



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 07:49 PM BST

PDB ID : 1GMO
Title : CRYSTAL STRUCTURES OF NK1-HEPARIN COMPLEXES REVEAL THE BASIS FOR NK1 ACTIVITY AND ENABLE ENGINEERING OF POTENT AGONISTS OF THE MET RECEPTOR
Authors : Lietha, D.; Chirgadze, D.Y.; Mulloy, B.; Blundell, T.L.; Gherardi, E.
Deposited on : 2001-09-20
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

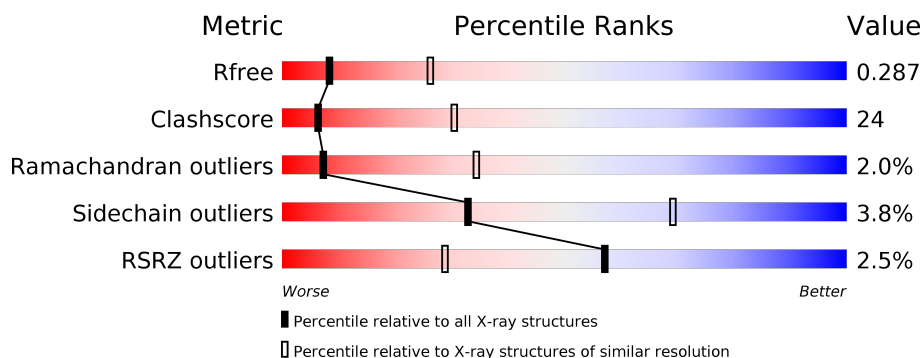
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	183	<div> <div>3%</div> <div> <div></div> <div>56%</div> <div>34%</div> <div>• • 5%</div> </div> </div>
1	B	183	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>34%</div> <div>• 5%</div> </div> </div>
1	C	183	<div> <div>%</div> <div> <div></div> <div>55%</div> <div>37%</div> <div>• 5%</div> </div> </div>
1	D	183	<div> <div>%</div> <div> <div></div> <div>52%</div> <div>38%</div> <div>• 5%</div> </div> </div>
1	E	183	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>32%</div> <div>• • 5%</div> </div> </div>
1	F	183	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>28%</div> <div>• 5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	183	
1	H	183	
2	I	6	
3	J	7	
4	K	8	
5	L	9	
6	M	6	
6	N	6	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IDS	I	1	-	-	-	X
2	SGN	I	4	-	-	-	X
2	IDS	I	5	X	-	-	-
2	SGN	I	6	-	-	-	X
3	IDS	J	1	-	-	-	X
3	SGN	J	2	-	-	-	X
3	IDS	J	3	-	-	-	X
3	IDS	J	5	-	-	-	X
3	SGN	J	6	-	-	-	X
3	IDS	J	7	-	-	-	X
4	IDS	K	7	X	-	-	-
6	SGN	M	1	-	-	-	X
6	IDS	M	2	-	-	-	X
6	SGN	N	1	-	-	-	X
6	SGN	N	5	-	-	-	X
6	IDS	N	6	-	-	-	X
7	SO4	C	301	-	-	X	-
7	SO4	F	307	-	-	X	-
8	EPE	F	309	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11555 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HEPATOCYTE GROWTH FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	0	1
			1324	833	229	250	12			
1	B	173	Total	C	N	O	S	0	0	1
			1339	843	232	252	12			
1	C	173	Total	C	N	O	S	0	0	1
			1341	846	232	251	12			
1	D	173	Total	C	N	O	S	0	0	1
			1305	821	224	248	12			
1	E	174	Total	C	N	O	S	0	0	1
			1297	812	223	250	12			
1	F	174	Total	C	N	O	S	0	0	1
			1331	836	232	251	12			
1	G	165	Total	C	N	O	S	0	0	1
			1241	783	213	233	12			
1	H	172	Total	C	N	O	S	0	0	1
			1299	814	225	248	12			

There are 16 discrepancies between the modelled and reference sequences:

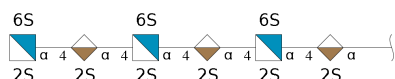
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	VAL	ALA	engineered mutation	UNP P14210
A	72	ASP	ASN	engineered mutation	UNP P14210
B	29	VAL	ALA	engineered mutation	UNP P14210
B	72	ASP	ASN	engineered mutation	UNP P14210
C	29	VAL	ALA	engineered mutation	UNP P14210
C	72	ASP	ASN	engineered mutation	UNP P14210
D	29	VAL	ALA	engineered mutation	UNP P14210
D	72	ASP	ASN	engineered mutation	UNP P14210
E	29	VAL	ALA	engineered mutation	UNP P14210
E	72	ASP	ASN	engineered mutation	UNP P14210
F	29	VAL	ALA	engineered mutation	UNP P14210
F	72	ASP	ASN	engineered mutation	UNP P14210
G	29	VAL	ALA	engineered mutation	UNP P14210

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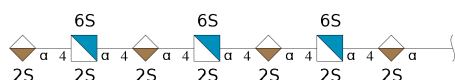
Chain	Residue	Modelled	Actual	Comment	Reference
G	72	ASP	ASN	engineered mutation	UNP P14210
H	29	VAL	ALA	engineered mutation	UNP P14210
H	72	ASP	ASN	engineered mutation	UNP P14210

- Molecule 2 is an oligosaccharide called 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid.



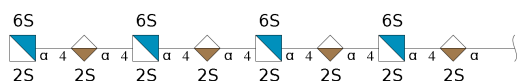
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	6	Total	C	N	O	S	0	0	0
			105	36	3	57	9			

- Molecule 3 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid.



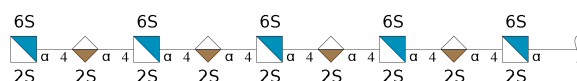
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	7	Total	C	N	O	S	0	0	0
			121	42	3	66	10			

- Molecule 4 is an oligosaccharide called 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid.



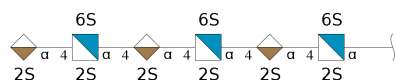
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	8	Total	C	N	O	S	0	0	0
			140	48	4	76	12			

- Molecule 5 is an oligosaccharide called 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	9	Total	C	N	O	S	0	0	0
			159	54	5	86	14			

- Molecule 6 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose.



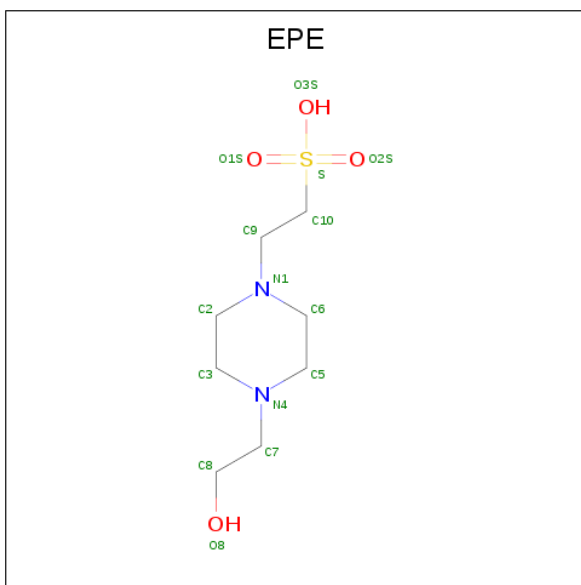
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	6	Total	C	N	O	S	0	0	0
			105	36	3	57	9			
6	N	6	Total	C	N	O	S	0	0	0
			105	36	3	57	9			

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	G	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	H	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	21	Total	O	0	0
			21	21		
9	B	34	Total	O	0	0
			34	34		
9	C	27	Total	O	0	0
			27	27		
9	D	22	Total	O	0	0
			22	22		

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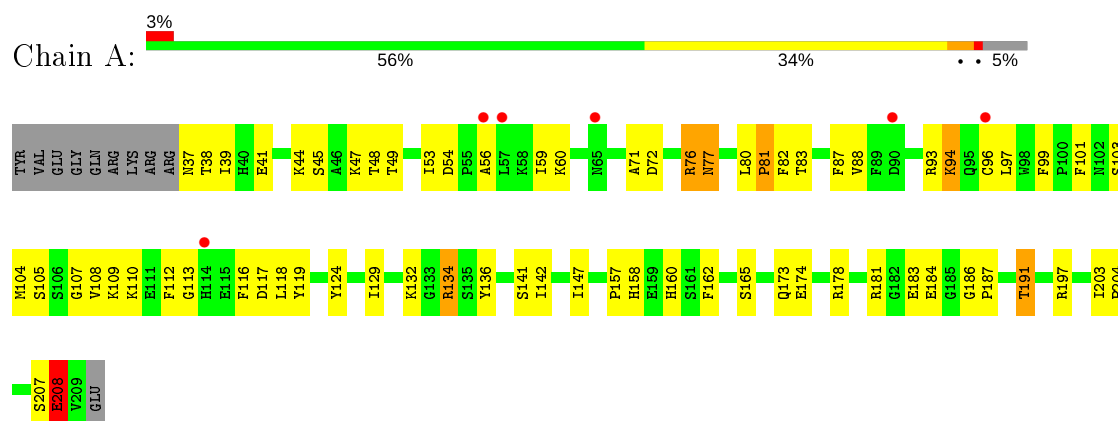
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	28	Total 28	O 28	0	0
9	F	20	Total 20	O 20	0	0
9	G	17	Total 17	O 17	0	0
9	H	14	Total 14	O 14	0	0

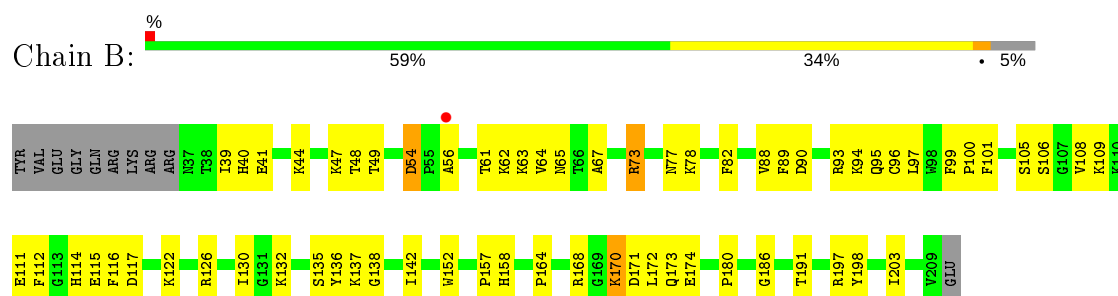
3 Residue-property plots

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.

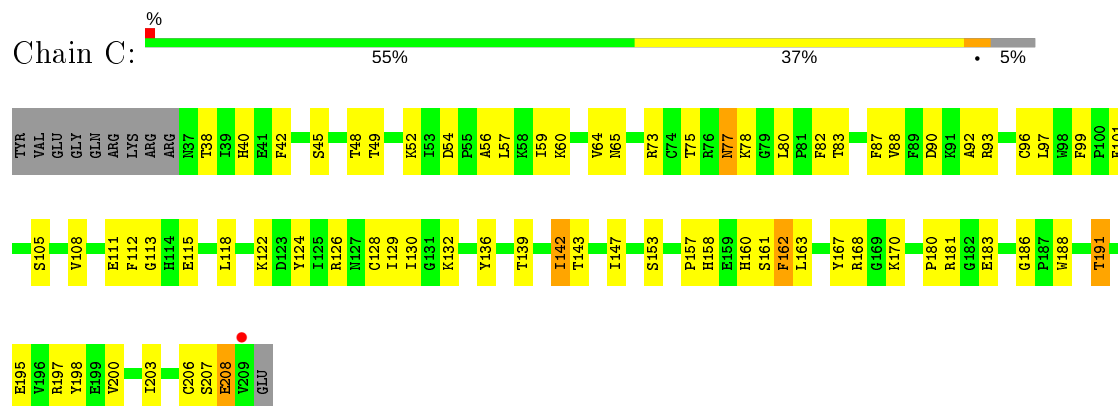
• Molecule 1: HEPATOCYTE GROWTH FACTOR



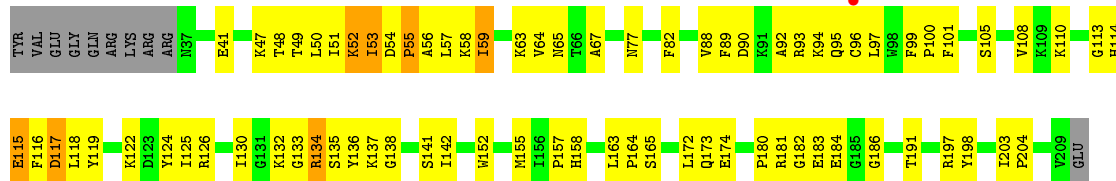
• Molecule 1: HEPATOCYTE GROWTH FACTOR



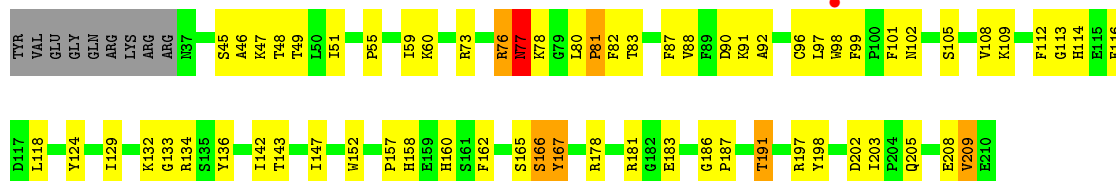
• Molecule 1: HEPATOCYTE GROWTH FACTOR



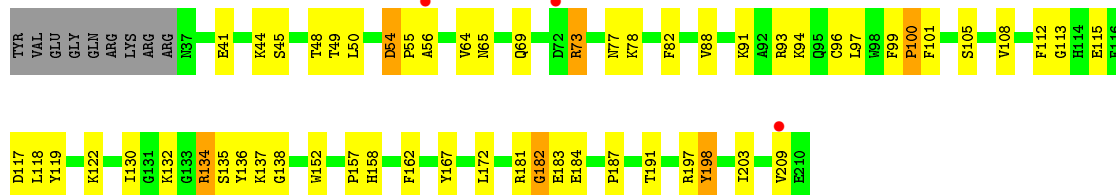
• Molecule 1: HEPATOCYTE GROWTH FACTOR



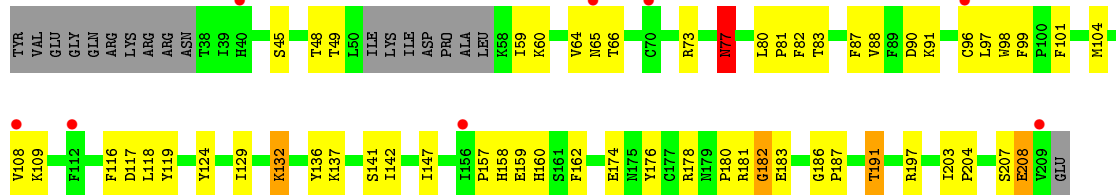
• Molecule 1: HEPATOCYTE GROWTH FACTOR



• Molecule 1: HEPATOCYTE GROWTH FACTOR

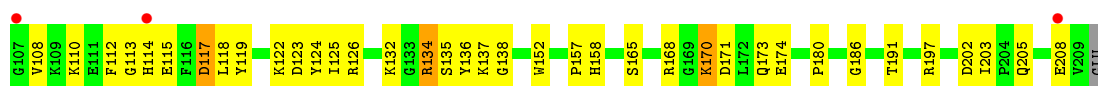


• Molecule 1: HEPATOCYTE GROWTH FACTOR



• Molecule 1: HEPATOCYTE GROWTH FACTOR



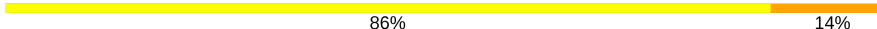



- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

Chain I:  100%



- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

Chain J:  86%  14%





- Molecule 4: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

Chain K:  63%  38%




- Molecule 5: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain L:  78%  22%



- Molecule 6: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain M:  83% 17%

SGH1
IDS2
SGH3
IDS4
SGH5
IDS6

- Molecule 6: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain N:  100%

SGH1
IDS2
SGH3
IDS4
SGH5
IDS6

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	179.70 Å 174.10 Å 59.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 19.97 – 2.97	Depositor EDS
% Data completeness (in resolution range)	95.3 (20.00-3.00) 94.6 (19.97-2.97)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.26 (at 2.98 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.254 , 0.295 0.248 , 0.287	Depositor DCC
R_{free} test set	1885 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for k,h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11555	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EPE, IDS, SGN

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	0.45	0/1358	0.67	0/1837
1	B	0.45	0/1374	0.63	0/1857
1	C	0.51	0/1376	0.67	0/1861
1	D	0.46	0/1338	0.63	0/1815
1	E	0.46	0/1331	0.66	0/1810
1	F	0.46	0/1365	0.66	0/1850
1	G	0.40	0/1273	0.62	0/1726
1	H	0.41	0/1334	0.59	0/1810
All	All	0.45	0/10749	0.64	0/14566

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	1324	0	1221	73	0
1	B	1339	0	1248	62	0
1	C	1341	0	1257	71	0
1	D	1305	0	1193	73	0
1	E	1297	0	1140	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1331	0	1223	56	0
1	G	1241	0	1121	55	0
1	H	1299	0	1162	55	0
2	I	105	0	33	0	0
3	J	121	0	38	1	0
4	K	140	0	44	3	0
5	L	159	0	51	2	0
6	M	105	0	34	1	0
6	N	105	0	34	0	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
7	C	5	0	0	2	0
7	D	5	0	0	1	0
7	E	5	0	0	0	0
7	F	10	0	0	2	0
7	H	5	0	0	1	0
8	A	15	0	17	1	0
8	B	15	0	17	2	0
8	C	15	0	17	3	0
8	D	15	0	17	1	0
8	E	15	0	17	1	0
8	F	15	0	17	1	0
8	G	15	0	17	0	0
8	H	15	0	17	0	0
9	A	21	0	0	0	0
9	B	34	0	0	5	0
9	C	27	0	0	6	0
9	D	22	0	0	7	0
9	E	28	0	0	7	0
9	F	20	0	0	3	0
9	G	17	0	0	3	0
9	H	14	0	0	1	0
All	All	11555	0	9935	513	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (513) 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:E:181:ARG:NH2	1:H:165:SER:HB3	1.63	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:LYS:H	1:D:52:LYS:HD3	1.22	1.01
1:A:134:ARG:HD2	1:A:134:ARG:H	1.26	0.98
1:F:64:VAL:HG13	1:F:69:GLN:OE1	1.64	0.96
1:G:132:LYS:H	1:G:132:LYS:HD2	1.31	0.96
1:H:134:ARG:HD2	1:H:134:ARG:H	1.32	0.94
1:D:97:LEU:HD23	9:D:407:HOH:O	1.69	0.92
1:G:207:SER:O	1:G:208:GLU:HB2	1.67	0.91
1:C:93:ARG:HH11	1:C:93:ARG:HG3	1.35	0.90
1:C:122:LYS:HE2	1:C:139:THR:HG21	1.54	0.89
1:E:181:ARG:HH21	1:H:165:SER:HB3	1.36	0.88
1:F:134:ARG:HD2	1:F:134:ARG:H	1.40	0.87
1:H:170:LYS:HG2	1:H:180:PRO:HA	1.57	0.86
1:E:101:PHE:HB2	1:E:105:SER:OG	1.76	0.85
1:A:103:SER:HB2	1:A:110:LYS:HE2	1.59	0.82
1:A:207:SER:O	1:A:208:GLU:HB2	1.79	0.82
1:A:72:ASP:OD1	1:A:76:ARG:HD2	1.79	0.82
1:F:132:LYS:HB2	1:F:134:ARG:HE	1.44	0.81
1:H:132:LYS:HB2	1:H:134:ARG:HE	1.46	0.80
1:E:181:ARG:HH21	1:H:165:SER:CB	1.94	0.80
1:C:38:THR:HG21	1:C:75:THR:OG1	1.81	0.80
1:F:73:ARG:HH11	1:F:73:ARG:HG3	1.48	0.79
8:B:317:EPE:H21	9:B:407:HOH:O	1.86	0.76
1:G:66:THR:HB	9:G:404:HOH:O	1.85	0.75
1:B:88:VAL:HG23	1:B:99:PHE:HE1	1.51	0.75
1:A:160:HIS:HD2	1:A:162:PHE:H	1.32	0.75
1:D:52:LYS:HD3	1:D:52:LYS:N	2.00	0.74
1:D:181:ARG:HB2	1:D:183:GLU:HG3	1.70	0.74
1:A:37:ASN:O	1:A:39:ILE:N	2.21	0.74
1:B:73:ARG:NH2	4:K:6:SGN:H62	2.01	0.74
1:C:183:GLU:OE1	8:C:311:EPE:H51	1.87	0.74
1:B:126:ARG:NH1	1:B:130:ILE:HD11	2.02	0.73
1:F:64:VAL:HG11	1:F:69:GLN:HB2	1.69	0.73
1:G:132:LYS:HA	9:G:402:HOH:O	1.86	0.73
1:A:96:CYS:C	1:A:97:LEU:HD12	2.09	0.72
1:E:59:ILE:HG22	1:E:60:LYS:N	2.04	0.72
1:A:160:HIS:CD2	1:A:162:PHE:H	2.06	0.72
1:B:73:ARG:HG3	1:B:73:ARG:HH11	1.53	0.72
1:B:54:ASP:HB3	9:B:402:HOH:O	1.89	0.71
1:G:160:HIS:HD2	1:G:162:PHE:H	1.36	0.71
1:C:93:ARG:HG3	1:C:93:ARG:NH1	2.00	0.71
1:B:170:LYS:HG2	1:B:180:PRO:HA	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:ILE:N	7:D:301:SO4:O2	2.22	0.70
1:H:64:VAL:HG13	1:H:69:GLN:OE1	1.92	0.70
1:E:96:CYS:C	1:E:97:LEU:HD12	2.13	0.69
1:E:158:HIS:NE2	1:E:197:ARG:HA	2.06	0.69
1:A:158:HIS:NE2	1:A:197:ARG:HA	2.08	0.69
1:G:132:LYS:N	1:G:132:LYS:HD2	2.07	0.69
1:E:181:ARG:HH22	1:H:165:SER:HB3	1.55	0.69
1:C:96:CYS:C	1:C:97:LEU:HD12	2.13	0.69
1:G:96:CYS:C	1:G:97:LEU:HD12	2.13	0.68
1:A:59:ILE:HG22	1:A:60:LYS:N	2.09	0.68
1:C:59:ILE:HG22	1:C:60:LYS:N	2.09	0.67
1:E:205:GLN:HG2	9:E:411:HOH:O	1.94	0.67
1:C:158:HIS:NE2	1:C:197:ARG:HA	2.10	0.66
1:A:101:PHE:HB2	1:A:105:SER:CB	2.26	0.66
1:E:181:ARG:NH2	1:H:165:SER:CB	2.48	0.66
1:A:93:ARG:O	1:A:94:LYS:HB2	1.95	0.66
1:B:73:ARG:HH22	4:K:6:SGN:H62	1.60	0.66
1:G:160:HIS:CD2	1:G:162:PHE:H	2.13	0.66
1:G:45:SER:HB2	1:G:118:LEU:HB3	1.77	0.65
1:G:88:VAL:HG23	1:G:99:PHE:HE2	1.60	0.65
1:A:134:ARG:HD2	1:A:134:ARG:N	2.06	0.65
1:H:63:LYS:O	1:H:64:VAL:HG23	1.97	0.65
1:D:59:ILE:HG22	1:D:59:ILE:O	1.97	0.65
1:F:105:SER:O	1:F:108:VAL:HG22	1.97	0.65
1:A:132:LYS:HB2	1:A:134:ARG:NE	2.12	0.65
1:H:105:SER:O	1:H:108:VAL:HG22	1.97	0.65
1:B:111:GLU:CD	1:B:112:PHE:H	1.99	0.65
1:B:105:SER:O	1:B:108:VAL:HG22	1.98	0.64
9:C:418:HOH:O	5:L:4:IDS:H2	1.97	0.64
1:E:88:VAL:HG23	1:E:99:PHE:HE2	1.61	0.64
1:A:45:SER:HB2	1:A:118:LEU:HB3	1.78	0.64
1:A:141:SER:O	1:A:142:ILE:HD12	1.98	0.64
1:H:132:LYS:HB2	1:H:134:ARG:NE	2.12	0.64
1:G:59:ILE:HG22	1:G:60:LYS:N	2.13	0.63
1:C:88:VAL:HG23	1:C:99:PHE:HE2	1.63	0.63
1:D:47:LYS:N	1:D:116:PHE:O	2.31	0.63
1:A:88:VAL:HG23	1:A:99:PHE:HE2	1.63	0.63
1:C:45:SER:HB2	1:C:118:LEU:HB3	1.81	0.63
1:G:158:HIS:NE2	1:G:197:ARG:HA	2.13	0.62
1:E:132:LYS:O	1:E:186:GLY:HA2	1.99	0.62
1:H:170:LYS:HE3	1:H:170:LYS:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:SER:O	1:D:108:VAL:HG22	1.99	0.62
1:D:184:GLU:O	8:D:302:EPE:H81	1.99	0.62
1:D:64:VAL:CG1	1:D:65:ASN:N	2.63	0.62
1:D:63:LYS:O	1:D:64:VAL:HG23	1.99	0.62
1:E:45:SER:HB2	1:E:118:LEU:HB3	1.80	0.61
1:D:158:HIS:CE1	1:D:197:ARG:HA	2.35	0.61
1:E:96:CYS:HB3	9:E:403:HOH:O	1.99	0.61
1:E:114:HIS:HA	9:E:408:HOH:O	2.00	0.61
1:G:207:SER:O	1:G:208:GLU:CB	2.43	0.61
1:H:64:VAL:HG11	1:H:69:GLN:HB2	1.83	0.61
1:A:184:GLU:O	8:A:308:EPE:H81	1.99	0.61
1:C:170:LYS:HD2	1:C:180:PRO:HA	1.82	0.61
1:E:152:TRP:N	9:E:402:HOH:O	2.33	0.61
1:B:64:VAL:CG1	1:B:65:ASN:N	2.64	0.61
1:E:47:LYS:HA	1:E:113:GLY:O	2.01	0.61
1:B:106:SER:HA	9:B:415:HOH:O	2.01	0.60
1:C:160:HIS:HD2	1:C:162:PHE:HB2	1.66	0.60
1:E:208:GLU:O	1:E:209:VAL:HG23	2.01	0.60
1:G:181:ARG:HB2	1:G:183:GLU:HG3	1.83	0.60
1:C:126:ARG:HD3	1:C:206:CYS:SG	2.40	0.60
1:C:130:ILE:N	7:C:301:SO4:O1	2.34	0.60
1:G:132:LYS:H	1:G:132:LYS:CD	2.11	0.60
1:D:52:LYS:H	1:D:52:LYS:CD	1.99	0.60
1:H:88:VAL:HG23	1:H:99:PHE:HE2	1.64	0.60
1:A:96:CYS:O	1:A:97:LEU:HD12	2.01	0.60
1:B:88:VAL:HG23	1:B:99:PHE:CE1	2.35	0.60
1:F:198:TYR:CD1	8:F:309:EPE:H22	2.36	0.60
1:G:160:HIS:CD2	1:G:162:PHE:HB2	2.37	0.60
8:C:311:EPE:H61	9:C:407:HOH:O	2.03	0.59
1:E:59:ILE:CG2	1:E:60:LYS:N	2.65	0.59
1:H:170:LYS:HE3	1:H:170:LYS:CA	2.32	0.59
1:B:126:ARG:NH1	1:B:130:ILE:CD1	2.66	0.59
1:G:48:THR:HG22	1:G:49:THR:N	2.18	0.59
1:C:198:TYR:CD1	1:C:198:TYR:C	2.77	0.58
1:A:132:LYS:O	1:A:186:GLY:HA2	2.03	0.58
1:A:41:GLU:HG2	1:B:41:GLU:HG2	1.85	0.58
1:D:48:THR:O	1:D:116:PHE:HB3	2.03	0.58
1:F:73:ARG:NH1	1:F:73:ARG:HG3	2.17	0.58
1:F:88:VAL:HG23	1:F:99:PHE:CE2	2.38	0.58
1:A:39:ILE:HD11	1:A:119:TYR:CE2	2.39	0.58
1:B:126:ARG:HH12	1:B:130:ILE:CD1	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:ASN:N	1:E:105:SER:OG	2.35	0.58
1:D:58:LYS:N	9:D:402:HOH:O	2.36	0.58
1:G:132:LYS:O	1:G:186:GLY:HA2	2.03	0.58
1:G:160:HIS:HD2	1:G:162:PHE:HB2	1.68	0.58
1:H:158:HIS:CE1	1:H:197:ARG:HA	2.38	0.58
1:B:126:ARG:HH12	1:B:130:ILE:HD11	1.68	0.58
1:D:96:CYS:C	1:D:97:LEU:HD12	2.24	0.58
1:D:117:ASP:HB3	1:D:119:TYR:CE1	2.39	0.58
1:F:158:HIS:CE1	1:F:197:ARG:HA	2.38	0.58
1:F:88:VAL:HG23	1:F:99:PHE:HE2	1.69	0.58
1:H:64:VAL:CG1	1:H:65:ASN:N	2.67	0.58
1:A:118:LEU:HD12	1:A:119:TYR:H	1.69	0.58
1:G:141:SER:C	1:G:142:ILE:HD12	2.25	0.58
1:A:117:ASP:HB3	1:A:119:TYR:HE1	1.69	0.57
1:G:141:SER:O	1:G:142:ILE:HD12	2.04	0.57
1:B:96:CYS:C	1:B:97:LEU:HD12	2.25	0.57
1:B:158:HIS:CE1	1:B:197:ARG:HA	2.39	0.57
1:C:200:VAL:HG13	9:C:422:HOH:O	2.04	0.57
1:C:48:THR:HG22	1:C:49:THR:N	2.19	0.57
1:F:64:VAL:CG1	1:F:65:ASN:N	2.67	0.57
1:A:48:THR:HG22	1:A:49:THR:N	2.20	0.57
1:F:122:LYS:HE3	9:F:406:HOH:O	2.05	0.57
1:H:157:PRO:HG2	1:H:158:HIS:CD2	2.40	0.57
1:A:39:ILE:HD11	1:A:119:TYR:HE2	1.68	0.57
1:D:88:VAL:HG23	1:D:99:PHE:HE2	1.69	0.57
1:G:73:ARG:HD3	1:G:98:TRP:CH2	2.40	0.56
1:E:101:PHE:HB2	1:E:105:SER:CB	2.35	0.56
1:G:73:ARG:HD3	1:G:98:TRP:CZ2	2.39	0.56
1:D:41:GLU:O	1:D:122:LYS:HG3	2.06	0.56
1:F:50:LEU:HD22	1:F:99:PHE:CD2	2.41	0.56
1:H:64:VAL:HG13	1:H:69:GLN:CD	2.26	0.56
1:E:165:SER:C	1:E:167:TYR:H	2.09	0.56
1:F:134:ARG:CD	1:F:134:ARG:H	2.11	0.56
1:A:44:LYS:HE3	1:A:119:TYR:OH	2.04	0.56
1:D:50:LEU:C	1:D:51:ILE:HD12	2.25	0.56
1:E:208:GLU:O	1:E:209:VAL:HB	2.04	0.56
1:C:59:ILE:CG2	1:C:60:LYS:N	2.69	0.56
1:C:83:THR:HG21	1:C:124:TYR:OH	2.06	0.56
1:E:48:THR:HG22	1:E:49:THR:N	2.21	0.56
1:H:47:LYS:HG3	1:H:114:HIS:HA	1.88	0.56
1:D:50:LEU:CD1	1:D:118:LEU:HD22	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:GLU:O	1:E:209:VAL:CB	2.52	0.55
1:F:157:PRO:HG2	1:F:158:HIS:CD2	2.41	0.55
1:F:41:GLU:O	1:F:122:LYS:HG3	2.06	0.55
1:B:73:ARG:HG3	1:B:73:ARG:NH1	2.21	0.55
1:D:157:PRO:HG2	1:D:158:HIS:CD2	2.41	0.55
1:B:41:GLU:O	1:B:122:LYS:HG3	2.05	0.55
1:C:105:SER:O	1:C:108:VAL:HB	2.06	0.55
1:C:207:SER:O	1:C:208:GLU:CB	2.54	0.55
1:D:53:ILE:O	1:D:54:ASP:C	2.45	0.55
1:F:96:CYS:C	1:F:97:LEU:HD12	2.27	0.55
1:G:117:ASP:HB3	1:G:119:TYR:CE1	2.41	0.55
1:A:83:THR:HG21	1:A:124:TYR:OH	2.06	0.55
1:C:122:LYS:HD3	1:C:139:THR:OG1	2.06	0.55
1:C:160:HIS:CD2	1:C:162:PHE:HB2	2.42	0.55
1:E:158:HIS:CD2	1:E:197:ARG:HA	2.41	0.55
1:F:45:SER:HB2	1:F:118:LEU:HB3	1.89	0.55
1:B:93:ARG:HH11	1:B:93:ARG:HG3	1.71	0.55
1:C:207:SER:O	1:C:208:GLU:HB3	2.08	0.54
1:C:38:THR:CG2	1:C:75:THR:OG1	2.54	0.54
1:G:90:ASP:OD2	1:G:116:PHE:HE1	1.90	0.54
1:C:158:HIS:CD2	1:C:197:ARG:HA	2.42	0.54
1:G:147:ILE:HG21	1:G:191:THR:HB	1.90	0.54
1:E:147:ILE:HG21	1:E:191:THR:HB	1.90	0.54
1:F:136:TYR:CZ	1:F:138:GLY:HA3	2.43	0.54
1:B:61:THR:O	1:B:62:LYS:HB2	2.08	0.54
1:A:162:PHE:CE1	1:A:181:ARG:HD2	2.42	0.54
1:H:41:GLU:O	1:H:122:LYS:HG3	2.08	0.54
1:A:59:ILE:CG2	1:A:60:LYS:N	2.70	0.53
1:B:170:LYS:CG	1:B:180:PRO:HA	2.38	0.53
1:H:96:CYS:C	1:H:97:LEU:HD12	2.28	0.53
1:D:134:ARG:HD2	9:D:401:HOH:O	2.07	0.53
1:D:49:THR:O	1:D:110:LYS:HA	2.08	0.53
1:G:83:THR:HG21	1:G:124:TYR:OH	2.08	0.53
1:C:161:SER:O	1:C:163:LEU:N	2.41	0.53
1:A:162:PHE:HE1	1:A:181:ARG:HD2	1.73	0.53
1:F:93:ARG:O	1:F:94:LYS:HB2	2.08	0.53
1:A:158:HIS:CD2	1:A:197:ARG:HA	2.43	0.53
1:H:135:SER:O	1:H:137:LYS:HG3	2.09	0.53
1:A:118:LEU:HD12	1:A:119:TYR:N	2.23	0.53
1:B:82:PHE:CD1	1:B:100:PRO:HB3	2.43	0.53
1:C:147:ILE:HG21	1:C:191:THR:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:TYR:CE2	8:B:317:EPE:H52	2.44	0.53
1:E:59:ILE:HG22	1:E:60:LYS:H	1.74	0.53
1:E:76:ARG:O	1:E:78:LYS:N	2.42	0.53
1:G:160:HIS:HD2	1:G:162:PHE:N	2.06	0.52
1:E:96:CYS:O	1:E:97:LEU:HD12	2.09	0.52
1:F:44:LYS:HD3	1:F:119:TYR:CE2	2.44	0.52
1:E:59:ILE:CG2	1:E:60:LYS:H	2.22	0.52
1:A:108:VAL:HG12	1:A:109:LYS:N	2.24	0.52
1:H:90:ASP:OD1	1:H:115:GLU:OE1	2.28	0.52
1:C:132:LYS:O	1:C:186:GLY:HA2	2.10	0.52
1:D:135:SER:O	1:D:137:LYS:HG3	2.08	0.52
1:B:97:LEU:HB3	1:B:99:PHE:CZ	2.45	0.52
1:D:64:VAL:HG12	1:D:65:ASN:N	2.24	0.52
1:F:73:ARG:HH22	6:M:5:SGN:H62	1.73	0.52
1:H:112:PHE:CD1	1:H:113:GLY:N	2.76	0.52
1:A:77:ASN:O	1:A:77:ASN:ND2	2.42	0.52
1:G:59:ILE:CG2	1:G:60:LYS:N	2.73	0.52
1:B:82:PHE:CG	1:B:100:PRO:HB3	2.45	0.51
1:C:73:ARG:NE	1:C:78:LYS:O	2.43	0.51
1:A:160:HIS:CD2	1:A:162:PHE:HB2	2.45	0.51
1:B:73:ARG:NE	1:B:78:LYS:O	2.43	0.51
1:F:132:LYS:HB2	1:F:134:ARG:NE	2.20	0.51
1:B:135:SER:O	1:B:137:LYS:HG3	2.10	0.51
1:B:54:ASP:OD1	1:B:56:ALA:CB	2.58	0.51
1:F:54:ASP:O	1:F:56:ALA:N	2.44	0.51
1:B:136:TYR:CZ	1:B:138:GLY:HA3	2.45	0.51
1:D:117:ASP:HB3	1:D:119:TYR:HE1	1.75	0.51
1:D:132:LYS:O	1:D:186:GLY:HA2	2.11	0.51
1:D:155:MET:CE	1:D:163:LEU:HD21	2.40	0.51
1:G:96:CYS:O	1:G:97:LEU:HD12	2.09	0.51
1:H:168:ARG:O	1:H:170:LYS:NZ	2.43	0.51
1:B:48:THR:O	1:B:116:PHE:HB3	2.11	0.51
1:C:38:THR:HG21	1:C:75:THR:CB	2.40	0.51
1:D:118:LEU:HD12	1:D:119:TYR:H	1.76	0.51
1:H:171:ASP:HA	7:H:301:SO4:O1	2.10	0.51
1:H:205:GLN:HB2	1:H:208:GLU:HG2	1.94	0.50
1:C:77:ASN:ND2	1:C:77:ASN:O	2.44	0.50
1:G:158:HIS:CD2	1:G:197:ARG:HA	2.45	0.50
1:H:173:GLN:O	1:H:174:GLU:C	2.49	0.50
1:B:157:PRO:HG2	1:B:158:HIS:CD2	2.45	0.50
1:C:153:SER:HA	9:C:402:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:136:TYR:CZ	1:H:138:GLY:HA3	2.47	0.50
1:A:54:ASP:OD1	1:A:56:ALA:HB3	2.12	0.50
1:D:164:PRO:HD2	9:D:414:HOH:O	2.10	0.50
1:H:82:PHE:CD1	1:H:100:PRO:HB3	2.47	0.50
1:B:64:VAL:HG12	1:B:65:ASN:N	2.26	0.50
1:C:96:CYS:O	1:C:97:LEU:HD12	2.10	0.50
1:E:208:GLU:O	1:E:209:VAL:CG2	2.59	0.50
1:E:142:ILE:HG22	1:E:143:THR:O	2.12	0.50
1:F:88:VAL:HG13	1:F:117:ASP:O	2.12	0.50
1:D:58:LYS:CB	9:D:402:HOH:O	2.60	0.50
1:H:45:SER:HB2	1:H:118:LEU:HB3	1.92	0.50
1:C:49:THR:HG22	1:C:111:GLU:O	2.11	0.49
1:G:132:LYS:N	1:G:132:LYS:CD	2.72	0.49
1:B:109:LYS:HA	9:B:408:HOH:O	2.11	0.49
1:E:166:SER:O	1:E:167:TYR:CG	2.65	0.49
1:H:132:LYS:O	1:H:186:GLY:HA2	2.12	0.49
1:B:54:ASP:OD1	1:B:56:ALA:HB3	2.13	0.49
1:B:93:ARG:NH1	1:B:115:GLU:OE1	2.45	0.49
1:F:134:ARG:HD2	1:F:134:ARG:N	2.20	0.49
1:F:91:LYS:N	1:F:115:GLU:O	2.44	0.49
1:A:132:LYS:HB2	1:A:134:ARG:CZ	2.42	0.49
1:C:93:ARG:CG	1:C:93:ARG:HH11	2.14	0.49
1:D:63:LYS:HA	1:D:95:GLN:HB2	1.94	0.49
1:A:97:LEU:HB3	1:A:99:PHE:CZ	2.48	0.49
1:F:187:PRO:O	9:F:401:HOH:O	2.20	0.49
1:F:181:ARG:O	1:F:182:GLY:C	2.50	0.49
1:A:160:HIS:HD2	1:A:162:PHE:HB2	1.77	0.49
1:B:171:ASP:OD1	1:B:173:GLN:HG2	2.13	0.49
1:H:64:VAL:HG12	1:H:65:ASN:N	2.28	0.49
1:B:173:GLN:O	1:B:174:GLU:C	2.51	0.49
1:C:126:ARG:HG2	1:C:128:CYS:H	1.78	0.49
1:D:90:ASP:OD1	1:D:93:ARG:N	2.44	0.48
1:H:82:PHE:CG	1:H:100:PRO:HB3	2.48	0.48
1:A:39:ILE:CG1	1:A:119:TYR:HE2	2.26	0.48
1:B:132:LYS:O	1:B:186:GLY:HA2	2.14	0.48
1:F:73:ARG:NE	1:F:78:LYS:O	2.45	0.48
1:A:99:PHE:HB3	1:A:101:PHE:CZ	2.49	0.48
1:C:168:ARG:C	1:C:170:LYS:H	2.17	0.48
1:D:64:VAL:O	1:D:94:LYS:O	2.31	0.48
1:D:82:PHE:CD1	1:D:100:PRO:HB3	2.48	0.48
1:E:162:PHE:HE1	1:E:181:ARG:HD2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:THR:HG21	1:E:124:TYR:OH	2.14	0.48
1:D:52:LYS:CD	1:D:52:LYS:N	2.69	0.48
1:E:97:LEU:HB3	1:E:99:PHE:CZ	2.49	0.48
1:F:135:SER:O	1:F:137:LYS:HG3	2.13	0.48
1:C:129:ILE:HG22	1:C:136:TYR:HB2	1.96	0.48
1:C:54:ASP:HB3	1:C:57:LEU:CD1	2.43	0.48
1:D:50:LEU:HD11	1:D:118:LEU:HD22	1.94	0.48
1:A:207:SER:O	1:A:208:GLU:CB	2.59	0.48
1:G:97:LEU:HB3	1:G:99:PHE:CZ	2.49	0.48
1:G:157:PRO:HG2	1:G:158:HIS:CE1	2.49	0.47
1:B:101:PHE:CE1	1:B:108:VAL:HG11	2.49	0.47
1:D:113:GLY:C	1:D:115:GLU:H	2.18	0.47
1:D:136:TYR:CZ	1:D:203:ILE:HD13	2.49	0.47
1:F:122:LYS:CE	9:F:406:HOH:O	2.62	0.47
1:A:147:ILE:HG21	1:A:191:THR:HB	1.94	0.47
1:B:54:ASP:O	1:B:56:ALA:N	2.44	0.47
1:D:125:ILE:O	1:D:126:ARG:C	2.50	0.47
1:F:184:GLU:OE1	1:F:184:GLU:HA	2.14	0.47
1:E:55:PRO:HA	9:E:420:HOH:O	2.13	0.47
1:E:160:HIS:HD2	1:E:162:PHE:H	1.61	0.47
1:C:122:LYS:HE2	1:C:139:THR:CG2	2.36	0.47
1:E:157:PRO:HG2	1:E:158:HIS:CE1	2.49	0.47
1:B:136:TYR:CE1	1:B:138:GLY:HA3	2.50	0.47
1:C:52:LYS:HB2	1:C:57:LEU:HD12	1.95	0.47
1:E:198:TYR:CE2	8:E:302:EPE:H32	2.49	0.47
1:F:64:VAL:HG12	1:F:65:ASN:N	2.30	0.47
1:A:134:ARG:H	1:A:134:ARG:CD	2.05	0.47
1:D:136:TYR:CZ	1:D:138:GLY:HA3	2.49	0.47
1:D:181:ARG:HB2	1:D:183:GLU:CG	2.41	0.47
1:E:202:ASP:HA	9:E:424:HOH:O	2.14	0.47
1:C:167:TYR:O	1:C:170:LYS:HB2	2.15	0.46
1:C:59:ILE:CG2	1:C:60:LYS:H	2.27	0.46
1:G:129:ILE:HG22	1:G:136:TYR:HB2	1.97	0.46
1:A:80:LEU:C	1:A:82:PHE:H	2.19	0.46
1:C:97:LEU:HB3	1:C:99:PHE:CZ	2.50	0.46
1:E:129:ILE:HG22	1:E:136:TYR:HB2	1.98	0.46
1:H:49:THR:O	1:H:110:LYS:HA	2.15	0.46
1:E:99:PHE:HB3	1:E:101:PHE:CZ	2.51	0.46
1:A:173:GLN:O	1:A:174:GLU:C	2.54	0.46
1:B:99:PHE:HB3	1:B:101:PHE:CZ	2.49	0.46
1:C:101:PHE:HB2	1:C:105:SER:OG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:HIS:CD2	1:E:162:PHE:HB2	2.51	0.46
1:A:181:ARG:HD3	1:A:183:GLU:OE2	2.16	0.46
1:D:55:PRO:O	1:D:56:ALA:HB3	2.15	0.46
1:F:82:PHE:CD1	1:F:100:PRO:HB3	2.51	0.46
1:G:136:TYR:CZ	1:G:203:ILE:HD13	2.51	0.46
1:G:48:THR:HG22	1:G:49:THR:H	1.80	0.46
1:H:125:ILE:O	1:H:126:ARG:C	2.53	0.46
1:G:80:LEU:C	1:G:82:PHE:H	2.19	0.46
1:H:48:THR:HG22	1:H:49:THR:N	2.31	0.46
1:B:47:LYS:HG2	1:B:114:HIS:HA	1.97	0.46
1:C:80:LEU:C	1:C:82:PHE:H	2.19	0.46
1:D:101:PHE:CE1	1:D:108:VAL:HG11	2.51	0.46
1:D:203:ILE:HA	1:D:204:PRO:HD2	1.78	0.46
1:C:99:PHE:HB3	1:C:101:PHE:CZ	2.50	0.46
1:D:82:PHE:CG	1:D:100:PRO:HB3	2.50	0.46
1:G:99:PHE:HB3	1:G:101:PHE:CZ	2.51	0.46
1:B:64:VAL:O	1:B:94:LYS:HB3	2.16	0.46
1:C:157:PRO:HG2	1:C:158:HIS:CE1	2.51	0.46
1:C:181:ARG:NH2	1:C:183:GLU:OE1	2.49	0.46
1:G:77:ASN:O	1:G:77:ASN:ND2	2.48	0.46
1:D:118:LEU:HD12	1:D:119:TYR:N	2.31	0.45
1:G:108:VAL:C	1:G:109:LYS:HG3	2.36	0.45
1:F:181:ARG:O	1:F:183:GLU:N	2.50	0.45
1:A:101:PHE:HB2	1:A:105:SER:OG	2.17	0.45
1:A:72:ASP:O	1:A:76:ARG:HD2	2.17	0.45
1:E:157:PRO:HG2	1:E:158:HIS:ND1	2.31	0.45
1:C:59:ILE:HG22	1:C:60:LYS:H	1.82	0.45
1:D:52:LYS:HG3	1:D:59:ILE:HD11	1.98	0.45
1:E:160:HIS:HD2	1:E:162:PHE:HB2	1.82	0.45
1:E:181:ARG:HD3	1:E:183:GLU:OE2	2.17	0.45
1:G:181:ARG:HB2	1:G:183:GLU:CG	2.47	0.45
1:A:112:PHE:CD2	1:A:113:GLY:N	2.84	0.45
1:C:162:PHE:CE2	1:C:188:TRP:HH2	2.34	0.45
1:C:54:ASP:OD1	1:C:56:ALA:HB3	2.17	0.45
1:D:181:ARG:O	1:D:182:GLY:C	2.54	0.45
1:E:108:VAL:HG12	1:E:109:LYS:N	2.32	0.45
1:A:47:LYS:HA	1:A:116:PHE:O	2.16	0.45
1:C:130:ILE:O	7:C:301:SO4:O1	2.35	0.45
1:E:80:LEU:C	1:E:82:PHE:H	2.20	0.45
1:F:136:TYR:CE1	1:F:138:GLY:HA3	2.51	0.45
1:A:39:ILE:CD1	1:A:119:TYR:HE2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:ILE:HG22	1:C:143:THR:O	2.17	0.45
1:C:40:HIS:C	1:C:42:PHE:H	2.19	0.45
1:D:173:GLN:O	1:D:174:GLU:C	2.55	0.45
1:E:73:ARG:HD3	1:E:98:TRP:CZ2	2.52	0.45
1:E:87:PHE:C	1:E:87:PHE:CD1	2.91	0.45
1:H:136:TYR:CE1	1:H:138:GLY:HA3	2.52	0.45
1:H:83:THR:HG21	1:H:124:TYR:OH	2.16	0.45
1:E:136:TYR:CZ	1:E:203:ILE:HD13	2.51	0.45
1:F:101:PHE:CE1	1:F:108:VAL:HG11	2.52	0.45
1:G:157:PRO:HG2	1:G:158:HIS:ND1	2.31	0.45
1:F:82:PHE:CG	1:F:100:PRO:HB3	2.51	0.44
1:A:48:THR:HG22	1:A:49:THR:H	1.82	0.44
1:C:113:GLY:HA2	9:C:414:HOH:O	2.17	0.44
1:F:44:LYS:HD3	1:F:119:TYR:CZ	2.51	0.44
1:A:157:PRO:HG2	1:A:158:HIS:CE1	2.52	0.44
1:D:155:MET:HE3	1:D:163:LEU:HD21	1.99	0.44
1:E:51:ILE:O	1:E:109:LYS:N	2.48	0.44
1:H:171:ASP:OD1	1:H:173:GLN:HG2	2.17	0.44
1:H:47:LYS:HD2	1:H:47:LYS:N	2.32	0.44
1:A:129:ILE:HG22	1:A:136:TYR:HB2	1.98	0.44
1:D:115:GLU:HG2	1:D:116:PHE:N	2.31	0.44
1:D:48:THR:HG22	1:D:49:THR:N	2.33	0.44
1:D:50:LEU:HD11	1:D:118:LEU:CD2	2.47	0.44
1:G:101:PHE:CD1	1:G:108:VAL:HG21	2.53	0.44
1:G:108:VAL:HG12	1:G:109:LYS:N	2.33	0.44
1:G:104:MET:CE	1:G:137:LYS:HB2	2.47	0.44
1:B:170:LYS:HD2	3:J:1:IDS:O3S	2.17	0.44
1:F:48:THR:HG22	1:F:49:THR:N	2.33	0.44
1:A:203:ILE:HA	1:A:204:PRO:HD2	1.87	0.44
1:E:165:SER:O	1:E:167:TYR:N	2.47	0.44
1:E:77:ASN:O	1:E:77:ASN:ND2	2.48	0.44
1:F:50:LEU:HD22	1:F:99:PHE:CE2	2.52	0.44
1:A:53:ILE:N	1:A:107:GLY:O	2.46	0.44
1:E:48:THR:O	1:E:116:PHE:HB3	2.17	0.44
1:H:101:PHE:CE1	1:H:108:VAL:HG11	2.52	0.44
1:B:48:THR:HG22	1:B:49:THR:N	2.33	0.43
1:D:51:ILE:N	1:D:51:ILE:HD12	2.33	0.43
1:F:93:ARG:HE	1:F:93:ARG:HB2	1.44	0.43
1:H:136:TYR:CZ	1:H:203:ILE:HD13	2.53	0.43
1:H:63:LYS:HA	1:H:95:GLN:CB	2.48	0.43
1:A:181:ARG:HB2	1:A:183:GLU:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:TYR:CE2	8:C:311:EPE:H102	2.52	0.43
1:A:87:PHE:CD1	1:A:87:PHE:C	2.91	0.43
1:G:147:ILE:CG2	1:G:191:THR:HB	2.49	0.43
1:H:117:ASP:HB3	1:H:119:TYR:CE1	2.53	0.43
1:H:152:TRP:N	9:H:2003:HOH:O	2.50	0.43
1:A:80:LEU:HA	1:A:81:PRO:HD2	1.90	0.43
1:B:93:ARG:HG3	1:B:93:ARG:NH1	2.32	0.43
1:H:99:PHE:HB3	1:H:101:PHE:CZ	2.54	0.43
1:D:113:GLY:C	1:D:115:GLU:N	2.72	0.43
1:A:160:HIS:HD2	1:A:162:PHE:N	2.06	0.43
1:D:47:LYS:CA	1:D:116:PHE:O	2.66	0.43
1:D:180:PRO:HD2	9:D:412:HOH:O	2.19	0.43
1:G:64:VAL:HG23	1:G:65:ASN:N	2.34	0.43
1:A:48:THR:O	1:A:116:PHE:HB3	2.18	0.43
1:A:59:ILE:CG2	1:A:60:LYS:H	2.32	0.43
1:E:80:LEU:HA	1:E:81:PRO:HD2	1.91	0.43
1:G:181:ARG:O	1:G:182:GLY:C	2.57	0.43
1:H:85:LYS:HE2	1:H:124:TYR:CE2	2.54	0.43
1:F:130:ILE:HD12	7:F:307:SO4:O1	2.19	0.42
1:D:113:GLY:O	1:D:115:GLU:N	2.52	0.42
1:E:76:ARG:O	1:E:77:ASN:C	2.58	0.42
1:A:118:LEU:C	1:A:119:TYR:HD1	2.22	0.42
1:B:90:ASP:OD2	1:B:116:PHE:HE1	2.01	0.42
1:B:136:TYR:CZ	1:B:203:ILE:HD13	2.54	0.42
1:B:39:ILE:HG13	1:B:40:HIS:ND1	2.35	0.42
1:C:147:ILE:CG2	1:C:191:THR:HB	2.49	0.42
1:D:198:TYR:C	1:D:198:TYR:CD2	2.92	0.42
1:E:112:PHE:CG	1:E:113:GLY:N	2.87	0.42
1:G:203:ILE:HA	1:G:204:PRO:HD2	1.87	0.42
1:F:136:TYR:CZ	1:F:203:ILE:HD13	2.54	0.42
1:B:44:LYS:HE3	1:B:117:ASP:OD2	2.19	0.42
1:B:40:HIS:NE2	9:B:405:HOH:O	2.37	0.42
1:D:90:ASP:OD1	1:D:92:ALA:HB3	2.20	0.42
1:E:114:HIS:CA	9:E:408:HOH:O	2.62	0.42
1:E:147:ILE:CG2	1:E:191:THR:HB	2.49	0.42
1:G:178:ARG:O	1:G:187:PRO:HA	2.20	0.42
1:H:170:LYS:CE	1:H:170:LYS:N	2.82	0.42
1:D:90:ASP:O	1:D:94:LYS:N	2.52	0.42
1:F:112:PHE:CD1	1:F:113:GLY:N	2.88	0.42
1:C:115:GLU:OE1	1:C:115:GLU:N	2.41	0.42
1:C:136:TYR:CZ	1:C:203:ILE:HD13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:ASP:OD1	1:C:92:ALA:HB3	2.20	0.42
1:H:90:ASP:O	1:H:94:LYS:HA	2.19	0.42
1:B:67:ALA:HB2	1:B:89:PHE:CD2	2.55	0.42
1:B:63:LYS:HA	1:B:95:GLN:HB3	2.01	0.42
1:C:161:SER:O	1:C:163:LEU:HG	2.19	0.42
1:E:181:ARG:HB2	1:E:183:GLU:HG3	2.02	0.42
1:F:134:ARG:HG2	5:L:3:SGN:O4S	2.20	0.42
1:F:64:VAL:CG1	1:F:69:GLN:HB2	2.46	0.42
1:D:67:ALA:HB2	1:D:89:PHE:CD2	2.55	0.42
1:E:48:THR:HG22	1:E:49:THR:H	1.85	0.42
1:H:170:LYS:HE3	1:H:170:LYS:HA	2.02	0.42
1:D:57:LEU:HA	1:D:57:LEU:HD23	1.85	0.42
1:D:122:LYS:C	1:D:124:TYR:H	2.23	0.41
1:D:52:LYS:CG	1:D:59:ILE:HD11	2.50	0.41
1:E:178:ARG:O	1:E:187:PRO:HA	2.20	0.41
1:E:73:ARG:HD3	1:E:98:TRP:CH2	2.55	0.41
1:A:157:PRO:HG2	1:A:158:HIS:ND1	2.35	0.41
1:C:87:PHE:C	1:C:87:PHE:CD1	2.94	0.41
1:E:181:ARG:NH1	1:E:183:GLU:OE2	2.53	0.41
1:E:46:ALA:O	1:E:47:LYS:C	2.59	0.41
1:B:152:TRP:CD2	1:B:172:LEU:HD22	2.55	0.41
1:C:181:ARG:HH21	1:C:183:GLU:CD	2.23	0.41
1:F:99:PHE:HB3	1:F:101:PHE:CZ	2.55	0.41
1:C:112:PHE:CD2	1:C:113:GLY:N	2.89	0.41
1:C:48:THR:HG22	1:C:49:THR:H	1.84	0.41
1:E:102:ASN:O	1:E:105:SER:OG	2.38	0.41
1:G:180:PRO:HD2	9:G:403:HOH:O	2.20	0.41
1:A:71:ALA:HA	1:A:87:PHE:CE2	2.55	0.41
1:C:64:VAL:HG23	1:C:65:ASN:N	2.36	0.41
1:D:47:LYS:HA	1:D:116:PHE:O	2.21	0.41
1:F:162:PHE:HA	1:F:167:TYR:HE2	1.86	0.41
1:G:87:PHE:CD1	1:G:87:PHE:C	2.94	0.41
1:H:67:ALA:HB2	1:H:89:PHE:CD2	2.56	0.41
1:D:181:ARG:O	1:D:183:GLU:N	2.53	0.41
1:E:133:GLY:O	1:E:134:ARG:C	2.56	0.41
1:A:132:LYS:HG3	1:A:134:ARG:NH2	2.34	0.41
1:A:41:GLU:HG2	1:B:41:GLU:CG	2.49	0.41
1:E:47:LYS:CA	1:E:113:GLY:O	2.67	0.41
1:G:174:GLU:HB2	1:G:176:TYR:CE2	2.56	0.41
1:G:48:THR:CG2	1:G:49:THR:N	2.84	0.41
1:B:61:THR:HA	1:B:96:CYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:PRO:HG2	1:C:158:HIS:ND1	2.36	0.41
1:C:197:ARG:HD3	9:C:410:HOH:O	2.21	0.41
1:D:152:TRP:CD2	1:D:172:LEU:HD22	2.56	0.41
1:F:198:TYR:C	1:F:198:TYR:CD1	2.95	0.41
1:F:44:LYS:HA	1:F:118:LEU:O	2.21	0.41
1:C:48:THR:CG2	1:C:49:THR:N	2.85	0.40
1:H:44:LYS:HA	1:H:118:LEU:O	2.21	0.40
4:K:7:IDS:O6A	4:K:8:SGN:H3	2.21	0.40
1:A:178:ARG:O	1:A:187:PRO:HA	2.21	0.40
1:A:77:ASN:CB	1:B:142:ILE:HG12	2.51	0.40
1:B:64:VAL:HG13	1:B:65:ASN:H	1.86	0.40
1:D:133:GLY:N	9:D:401:HOH:O	2.35	0.40
1:D:141:SER:C	1:D:142:ILE:HD12	2.41	0.40
1:F:135:SER:OG	7:F:307:SO4:S	2.78	0.40
1:A:108:VAL:C	1:A:109:LYS:HG3	2.42	0.40
1:A:136:TYR:CZ	1:A:203:ILE:HD13	2.57	0.40
1:F:100:PRO:HD2	1:F:101:PHE:CE2	2.57	0.40
1:F:152:TRP:CD2	1:F:172:LEU:HD22	2.57	0.40
1:B:164:PRO:O	1:B:168:ARG:N	2.55	0.40
1:E:90:ASP:O	1:E:92:ALA:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	171/183 (93%)	152 (89%)	15 (9%)	4 (2%)	6	30
1	B	171/183 (93%)	152 (89%)	18 (10%)	1 (1%)	25	64
1	C	171/183 (93%)	147 (86%)	22 (13%)	2 (1%)	13	48
1	D	171/183 (93%)	148 (86%)	19 (11%)	4 (2%)	6	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	172/183 (94%)	148 (86%)	18 (10%)	6 (4%)	3	20
1	F	172/183 (94%)	149 (87%)	19 (11%)	4 (2%)	6	30
1	G	161/183 (88%)	142 (88%)	14 (9%)	5 (3%)	4	23
1	H	170/183 (93%)	147 (86%)	22 (13%)	1 (1%)	25	64
All	All	1359/1464 (93%)	1185 (87%)	147 (11%)	27 (2%)	7	34

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	THR
1	A	208	GLU
1	C	208	GLU
1	E	77	ASN
1	E	209	VAL
1	G	208	GLU
1	E	91	LYS
1	F	55	PRO
1	F	182	GLY
1	H	94	LYS
1	A	94	LYS
1	D	55	PRO
1	E	167	TYR
1	C	162	PHE
1	D	114	HIS
1	F	54	ASP
1	B	54	ASP
1	E	166	SER
1	G	77	ASN
1	G	91	LYS
1	D	53	ILE
1	D	59	ILE
1	F	100	PRO
1	G	182	GLY
1	A	81	PRO
1	E	81	PRO
1	G	81	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	140/165 (85%)	133 (95%)	7 (5%)	24	60
1	B	144/165 (87%)	140 (97%)	4 (3%)	43	77
1	C	145/165 (88%)	141 (97%)	4 (3%)	43	77
1	D	137/165 (83%)	130 (95%)	7 (5%)	24	60
1	E	132/165 (80%)	129 (98%)	3 (2%)	50	80
1	F	141/165 (86%)	135 (96%)	6 (4%)	29	66
1	G	129/165 (78%)	125 (97%)	4 (3%)	40	75
1	H	135/165 (82%)	128 (95%)	7 (5%)	23	59
All	All	1103/1320 (84%)	1061 (96%)	42 (4%)	33	69

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ARG
1	A	77	ASN
1	A	104	MET
1	A	134	ARG
1	A	165	SER
1	A	191	THR
1	A	208	GLU
1	B	73	ARG
1	B	77	ASN
1	B	170	LYS
1	B	191	THR
1	C	77	ASN
1	C	142	ILE
1	C	191	THR
1	C	195	GLU
1	D	52	LYS
1	D	77	ASN
1	D	115	GLU
1	D	117	ASP

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Mol	Chain	Res	Type
1	D	134	ARG
1	D	165	SER
1	D	191	THR
1	E	76	ARG
1	E	77	ASN
1	E	191	THR
1	F	73	ARG
1	F	77	ASN
1	F	134	ARG
1	F	191	THR
1	F	198	TYR
1	F	209	VAL
1	G	77	ASN
1	G	132	LYS
1	G	159	GLU
1	G	191	THR
1	H	77	ASN
1	H	117	ASP
1	H	123	ASP
1	H	134	ARG
1	H	170	LYS
1	H	191	THR
1	H	202	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	160	HIS
1	B	65	ASN
1	B	158	HIS
1	C	160	HIS
1	C	173	GLN
1	D	65	ASN
1	D	158	HIS
1	E	160	HIS
1	F	40	HIS
1	F	65	ASN
1	F	158	HIS
1	G	65	ASN
1	G	160	HIS
1	G	205	GLN

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Mol	Chain	Res	Type
1	H	158	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

42 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	IDS	I	1	2	14,17,17	1.10	1 (7%)	17,26,26	1.57	3 (17%)
2	SGN	I	2	2	18,19,20	1.32	2 (11%)	22,29,31	2.00	4 (18%)
2	IDS	I	3	2	13,16,17	1.39	1 (7%)	15,24,26	3.82	5 (33%)
2	SGN	I	4	2	18,19,20	1.59	4 (22%)	22,29,31	1.92	5 (22%)
2	IDS	I	5	2	13,16,17	1.30	3 (23%)	15,24,26	4.75	3 (20%)
2	SGN	I	6	2	17,18,20	1.71	2 (11%)	18,27,31	1.34	3 (16%)
3	IDS	J	1	3	14,17,17	1.43	1 (7%)	17,26,26	2.75	4 (23%)
3	SGN	J	2	3	18,19,20	1.40	2 (11%)	22,29,31	1.68	3 (13%)
3	IDS	J	3	3	13,16,17	1.46	2 (15%)	15,24,26	3.02	6 (40%)
3	SGN	J	4	3	18,19,20	1.23	1 (5%)	22,29,31	1.89	5 (22%)
3	IDS	J	5	3	13,16,17	1.46	2 (15%)	15,24,26	2.93	5 (33%)
3	SGN	J	6	3	18,19,20	1.54	3 (16%)	22,29,31	1.83	4 (18%)
3	IDS	J	7	3	12,15,17	1.59	3 (25%)	12,22,26	2.57	1 (8%)
4	IDS	K	1	4	14,17,17	1.53	3 (21%)	17,26,26	2.63	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SGN	K	2	4	18,19,20	1.46	2 (11%)	22,29,31	1.56	4 (18%)
4	IDS	K	3	4	13,16,17	1.36	2 (15%)	15,24,26	2.43	3 (20%)
4	SGN	K	4	4	18,19,20	1.07	1 (5%)	22,29,31	1.57	6 (27%)
4	IDS	K	5	4	13,16,17	1.39	2 (15%)	15,24,26	3.64	5 (33%)
4	SGN	K	6	4	18,19,20	1.54	4 (22%)	22,29,31	2.10	4 (18%)
4	IDS	K	7	4	13,16,17	1.45	3 (23%)	15,24,26	4.72	3 (20%)
4	SGN	K	8	4	17,18,20	1.71	3 (17%)	18,27,31	1.35	2 (11%)
5	SGN	L	1	5	19,20,20	1.60	4 (21%)	24,31,31	2.51	6 (25%)
5	IDS	L	2	5	13,16,17	1.53	3 (23%)	15,24,26	3.25	4 (26%)
5	SGN	L	3	5	18,19,20	1.36	1 (5%)	22,29,31	1.90	5 (22%)
5	IDS	L	4	5	13,16,17	1.21	2 (15%)	15,24,26	2.72	3 (20%)
5	SGN	L	5	5	18,19,20	0.94	0	22,29,31	1.47	4 (18%)
5	IDS	L	6	5	13,16,17	1.35	2 (15%)	15,24,26	2.40	4 (26%)
5	SGN	L	7	5	18,19,20	1.31	2 (11%)	22,29,31	2.16	7 (31%)
5	IDS	L	8	5	13,16,17	1.38	2 (15%)	15,24,26	2.41	2 (13%)
5	SGN	L	9	5	17,18,20	1.48	3 (17%)	18,27,31	1.46	3 (16%)
6	SGN	M	1	6	19,20,20	1.64	3 (15%)	24,31,31	1.43	2 (8%)
6	IDS	M	2	6	13,16,17	1.40	2 (15%)	15,24,26	2.89	5 (33%)
6	SGN	M	3	6	18,19,20	1.37	2 (11%)	22,29,31	1.96	5 (22%)
6	IDS	M	4	6	13,16,17	1.39	2 (15%)	15,24,26	3.23	5 (33%)
6	SGN	M	5	6	18,19,20	1.47	2 (11%)	22,29,31	2.00	4 (18%)
6	IDS	M	6	6	12,15,17	1.54	2 (16%)	12,22,26	3.37	1 (8%)
6	SGN	N	1	6	19,20,20	1.53	3 (15%)	24,31,31	2.53	4 (16%)
6	IDS	N	2	6	13,16,17	1.40	1 (7%)	15,24,26	2.76	3 (20%)
6	SGN	N	3	6	18,19,20	1.49	3 (16%)	22,29,31	2.24	5 (22%)
6	IDS	N	4	6	13,16,17	1.45	2 (15%)	15,24,26	3.81	6 (40%)
6	SGN	N	5	6	18,19,20	1.80	4 (22%)	22,29,31	1.92	4 (18%)
6	IDS	N	6	6	12,15,17	1.49	2 (16%)	12,22,26	3.63	1 (8%)

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	IDS	I	1	2	-	0/5/29/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SGN	I	2	2	-	1/11/28/31	0/1/1/1
2	IDS	I	3	2	-	0/5/26/29	0/1/1/1
2	SGN	I	4	2	-	1/11/28/31	0/1/1/1
2	IDS	I	5	2	1/1/6/7	1/5/26/29	0/1/1/1
2	SGN	I	6	2	-	6/11/24/31	0/1/1/1
3	IDS	J	1	3	-	1/5/29/29	0/1/1/1
3	SGN	J	2	3	-	5/11/28/31	0/1/1/1
3	IDS	J	3	3	-	0/5/26/29	0/1/1/1
3	SGN	J	4	3	-	0/11/28/31	0/1/1/1
3	IDS	J	5	3	-	0/5/26/29	0/1/1/1
3	SGN	J	6	3	-	2/11/28/31	0/1/1/1
3	IDS	J	7	3	-	1/5/22/29	1/1/1/1
4	IDS	K	1	4	-	1/5/29/29	0/1/1/1
4	SGN	K	2	4	-	1/11/28/31	0/1/1/1
4	IDS	K	3	4	-	0/5/26/29	0/1/1/1
4	SGN	K	4	4	-	1/11/28/31	0/1/1/1
4	IDS	K	5	4	-	2/5/26/29	0/1/1/1
4	SGN	K	6	4	-	1/11/28/31	0/1/1/1
4	IDS	K	7	4	1/1/6/7	1/5/26/29	0/1/1/1
4	SGN	K	8	4	-	5/11/24/31	0/1/1/1
5	SGN	L	1	5	-	5/11/31/31	0/1/1/1
5	IDS	L	2	5	-	4/5/26/29	0/1/1/1
5	SGN	L	3	5	-	5/11/28/31	0/1/1/1
5	IDS	L	4	5	-	0/5/26/29	0/1/1/1
5	SGN	L	5	5	-	3/11/28/31	0/1/1/1
5	IDS	L	6	5	-	0/5/26/29	0/1/1/1
5	SGN	L	7	5	-	4/11/28/31	0/1/1/1
5	IDS	L	8	5	-	0/5/26/29	0/1/1/1
5	SGN	L	9	5	-	5/11/24/31	0/1/1/1
6	SGN	M	1	6	-	2/11/31/31	0/1/1/1
6	IDS	M	2	6	-	0/5/26/29	0/1/1/1
6	SGN	M	3	6	-	1/11/28/31	0/1/1/1
6	IDS	M	4	6	-	3/5/26/29	0/1/1/1
6	SGN	M	5	6	-	1/11/28/31	0/1/1/1
6	IDS	M	6	6	-	1/5/22/29	0/1/1/1
6	SGN	N	1	6	-	5/11/31/31	0/1/1/1
6	IDS	N	2	6	-	0/5/26/29	0/1/1/1
6	SGN	N	3	6	-	3/11/28/31	0/1/1/1
6	IDS	N	4	6	-	1/5/26/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SGN	N	5	6	-	0/11/28/31	0/1/1/1
6	IDS	N	6	6	-	1/5/22/29	1/1/1/1

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	5	SGN	S1-N2	5.08	1.66	1.59
6	M	1	SGN	S1-N2	4.74	1.65	1.59
2	I	6	SGN	S1-N2	4.44	1.65	1.59
2	I	4	SGN	S1-N2	4.44	1.65	1.59
4	K	8	SGN	S1-N2	4.23	1.65	1.59
3	J	6	SGN	S1-N2	4.15	1.65	1.59
5	L	1	SGN	S1-N2	4.15	1.65	1.59
6	M	5	SGN	S1-N2	3.94	1.64	1.59
6	N	1	SGN	S1-N2	3.93	1.64	1.59
6	N	3	SGN	S1-N2	3.83	1.64	1.59
4	K	6	SGN	S1-N2	3.82	1.64	1.59
3	J	2	SGN	S1-N2	3.78	1.64	1.59
3	J	1	IDS	C1-C2	3.76	1.56	1.52
5	L	3	SGN	S1-N2	3.73	1.64	1.59
6	N	2	IDS	O2-C2	-3.69	1.41	1.47
4	K	5	IDS	O2-C2	-3.66	1.41	1.47
3	J	3	IDS	C1-C2	3.58	1.57	1.51
2	I	6	SGN	C1-C2	3.58	1.57	1.52
2	I	3	IDS	O2-C2	-3.57	1.41	1.47
4	K	2	SGN	S1-N2	3.54	1.64	1.59
6	M	3	SGN	S1-N2	3.54	1.64	1.59
5	L	9	SGN	S1-N2	3.51	1.64	1.59
6	N	4	IDS	O2-C2	-3.49	1.41	1.47
4	K	1	IDS	C1-C2	3.46	1.55	1.52
6	M	4	IDS	O2-C2	-3.44	1.42	1.47
4	K	3	IDS	O2-C2	-3.43	1.42	1.47
5	L	6	IDS	O2-C2	-3.43	1.42	1.47
4	K	8	SGN	C1-C2	3.38	1.57	1.52
6	M	2	IDS	C1-C2	3.35	1.57	1.51
6	N	6	IDS	C1-C2	3.30	1.57	1.51
5	L	7	SGN	S1-N2	3.27	1.64	1.59
3	J	4	SGN	S1-N2	3.18	1.63	1.59
3	J	5	IDS	C1-C2	3.15	1.56	1.51
2	I	2	SGN	S1-N2	3.01	1.63	1.59
3	J	5	IDS	O2-C2	-3.00	1.42	1.47
5	L	8	IDS	C1-C2	2.96	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	7	IDS	O2-C2	-2.96	1.42	1.47
6	M	1	SGN	C1-C2	2.92	1.56	1.52
6	M	6	IDS	C1-C2	2.91	1.56	1.51
5	L	2	IDS	O2-C2	-2.89	1.42	1.47
5	L	2	IDS	C1-C2	2.85	1.56	1.51
2	I	1	IDS	C1-C2	2.83	1.55	1.52
3	J	6	SGN	C1-C2	2.80	1.56	1.52
3	J	7	IDS	C4-C5	2.76	1.56	1.52
6	N	3	SGN	C1-C2	2.75	1.56	1.52
6	M	6	IDS	C4-C5	2.73	1.56	1.52
5	L	4	IDS	C1-C2	2.72	1.56	1.51
6	N	1	SGN	C1-C2	2.72	1.56	1.52
6	M	4	IDS	C1-C2	2.72	1.56	1.51
4	K	7	IDS	C1-C2	2.71	1.56	1.51
2	I	4	SGN	C1-C2	2.69	1.56	1.52
4	K	6	SGN	C1-C2	2.68	1.56	1.52
4	K	2	SGN	C1-C2	2.66	1.56	1.52
5	L	8	IDS	O2-C2	-2.64	1.43	1.47
6	N	5	SGN	C1-C2	2.62	1.56	1.52
6	M	2	IDS	O2-C2	-2.62	1.43	1.47
4	K	7	IDS	C4-C5	2.61	1.59	1.53
5	L	1	SGN	O1S-S1	2.60	1.45	1.42
4	K	3	IDS	C1-C2	2.59	1.55	1.51
6	N	6	IDS	C4-C5	2.57	1.56	1.52
2	I	5	IDS	C1-C2	2.56	1.55	1.51
3	J	7	IDS	C1-C2	2.49	1.55	1.51
5	L	4	IDS	O2-C2	-2.49	1.43	1.47
5	L	6	IDS	C1-C2	2.48	1.55	1.51
4	K	1	IDS	C4-C5	2.47	1.59	1.53
6	N	4	IDS	C1-C2	2.46	1.55	1.51
5	L	1	SGN	O2S-S1	2.45	1.44	1.42
6	M	3	SGN	C1-C2	2.43	1.56	1.52
3	J	3	IDS	O2-C2	-2.41	1.43	1.47
5	L	1	SGN	C1-C2	2.40	1.55	1.52
4	K	6	SGN	O2S-S1	2.39	1.44	1.42
4	K	4	SGN	S1-N2	2.34	1.62	1.59
4	K	8	SGN	C3-C2	2.34	1.55	1.52
5	L	9	SGN	O1S-S1	2.32	1.44	1.42
6	M	5	SGN	C1-C2	2.31	1.55	1.52
6	N	5	SGN	C4-C5	2.30	1.57	1.53
6	M	1	SGN	O2S-S1	2.27	1.44	1.42
5	L	2	IDS	C4-C5	2.26	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	5	IDS	C1-C2	2.26	1.55	1.51
6	N	1	SGN	O2S-S1	2.25	1.44	1.42
2	I	2	SGN	O2S-S1	2.22	1.44	1.42
3	J	2	SGN	C1-C2	2.13	1.55	1.52
6	N	5	SGN	O2S-S1	2.12	1.44	1.42
2	I	4	SGN	O1S-S1	2.10	1.44	1.42
2	I	5	IDS	C4-C5	2.09	1.58	1.53
5	L	9	SGN	C1-C2	2.08	1.55	1.52
5	L	7	SGN	C1-C2	2.07	1.55	1.52
2	I	4	SGN	O2S-S1	2.06	1.44	1.42
3	J	6	SGN	C4-C5	2.06	1.57	1.53
4	K	7	IDS	C4-C3	2.05	1.57	1.52
4	K	6	SGN	C4-C5	2.05	1.57	1.53
2	I	5	IDS	C4-C3	2.03	1.57	1.52
4	K	1	IDS	C4-C3	2.03	1.57	1.52
6	N	3	SGN	O2S-S1	2.01	1.44	1.42

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	7	IDS	O4-C4-C3	14.47	143.81	110.35
2	I	5	IDS	O4-C4-C3	14.12	142.99	110.35
6	N	6	IDS	C2-O2-S	12.28	133.93	117.91
6	M	6	IDS	C2-O2-S	11.35	132.71	117.91
2	I	5	IDS	C2-O2-S	11.08	132.36	117.91
6	N	1	SGN	O4-C4-C3	-11.08	84.74	110.35
4	K	7	IDS	C2-O2-S	10.24	131.26	117.91
5	L	1	SGN	O4-C4-C3	-9.98	87.27	110.35
2	I	3	IDS	O4-C4-C5	9.24	127.70	110.05
4	K	5	IDS	O4-C4-C5	8.82	126.90	110.05
3	J	5	IDS	C2-O2-S	8.77	129.34	117.91
5	L	2	IDS	C2-O2-S	8.73	129.29	117.91
6	M	2	IDS	C2-O2-S	8.66	129.21	117.91
3	J	1	IDS	O4-C4-C3	8.61	130.25	110.35
6	N	4	IDS	O4-C4-C5	8.60	126.49	110.05
6	N	4	IDS	C2-O2-S	8.53	129.03	117.91
3	J	7	IDS	C2-O2-S	8.51	129.01	117.91
2	I	3	IDS	C2-O2-S	8.41	128.87	117.91
6	M	4	IDS	C2-O2-S	8.29	128.73	117.91
3	J	3	IDS	C2-O2-S	8.28	128.71	117.91
5	L	8	IDS	C2-O2-S	8.17	128.56	117.91
4	K	1	IDS	C2-O2-S	8.16	134.64	118.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	2	IDS	C2-O2-S	8.14	128.53	117.91
4	K	3	IDS	C2-O2-S	7.94	128.27	117.91
4	K	5	IDS	C2-O2-S	7.82	128.11	117.91
5	L	4	IDS	C2-O2-S	7.57	127.78	117.91
5	L	6	IDS	C2-O2-S	7.37	127.53	117.91
6	N	3	SGN	O4-C4-C5	7.34	127.53	109.30
5	L	2	IDS	O4-C4-C5	7.05	123.52	110.05
6	M	4	IDS	O4-C4-C5	6.87	123.18	110.05
2	I	2	SGN	O4-C4-C5	6.56	125.58	109.30
5	L	7	SGN	O4-C4-C5	6.16	124.60	109.30
6	N	4	IDS	O4-C4-C3	-5.98	96.53	110.35
2	I	3	IDS	O4-C4-C3	-5.94	96.62	110.35
3	J	4	SGN	O4-C4-C3	-5.74	97.07	110.35
2	I	4	SGN	O4-C4-C3	-5.74	97.09	110.35
4	K	6	SGN	O4-C4-C3	-5.72	97.14	110.35
6	M	3	SGN	O4-C4-C5	5.69	123.43	109.30
4	K	5	IDS	O4-C4-C3	-5.68	97.22	110.35
6	M	5	SGN	O4-C4-C3	-5.48	97.68	110.35
4	K	1	IDS	O4-C4-C3	5.38	122.78	110.35
6	N	5	SGN	O4-C4-C5	5.31	122.48	109.30
4	K	6	SGN	O4-C4-C5	5.26	122.37	109.30
3	J	1	IDS	C2-O2-S	5.21	128.94	118.88
3	J	6	SGN	O4-C4-C5	5.12	122.00	109.30
5	L	3	SGN	O4-C4-C5	5.05	121.84	109.30
6	N	2	IDS	C1-C2-C3	5.05	116.95	109.40
3	J	3	IDS	O4-C4-C3	4.99	121.88	110.35
5	L	4	IDS	O4-C4-C3	4.97	121.83	110.35
3	J	2	SGN	O4-C4-C3	-4.75	99.36	110.35
5	L	7	SGN	O4-C4-C3	-4.71	99.46	110.35
2	I	1	IDS	C2-O2-S	4.65	127.86	118.88
6	M	5	SGN	O4-C4-C5	4.64	120.82	109.30
6	N	3	SGN	O4-C4-C3	-4.57	99.78	110.35
3	J	3	IDS	C1-C2-C3	4.46	116.07	109.40
3	J	5	IDS	O4-C4-C3	-4.37	100.26	110.35
6	N	4	IDS	C1-C2-C3	4.36	115.92	109.40
6	M	1	SGN	O4-C4-C3	-4.07	100.95	110.35
6	M	3	SGN	O4-C4-C3	-4.06	100.96	110.35
4	K	2	SGN	C1-O5-C5	3.91	117.49	112.19
6	M	2	IDS	C1-C2-C3	3.90	115.23	109.40
2	I	4	SGN	O4-C4-C5	3.84	118.83	109.30
5	L	2	IDS	O4-C4-C3	3.78	119.08	110.35
6	M	4	IDS	O4-C4-C3	-3.76	101.66	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	4	IDS	C1-C2-C3	3.72	114.97	109.40
2	I	3	IDS	C1-C2-C3	3.67	114.89	109.40
5	L	9	SGN	O2S-S1-O1S	-3.62	111.59	120.16
2	I	6	SGN	O2S-S1-O1S	-3.56	111.74	120.16
3	J	6	SGN	O4-C4-C3	-3.55	102.15	110.35
2	I	2	SGN	O4-C4-C3	-3.54	102.16	110.35
5	L	4	IDS	C1-C2-C3	3.52	114.66	109.40
4	K	8	SGN	O2S-S1-O1S	-3.51	111.87	120.16
6	M	2	IDS	O4-C4-C5	3.50	116.75	110.05
4	K	5	IDS	C1-C2-C3	3.48	114.60	109.40
3	J	1	IDS	O4-C4-C5	3.48	116.70	110.05
5	L	3	SGN	C1-O5-C5	3.41	116.81	112.19
4	K	3	IDS	C1-C2-C3	3.40	114.48	109.40
5	L	3	SGN	O2S-S1-O1S	-3.31	112.33	120.16
3	J	5	IDS	C1-C2-C3	3.30	114.33	109.40
6	N	5	SGN	C1-O5-C5	3.29	116.65	112.19
3	J	2	SGN	C1-O5-C5	3.24	116.58	112.19
4	K	2	SGN	O2S-S1-O1S	-3.20	112.60	120.16
5	L	3	SGN	O4-C4-C3	-3.12	103.14	110.35
2	I	4	SGN	O2S-S1-O1S	-3.11	112.80	120.16
6	N	5	SGN	O2S-S1-O1S	-3.10	112.83	120.16
6	M	1	SGN	O2S-S1-O1S	-3.09	112.85	120.16
4	K	4	SGN	O4-C4-C3	-3.06	103.26	110.35
3	J	4	SGN	O2S-S1-O1S	-3.06	112.92	120.16
6	N	5	SGN	O4-C4-C3	-3.06	103.28	110.35
6	N	3	SGN	O2S-S1-O1S	-3.04	112.98	120.16
6	N	1	SGN	O2S-S1-O1S	-3.03	112.99	120.16
6	M	2	IDS	O4-C4-C3	-3.03	103.33	110.35
3	J	6	SGN	O2S-S1-O1S	-3.03	112.99	120.16
4	K	6	SGN	C1-O5-C5	3.03	116.30	112.19
6	N	2	IDS	C1-O5-C5	3.02	117.50	112.17
4	K	4	SGN	C1-O5-C5	3.02	116.28	112.19
3	J	2	SGN	O2S-S1-O1S	-3.00	113.07	120.16
6	M	3	SGN	O2S-S1-O1S	-3.00	113.07	120.16
3	J	4	SGN	O4-C4-C5	3.00	116.74	109.30
5	L	6	IDS	C1-C2-C3	2.98	113.86	109.40
4	K	2	SGN	O4-C4-C3	-2.96	103.50	110.35
6	M	5	SGN	C1-O5-C5	2.95	116.19	112.19
6	M	5	SGN	O2S-S1-O1S	-2.95	113.20	120.16
3	J	4	SGN	C1-O5-C5	2.93	116.16	112.19
5	L	7	SGN	O2S-S1-O1S	-2.92	113.26	120.16
5	L	1	SGN	O2S-S1-O1S	-2.89	113.33	120.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	5	SGN	O4-C4-C3	-2.89	103.67	110.35
5	L	3	SGN	C4-C3-C2	-2.87	106.81	111.02
4	K	6	SGN	O2S-S1-O1S	-2.87	113.39	120.16
5	L	7	SGN	C1-O5-C5	2.85	116.06	112.19
5	L	2	IDS	C1-O5-C5	2.85	117.19	112.17
6	M	3	SGN	C1-O5-C5	2.83	116.03	112.19
5	L	5	SGN	O2S-S1-O1S	-2.80	113.55	120.16
5	L	6	IDS	O4-C4-C3	-2.79	103.90	110.35
5	L	5	SGN	C1-O5-C5	2.77	115.94	112.19
2	I	2	SGN	O2S-S1-O1S	-2.77	113.62	120.16
4	K	1	IDS	C1-O5-C5	2.76	116.43	112.31
6	N	3	SGN	C1-O5-C5	2.74	115.90	112.19
5	L	8	IDS	O4-C4-C3	-2.73	104.03	110.35
3	J	5	IDS	O4-C4-C5	2.73	115.26	110.05
5	L	1	SGN	O4-C4-C5	-2.72	102.53	109.30
5	L	1	SGN	O6-C6-C5	2.72	112.70	107.62
4	K	1	IDS	O2-C2-C1	2.68	111.19	107.58
2	I	1	IDS	C1-O5-C5	2.65	116.26	112.31
3	J	6	SGN	C1-O5-C5	2.62	115.75	112.19
2	I	4	SGN	C1-O5-C5	2.61	115.73	112.19
3	J	5	IDS	C1-O5-C5	2.57	116.70	112.17
3	J	1	IDS	C1-O5-C5	2.54	116.11	112.31
3	J	3	IDS	C4-C3-C2	2.52	114.73	110.24
4	K	2	SGN	C4-C3-C2	-2.52	107.33	111.02
5	L	5	SGN	C4-C3-C2	-2.49	107.36	111.02
4	K	3	IDS	C1-O5-C5	2.47	116.53	112.17
4	K	8	SGN	O1S-S1-N2	-2.47	104.37	108.87
4	K	4	SGN	O2S-S1-O1S	-2.47	114.33	120.16
6	M	4	IDS	C1-O5-C5	2.43	116.46	112.17
4	K	4	SGN	O2S-S1-N2	-2.42	104.46	108.87
3	J	3	IDS	C1-O5-C5	2.42	116.43	112.17
5	L	1	SGN	C1-C2-N2	-2.35	107.86	110.67
2	I	2	SGN	C1-O5-C5	2.33	115.35	112.19
2	I	1	IDS	O4-C4-C5	2.33	114.50	110.05
2	I	3	IDS	C1-O5-C5	2.32	116.27	112.17
5	L	7	SGN	O2S-S1-N2	-2.32	104.64	108.87
3	J	4	SGN	C4-C3-C2	-2.32	107.62	111.02
4	K	4	SGN	O4-C4-C5	2.30	115.01	109.30
4	K	5	IDS	C1-O5-C5	2.30	116.23	112.17
4	K	7	IDS	C6-C5-C4	2.28	118.76	113.04
6	N	4	IDS	C1-O5-C5	2.28	116.19	112.17
2	I	6	SGN	O1S-S1-N2	-2.27	104.72	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	9	SGN	C4-C3-C2	-2.26	107.38	110.84
6	N	4	IDS	C4-C3-C2	2.25	114.24	110.24
5	L	9	SGN	O1S-S1-N2	-2.24	104.78	108.87
6	N	3	SGN	C4-C3-C2	-2.24	107.74	111.02
5	L	1	SGN	C6-C5-C4	2.23	116.76	112.09
2	I	4	SGN	C4-C3-C2	-2.22	107.77	111.02
5	L	7	SGN	C3-C4-C5	-2.21	106.30	110.24
6	M	2	IDS	C1-O5-C5	2.19	116.04	112.17
5	L	7	SGN	O6-C6-C5	2.18	111.70	107.62
6	M	3	SGN	C4-C3-C2	-2.11	107.93	111.02
6	N	1	SGN	C1-C2-N2	-2.08	108.19	110.67
4	K	4	SGN	O6-C6-C5	2.08	111.50	107.62
2	I	6	SGN	C4-C3-C2	-2.08	107.66	110.84
6	N	1	SGN	C3-C4-C5	-2.07	106.54	110.24
3	J	3	IDS	O4-C4-C5	-2.07	106.09	110.05
2	I	5	IDS	C1-O5-C5	2.02	115.72	112.17
5	L	6	IDS	C1-O5-C5	2.01	115.72	112.17

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	K	7	IDS	C4
2	I	5	IDS	C4

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	1	SGN	C4-C5-C6-O6
5	L	1	SGN	O5-C5-C6-O6
5	L	1	SGN	C2-N2-S1-O2S
5	L	1	SGN	C2-N2-S1-O3S
2	I	6	SGN	O5-C5-C6-O6
2	I	6	SGN	C6-O6-S2-O6S
5	L	7	SGN	C2-N2-S1-O3S
6	M	6	IDS	C1-C2-O2-S
3	J	2	SGN	O5-C5-C6-O6
3	J	2	SGN	C2-N2-S1-O2S
3	J	2	SGN	C2-N2-S1-O3S
6	N	6	IDS	C1-C2-O2-S
4	K	1	IDS	C1-C2-O2-S
5	L	2	IDS	C1-C2-O2-S
5	L	2	IDS	C2-O2-S-O3S

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Mol	Chain	Res	Type	Atoms
5	L	5	SGN	C2-N2-S1-O3S
4	K	7	IDS	C1-C2-O2-S
2	I	2	SGN	C2-N2-S1-O1S
6	M	4	IDS	C2-O2-S-O3S
5	L	3	SGN	C2-N2-S1-O2S
5	L	3	SGN	C2-N2-S1-O3S
5	L	9	SGN	C4-C5-C6-O6
5	L	9	SGN	C2-N2-S1-O1S
5	L	9	SGN	C2-N2-S1-O3S
3	J	6	SGN	C2-N2-S1-O3S
2	I	5	IDS	C1-C2-O2-S
2	I	6	SGN	C6-O6-S2-O5S
6	N	1	SGN	O5-C5-C6-O6
6	N	3	SGN	O5-C5-C6-O6
5	L	3	SGN	O5-C5-C6-O6
5	L	3	SGN	C4-C5-C6-O6
4	K	8	SGN	C6-O6-S2-O6S
2	I	6	SGN	C4-C5-C6-O6
4	K	5	IDS	C2-O2-S-O2S
6	M	4	IDS	C2-O2-S-O2S
2	I	6	SGN	C6-O6-S2-O4S
4	K	8	SGN	C6-O6-S2-O4S
5	L	1	SGN	C2-N2-S1-O1S
5	L	7	SGN	C2-N2-S1-O2S
4	K	4	SGN	C2-N2-S1-O1S
5	L	5	SGN	C2-N2-S1-O2S
4	K	8	SGN	C2-N2-S1-O2S
3	J	6	SGN	C2-N2-S1-O2S
6	N	1	SGN	C6-O6-S2-O4S
6	N	1	SGN	C6-O6-S2-O5S
4	K	8	SGN	C6-O6-S2-O5S
5	L	9	SGN	O5-C5-C6-O6
4	K	8	SGN	O5-C5-C6-O6
4	K	5	IDS	C2-O2-S-O3S
3	J	7	IDS	C2-O2-S-O3S
6	M	1	SGN	C6-O6-S2-O5S
3	J	2	SGN	C4-C5-C6-O6
6	N	1	SGN	C4-C5-C6-O6
6	N	3	SGN	C4-C5-C6-O6
6	N	1	SGN	C6-O6-S2-O6S
2	I	6	SGN	C2-N2-S1-O2S
3	J	2	SGN	C2-N2-S1-O1S

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Mol	Chain	Res	Type	Atoms
6	N	3	SGN	C2-N2-S1-O1S
5	L	2	IDS	C2-O2-S-O1S
5	L	3	SGN	C2-N2-S1-O1S
5	L	9	SGN	C2-N2-S1-O2S
6	M	1	SGN	C6-O6-S2-O4S
5	L	2	IDS	C3-C2-O2-S
5	L	7	SGN	C6-O6-S2-O4S
5	L	5	SGN	C6-O6-S2-O4S
6	N	4	IDS	C2-O2-S-O2S
3	J	1	IDS	C2-O2-S-O3S
6	M	4	IDS	C2-O2-S-O1S
5	L	7	SGN	C2-N2-S1-O1S
2	I	4	SGN	C2-N2-S1-O1S
6	M	3	SGN	C2-N2-S1-O1S
4	K	6	SGN	C2-N2-S1-O1S
4	K	2	SGN	C2-N2-S1-O2S
6	M	5	SGN	C2-N2-S1-O1S

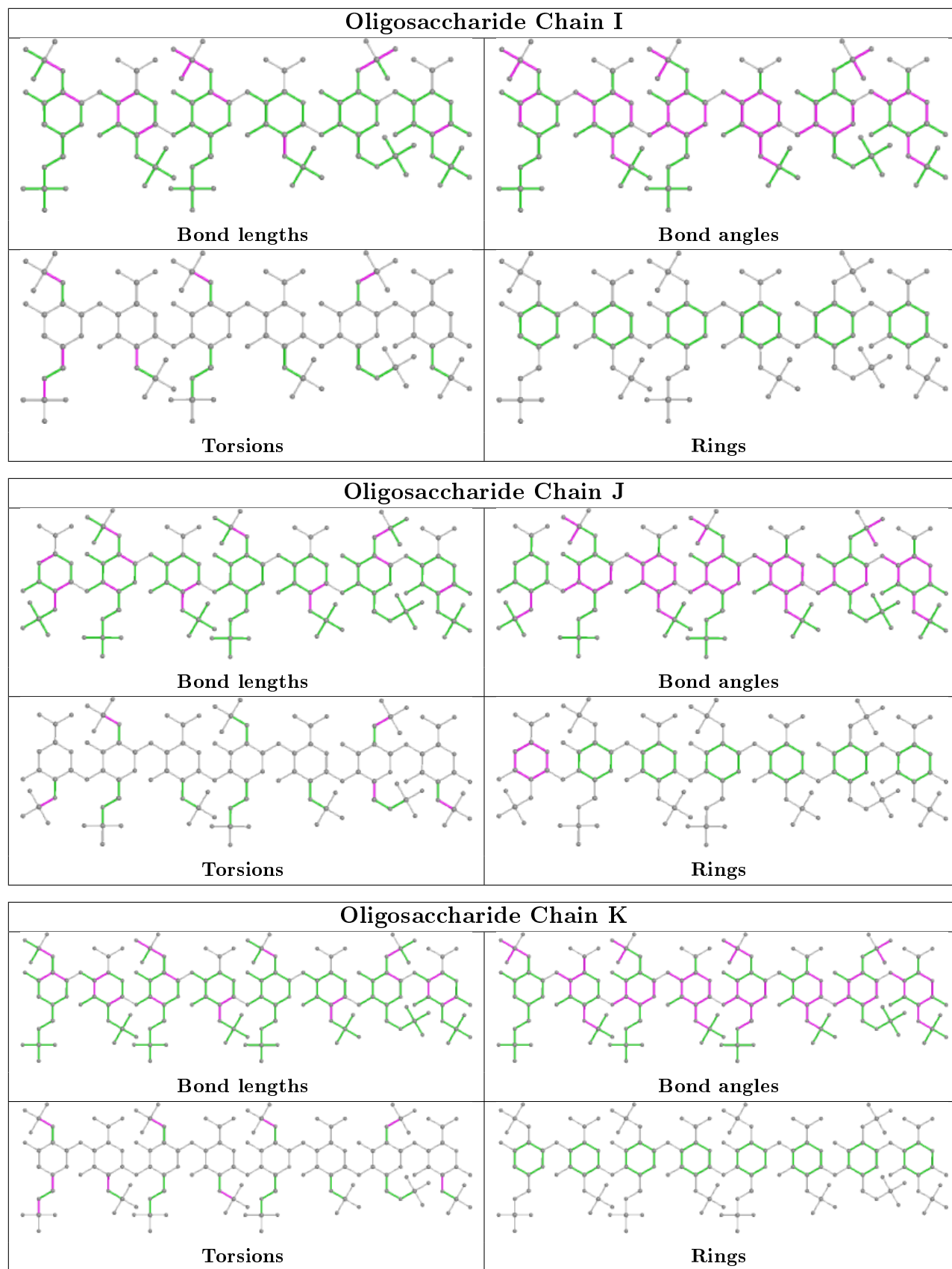
All (2) ring outliers are listed below:

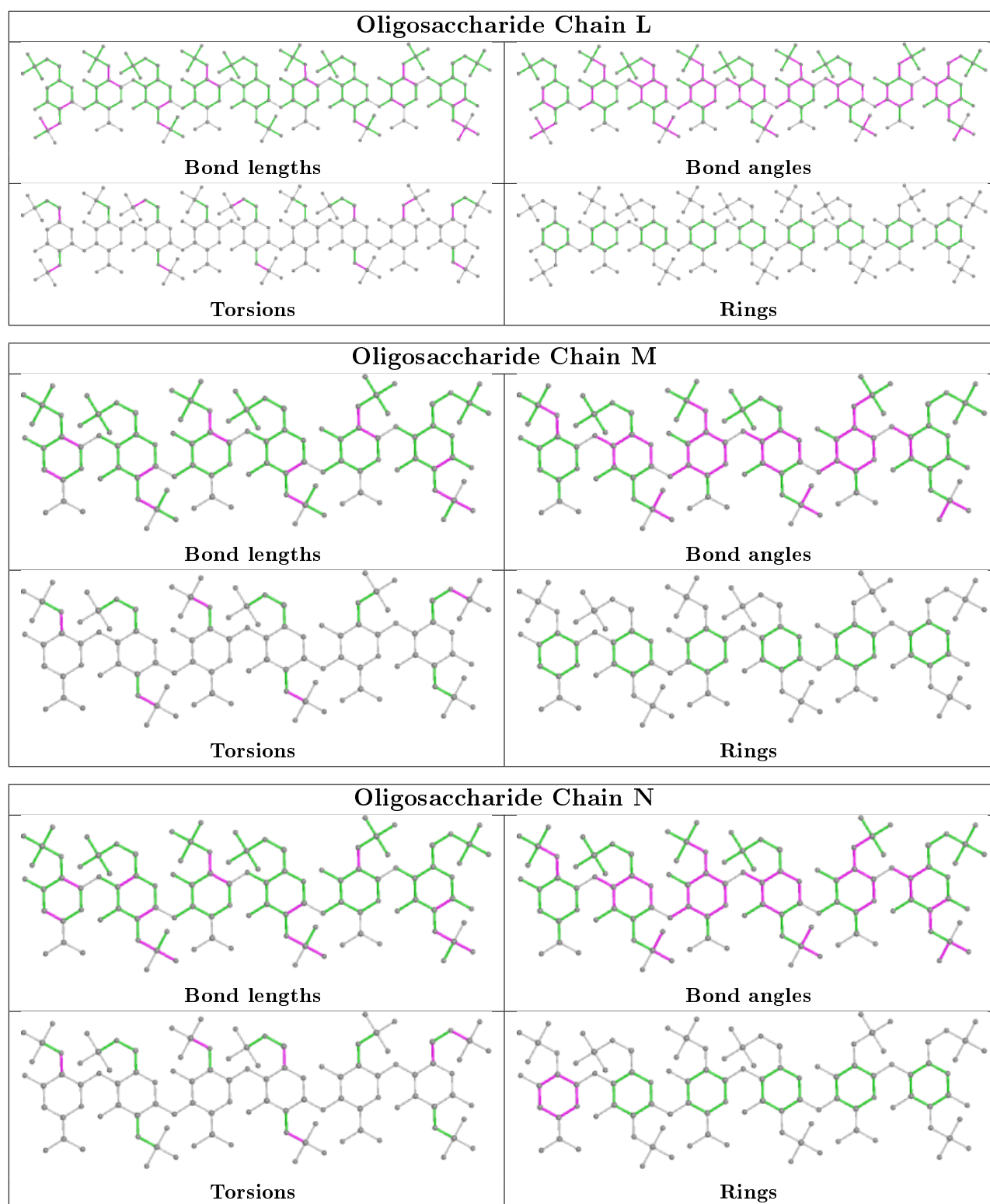
Mol	Chain	Res	Type	Atoms
6	N	6	IDS	C1-C2-C3-C4-C5-O5
3	J	7	IDS	C1-C2-C3-C4-C5-O5

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	4	IDS	1	0
4	K	6	SGN	2	0
4	K	7	IDS	1	0
6	M	5	SGN	1	0
3	J	1	IDS	1	0
5	L	3	SGN	1	0
4	K	8	SGN	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.





5.6 Ligand geometry [i](#)

16 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$
8	EPE	F	309	-	15,15,15	1.48	3 (20%)	18,20,20	0.80	0
7	SO4	A	307	-	4,4,4	1.87	2 (50%)	6,6,6	0.92	0
7	SO4	B	308	-	4,4,4	1.85	2 (50%)	6,6,6	0.86	0
8	EPE	B	317	-	15,15,15	1.38	3 (20%)	18,20,20	0.95	0
7	SO4	F	307	-	4,4,4	1.91	2 (50%)	6,6,6	0.91	0
8	EPE	A	308	-	15,15,15	1.11	1 (6%)	18,20,20	0.97	1 (5%)
8	EPE	G	307	-	15,15,15	1.28	2 (13%)	18,20,20	0.89	0
8	EPE	E	302	-	15,15,15	1.12	1 (6%)	18,20,20	1.06	1 (5%)
7	SO4	H	301	-	4,4,4	1.88	2 (50%)	6,6,6	0.90	0
7	SO4	E	301	-	4,4,4	1.89	1 (25%)	6,6,6	0.98	0
8	EPE	C	311	-	15,15,15	0.97	1 (6%)	18,20,20	0.96	0
7	SO4	F	308	-	4,4,4	1.90	2 (50%)	6,6,6	0.90	0
7	SO4	D	301	-	4,4,4	1.94	2 (50%)	6,6,6	0.86	0
8	EPE	D	302	-	15,15,15	1.25	2 (13%)	18,20,20	0.87	0
7	SO4	C	301	-	4,4,4	1.67	1 (25%)	6,6,6	1.12	0
8	EPE	H	302	-	15,15,15	1.14	1 (6%)	18,20,20	0.90	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
8	EPE	F	309	-	-	3/9/19/19	0/1/1/1
8	EPE	B	317	-	-	1/9/19/19	0/1/1/1
8	EPE	A	308	-	-	3/9/19/19	0/1/1/1
8	EPE	G	307	-	-	3/9/19/19	0/1/1/1
8	EPE	E	302	-	-	3/9/19/19	0/1/1/1
8	EPE	C	311	-	-	3/9/19/19	0/1/1/1
8	EPE	D	302	-	-	3/9/19/19	0/1/1/1
8	EPE	H	302	-	-	3/9/19/19	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	301	SO4	O1-S	3.20	1.63	1.46
7	F	307	SO4	O1-S	3.19	1.63	1.46
7	F	308	SO4	O1-S	3.16	1.63	1.46
7	D	301	SO4	O1-S	3.14	1.63	1.46
7	A	307	SO4	O1-S	3.09	1.62	1.46
7	H	301	SO4	O1-S	3.04	1.62	1.46
8	F	309	EPE	C10-S	3.03	1.81	1.77
7	B	308	SO4	O1-S	2.97	1.62	1.46
7	C	301	SO4	O1-S	2.71	1.60	1.46
8	E	302	EPE	C6-N1	2.45	1.53	1.46
8	A	308	EPE	C6-N1	2.43	1.53	1.46
8	D	302	EPE	C6-N1	2.38	1.53	1.46
8	B	317	EPE	C10-S	2.34	1.80	1.77
8	G	307	EPE	C6-N1	2.29	1.53	1.46
8	F	309	EPE	C6-N1	2.28	1.53	1.46
8	F	309	EPE	C2-N1	2.23	1.53	1.46
8	B	317	EPE	C2-N1	2.19	1.53	1.46
8	D	302	EPE	C10-S	2.18	1.80	1.77
8	B	317	EPE	C6-N1	2.17	1.52	1.46
7	D	301	SO4	O3-S	-2.16	1.30	1.47
7	H	301	SO4	O3-S	-2.15	1.30	1.47
7	B	308	SO4	O3-S	-2.11	1.30	1.47
7	F	308	SO4	O3-S	-2.07	1.30	1.47
8	H	302	EPE	C6-N1	2.07	1.52	1.46
7	F	307	SO4	O3-S	-2.05	1.31	1.47
7	A	307	SO4	O3-S	-2.05	1.31	1.47
8	G	307	EPE	C10-S	2.00	1.80	1.77
8	C	311	EPE	C6-N1	2.00	1.52	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	302	EPE	C7-N4-C5	-2.07	105.94	111.23
8	A	308	EPE	C7-N4-C5	-2.04	106.03	111.23

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	309	EPE	C10-C9-N1-C2
8	B	317	EPE	N4-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
8	A	308	EPE	N4-C7-C8-O8
8	G	307	EPE	C10-C9-N1-C2
8	G	307	EPE	C10-C9-N1-C6
8	E	302	EPE	C10-C9-N1-C6
8	C	311	EPE	C10-C9-N1-C2
8	C	311	EPE	C10-C9-N1-C6
8	E	302	EPE	N4-C7-C8-O8
8	F	309	EPE	N4-C7-C8-O8
8	G	307	EPE	N4-C7-C8-O8
8	F	309	EPE	C10-C9-N1-C6
8	E	302	EPE	C10-C9-N1-C2
8	D	302	EPE	C10-C9-N1-C2
8	D	302	EPE	C10-C9-N1-C6
8	H	302	EPE	C10-C9-N1-C2
8	H	302	EPE	C10-C9-N1-C6
8	D	302	EPE	N4-C7-C8-O8
8	H	302	EPE	N4-C7-C8-O8
8	C	311	EPE	N4-C7-C8-O8
8	A	308	EPE	C10-C9-N1-C2
8	A	308	EPE	C10-C9-N1-C6

There are no ring outliers.

10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	309	EPE	1	0
8	B	317	EPE	2	0
7	F	307	SO4	2	0
8	A	308	EPE	1	0
8	E	302	EPE	1	0
7	H	301	SO4	1	0
8	C	311	EPE	3	0
7	D	301	SO4	1	0
8	D	302	EPE	1	0
7	C	301	SO4	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	173/183 (94%)	0.03	6 (3%)	44	18	22, 50, 91, 102	0
1	B	173/183 (94%)	-0.23	1 (0%)	89	72	18, 47, 84, 94	0
1	C	173/183 (94%)	-0.36	1 (0%)	89	72	10, 35, 57, 72	0
1	D	173/183 (94%)	-0.16	1 (0%)	89	72	17, 48, 87, 90	0
1	E	174/183 (95%)	-0.03	1 (0%)	89	72	22, 54, 88, 98	0
1	F	174/183 (95%)	-0.12	3 (1%)	70	41	18, 50, 92, 109	0
1	G	165/183 (90%)	0.30	8 (4%)	30	11	43, 69, 95, 103	0
1	H	172/183 (93%)	0.25	13 (7%)	13	4	24, 65, 114, 129	0
All	All	1377/1464 (94%)	-0.04	34 (2%)	57	29	10, 52, 94, 129	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	209	VAL	4.1
1	H	66	THR	3.9
1	F	209	VAL	3.5
1	H	65	ASN	3.1
1	A	57	LEU	3.0
1	H	107	GLY	2.9
1	A	96	CYS	2.9
1	G	65	ASN	2.9
1	F	56	ALA	2.8
1	G	112	PHE	2.8
1	B	56	ALA	2.7
1	H	88	VAL	2.7
1	A	65	ASN	2.6
1	A	90	ASP	2.6
1	D	96	CYS	2.4
1	A	114	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	108	VAL	2.4
1	F	72	ASP	2.3
1	G	96	CYS	2.3
1	H	57	LEU	2.3
1	C	209	VAL	2.3
1	H	106	SER	2.3
1	G	70	CYS	2.3
1	H	70	CYS	2.2
1	G	156	ILE	2.2
1	H	91	LYS	2.2
1	A	56	ALA	2.2
1	H	59	ILE	2.1
1	G	40	HIS	2.1
1	E	98	TRP	2.1
1	H	114	HIS	2.1
1	H	56	ALA	2.1
1	H	72	ASP	2.0
1	H	208	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	IDS	J	3	16/17	0.56	0.42	138,140,142,142	0
6	SGN	M	1	20/20	0.56	0.50	143,150,155,155	0
6	IDS	M	2	16/17	0.61	0.45	134,140,143,143	0
3	IDS	J	1	17/17	0.61	0.47	142,145,146,146	0
2	SGN	I	6	18/20	0.62	0.43	132,134,142,142	0
6	SGN	N	5	19/20	0.64	0.44	125,126,129,129	0
6	SGN	N	1	20/20	0.65	0.50	131,137,140,140	0
5	SGN	L	9	18/20	0.67	0.38	118,126,130,130	0
3	SGN	J	2	19/20	0.69	0.42	138,141,143,143	0
3	SGN	J	6	19/20	0.69	0.42	143,145,146,147	0

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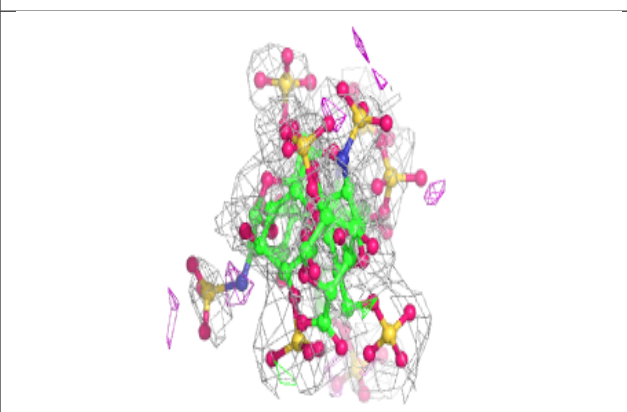
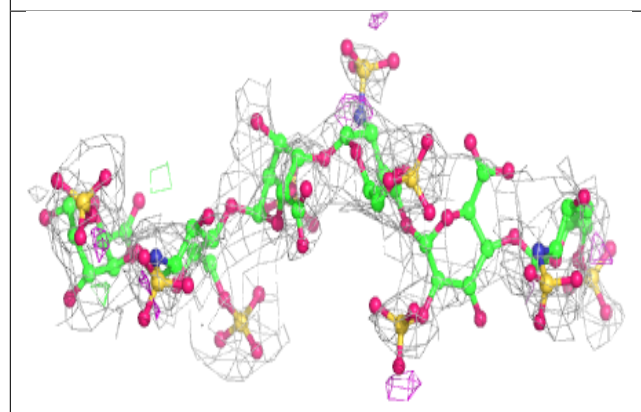
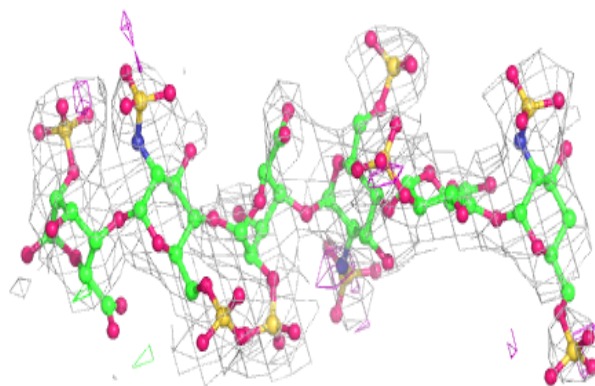
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SGN	I	2	19/20	0.70	0.34	120,121,124,124	0
2	IDS	I	3	16/17	0.71	0.28	118,121,122,122	0
5	SGN	L	1	20/20	0.71	0.22	105,112,122,122	0
6	IDS	N	2	16/17	0.72	0.39	122,129,131,131	0
2	SGN	I	4	19/20	0.74	0.46	123,125,127,127	0
2	IDS	I	1	17/17	0.74	0.49	121,122,123,123	0
4	IDS	K	1	17/17	0.75	0.34	106,114,118,118	0
6	IDS	N	6	15/17	0.75	0.44	125,125,126,127	0
6	SGN	M	5	19/20	0.76	0.32	132,135,137,137	0
3	IDS	J	5	16/17	0.76	0.45	139,140,141,144	0
4	SGN	K	8	18/20	0.77	0.34	124,127,129,129	0
3	IDS	J	7	15/17	0.77	0.48	144,144,145,145	0
6	IDS	N	4	16/17	0.77	0.30	123,124,126,127	0
6	IDS	M	6	15/17	0.78	0.30	127,130,132,132	0
3	SGN	J	4	19/20	0.78	0.25	134,137,138,138	0
5	IDS	L	2	16/17	0.80	0.27	103,106,106,106	0
5	SGN	L	3	19/20	0.81	0.30	94,101,106,106	0
6	SGN	M	3	19/20	0.81	0.24	127,131,132,133	0
2	IDS	I	5	16/17	0.82	0.36	125,127,130,131	0
5	IDS	L	4	16/17	0.83	0.19	71,87,89,91	0
4	IDS	K	7	16/17	0.83	0.28	106,112,115,123	0
4	SGN	K	6	19/20	0.84	0.20	97,103,107,109	0
6	SGN	N	3	19/20	0.84	0.18	119,120,121,122	0
6	IDS	M	4	16/17	0.85	0.26	134,135,136,137	0
4	IDS	K	5	16/17	0.88	0.18	93,97,102,102	0
4	SGN	K	2	19/20	0.88	0.21	95,103,105,105	0
5	SGN	L	5	19/20	0.89	0.20	55,60,67,74	0
4	IDS	K	3	16/17	0.89	0.26	82,90,92,93	0
4	SGN	K	4	19/20	0.90	0.22	70,79,82,89	0
5	IDS	L	8	16/17	0.91	0.17	90,95,101,114	0
5	SGN	L	7	19/20	0.92	0.18	75,79,81,89	0
5	IDS	L	6	16/17	0.94	0.13	76,78,82,82	0

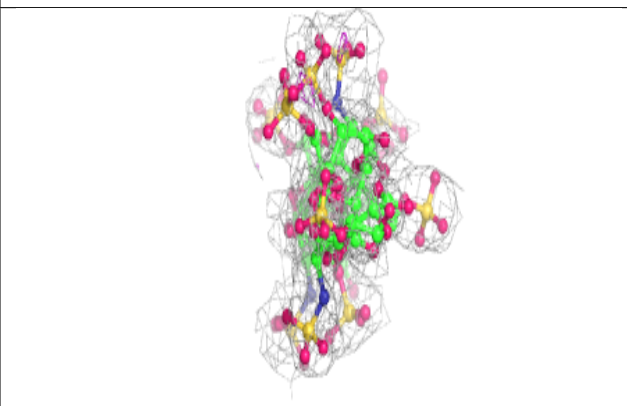
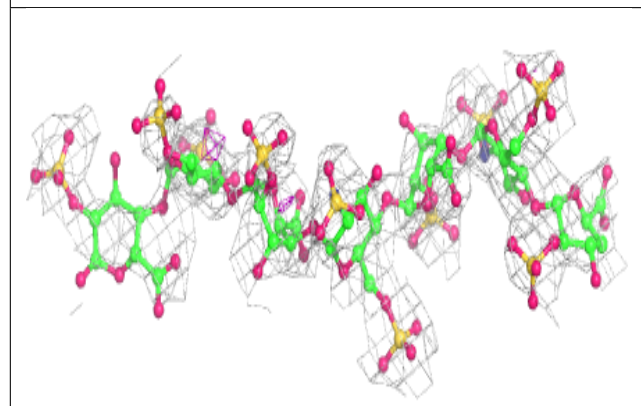
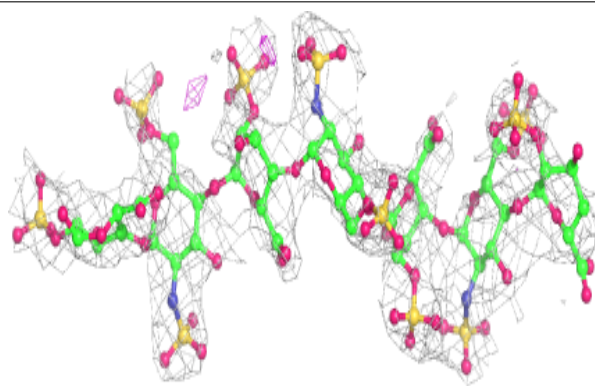
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

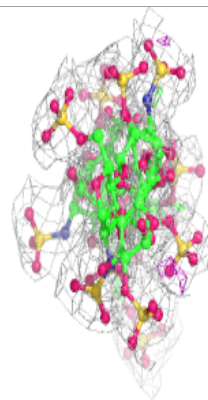
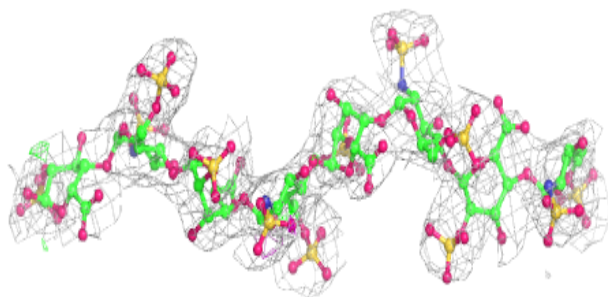
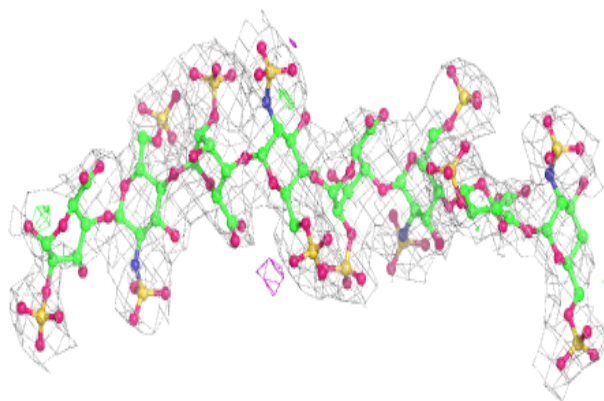
**Electron density around Chain J:**

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

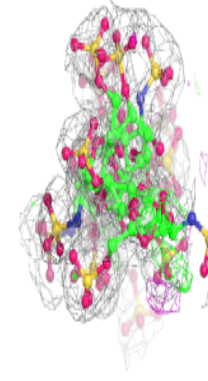
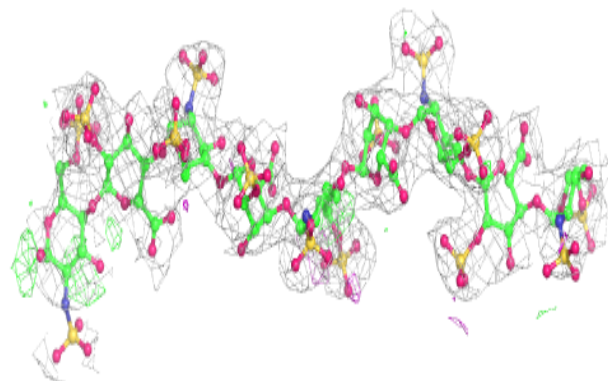
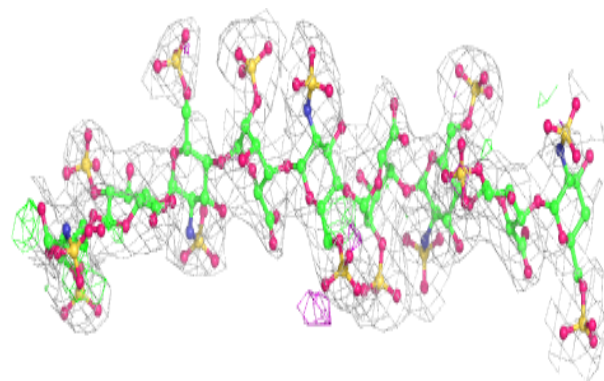


Electron density around Chain K:

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

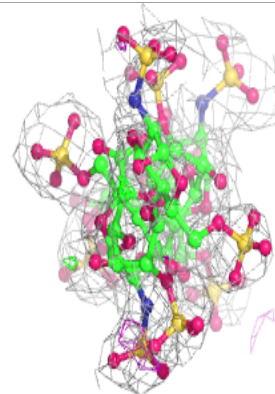
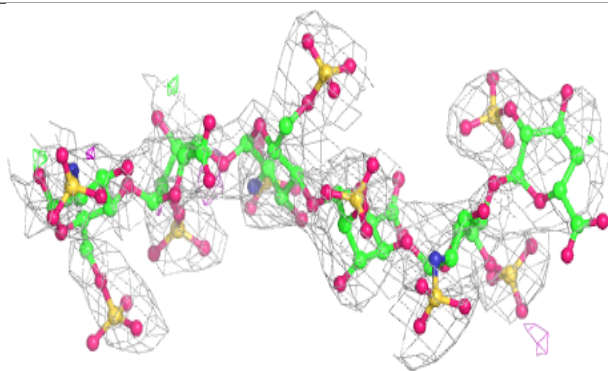
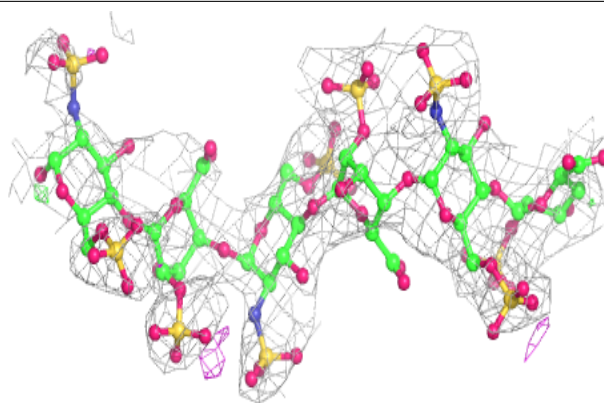
**Electron density around Chain L:**

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

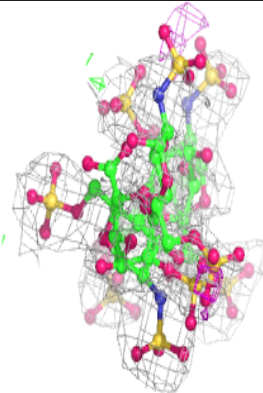
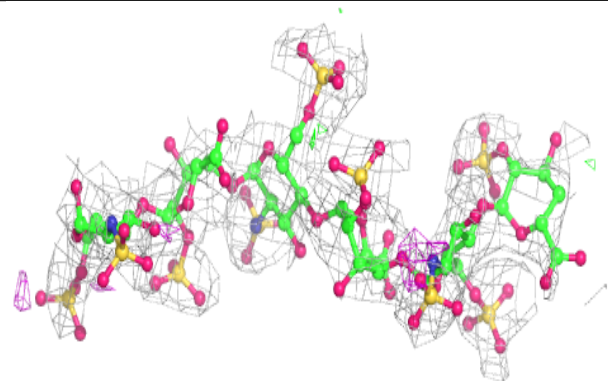
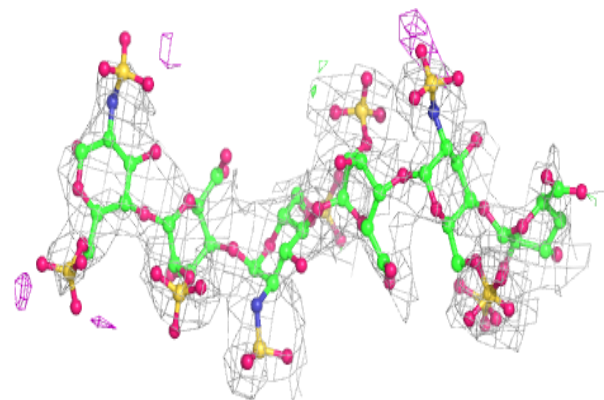


Electron density around Chain M:

$2mF_o-DF_c$ (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)



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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	EPE	F	309	15/15	0.78	0.41	102,103,104,105	0
7	SO4	A	307	5/5	0.88	0.27	126,126,127,127	0
8	EPE	G	307	15/15	0.90	0.28	73,80,86,86	0
7	SO4	C	301	5/5	0.90	0.22	108,108,109,110	0
7	SO4	F	308	5/5	0.91	0.26	133,133,133,134	0
8	EPE	C	311	15/15	0.93	0.26	46,50,53,53	0
7	SO4	F	307	5/5	0.93	0.17	111,112,112,112	0
8	EPE	D	302	15/15	0.93	0.20	62,67,68,68	0
8	EPE	E	302	15/15	0.93	0.25	64,69,70,70	0
7	SO4	E	301	5/5	0.94	0.17	94,94,95,95	0
7	SO4	D	301	5/5	0.94	0.21	102,102,102,103	0
8	EPE	H	302	15/15	0.94	0.16	54,55,57,58	0
7	SO4	H	301	5/5	0.95	0.14	82,83,83,83	0
8	EPE	A	308	15/15	0.95	0.20	35,37,43,44	0
8	EPE	B	317	15/15	0.95	0.18	35,46,53,53	0
7	SO4	B	308	5/5	0.95	0.15	101,101,101,101	0

6.5 Other polymers ⓘ

There are no such residues in this entry.