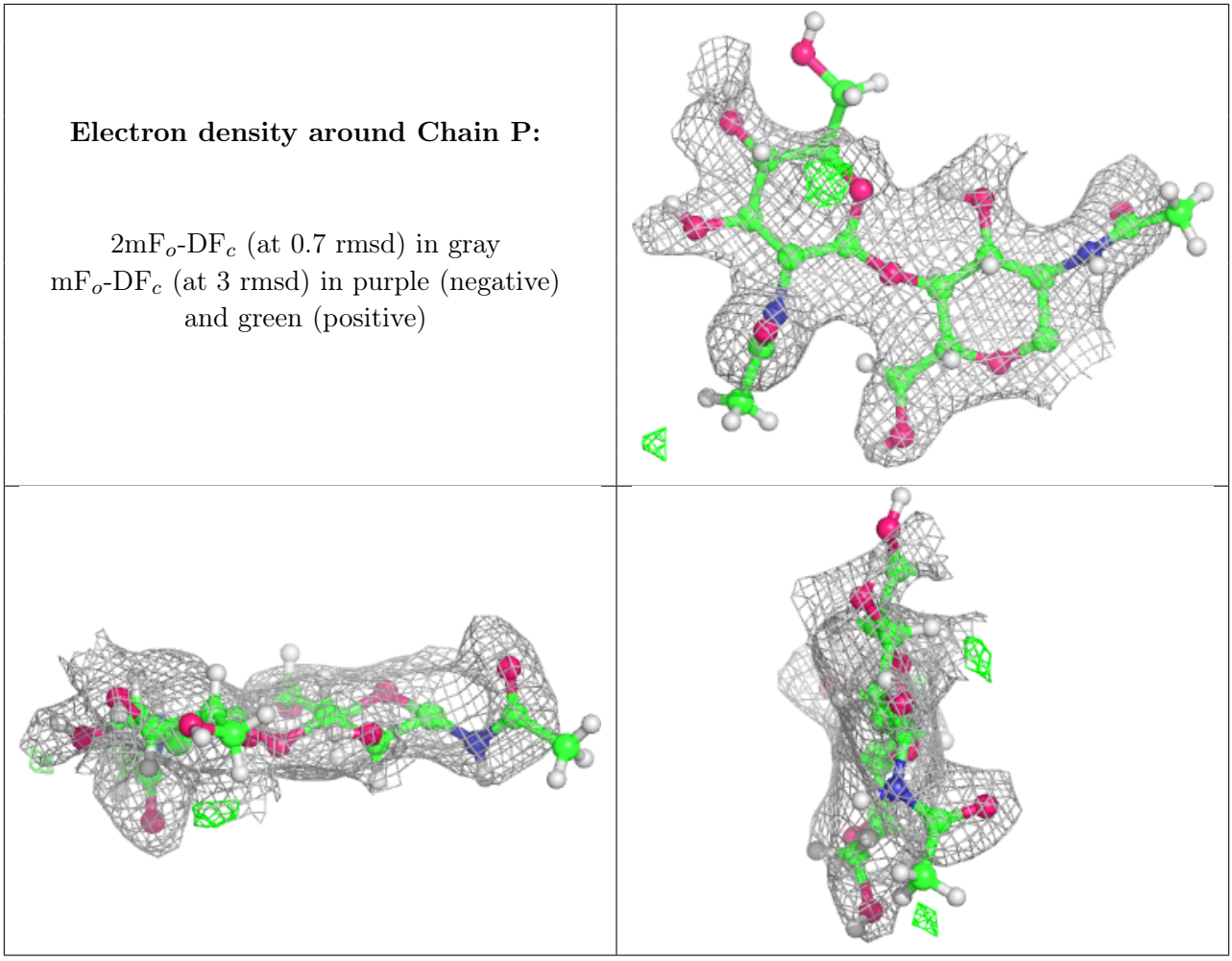






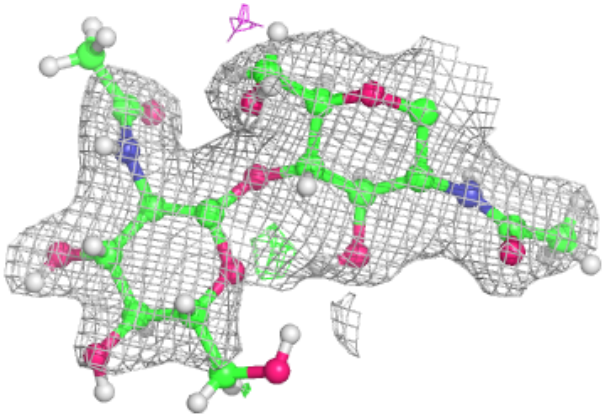
Electron density around Chain P:

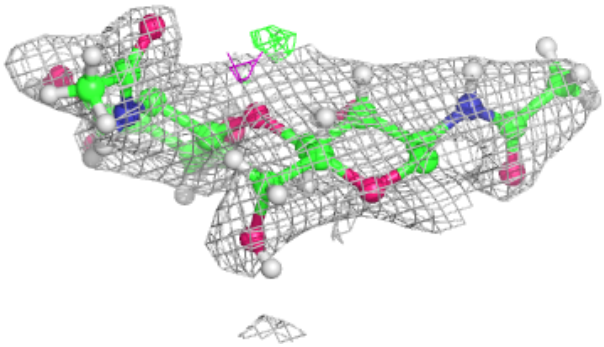
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

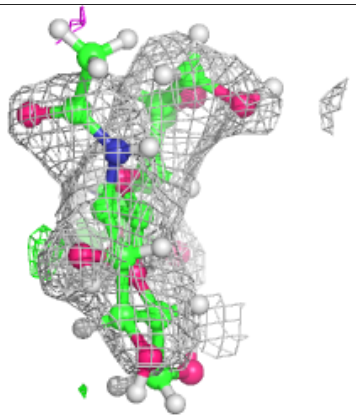


Electron density around Chain Q:

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

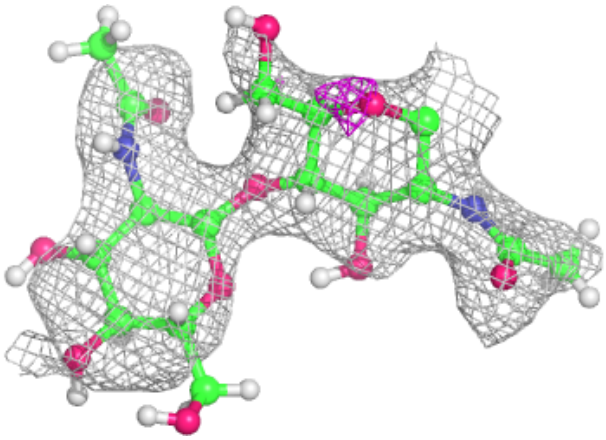


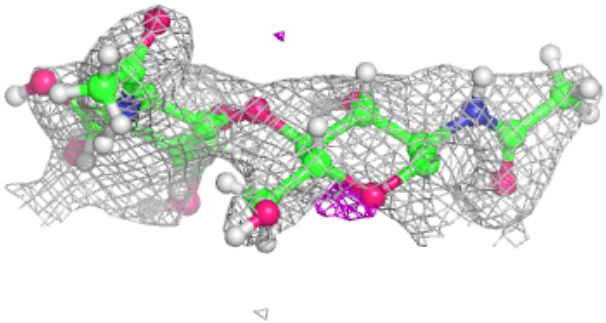


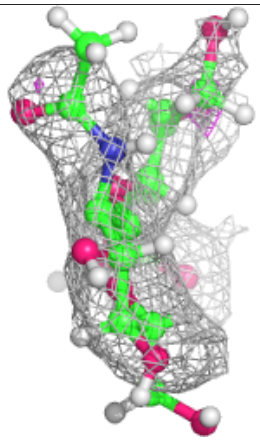


Electron density around Chain R:

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

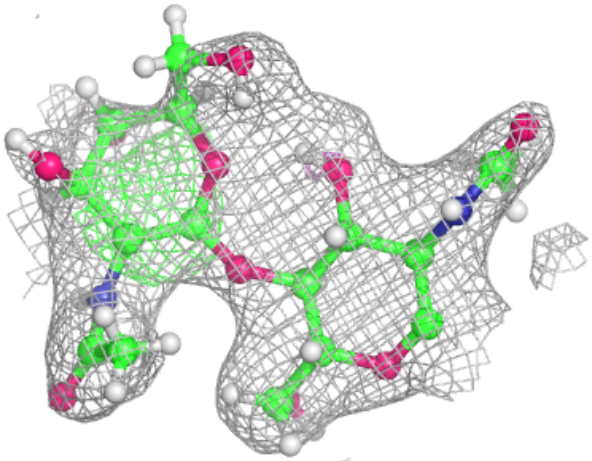


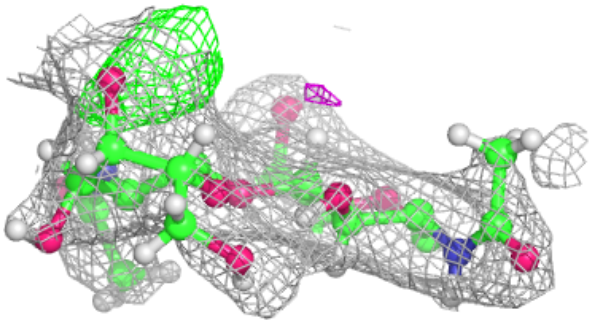


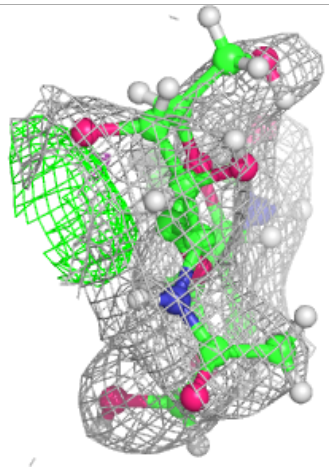


Electron density around Chain S:

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

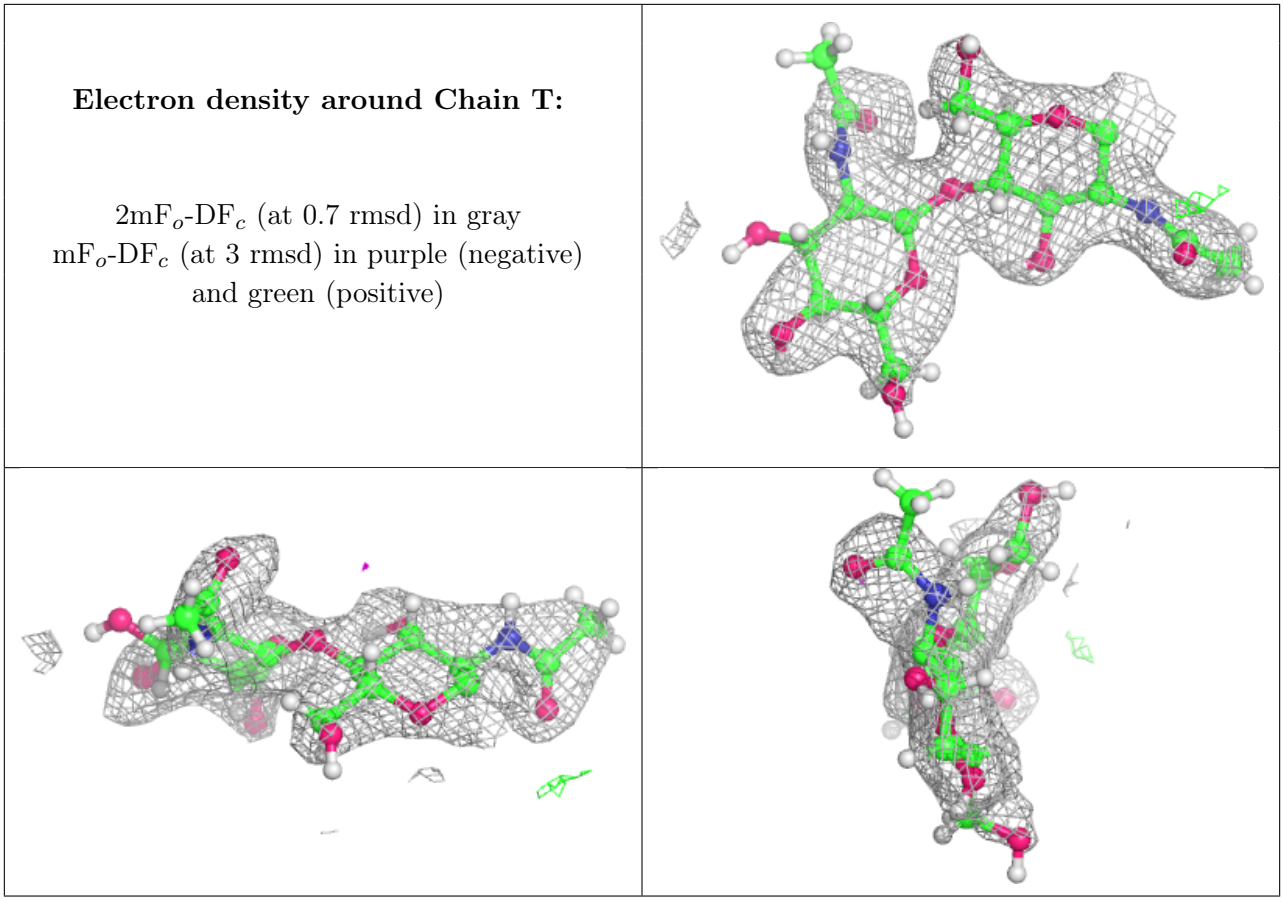






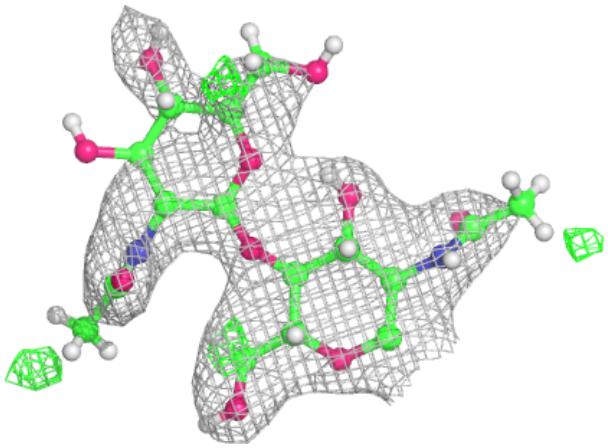
Electron density around Chain T:

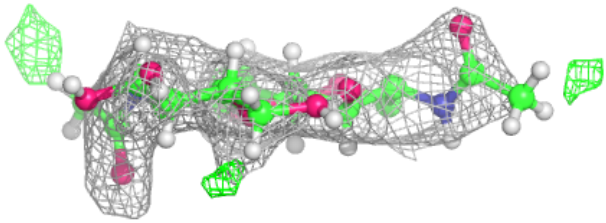
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

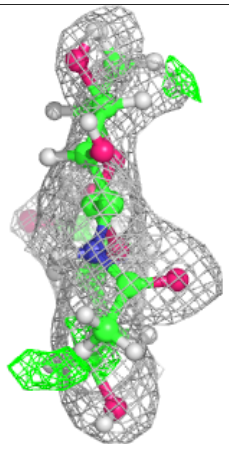


Electron density around Chain U:

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

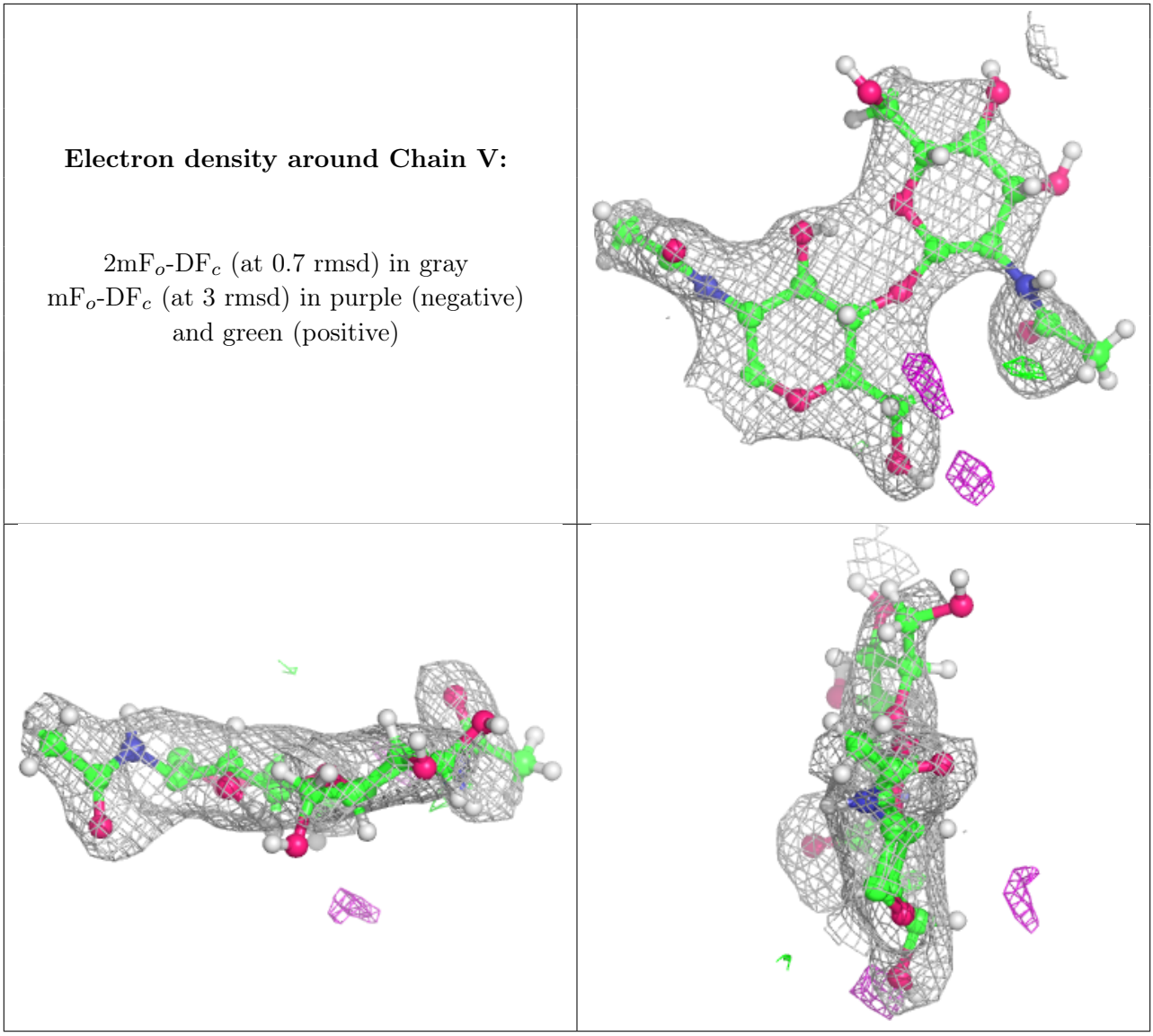






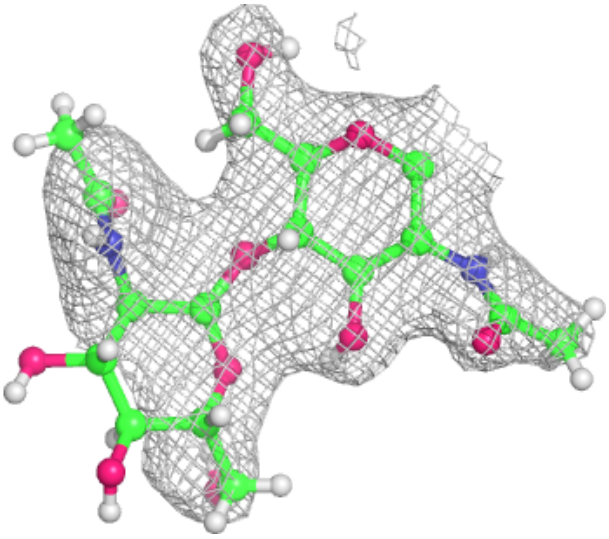
Electron density around Chain V:

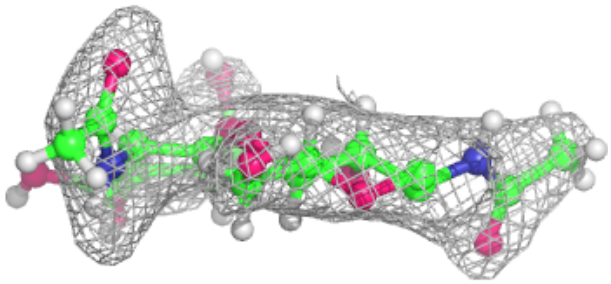
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

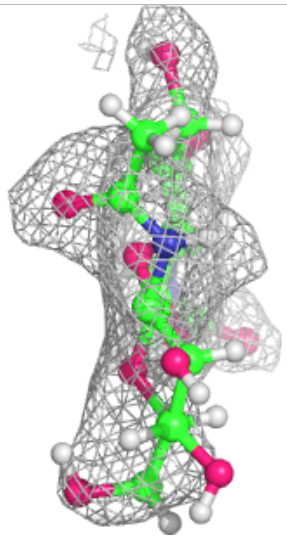


Electron density around Chain W:

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

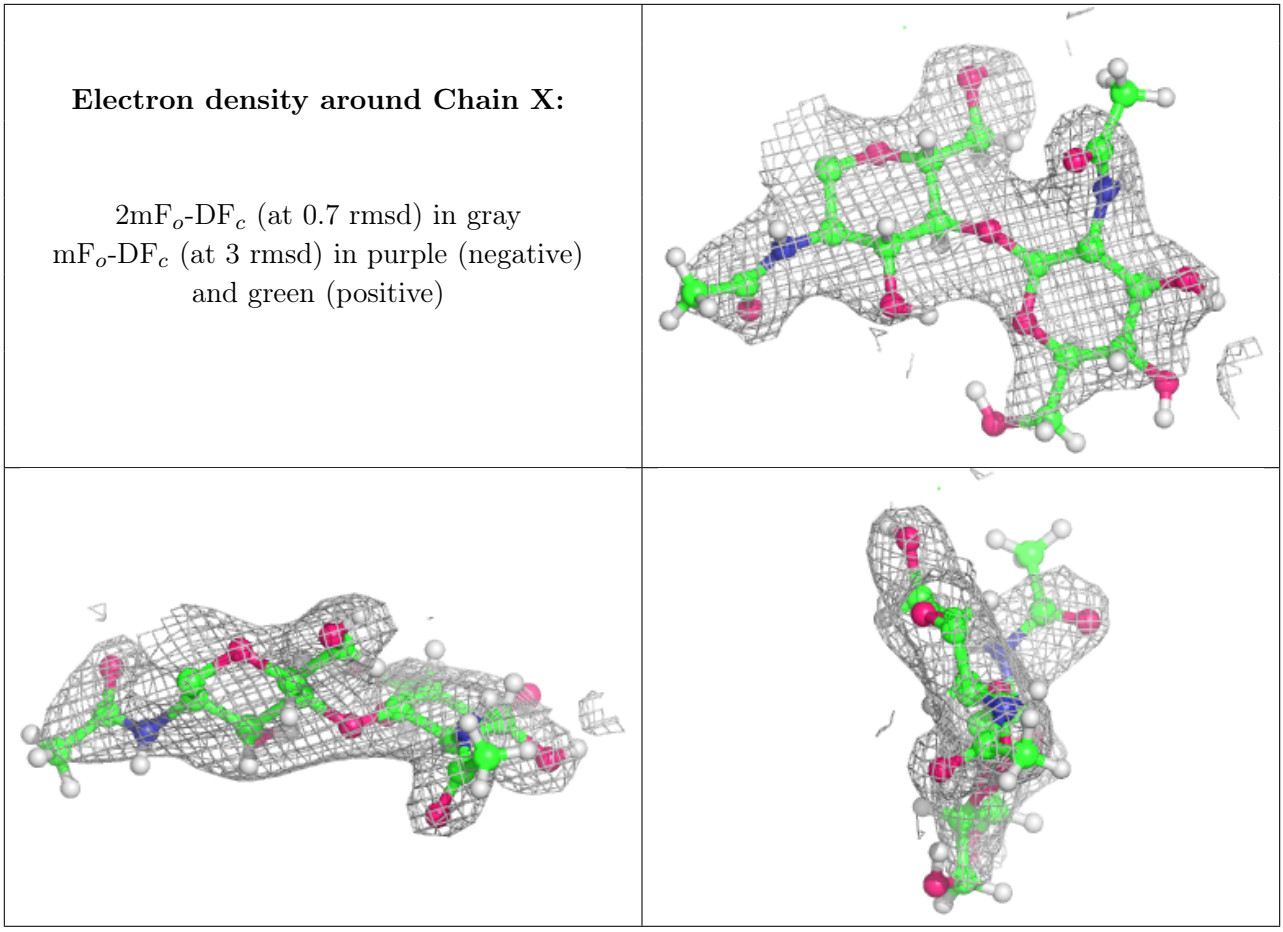






Electron density around Chain X:

$2mF_o$-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
3	SO4	E	508	5/5	0.85	0.21	45,46,72,103	0
4	CIT	E	507	13/13	0.85	0.33	42,60,76,91	16
3	SO4	I	504	5/5	0.87	0.18	44,50,71,86	0
3	SO4	E	506	5/5	0.90	0.14	42,48,53,70	5
3	SO4	A	506	5/5	0.91	0.20	44,53,59,60	5
3	SO4	K	505	5/5	0.93	0.13	43,47,57,73	0
3	SO4	L	505	5/5	0.93	0.14	38,43,46,46	5
3	SO4	L	506	5/5	0.93	0.12	55,56,60,69	5
3	SO4	J	506	5/5	0.93	0.19	47,54,57,61	5
3	SO4	E	505	5/5	0.94	0.14	43,43,58,59	5
3	SO4	J	507	5/5	0.94	0.16	40,41,61,65	5
3	SO4	G	505	5/5	0.94	0.10	42,53,59,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	H	508	5/5	0.94	0.14	56,59,73,78	0
3	SO4	E	504	5/5	0.94	0.11	58,63,76,87	0
3	SO4	J	505	5/5	0.94	0.09	46,49,55,57	0
3	SO4	K	507	5/5	0.95	0.11	43,45,58,64	5
3	SO4	C	506	5/5	0.95	0.10	46,62,66,68	0
3	SO4	J	504	5/5	0.95	0.15	48,49,54,75	0
3	SO4	F	506	5/5	0.95	0.11	51,57,66,74	0
3	SO4	I	510	5/5	0.96	0.10	47,51,65,67	5
3	SO4	B	505	5/5	0.96	0.10	53,57,71,73	0
3	SO4	F	507	5/5	0.96	0.09	39,47,57,65	0
3	SO4	F	508	5/5	0.96	0.12	49,52,56,57	5
3	SO4	G	504	5/5	0.96	0.11	49,55,64,72	0
3	SO4	K	501	5/5	0.96	0.09	56,56,61,67	0
3	SO4	C	507	5/5	0.96	0.10	41,47,50,52	5
3	SO4	G	506	5/5	0.96	0.07	50,51,55,68	5
3	SO4	C	504	5/5	0.96	0.10	52,54,66,71	0
3	SO4	F	503	5/5	0.96	0.14	34,34,39,49	5
3	SO4	I	506	5/5	0.96	0.09	50,55,60,65	0
3	SO4	I	505	5/5	0.97	0.10	49,51,60,63	0
3	SO4	B	503	5/5	0.97	0.09	54,60,62,76	0
3	SO4	D	504	5/5	0.97	0.10	53,57,61,66	0
3	SO4	D	505	5/5	0.97	0.11	39,55,62,63	0
3	SO4	G	503	5/5	0.97	0.16	34,34,48,53	5
3	SO4	B	504	5/5	0.97	0.10	45,48,56,57	0
3	SO4	A	504	5/5	0.97	0.07	46,49,65,71	0
3	SO4	A	503	5/5	0.97	0.12	49,56,61,62	0
3	SO4	H	504	5/5	0.97	0.12	32,39,42,48	0
3	SO4	H	506	5/5	0.97	0.09	49,49,59,69	0
3	SO4	C	505	5/5	0.97	0.11	39,51,57,67	0
3	SO4	H	509	5/5	0.97	0.14	51,58,59,62	5
3	SO4	A	507	5/5	0.97	0.13	46,49,52,55	5
3	SO4	C	503	5/5	0.98	0.11	32,33,35,49	5
3	SO4	I	507	5/5	0.98	0.10	51,59,65,68	0
3	SO4	I	509	5/5	0.98	0.14	31,37,43,44	0
3	SO4	D	506	5/5	0.98	0.09	44,45,54,56	5
3	SO4	J	503	5/5	0.98	0.11	31,37,41,43	5
3	SO4	F	504	5/5	0.98	0.10	51,54,57,62	0
3	SO4	F	505	5/5	0.98	0.10	47,55,59,67	0
3	SO4	H	505	5/5	0.98	0.08	50,50,61,62	0
3	SO4	E	503	5/5	0.98	0.13	34,39,40,50	0
3	SO4	H	507	5/5	0.98	0.10	49,54,57,65	0
3	SO4	K	504	5/5	0.98	0.11	33,34,39,44	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	B	507	5/5	0.98	0.11	43,45,48,60	5
3	SO4	K	506	5/5	0.98	0.08	30,30,30,30	0
3	SO4	D	503	5/5	0.98	0.13	32,34,37,39	0
3	SO4	L	504	5/5	0.98	0.14	34,37,42,43	5
3	SO4	I	501	5/5	0.98	0.11	48,49,53,61	0
3	SO4	F	509	5/5	0.98	0.09	41,42,51,56	0
3	SO4	B	508	5/5	0.98	0.08	50,52,60,67	0
3	SO4	C	508	5/5	0.99	0.07	48,49,52,59	0
3	SO4	L	501	5/5	0.99	0.09	46,47,52,57	0
3	SO4	B	506	5/5	0.99	0.09	30,31,35,37	0
3	SO4	A	505	5/5	0.99	0.11	27,33,34,36	5
3	SO4	I	508	5/5	0.99	0.06	46,50,61,69	0
3	SO4	H	501	5/5	0.99	0.10	41,43,47,55	0

6.5 Other polymers

There are no such residues in this entry.