Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 10:29 AM BST

PDB ID	:	1YWH
Title	:	crystal structure of urokinase plasminogen activator receptor
Authors	:	Llinas, P.; Le Du, M.H.; Gardsvoll, H.; Dano, K.; Ploug, M.; Gilquin, B.; Stura, E.A.; Menez, A.
Deposited on	:	2005-02-18
Resolution	:	2.70 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:

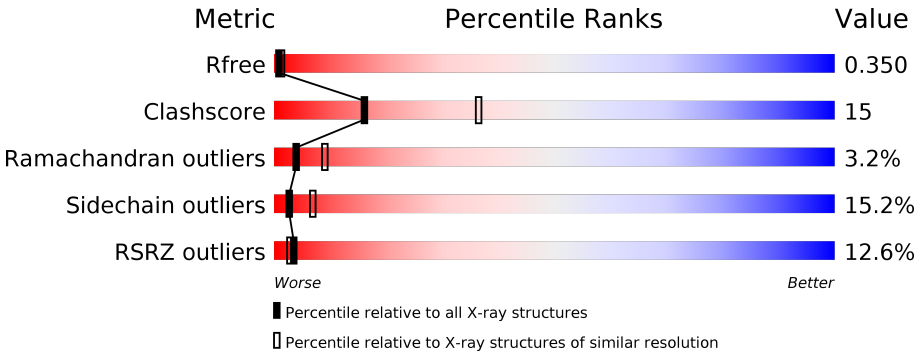
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	313	11% 51% 26% 6% • 14%
1	C	313	11% 51% 25% 6% • 17%
1	E	313	10% 53% 25% 5% 16%
1	G	313	8% 50% 27% 6% 18%
1	I	313	14% 47% 29% 9% 16%
1	K	313	10% 52% 23% 6% • 18%

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Mol	Chain	Length	Quality of chain
1	M	313	10% 50% 27% 7% 16%
1	O	313	10% 52% 26% 18%
2	B	13	8% 31% 54% 15%
2	D	13	8% 38% 62%
2	F	13	15% 69% 31%
2	H	13	8% 46% 54%
2	J	13	15% 54% 46%
2	L	13	15% 38% 38% 15% 8%
2	N	13	8% 69% 31%
2	P	13	15% 54% 38% 8%
3	Q	3	67% 33%
3	S	3	100%
3	T	3	67% 33%
3	b	3	100%
4	R	2	100%
4	U	2	100%
4	V	2	50% 50%
4	X	2	50% 50%
4	Y	2	100%
4	a	2	50% 50%
4	d	2	50% 50%
4	g	2	50% 50%
5	W	2	100%
5	f	2	100%
6	Z	5	20% 80%

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Mol	Chain	Length	Quality of chain
6	c	5	100%
6	e	5	100%
6	h	5	20% 80%

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	FUC	Q	3	X	-	-	-
3	NAG	S	1	X	-	-	-
3	NAG	S	2	-	-	-	X
3	FUC	S	3	X	-	-	-
3	FUC	T	3	X	-	-	-
3	NAG	b	2	-	-	-	X
3	FUC	b	3	X	-	-	-
4	FUC	R	2	X	-	-	-
4	NAG	U	1	-	-	-	X
4	FUC	U	2	X	-	-	X
4	FUC	V	2	X	-	-	-
4	NAG	X	1	X	-	-	X
4	FUC	X	2	X	-	-	X
4	FUC	Y	2	X	-	-	-
4	FUC	a	2	X	-	-	X
4	FUC	d	2	X	-	-	-
4	FUC	g	2	X	-	-	-
5	NAG	W	1	-	-	-	X
5	NAG	W	2	-	-	-	X
5	NAG	f	1	-	-	-	X
5	NAG	f	2	-	-	-	X
6	NAG	Z	1	X	-	-	-
6	NAG	c	1	X	-	-	-
6	NAG	e	1	X	-	-	-
6	NAG	h	1	X	-	-	-
7	NAG	A	317	X	-	-	-
7	NAG	A	321	X	-	-	X
7	NAG	C	316	X	-	-	-
7	NAG	C	321	X	-	-	-
7	NAG	G	321	-	-	-	X
7	NAG	I	321	-	-	-	X
7	NAG	K	322	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	K	331	X	-	-	X
7	NAG	O	321	X	-	-	-
8	SO4	K	810	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18552 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 Urokinase plasminogen activator surface receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2040	1222	377	407	34			
1	C	259	Total	C	N	O	S	0	0	0
			1985	1188	368	395	34			
1	E	262	Total	C	N	O	S	0	0	0
			2006	1202	370	400	34			
1	G	258	Total	C	N	O	S	0	0	0
			1978	1186	363	395	34			
1	I	264	Total	C	N	O	S	0	0	0
			2008	1201	372	401	34			
1	K	257	Total	C	N	O	S	0	0	0
			1969	1180	363	392	34			
1	M	263	Total	C	N	O	S	0	0	0
			2016	1204	374	404	34			
1	O	258	Total	C	N	O	S	0	0	0
			1970	1180	362	394	34			

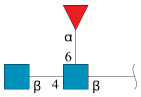
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	GLN	ASN	conflict	UNP Q9UMV0
C	200	GLN	ASN	conflict	UNP Q9UMV0
E	200	GLN	ASN	conflict	UNP Q9UMV0
G	200	GLN	ASN	conflict	UNP Q9UMV0
I	200	GLN	ASN	conflict	UNP Q9UMV0
K	200	GLN	ASN	conflict	UNP Q9UMV0
M	200	GLN	ASN	conflict	UNP Q9UMV0
O	200	GLN	ASN	conflict	UNP Q9UMV0

- Molecule 2 is a protein called antagonist peptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	B	13	Total C N O 116 78 17 21	0	0	0
2	D	13	Total C N O 116 78 17 21	0	0	0
2	F	13	Total C N O 116 78 17 21	0	0	0
2	H	13	Total C N O 116 78 17 21	0	0	0
2	J	13	Total C N O 116 78 17 21	0	0	0
2	L	13	Total C N O 116 78 17 21	0	0	0
2	N	13	Total C N O 116 78 17 21	0	0	0
2	P	13	Total C N O 116 78 17 21	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	Q	3	Total C N O 38 22 2 14	0	0	0
3	S	3	Total C N O 38 22 2 14	0	0	0
3	T	3	Total C N O 38 22 2 14	0	0	0
3	b	3	Total C N O 38 22 2 14	0	0	0

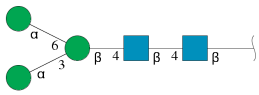
- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	R	2	Total C N O 24 14 1 9	0	0	0
4	U	2	Total C N O 24 14 1 9	0	0	0
4	V	2	Total C N O 24 14 1 9	0	0	0
4	X	2	Total C N O 24 14 1 9	0	0	0
4	Y	2	Total C N O 24 14 1 9	0	0	0
4	a	2	Total C N O 24 14 1 9	0	0	0
4	d	2	Total C N O 24 14 1 9	0	0	0
4	g	2	Total C N O 24 14 1 9	0	0	0

- Molecule 5 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
5	W	2	Total C N O 28 16 2 10	0	0	0
5	f	2	Total C N O 28 16 2 10	0	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	Z	5	Total C N O 61 34 2 25	0	0	0
6	c	5	Total C N O 61 34 2 25	0	0	0

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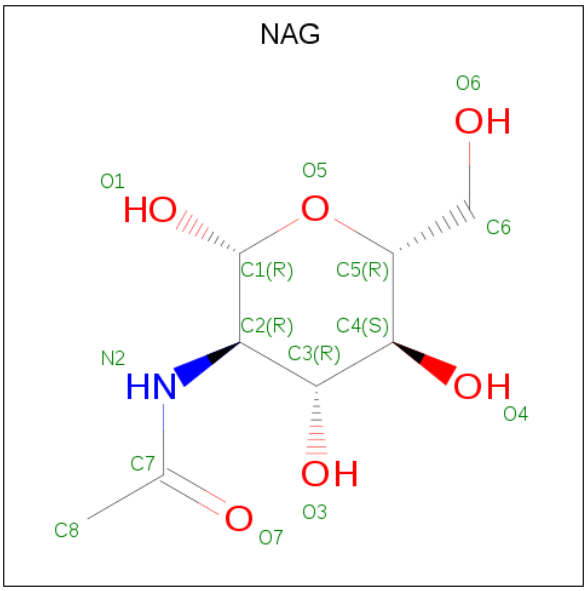
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	e	5	Total C N O 61 34 2 25	0	0	0
6	h	5	Total C N O 61 34 2 25	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0
7	E	1	Total C N O 14 8 1 5	0	0
7	G	1	Total C N O 14 8 1 5	0	0
7	I	1	Total C N O 14 8 1 5	0	0
7	K	1	Total C N O 14 8 1 5	0	0
7	K	1	Total C N O 14 8 1 5	0	0

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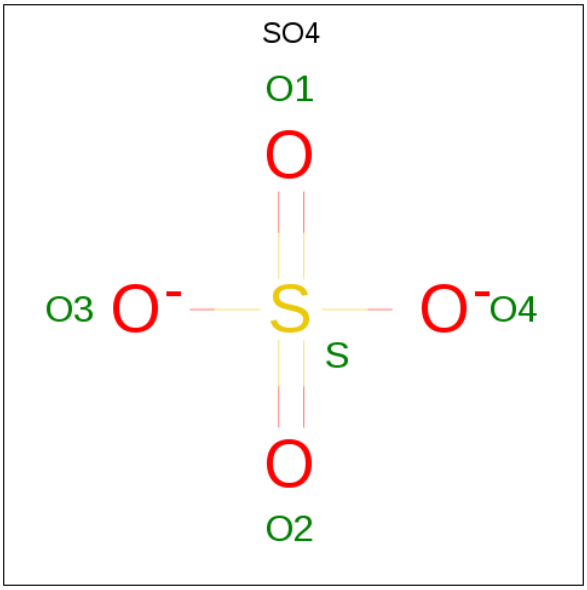
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	M	1	Total C N O 14 8 1 5	0	0
7	O	1	Total C N O 14 8 1 5	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	1	Total O S 5 4 1	0	0
8	G	1	Total O S 5 4 1	0	0
8	G	1	Total O S 5 4 1	0	0
8	G	1	Total O S 5 4 1	0	0
8	I	1	Total O S 5 4 1	0	0
8	I	1	Total O S 5 4 1	0	0
8	I	1	Total O S 5 4 1	0	0
8	K	1	Total O S 5 4 1	0	0
8	K	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	O	1	Total O S 5 4 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	81	Total O 81 81	0	0
9	B	5	Total O 5 5	0	0
9	C	85	Total O 85 85	0	0
9	D	2	Total O 2 2	0	0
9	E	98	Total O 98 98	0	0
9	F	8	Total O 8 8	0	0
9	G	88	Total O 88 88	0	0

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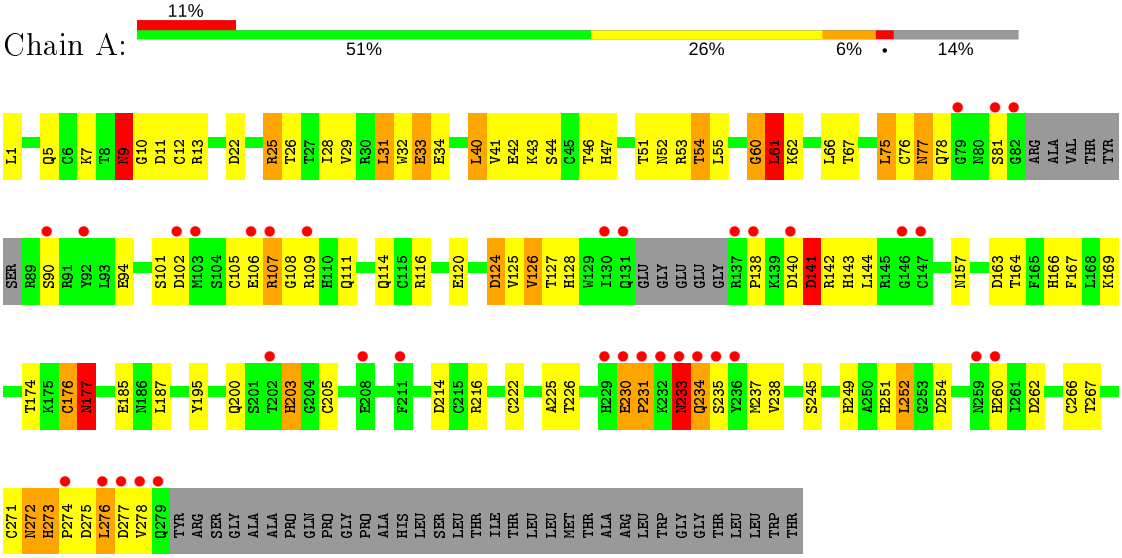
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	H	4	Total O 4 4	0	0
9	I	87	Total O 87 87	0	0
9	J	3	Total O 3 3	0	0
9	K	83	Total O 83 83	0	0
9	L	2	Total O 2 2	0	0
9	M	91	Total O 91 91	0	0
9	N	1	Total O 1 1	0	0
9	O	106	Total O 106 106	0	0
9	P	5	Total O 5 5	0	0

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.

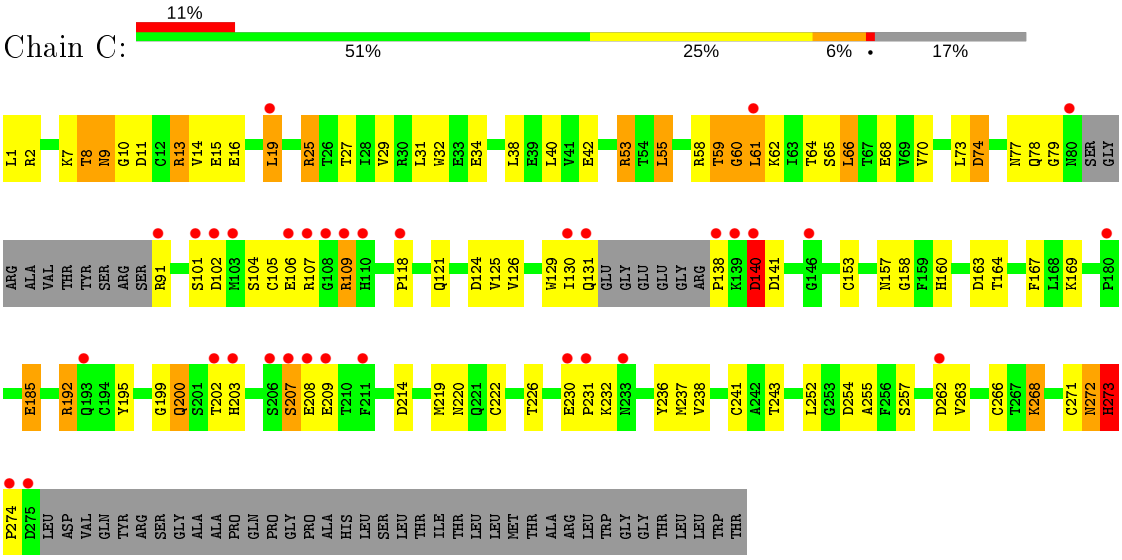
- Molecule 1: Urokinase plasminogen activator surface receptor

Chain A:



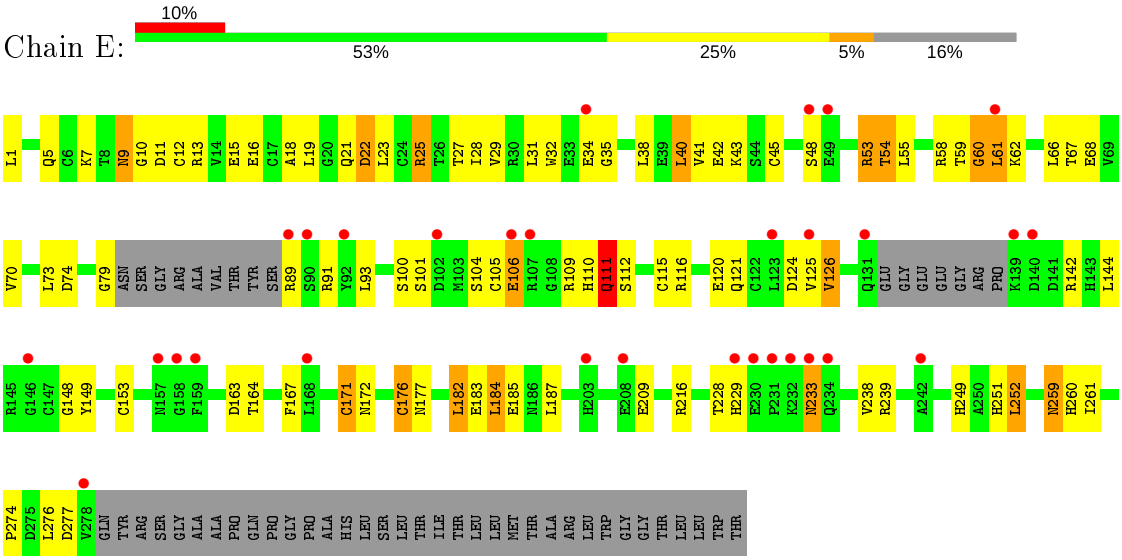
- Molecule 1: Urokinase plasminogen activator surface receptor

Chain C:



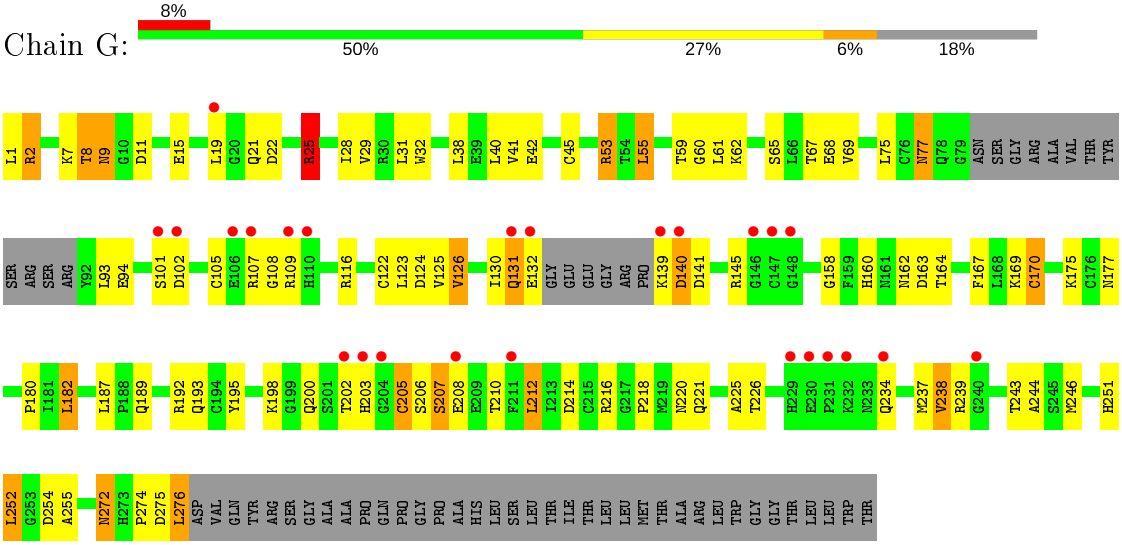
- Molecule 1: Urokinase plasminogen activator surface receptor

Chain E:



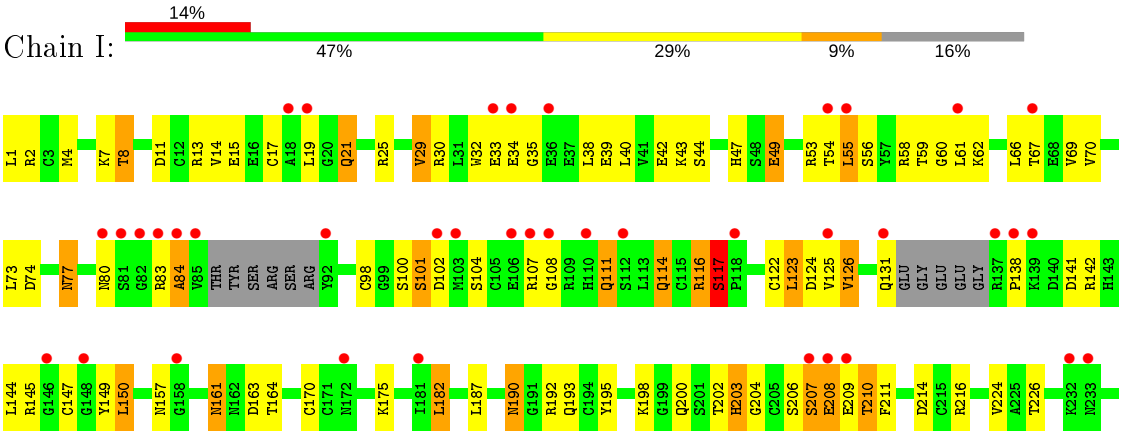
• Molecule 1: Urokinase plasminogen activator surface receptor

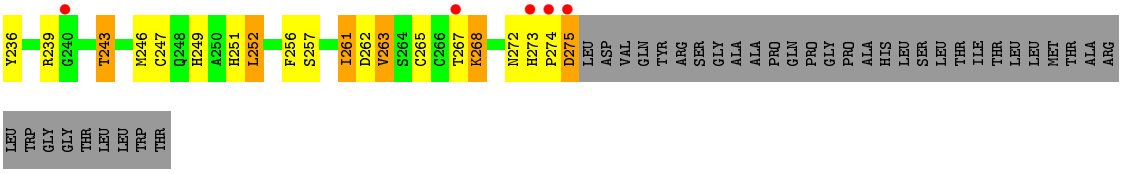
Chain G:



• Molecule 1: Urokinase plasminogen activator surface receptor

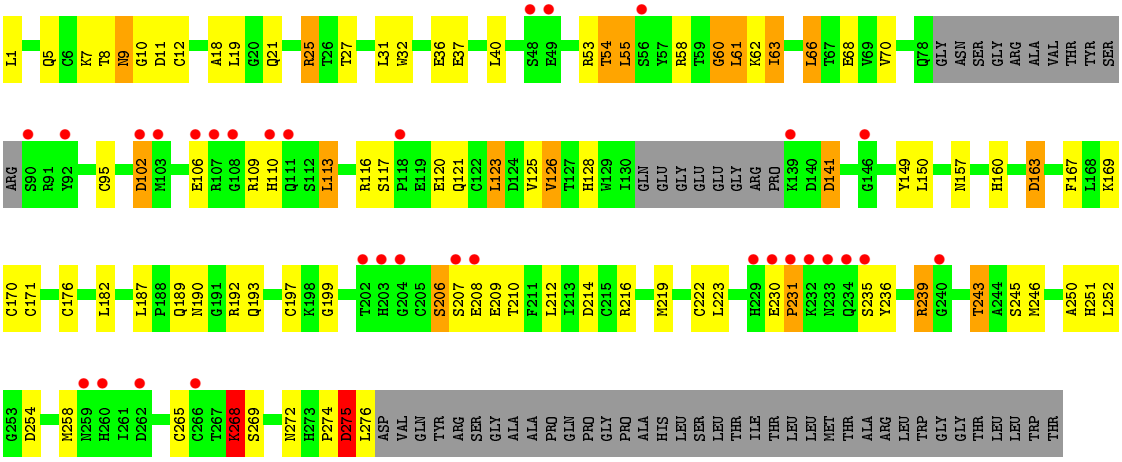
Chain I:





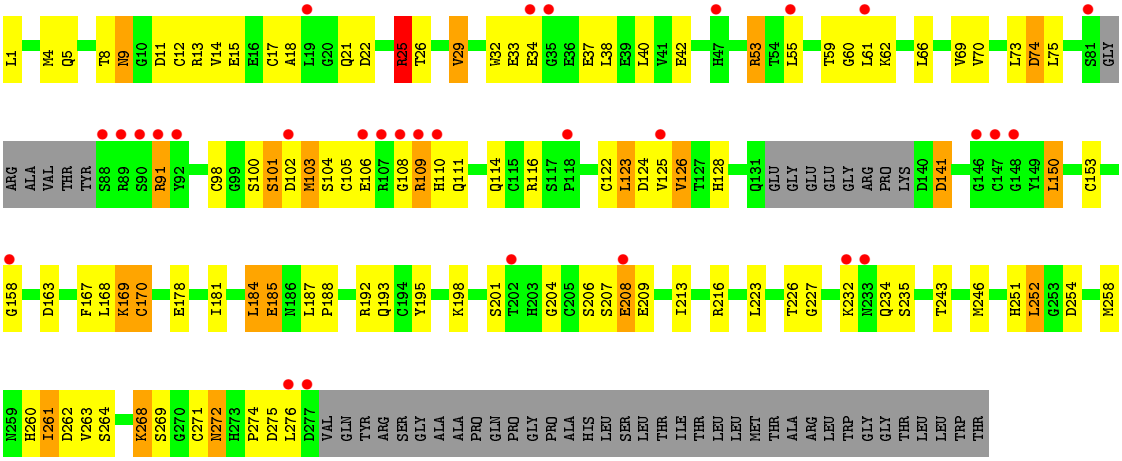
• Molecule 1: Urokinase plasminogen activator surface receptor

Chain K:



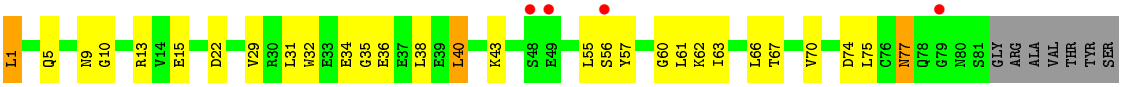
• Molecule 1: Urokinase plasminogen activator surface receptor

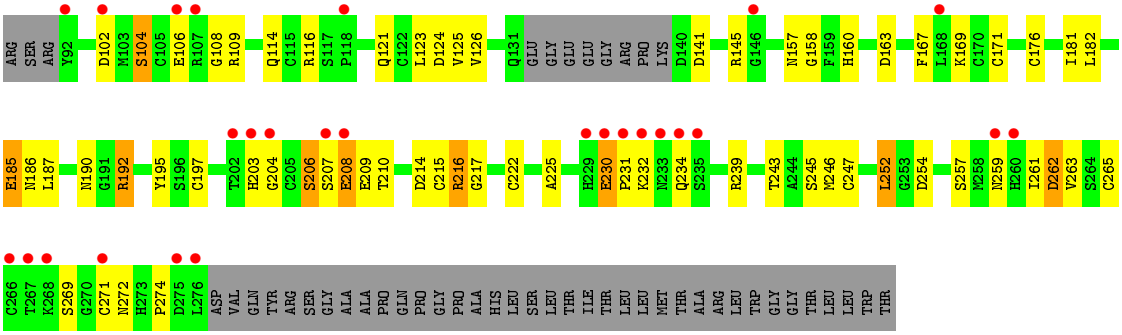
Chain M:



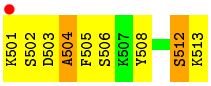
• Molecule 1: Urokinase plasminogen activator surface receptor

Chain O:

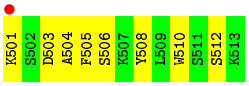




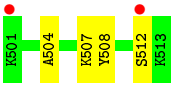
• Molecule 2: antagonist peptide



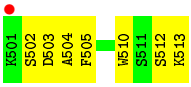
• Molecule 2: antagonist peptide



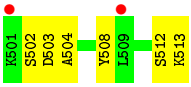
• Molecule 2: antagonist peptide



• Molecule 2: antagonist peptide

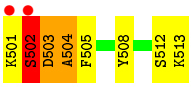


• Molecule 2: antagonist peptide



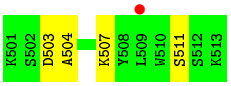
• Molecule 2: antagonist peptide

Chain L:



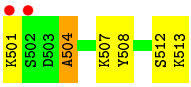
• Molecule 2: antagonist peptide

Chain N:



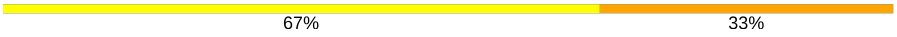
• Molecule 2: antagonist peptide

Chain P:



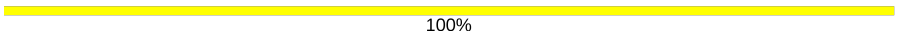
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

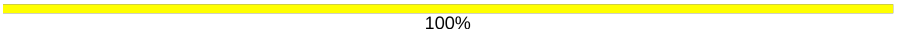


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



- Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

- Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

- Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

- Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

- Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

- Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:

- Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:

- Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

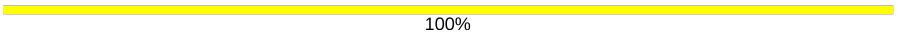
Chain g:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:

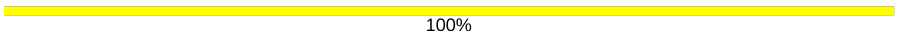


• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:

• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:

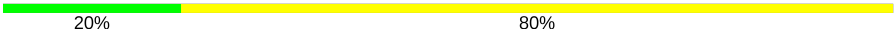


• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:

• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	106.93Å 136.83Å 140.54Å 90.00° 97.27° 90.00°	Depositor
Resolution (Å)	24.85 – 2.70 24.85 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (24.85-2.70) 97.2 (24.85-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.245 , 0.315 0.282 , 0.350	Depositor DCC
R_{free} test set	5335 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	50.6	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 58.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	18552	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 13.00% 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: BMA, NAG, ALC, DSN, FUC, DLY, MAN, SO4

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	0.55	2/2072 (0.1%)	0.87	11/2791 (0.4%)
1	C	0.62	3/2016 (0.1%)	0.87	10/2713 (0.4%)
1	E	0.54	0/2037	0.85	4/2742 (0.1%)
1	G	0.54	0/2009	0.90	10/2704 (0.4%)
1	I	0.53	1/2039 (0.0%)	0.85	9/2746 (0.3%)
1	K	0.60	1/2000 (0.1%)	0.85	6/2693 (0.2%)
1	M	0.52	0/2047	0.87	7/2755 (0.3%)
1	O	0.50	0/2001	0.82	7/2695 (0.3%)
2	B	0.63	0/91	0.86	1/116 (0.9%)
2	D	0.56	0/91	0.82	1/116 (0.9%)
2	F	0.61	0/91	0.82	0/116
2	H	0.67	0/91	0.88	1/116 (0.9%)
2	J	0.71	0/91	0.96	1/116 (0.9%)
2	L	0.54	0/91	0.86	0/116
2	N	0.56	0/91	0.92	1/116 (0.9%)
2	P	0.49	0/91	0.84	0/116
All	All	0.55	7/16949 (0.0%)	0.86	69/22767 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	E	0	1
1	G	0	1
1	I	0	1
1	K	0	2
All	All	0	8

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	268	LYS	CE-NZ	14.47	1.85	1.49
1	C	273	HIS	CE1-NE2	13.68	1.64	1.32
1	C	273	HIS	CG-ND1	11.19	1.63	1.38
1	A	233	ASN	CG-ND2	6.80	1.49	1.32
1	I	268	LYS	CE-NZ	5.75	1.63	1.49
1	C	273	HIS	CG-CD2	5.33	1.44	1.35
1	A	233	ASN	CG-OD1	5.20	1.35	1.24

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	141	ASP	CB-CG-OD2	7.49	125.04	118.30
1	A	102	ASP	CB-CG-OD2	6.97	124.57	118.30
1	A	262	ASP	CB-CG-OD2	6.68	124.31	118.30
1	I	141	ASP	CB-CG-OD2	6.54	124.19	118.30
2	H	503	ASP	CB-CG-OD2	6.45	124.10	118.30
1	I	124	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	141	ASP	CB-CG-OD2	6.30	123.97	118.30
1	G	22	ASP	CB-CG-OD2	6.27	123.94	118.30
1	E	124	ASP	CB-CG-OD2	6.18	123.87	118.30
1	K	275	ASP	CB-CG-OD2	6.16	123.84	118.30
1	C	124	ASP	CB-CG-OD2	6.11	123.80	118.30
1	C	138	PRO	N-CA-CB	6.08	110.60	103.30
1	C	262	ASP	CB-CG-OD2	6.05	123.75	118.30
1	E	176	CYS	CA-CB-SG	-6.05	103.11	114.00
1	O	22	ASP	CB-CG-OD2	6.04	123.73	118.30
1	M	141	ASP	CB-CG-OD2	6.03	123.72	118.30
1	I	138	PRO	N-CA-CB	6.02	110.53	103.30
1	I	74	ASP	CB-CG-OD2	6.00	123.70	118.30
1	G	102	ASP	CB-CG-OD2	5.97	123.67	118.30
2	N	503	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	31	LEU	CA-CB-CG	5.88	128.83	115.30
1	G	212	LEU	CA-CB-CG	5.88	128.82	115.30
1	C	74	ASP	CB-CG-OD2	5.84	123.56	118.30
1	K	214	ASP	CB-CG-OD2	5.76	123.48	118.30
1	O	163	ASP	CB-CG-OD2	5.70	123.43	118.30
1	M	124	ASP	CB-CG-OD2	5.69	123.42	118.30
1	O	214	ASP	CB-CG-OD2	5.68	123.41	118.30
1	C	163	ASP	CB-CG-OD2	5.66	123.40	118.30
1	K	102	ASP	CB-CG-OD2	5.63	123.37	118.30
1	G	141	ASP	CB-CG-OD2	5.63	123.37	118.30
1	G	140	ASP	CB-CG-OD2	5.61	123.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	124	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	214	ASP	CB-CG-OD2	5.58	123.32	118.30
1	O	254	ASP	CB-CG-OD2	5.57	123.31	118.30
1	C	273	HIS	CG-ND1-CE1	-5.57	98.47	105.70
1	G	254	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	163	ASP	CB-CG-OD2	5.49	123.24	118.30
1	I	102	ASP	CB-CG-OD2	5.47	123.23	118.30
1	M	163	ASP	CB-CG-OD2	5.47	123.22	118.30
1	C	254	ASP	CB-CG-OD2	5.47	123.22	118.30
1	K	163	ASP	CB-CG-OD2	5.46	123.22	118.30
1	I	275	ASP	CB-CG-OD2	5.46	123.21	118.30
2	J	503	ASP	CB-CG-OD2	5.46	123.21	118.30
1	E	74	ASP	CB-CG-OD2	5.46	123.21	118.30
1	K	141	ASP	CB-CG-OD2	5.43	123.18	118.30
1	A	22	ASP	CB-CG-OD2	5.40	123.16	118.30
1	C	102	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	9	ASN	CB-CA-C	-5.35	99.69	110.40
1	C	140	ASP	CB-CG-OD2	5.34	123.11	118.30
1	M	275	ASP	CB-CG-OD2	5.33	123.10	118.30
1	I	214	ASP	CB-CG-OD2	5.32	123.09	118.30
1	E	277	ASP	CB-CG-OD2	5.31	123.08	118.30
1	M	25	ARG	NE-CZ-NH1	-5.31	117.65	120.30
2	B	503	ASP	CB-CG-OD2	5.29	123.06	118.30
1	G	25	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	O	262	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	124	ASP	CB-CG-OD2	5.25	123.02	118.30
1	M	74	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	277	ASP	CB-CG-OD2	5.21	122.99	118.30
1	I	55	LEU	CA-CB-CG	5.20	127.26	115.30
1	G	214	ASP	CB-CG-OD2	5.19	122.97	118.30
1	I	11	ASP	CB-CG-OD2	5.15	122.94	118.30
2	D	503	ASP	CB-CG-OD2	5.12	122.91	118.30
1	G	124	ASP	CB-CG-OD2	5.11	122.90	118.30
1	M	22	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	214	ASP	CB-CG-OD2	5.09	122.89	118.30
1	G	163	ASP	CB-CG-OD2	5.08	122.87	118.30
1	K	254	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	254	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	230	GLU	Peptide
1	A	272	ASN	Peptide
1	A	61	LEU	Peptide
1	E	61	LEU	Peptide
1	G	208	GLU	Peptide
1	I	80	ASN	Peptide
1	K	102	ASP	Peptide
1	K	61	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2040	0	1885	59	0
1	C	1985	0	1840	72	0
1	E	2006	0	1864	66	0
1	G	1978	0	1836	62	0
1	I	2008	0	1850	67	0
1	K	1969	0	1825	65	0
1	M	2016	0	1868	56	0
1	O	1970	0	1823	55	0
2	B	116	0	112	9	0
2	D	116	0	112	7	0
2	F	116	0	112	3	0
2	H	116	0	112	3	0
2	J	116	0	112	2	0
2	L	116	0	112	7	0
2	N	116	0	112	2	0
2	P	116	0	112	6	0
3	Q	38	0	34	0	0
3	S	38	0	34	0	0
3	T	38	0	34	0	0
3	b	38	0	34	0	0
4	R	24	0	22	0	0
4	U	24	0	22	1	0
4	V	24	0	22	0	0
4	X	24	0	22	0	0
4	Y	24	0	22	1	0
4	a	24	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	d	24	0	22	0	0
4	g	24	0	22	0	0
5	W	28	0	25	2	0
5	f	28	0	25	0	0
6	Z	61	0	52	0	0
6	c	61	0	52	0	0
6	e	61	0	52	0	0
6	h	61	0	52	0	0
7	A	28	0	26	0	0
7	C	28	0	26	0	0
7	E	14	0	13	0	0
7	G	14	0	13	0	0
7	I	14	0	13	0	0
7	K	28	0	26	0	0
7	M	14	0	13	0	0
7	O	14	0	13	0	0
8	A	15	0	0	1	0
8	C	15	0	0	1	0
8	E	15	0	0	0	0
8	G	20	0	0	1	0
8	I	15	0	0	1	0
8	K	10	0	0	3	0
8	M	10	0	0	1	0
8	O	5	0	0	0	0
9	A	81	0	0	2	0
9	B	5	0	0	0	0
9	C	85	0	0	1	0
9	D	2	0	0	1	0
9	E	98	0	0	4	0
9	F	8	0	0	1	0
9	G	88	0	0	3	0
9	H	4	0	0	0	0
9	I	87	0	0	1	0
9	J	3	0	0	0	0
9	K	83	0	0	4	0
9	L	2	0	0	1	0
9	M	91	0	0	3	0
9	N	1	0	0	0	0
9	O	106	0	0	4	0
9	P	5	0	0	1	0
All	All	18552	0	16400	495	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 15.

All (495) 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:K:268:LYS:NZ	1:K:268:LYS:CE	1.85	1.38
1:C:273:HIS:HB3	1:C:274:PRO:HD3	1.11	1.10
1:C:273:HIS:HB3	1:C:274:PRO:CD	1.86	1.05
1:C:55:LEU:HB3	1:C:66:LEU:HD23	1.35	1.04
1:G:55:LEU:HD23	1:G:123:LEU:HD12	1.46	0.97
1:M:29:VAL:HB	1:M:66:LEU:HD13	1.45	0.96
1:M:4:MET:CE	1:M:75:LEU:HD22	2.00	0.91
1:C:273:HIS:CB	1:C:274:PRO:HD3	2.01	0.90
1:G:195:TYR:H	1:G:272:ASN:HD21	1.13	0.90
1:G:32:TRP:CE2	1:G:62:LYS:HB3	2.06	0.90
1:G:198:LYS:NZ	8:G:817:SO4:O2	2.05	0.90
1:O:32:TRP:CD1	1:O:62:LYS:HB3	2.08	0.89
1:G:55:LEU:HD23	1:G:123:LEU:CD1	2.05	0.87
1:K:27:THR:HG23	1:K:68:GLU:HG2	1.53	0.87
1:E:184:LEU:HD22	1:E:216:ARG:HD3	1.55	0.87
1:C:8:THR:HG21	1:E:12:CYS:H	1.40	0.86
1:C:32:TRP:CE2	1:C:62:LYS:HB3	2.09	0.86
1:G:7:LYS:HG3	1:G:9:ASN:HD21	1.42	0.84
1:A:32:TRP:CD1	1:A:62:LYS:HB3	2.12	0.84
1:I:4:MET:H	1:I:77:ASN:HD21	1.23	0.83
1:O:9:ASN:ND2	9:O:916:HOH:O	2.11	0.83
1:M:4:MET:HE2	1:M:75:LEU:HD22	1.58	0.83
1:C:8:THR:CG2	1:E:12:CYS:H	1.91	0.83
1:G:205:CYS:HB3	1:G:237:MET:HE2	1.61	0.82
1:E:91:ARG:NH1	1:E:116:ARG:HE	1.77	0.81
1:M:29:VAL:HB	1:M:66:LEU:CD1	2.11	0.80
2:P:508:TYR:HA	2:P:512:SER:HB3	1.63	0.80
1:I:32:TRP:CE2	1:I:62:LYS:HB3	2.17	0.80
1:C:195:TYR:H	1:C:272:ASN:HD21	1.25	0.80
1:E:32:TRP:CD1	1:E:62:LYS:HB3	2.16	0.80
1:E:54:THR:HG21	1:E:120:GLU:OE1	1.83	0.78
1:K:32:TRP:CD1	1:K:62:LYS:HB3	2.19	0.78
1:C:8:THR:HG21	1:E:12:CYS:N	1.99	0.77
2:F:508:TYR:HA	2:F:512:SER:HB3	1.65	0.77
2:B:508:TYR:HA	2:B:512:SER:HB3	1.67	0.77
1:I:239:ARG:HD3	1:I:272:ASN:HB3	1.67	0.75
1:C:268:LYS:HD3	1:C:268:LYS:H	1.51	0.75
1:K:157:ASN:ND2	1:K:245:SER:OG	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:123:LEU:HD22	1:M:170:CYS:HB3	1.69	0.75
1:M:195:TYR:H	1:M:272:ASN:HD21	1.36	0.74
1:O:29:VAL:HB	1:O:66:LEU:HD13	1.69	0.74
1:I:161:ASN:ND2	1:I:164:THR:H	1.85	0.74
1:I:123:LEU:HD22	1:I:170:CYS:HB3	1.70	0.73
1:M:98:CYS:HA	1:M:103:MET:HE3	1.70	0.73
1:A:275:ASP:O	1:A:276:LEU:HB2	1.88	0.73
1:A:75:LEU:C	1:A:77:ASN:H	1.90	0.73
2:J:508:TYR:CD2	2:J:512:SER:HB3	2.23	0.73
1:A:9:ASN:ND2	1:C:11:ASP:OD1	2.20	0.72
1:G:246:MET:HE2	1:G:252:LEU:HG	1.71	0.72
1:M:9:ASN:HD21	1:M:11:ASP:HB3	1.54	0.71
1:G:105:CYS:O	1:G:109:ARG:HG3	1.90	0.71
1:O:259:ASN:HD21	2:P:501:LYS:N	1.89	0.71
1:I:200:GLN:H	1:I:203:HIS:HD2	1.39	0.71
1:E:34:GLU:O	9:E:836:HOH:O	2.08	0.71
1:G:205:CYS:HB3	1:G:237:MET:CE	2.21	0.71
1:O:157:ASN:HA	1:O:243:THR:HG21	1.73	0.71
1:I:157:ASN:HA	1:I:243:THR:HG21	1.73	0.71
1:O:239:ARG:HD3	1:O:272:ASN:O	1.92	0.70
1:O:195:TYR:HB2	1:O:272:ASN:HB2	1.74	0.70
1:G:126:VAL:HG13	1:G:167:PHE:HB3	1.74	0.70
1:I:200:GLN:H	1:I:203:HIS:CD2	2.10	0.70
1:C:192:ARG:HD2	1:C:220:ASN:O	1.90	0.70
1:M:188:PRO:O	1:M:216:ARG:O	2.09	0.70
1:K:243:THR:HG22	1:K:246:MET:HG2	1.73	0.69
1:G:246:MET:CE	1:G:252:LEU:HG	2.23	0.69
1:G:274:PRO:C	1:G:276:LEU:H	1.96	0.69
8:K:810:SO4:O1	9:K:823:HOH:O	2.11	0.69
1:M:184:LEU:HD22	1:M:216:ARG:HG3	1.73	0.69
1:M:32:TRP:CE2	1:M:62:LYS:HB3	2.28	0.69
1:C:61:LEU:CA	1:O:61:LEU:CA	2.70	0.69
1:G:272:ASN:H	1:G:272:ASN:HD22	1.41	0.68
1:C:8:THR:HG22	9:E:822:HOH:O	1.91	0.68
1:A:53:ARG:NH1	1:A:251:HIS:HB3	2.09	0.68
1:A:230:GLU:HG2	1:A:233:ASN:H	1.57	0.68
1:E:9:ASN:ND2	1:G:11:ASP:OD1	2.22	0.67
1:C:268:LYS:H	1:C:268:LYS:CD	2.06	0.67
1:C:25:ARG:NH2	1:C:42:GLU:OE1	2.25	0.67
1:O:192:ARG:HG3	1:O:269:SER:HB3	1.77	0.66
1:C:10:GLY:O	9:C:860:HOH:O	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:25:ARG:NH2	1:G:42:GLU:OE1	2.24	0.66
1:I:195:TYR:HB2	1:I:272:ASN:HB2	1.78	0.65
1:C:157:ASN:HA	1:C:243:THR:HG21	1.79	0.65
1:K:109:ARG:O	1:K:110:HIS:HB2	1.97	0.65
1:M:226:THR:HG22	1:M:262:ASP:HB3	1.79	0.65
1:I:190:ASN:ND2	1:I:192:ARG:H	1.95	0.65
1:G:160:HIS:HE1	1:G:216:ARG:H	1.46	0.65
1:I:273:HIS:CD2	1:I:275:ASP:H	2.16	0.64
1:G:55:LEU:CD2	1:G:123:LEU:HD12	2.26	0.64
1:A:25:ARG:HG2	1:A:46:THR:HB	1.80	0.63
1:K:197:CYS:SG	1:K:239:ARG:HD2	2.38	0.63
1:K:66:LEU:HD23	2:L:505:PHE:CD1	2.33	0.63
1:E:185:GLU:CD	1:E:185:GLU:H	2.00	0.63
1:G:7:LYS:HG3	1:G:9:ASN:ND2	2.13	0.63
1:G:68:GLU:OE2	9:G:822:HOH:O	2.15	0.63
1:I:190:ASN:HD22	1:I:192:ARG:H	1.47	0.63
1:C:2:ARG:HD3	1:C:74:ASP:OD1	1.98	0.63
1:I:29:VAL:HB	1:I:66:LEU:HD13	1.80	0.63
1:M:104:SER:O	1:M:108:GLY:N	2.28	0.63
1:I:8:THR:HG22	1:K:10:GLY:O	1.99	0.63
8:A:801:SO4:O3	1:C:13:ARG:NH1	2.31	0.62
1:A:67:THR:OG1	1:A:81:SER:HB3	1.99	0.62
1:O:195:TYR:HB2	1:O:272:ASN:CB	2.28	0.62
1:K:246:MET:HE2	1:K:252:LEU:HD13	1.81	0.62
2:L:508:TYR:HA	2:L:512:SER:HB3	1.81	0.62
1:M:25:ARG:NH1	1:M:42:GLU:OE1	2.25	0.62
1:E:43:LYS:NZ	1:E:79:GLY:H	1.98	0.61
1:I:7:LYS:NZ	9:I:834:HOH:O	2.19	0.61
1:O:207:SER:C	1:O:209:GLU:H	2.04	0.61
1:M:246:MET:HE1	1:M:252:LEU:HG	1.81	0.61
1:I:13:ARG:HD2	8:I:804:SO4:O4	1.99	0.61
1:C:129:TRP:HZ3	1:C:140:ASP:O	1.83	0.61
1:G:60:GLY:O	1:K:61:LEU:O	2.18	0.61
1:M:25:ARG:HG2	1:M:26:THR:N	2.15	0.61
1:O:104:SER:O	1:O:108:GLY:HA3	2.01	0.61
1:O:247:CYS:HA	1:O:263:VAL:CG2	2.30	0.61
1:A:225:ALA:HB3	1:A:238:VAL:HG12	1.83	0.61
1:G:101:SER:OG	2:H:513:LYS:O	2.13	0.60
1:I:243:THR:HG22	1:I:246:MET:HG2	1.83	0.60
1:G:61:LEU:CA	1:K:61:LEU:CA	2.79	0.60
1:K:117:SER:HB2	1:K:120:GLU:HG3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:116:ARG:O	1:I:117:SER:HB3	2.02	0.60
1:M:254:ASP:O	2:N:507:DLY:HE3	2.00	0.60
1:A:105:CYS:O	1:A:109:ARG:HG3	2.02	0.60
1:M:185:GLU:H	1:M:185:GLU:CD	2.04	0.60
1:A:10:GLY:O	1:G:8:THR:HG22	2.02	0.59
1:A:108:GLY:O	1:A:111:GLN:HB2	2.03	0.59
1:I:17:CYS:HB3	1:I:21:GLN:HB2	1.84	0.59
1:C:272:ASN:H	1:C:272:ASN:HD22	1.51	0.59
1:C:160:HIS:CE1	1:C:241:CYS:HB2	2.38	0.58
1:K:210:THR:HG21	1:K:274:PRO:HG3	1.84	0.58
1:C:9:ASN:HD22	1:C:9:ASN:H	1.49	0.58
1:G:205:CYS:CB	1:G:237:MET:HE2	2.33	0.58
1:A:28:ILE:HG12	1:A:41:VAL:HG22	1.86	0.58
1:C:226:THR:HG23	1:C:237:MET:HB3	1.85	0.58
1:C:59:THR:HG21	1:C:64:THR:OG1	2.04	0.58
2:D:501:LYS:HG3	1:E:13:ARG:NH2	2.19	0.58
1:E:54:THR:HG22	1:E:148:GLY:HA2	1.86	0.58
1:K:192:ARG:HH11	1:K:269:SER:HB2	1.69	0.58
1:G:225:ALA:HB3	1:G:238:VAL:HG12	1.86	0.58
1:M:5:GLN:HB2	1:M:15:GLU:HG2	1.86	0.58
1:A:114:GLN:O	1:A:116:ARG:NH1	2.36	0.57
2:D:508:TYR:CD2	2:D:512:SER:HB3	2.39	0.57
1:E:104:SER:HB3	1:E:106:GLU:HG3	1.86	0.57
1:E:121:GLN:HB3	1:E:171:CYS:O	2.03	0.57
1:E:182:LEU:HD21	1:E:187:LEU:HD21	1.85	0.57
1:O:243:THR:HG23	1:O:245:SER:HB2	1.85	0.57
1:C:164:THR:HG21	8:C:818:SO4:O1	2.04	0.57
1:K:27:THR:HG23	1:K:68:GLU:CG	2.30	0.57
1:O:160:HIS:CE1	1:O:215:CYS:HA	2.38	0.57
1:C:268:LYS:N	1:C:268:LYS:HD3	2.18	0.57
1:E:34:GLU:HG3	1:E:35:GLY:H	1.69	0.57
1:G:251:HIS:CE1	1:G:252:LEU:HD13	2.39	0.57
2:F:507:DLY:HE3	9:F:421:HOH:O	2.03	0.57
1:G:192:ARG:HG3	1:G:220:ASN:O	2.05	0.57
1:I:207:SER:OG	1:I:274:PRO:HG3	2.05	0.57
1:K:9:ASN:HD22	1:K:10:GLY:N	2.03	0.56
1:A:195:TYR:HB2	1:A:272:ASN:HB2	1.87	0.56
1:M:246:MET:CE	1:M:252:LEU:HG	2.35	0.56
1:O:247:CYS:HA	1:O:263:VAL:HG23	1.86	0.56
1:E:105:CYS:O	1:E:109:ARG:HG3	2.05	0.56
1:C:32:TRP:CD2	1:C:62:LYS:HB3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:9:ASN:ND2	1:M:11:ASP:HB3	2.20	0.56
1:E:251:HIS:HB3	9:E:908:HOH:O	2.06	0.56
1:G:75:LEU:C	1:G:77:ASN:H	2.08	0.56
1:A:106:GLU:O	1:A:107:ARG:HB3	2.06	0.55
1:A:176:CYS:SG	1:A:177:ASN:N	2.79	0.55
1:K:121:GLN:HB3	1:K:171:CYS:O	2.05	0.55
1:A:75:LEU:C	1:A:77:ASN:N	2.60	0.55
2:B:501:LYS:HE3	1:C:13:ARG:HH22	1.70	0.55
1:E:228:THR:HG21	1:E:233:ASN:ND2	2.22	0.55
1:A:200:GLN:HG3	1:A:203:HIS:HD2	1.70	0.55
1:A:273:HIS:HB3	1:A:274:PRO:HD3	1.88	0.55
1:K:149:TYR:C	1:K:150:LEU:HD12	2.27	0.55
1:O:121:GLN:HB3	1:O:171:CYS:O	2.06	0.55
1:M:1:LEU:O	1:M:1:LEU:HD13	2.06	0.55
1:A:205:CYS:HB3	1:A:237:MET:HE2	1.87	0.55
1:M:126:VAL:HG13	1:M:167:PHE:HB3	1.89	0.55
1:K:275:ASP:OD2	1:K:276:LEU:N	2.40	0.55
1:E:29:VAL:CG1	1:E:40:LEU:HB2	2.37	0.55
1:K:25:ARG:HD3	9:K:817:HOH:O	2.07	0.55
1:K:192:ARG:NH1	1:K:269:SER:HB2	2.21	0.55
1:O:239:ARG:HD2	1:O:272:ASN:HB3	1.87	0.55
1:G:160:HIS:CE1	1:G:216:ARG:H	2.25	0.54
1:O:55:LEU:HD21	1:O:57:TYR:CE2	2.43	0.54
1:M:18:ALA:HB3	1:M:21:GLN:HE21	1.72	0.54
1:C:257:SER:HA	1:E:16:GLU:OE1	2.07	0.54
1:I:14:VAL:HG21	2:P:504:ALC:HE23	1.89	0.54
1:M:32:TRP:O	1:M:33:GLU:HB2	2.07	0.54
1:E:25:ARG:HH21	1:E:42:GLU:HG2	1.72	0.54
1:K:9:ASN:HD21	1:K:11:ASP:HB3	1.73	0.54
1:O:257:SER:OG	2:P:507:DLY:NZ	2.40	0.54
1:C:60:GLY:O	1:O:61:LEU:O	2.25	0.54
1:K:192:ARG:HH12	1:K:268:LYS:NZ	2.06	0.53
1:C:199:GLY:HA2	1:C:236:TYR:CZ	2.43	0.53
1:I:47:HIS:HB3	1:I:49:GLU:OE2	2.08	0.53
2:L:513:LYS:HD2	1:M:73:LEU:HD22	1.90	0.53
1:E:43:LYS:HZ1	1:E:79:GLY:H	1.57	0.53
1:I:83:ARG:O	1:I:84:ALA:HB2	2.08	0.53
1:O:32:TRP:CG	1:O:62:LYS:HB3	2.41	0.53
1:K:9:ASN:C	1:K:9:ASN:HD22	2.10	0.53
1:E:142:ARG:HG3	1:E:142:ARG:HH11	1.72	0.53
1:I:195:TYR:HB3	1:I:210:THR:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:245:SER:HB3	1:O:252:LEU:HD23	1.90	0.53
1:C:230:GLU:HB2	1:E:18:ALA:CB	2.38	0.53
1:E:53:ARG:NH2	1:E:68:GLU:OE2	2.39	0.53
1:E:15:GLU:HG2	1:E:45:CYS:SG	2.49	0.53
1:M:122:CYS:O	1:M:170:CYS:HA	2.09	0.53
1:A:9:ASN:HB3	1:A:11:ASP:H	1.73	0.52
1:M:227:GLY:HA2	1:M:260:HIS:O	2.09	0.52
1:A:126:VAL:HG13	1:A:167:PHE:HB3	1.90	0.52
1:K:160:HIS:HE1	1:K:216:ARG:H	1.57	0.52
1:C:130:ILE:O	1:C:131:GLN:HB2	2.10	0.52
1:A:124:ASP:HB3	1:A:169:LYS:HG3	1.90	0.52
1:K:207:SER:C	1:K:209:GLU:H	2.13	0.52
1:M:181:ILE:H	1:M:181:ILE:HD12	1.74	0.52
2:B:501:LYS:HD3	1:C:16:GLU:HB2	1.91	0.52
1:G:189:GLN:N	1:G:189:GLN:OE1	2.39	0.52
1:A:126:VAL:HB	1:A:143:HIS:HD2	1.74	0.51
1:G:182:LEU:HD11	1:G:187:LEU:HD21	1.91	0.51
2:L:501:LYS:O	2:L:502:SER:HB2	2.10	0.51
1:A:32:TRP:CG	1:A:62:LYS:HB3	2.45	0.51
1:O:38:LEU:HD12	9:O:828:HOH:O	2.10	0.51
1:G:123:LEU:HD23	1:G:170:CYS:HB3	1.91	0.51
1:I:30:ARG:NH1	1:I:39:GLU:OE1	2.44	0.51
1:O:230:GLU:HG3	1:O:231:PRO:HA	1.92	0.51
1:M:5:GLN:O	1:M:12:CYS:HA	2.11	0.51
1:G:131:GLN:HG2	1:G:132:GLU:H	1.75	0.51
1:C:91:ARG:HB2	1:C:118:PRO:HB3	1.92	0.50
1:E:121:GLN:HE22	1:E:153:CYS:HB3	1.76	0.50
1:G:9:ASN:ND2	1:G:9:ASN:H	2.09	0.50
1:K:18:ALA:H	1:K:21:GLN:HE21	1.60	0.50
1:C:9:ASN:HD22	1:C:9:ASN:N	2.08	0.50
1:E:142:ARG:HH12	2:F:512:SER:C	2.13	0.50
1:O:55:LEU:HD21	1:O:57:TYR:HE2	1.77	0.50
1:E:66:LEU:HD12	1:E:67:THR:N	2.27	0.50
1:G:162:ASN:HD22	5:W:1:NAG:H82	1.76	0.50
1:E:115:CYS:HB3	1:E:120:GLU:CG	2.42	0.50
1:I:29:VAL:HG13	1:I:40:LEU:HB3	1.93	0.50
1:C:200:GLN:HE21	1:C:203:HIS:HB2	1.77	0.50
1:E:110:HIS:O	1:E:111:GLN:HB2	2.10	0.50
1:G:274:PRO:C	1:G:276:LEU:N	2.64	0.50
1:K:251:HIS:HD2	9:K:823:HOH:O	1.93	0.50
1:I:256:PHE:HB2	1:I:261:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:259:ASN:ND2	2:P:501:LYS:N	2.60	0.50
1:I:161:ASN:HD21	1:I:164:THR:H	1.58	0.50
1:I:226:THR:HG22	1:I:262:ASP:HB3	1.94	0.50
1:O:246:MET:HE1	1:O:252:LEU:HG	1.94	0.50
1:E:32:TRP:CG	1:E:62:LYS:HB3	2.46	0.49
1:I:149:TYR:O	1:I:150:LEU:HD13	2.12	0.49
1:A:61:LEU:CA	1:I:61:LEU:CA	2.90	0.49
2:J:508:TYR:HD2	2:J:512:SER:HB3	1.76	0.49
1:C:104:SER:OG	1:C:106:GLU:HG2	2.13	0.49
1:K:190:ASN:HB3	1:K:192:ARG:H	1.76	0.49
1:C:121:GLN:NE2	1:C:153:CYS:HB3	2.27	0.49
1:E:54:THR:CG2	1:E:120:GLU:OE1	2.59	0.49
1:K:207:SER:HA	1:K:210:THR:HG22	1.93	0.49
1:C:268:LYS:O	1:C:271:CYS:SG	2.70	0.49
1:K:192:ARG:HH12	1:K:268:LYS:HZ3	1.60	0.49
1:G:53:ARG:HG3	2:H:505:PHE:CE2	2.48	0.49
1:K:126:VAL:HG13	1:K:167:PHE:HB3	1.94	0.49
1:M:33:GLU:O	1:M:34:GLU:HB2	2.12	0.49
1:K:7:LYS:HD3	8:K:803:SO4:O4	2.12	0.49
1:O:190:ASN:HD21	1:O:217:GLY:N	2.11	0.49
1:I:108:GLY:O	1:I:111:GLN:HB2	2.12	0.49
1:I:204:GLY:O	1:I:209:GLU:HB3	2.13	0.49
1:C:9:ASN:H	1:C:9:ASN:ND2	2.10	0.49
1:E:22:ASP:OD2	1:E:48:SER:HA	2.12	0.49
1:K:157:ASN:HA	1:K:243:THR:HG21	1.95	0.49
1:M:73:LEU:O	1:M:74:ASP:C	2.51	0.49
1:O:29:VAL:HG13	1:O:40:LEU:HB2	1.94	0.49
1:G:158:GLY:N	1:G:246:MET:HE3	2.28	0.48
1:G:25:ARG:HA	1:G:69:VAL:O	2.13	0.48
1:A:60:GLY:O	1:I:61:LEU:O	2.31	0.48
1:K:63:ILE:HD11	1:K:113:LEU:HD21	1.94	0.48
1:I:247:CYS:HA	1:I:263:VAL:CG2	2.43	0.48
2:L:504:ALC:HE23	1:M:14:VAL:HG21	1.94	0.48
1:A:231:PRO:HD3	1:C:19:LEU:HB2	1.96	0.48
1:K:243:THR:HG23	1:K:245:SER:OG	2.13	0.48
1:A:251:HIS:CE1	1:A:252:LEU:HD22	2.48	0.48
1:A:51:THR:HG21	9:A:815:HOH:O	2.13	0.48
1:G:94:GLU:CD	1:G:175:LYS:HD2	2.34	0.48
1:A:51:THR:HG22	1:A:52:ASN:N	2.29	0.48
1:A:54:THR:HG21	1:A:120:GLU:OE1	2.14	0.48
1:C:230:GLU:HB2	1:E:18:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:LEU:HB3	1:C:66:LEU:CD2	2.25	0.48
1:I:246:MET:CE	1:I:252:LEU:HG	2.43	0.48
1:E:27:THR:OG1	1:E:68:GLU:HG3	2.13	0.48
1:M:8:THR:HG22	1:O:10:GLY:O	2.14	0.48
1:K:222:CYS:HB3	1:K:272:ASN:HB3	1.95	0.48
1:O:43:LYS:NZ	9:O:879:HOH:O	2.46	0.48
1:O:55:LEU:C	1:O:55:LEU:HD23	2.34	0.47
1:I:203:HIS:CG	1:I:204:GLY:N	2.82	0.47
2:B:501:LYS:HB3	1:C:16:GLU:OE2	2.14	0.47
1:K:268:LYS:HA	1:K:268:LYS:HD2	1.51	0.47
1:G:61:LEU:O	1:K:60:GLY:O	2.33	0.47
1:C:27:THR:OG1	1:C:68:GLU:HG2	2.13	0.47
1:I:114:GLN:HB2	1:I:114:GLN:HE21	1.56	0.47
1:E:176:CYS:SG	1:E:177:ASN:N	2.85	0.47
1:K:190:ASN:ND2	1:K:219:MET:O	2.47	0.47
1:A:67:THR:OG1	1:A:81:SER:CB	2.63	0.47
1:O:123:LEU:O	1:O:145:ARG:HA	2.14	0.47
1:I:104:SER:O	1:I:108:GLY:HA3	2.14	0.47
1:M:251:HIS:CD2	1:M:252:LEU:HD13	2.50	0.47
1:E:239:ARG:NH2	1:E:274:PRO:HA	2.30	0.47
1:E:54:THR:HB	1:E:149:TYR:HB3	1.96	0.47
1:I:273:HIS:HD2	1:I:275:ASP:H	1.59	0.47
1:I:56:SER:HB2	1:I:147:CYS:HB2	1.96	0.47
2:N:507:DLY:O	2:N:511:SER:HB2	2.15	0.47
1:C:53:ARG:HG3	2:D:505:PHE:CE2	2.50	0.47
1:A:43:LYS:O	1:A:44:SER:HB3	2.15	0.46
1:G:21:GLN:HG2	1:G:45:CYS:HB3	1.96	0.46
1:G:218:PRO:O	1:G:243:THR:HG22	2.16	0.46
1:A:157:ASN:HD22	1:A:245:SER:CB	2.28	0.46
1:I:2:ARG:HA	1:I:15:GLU:O	2.16	0.46
1:O:5:GLN:NE2	9:O:898:HOH:O	2.48	0.46
1:G:2:ARG:HA	1:G:15:GLU:O	2.16	0.46
1:K:66:LEU:HD23	2:L:505:PHE:HD1	1.79	0.46
1:M:100:SER:O	1:M:101:SER:C	2.54	0.46
1:O:157:ASN:HD22	1:O:245:SER:CB	2.28	0.46
1:A:249:HIS:HB2	1:A:252:LEU:HD23	1.97	0.46
1:C:8:THR:HG23	1:E:11:ASP:HA	1.97	0.46
1:G:32:TRP:CD2	1:G:62:LYS:HB3	2.49	0.46
1:A:222:CYS:HB2	1:A:271:CYS:SG	2.56	0.46
1:G:122:CYS:O	1:G:170:CYS:HA	2.15	0.46
1:E:259:ASN:O	1:E:261:ILE:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:239:ARG:NH2	1:G:274:PRO:HA	2.31	0.46
1:C:8:THR:CG2	1:E:12:CYS:N	2.64	0.46
1:G:276:LEU:HD11	9:G:901:HOH:O	2.15	0.46
1:C:268:LYS:HG2	1:C:271:CYS:HB3	1.98	0.46
1:A:34:GLU:O	9:A:834:HOH:O	2.21	0.45
1:A:40:LEU:HD23	2:B:504:ALC:HZ2	1.97	0.45
1:K:9:ASN:ND2	1:K:11:ASP:H	2.15	0.45
1:M:272:ASN:H	1:M:272:ASN:HD22	1.63	0.45
1:C:266:CYS:HB2	1:C:268:LYS:HE2	1.98	0.45
1:C:29:VAL:HG13	1:C:66:LEU:CD1	2.46	0.45
1:K:53:ARG:HG2	1:K:68:GLU:HB2	1.97	0.45
2:L:503:ASP:HB3	9:L:745:HOH:O	2.15	0.45
1:G:255:ALA:HB2	2:H:510:TRP:CE2	2.52	0.45
1:I:246:MET:HE1	1:I:252:LEU:HG	1.98	0.45
1:K:123:LEU:HD22	1:K:123:LEU:HA	1.82	0.45
1:M:169:LYS:HE2	1:M:169:LYS:HB3	1.78	0.45
1:A:7:LYS:HB2	1:A:9:ASN:HB2	1.98	0.45
1:C:8:THR:HG23	1:E:10:GLY:O	2.16	0.45
1:E:34:GLU:HG3	1:E:35:GLY:N	2.31	0.45
1:E:7:LYS:HB2	1:E:9:ASN:HB2	1.98	0.45
1:I:25:ARG:HH22	1:I:42:GLU:CD	2.19	0.45
1:M:243:THR:O	1:M:246:MET:HB2	2.16	0.45
1:E:249:HIS:HB3	1:E:251:HIS:CD2	2.51	0.45
1:K:32:TRP:CG	1:K:62:LYS:HB3	2.52	0.45
1:A:33:GLU:HG2	1:C:78:GLN:O	2.16	0.45
1:A:230:GLU:HA	1:A:231:PRO:C	2.37	0.45
1:E:89:ARG:N	9:E:851:HOH:O	2.49	0.45
1:M:208:GLU:HG3	1:M:209:GLU:N	2.31	0.45
1:O:195:TYR:H	1:O:272:ASN:ND2	2.15	0.45
1:A:25:ARG:HH21	1:A:42:GLU:HG2	1.83	0.45
1:C:192:ARG:CD	1:C:220:ASN:O	2.64	0.45
1:C:158:GLY:H	1:C:243:THR:HG22	1.82	0.45
1:E:34:GLU:OE1	1:E:34:GLU:HA	2.17	0.45
1:K:223:LEU:HD12	1:K:265:CYS:SG	2.57	0.45
1:M:150:LEU:HB2	1:M:153:CYS:SG	2.57	0.45
1:K:230:GLU:HA	1:K:231:PRO:HA	1.77	0.44
1:O:181:ILE:H	1:O:181:ILE:HG13	1.64	0.44
1:O:246:MET:CE	1:O:252:LEU:HG	2.46	0.44
1:E:23:LEU:HB3	1:E:70:VAL:HG22	1.99	0.44
1:I:251:HIS:CD2	1:I:252:LEU:HD13	2.52	0.44
1:M:178:GLU:HB3	9:M:823:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:261:ILE:HG22	9:M:849:HOH:O	2.15	0.44
1:O:160:HIS:CE1	1:O:216:ARG:H	2.35	0.44
2:B:504:ALC:HE12	1:C:14:VAL:HG21	1.98	0.44
1:C:140:ASP:OD2	1:E:73:LEU:HD23	2.18	0.44
1:I:98:CYS:SG	1:I:145:ARG:HG3	2.57	0.44
1:A:29:VAL:CG1	1:A:40:LEU:HB2	2.47	0.44
1:C:7:LYS:HB2	1:C:9:ASN:ND2	2.32	0.44
1:I:239:ARG:HD3	1:I:272:ASN:CB	2.42	0.44
1:E:115:CYS:HB3	1:E:120:GLU:HG3	1.99	0.44
1:I:198:LYS:HG2	1:I:236:TYR:CE1	2.53	0.44
1:I:83:ARG:O	1:I:84:ALA:CB	2.65	0.44
1:O:158:GLY:H	1:O:243:THR:CG2	2.31	0.44
1:O:207:SER:C	1:O:209:GLU:N	2.70	0.44
1:O:225:ALA:HA	1:O:262:ASP:O	2.17	0.44
1:O:243:THR:CG2	1:O:245:SER:HB2	2.46	0.44
1:A:128:HIS:ND1	1:A:141:ASP:OD1	2.51	0.44
1:M:109:ARG:HB3	1:M:110:HIS:H	1.44	0.44
1:M:168:LEU:HD23	1:M:168:LEU:C	2.37	0.44
1:I:161:ASN:HD22	1:I:164:THR:H	1.64	0.44
1:K:243:THR:CG2	1:K:245:SER:OG	2.66	0.44
1:K:9:ASN:HD21	1:K:11:ASP:CB	2.30	0.44
1:E:5:GLN:O	1:E:12:CYS:HA	2.18	0.43
1:I:203:HIS:CD2	1:I:204:GLY:H	2.36	0.43
1:C:273:HIS:CB	1:C:274:PRO:CD	2.70	0.43
1:G:109:ARG:HH11	1:G:180:PRO:HA	1.83	0.43
1:A:5:GLN:O	1:A:12:CYS:HA	2.19	0.43
1:E:28:ILE:HG12	1:E:41:VAL:HG22	1.99	0.43
1:G:145:ARG:HD3	1:G:177:ASN:O	2.18	0.43
1:I:122:CYS:O	1:I:170:CYS:HA	2.19	0.43
1:G:221:GLN:NE2	1:G:244:ALA:HB2	2.34	0.43
1:K:109:ARG:O	1:K:110:HIS:CB	2.65	0.43
1:A:101:SER:N	2:B:513:LYS:O	2.51	0.43
1:A:28:ILE:O	1:A:66:LEU:HA	2.17	0.43
1:C:13:ARG:NH2	1:C:15:GLU:HA	2.34	0.43
1:O:167:PHE:HE2	1:O:169:LYS:HG3	1.83	0.43
2:B:508:TYR:CD2	2:B:512:SER:CB	3.01	0.43
1:K:55:LEU:O	1:K:66:LEU:N	2.42	0.43
1:M:223:LEU:HA	1:M:264:SER:O	2.19	0.43
1:O:158:GLY:CA	1:O:246:MET:HE3	2.49	0.43
1:A:75:LEU:O	1:A:77:ASN:N	2.51	0.43
1:C:185:GLU:CD	1:C:185:GLU:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1:LEU:HD23	1:O:74:ASP:OD1	2.19	0.43
2:D:505:PHE:O	2:D:506:DSN:C	2.66	0.43
1:I:126:VAL:HA	1:I:142:ARG:O	2.18	0.43
1:K:32:TRP:CZ2	1:K:37:GLU:HG2	2.54	0.43
1:M:158:GLY:O	1:M:246:MET:HG3	2.19	0.43
1:C:158:GLY:H	1:C:243:THR:CG2	2.32	0.43
2:D:501:LYS:NZ	9:D:350:HOH:O	0.58	0.43
1:E:228:THR:OG1	1:E:259:ASN:HB2	2.19	0.43
1:G:28:ILE:HG12	1:G:41:VAL:HG22	2.01	0.43
1:C:167:PHE:HE2	1:C:169:LYS:HB2	1.84	0.42
1:K:230:GLU:HG3	1:M:17:CYS:O	2.19	0.42
1:A:53:ARG:CZ	1:A:251:HIS:HB3	2.49	0.42
1:I:195:TYR:HA	1:I:211:PHE:O	2.19	0.42
1:K:54:THR:HB	1:K:149:TYR:HB3	2.01	0.42
1:A:200:GLN:N	1:A:203:HIS:O	2.52	0.42
1:A:187:LEU:O	1:A:216:ARG:HD3	2.19	0.42
1:C:222:CYS:HB2	1:C:271:CYS:SG	2.59	0.42
1:C:199:GLY:HA2	1:C:236:TYR:CE2	2.54	0.42
1:C:7:LYS:HB2	1:C:9:ASN:HD21	1.84	0.42
1:C:255:ALA:HB2	2:D:510:TRP:CE2	2.54	0.42
1:G:9:ASN:HD22	1:G:9:ASN:N	2.17	0.42
1:M:268:LYS:HE3	1:M:269:SER:H	1.84	0.42
1:E:251:HIS:CE1	1:E:252:LEU:HD13	2.55	0.42
1:K:150:LEU:HD23	1:K:251:HIS:CE1	2.55	0.42
5:W:1:NAG:H62	5:W:2:NAG:N2	2.35	0.42
1:C:272:ASN:N	1:C:272:ASN:HD22	2.13	0.42
1:I:123:LEU:CD2	1:I:170:CYS:HB3	2.45	0.42
1:K:251:HIS:CD2	9:K:823:HOH:O	2.70	0.42
1:A:127:THR:HG23	1:A:166:HIS:CE1	2.55	0.42
1:G:252:LEU:HA	1:G:252:LEU:HD12	1.90	0.42
1:O:222:CYS:O	1:O:265:CYS:HA	2.20	0.42
1:E:121:GLN:NE2	1:E:153:CYS:HB3	2.35	0.41
1:I:67:THR:HG21	1:I:84:ALA:HB1	2.01	0.41
1:A:94:GLU:HB3	1:A:174:THR:HG23	2.01	0.41
2:B:505:PHE:O	2:B:506:DSN:C	2.68	0.41
1:I:161:ASN:ND2	1:I:163:ASP:H	2.18	0.41
1:K:128:HIS:CD2	1:K:141:ASP:OD1	2.73	0.41
1:K:5:GLN:O	1:K:12:CYS:HA	2.19	0.41
1:O:252:LEU:HD12	1:O:252:LEU:HA	1.90	0.41
1:A:249:HIS:HB2	1:A:252:LEU:CD2	2.50	0.41
1:G:139:LYS:HD3	9:G:899:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:207:SER:O	1:K:208:GLU:HB3	2.20	0.41
1:E:126:VAL:HG13	1:E:167:PHE:HB3	2.03	0.41
1:G:145:ARG:HB3	1:G:177:ASN:ND2	2.36	0.41
1:M:116:ARG:HD3	9:M:863:HOH:O	2.21	0.41
1:E:172:ASN:OD1	4:U:1:NAG:O5	2.39	0.41
1:G:60:GLY:C	1:G:62:LYS:H	2.22	0.41
1:I:198:LYS:HG2	1:I:236:TYR:HE1	1.85	0.41
1:M:258:MET:HG3	1:M:261:ILE:HD12	2.03	0.41
1:O:185:GLU:HG2	1:O:186:ASN:N	2.36	0.41
1:O:230:GLU:HA	1:O:231:PRO:C	2.41	0.41
1:O:34:GLU:HB3	1:O:35:GLY:H	1.68	0.41
1:O:75:LEU:C	1:O:77:ASN:N	2.73	0.41
1:E:100:SER:O	1:E:101:SER:C	2.59	0.41
1:K:123:LEU:CD2	1:K:170:CYS:HB3	2.50	0.41
1:K:199:GLY:HA2	1:K:236:TYR:CE2	2.55	0.41
1:M:128:HIS:HD2	1:M:141:ASP:OD1	2.03	0.41
1:M:204:GLY:O	1:M:209:GLU:HB3	2.21	0.41
4:Y:1:NAG:H82	4:Y:1:NAG:H2	1.91	0.41
1:I:249:HIS:HB2	1:I:252:LEU:HD22	2.03	0.41
2:P:513:LYS:NZ	9:P:260:HOH:O	2.53	0.41
1:A:142:ARG:NH2	1:A:144:LEU:HD22	2.35	0.41
1:I:247:CYS:SG	1:I:265:CYS:N	2.94	0.41
1:M:53:ARG:NH2	8:M:811:SO4:O3	2.54	0.41
1:O:197:CYS:CB	1:O:210:THR:HG22	2.51	0.41
1:O:160:HIS:HE1	1:O:215:CYS:HA	1.85	0.41
1:A:47:HIS:CD2	1:A:47:HIS:H	2.39	0.41
1:C:200:GLN:H	1:C:200:GLN:CD	2.24	0.41
2:D:501:LYS:HB2	1:E:13:ARG:HH21	1.86	0.41
1:E:171:CYS:SG	1:E:172:ASN:N	2.90	0.41
1:E:60:GLY:O	1:M:61:LEU:CA	2.68	0.41
1:I:208:GLU:OE1	1:I:209:GLU:HB2	2.21	0.41
1:K:250:ALA:N	8:K:810:SO4:O1	2.54	0.41
1:A:5:GLN:OE1	1:A:13:ARG:HD2	2.21	0.40
1:I:43:LYS:O	1:I:44:SER:HB3	2.20	0.40
1:M:268:LYS:O	1:M:271:CYS:SG	2.79	0.40
1:I:100:SER:O	1:I:101:SER:C	2.59	0.40
1:I:243:THR:O	1:I:246:MET:HB2	2.21	0.40
1:I:239:ARG:CD	1:I:272:ASN:HB3	2.44	0.40
1:E:142:ARG:NH2	1:E:144:LEU:HG	2.35	0.40
1:E:53:ARG:HH11	1:E:251:HIS:HB3	1.86	0.40
1:G:182:LEU:HA	1:G:182:LEU:HD13	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:206:SER:O	1:G:207:SER:C	2.59	0.40
1:I:182:LEU:HD21	1:I:187:LEU:HD21	2.03	0.40
1:G:182:LEU:CD1	1:G:187:LEU:HD21	2.52	0.40
1:I:29:VAL:HB	1:I:66:LEU:CD1	2.50	0.40
1:K:32:TRP:CH2	1:K:37:GLU:HG2	2.56	0.40
1:K:95:CYS:O	1:K:113:LEU:N	2.51	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	262/313 (84%)	231 (88%)	16 (6%)	15 (6%)	1 2
1	C	253/313 (81%)	226 (89%)	16 (6%)	11 (4%)	2 5
1	E	256/313 (82%)	229 (90%)	22 (9%)	5 (2%)	7 19
1	G	252/313 (80%)	233 (92%)	16 (6%)	3 (1%)	13 32
1	I	258/313 (82%)	228 (88%)	23 (9%)	7 (3%)	5 12
1	K	251/313 (80%)	227 (90%)	20 (8%)	4 (2%)	9 24
1	M	257/313 (82%)	230 (90%)	15 (6%)	12 (5%)	2 4
1	O	252/313 (80%)	223 (88%)	20 (8%)	9 (4%)	3 7
2	B	8/13 (62%)	7 (88%)	1 (12%)	0	100 100
2	D	8/13 (62%)	7 (88%)	1 (12%)	0	100 100
2	F	8/13 (62%)	7 (88%)	1 (12%)	0	100 100
2	H	8/13 (62%)	7 (88%)	1 (12%)	0	100 100
2	J	8/13 (62%)	7 (88%)	0	1 (12%)	0 0
2	L	8/13 (62%)	7 (88%)	0	1 (12%)	0 0
2	N	8/13 (62%)	7 (88%)	1 (12%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	P	8/13 (62%)	8 (100%)	0	0	100 100
All	All	2105/2608 (81%)	1884 (90%)	153 (7%)	68 (3%)	4 9

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	PRO
1	A	231	PRO
1	A	276	LEU
1	C	208	GLU
1	C	273	HIS
1	E	111	GLN
1	E	259	ASN
1	I	33	GLU
1	I	101	SER
1	M	101	SER
1	O	203	HIS
1	O	206	SER
1	O	208	GLU
1	O	232	LYS
1	A	61	LEU
1	A	177	ASN
1	C	109	ARG
1	C	207	SER
1	G	275	ASP
1	I	84	ALA
1	I	208	GLU
1	K	275	ASP
1	M	91	ARG
1	M	207	SER
1	M	276	LEU
1	O	109	ARG
1	A	234	GLN
1	A	235	SER
1	A	278	VAL
1	E	61	LEU
1	K	206	SER
1	M	60	GLY
1	M	105	CYS
1	M	106	GLU
1	M	208	GLU
1	M	274	PRO

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Mol	Chain	Res	Type
1	A	90	SER
1	A	107	ARG
1	A	273	HIS
1	C	61	LEU
1	C	231	PRO
1	G	207	SER
1	I	60	GLY
1	I	117	SER
1	K	231	PRO
1	M	109	ARG
1	O	204	GLY
1	A	75	LEU
1	C	34	GLU
1	C	60	GLY
1	C	79	GLY
1	C	101	SER
1	C	107	ARG
1	I	35	GLY
1	O	106	GLU
1	A	76	CYS
1	A	233	ASN
1	E	260	HIS
2	J	502	SER
2	L	502	SER
1	M	111	GLN
1	M	206	SER
1	O	60	GLY
1	O	274	PRO
1	E	60	GLY
1	G	108	GLY
1	K	60	GLY
1	A	60	GLY

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	234/273 (86%)	208 (89%)	26 (11%)	6 14
1	C	229/273 (84%)	192 (84%)	37 (16%)	2 6
1	E	232/273 (85%)	200 (86%)	32 (14%)	3 8
1	G	229/273 (84%)	188 (82%)	41 (18%)	2 4
1	I	230/273 (84%)	183 (80%)	47 (20%)	1 3
1	K	228/273 (84%)	194 (85%)	34 (15%)	3 7
1	M	234/273 (86%)	196 (84%)	38 (16%)	2 6
1	O	228/273 (84%)	198 (87%)	30 (13%)	4 9
2	B	10/10 (100%)	8 (80%)	2 (20%)	1 3
2	D	10/10 (100%)	10 (100%)	0	100 100
2	F	10/10 (100%)	10 (100%)	0	100 100
2	H	10/10 (100%)	8 (80%)	2 (20%)	1 3
2	J	10/10 (100%)	9 (90%)	1 (10%)	7 18
2	L	10/10 (100%)	8 (80%)	2 (20%)	1 3
2	N	10/10 (100%)	10 (100%)	0	100 100
2	P	10/10 (100%)	10 (100%)	0	100 100
All	All	1924/2264 (85%)	1632 (85%)	292 (15%)	3 7

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	9	ASN
1	A	25	ARG
1	A	26	THR
1	A	31	LEU
1	A	33	GLU
1	A	40	LEU
1	A	54	THR
1	A	55	LEU
1	A	77	ASN
1	A	78	GLN
1	A	125	VAL
1	A	126	VAL
1	A	140	ASP
1	A	141	ASP
1	A	164	THR

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Mol	Chain	Res	Type
1	A	176	CYS
1	A	177	ASN
1	A	185	GLU
1	A	203	HIS
1	A	226	THR
1	A	234	GLN
1	A	252	LEU
1	A	260	HIS
1	A	266	CYS
1	A	267	THR
2	B	502	SER
2	B	512	SER
1	C	1	LEU
1	C	8	THR
1	C	9	ASN
1	C	13	ARG
1	C	19	LEU
1	C	25	ARG
1	C	31	LEU
1	C	38	LEU
1	C	40	LEU
1	C	53	ARG
1	C	55	LEU
1	C	58	ARG
1	C	59	THR
1	C	65	SER
1	C	66	LEU
1	C	70	VAL
1	C	73	LEU
1	C	77	ASN
1	C	105	CYS
1	C	109	ARG
1	C	125	VAL
1	C	126	VAL
1	C	140	ASP
1	C	141	ASP
1	C	185	GLU
1	C	192	ARG
1	C	200	GLN
1	C	202	THR
1	C	207	SER
1	C	209	GLU

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Mol	Chain	Res	Type
1	C	219	MET
1	C	232	LYS
1	C	238	VAL
1	C	252	LEU
1	C	263	VAL
1	C	268	LYS
1	C	272	ASN
1	E	1	LEU
1	E	9	ASN
1	E	19	LEU
1	E	21	GLN
1	E	22	ASP
1	E	25	ARG
1	E	31	LEU
1	E	38	LEU
1	E	40	LEU
1	E	53	ARG
1	E	54	THR
1	E	55	LEU
1	E	58	ARG
1	E	59	THR
1	E	93	LEU
1	E	106	GLU
1	E	111	GLN
1	E	112	SER
1	E	125	VAL
1	E	126	VAL
1	E	163	ASP
1	E	164	THR
1	E	171	CYS
1	E	182	LEU
1	E	183	GLU
1	E	184	LEU
1	E	209	GLU
1	E	229	HIS
1	E	233	ASN
1	E	238	VAL
1	E	252	LEU
1	E	276	LEU
1	G	1	LEU
1	G	2	ARG
1	G	8	THR

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Mol	Chain	Res	Type
1	G	9	ASN
1	G	19	LEU
1	G	25	ARG
1	G	29	VAL
1	G	31	LEU
1	G	38	LEU
1	G	40	LEU
1	G	53	ARG
1	G	55	LEU
1	G	59	THR
1	G	65	SER
1	G	67	THR
1	G	77	ASN
1	G	93	LEU
1	G	107	ARG
1	G	116	ARG
1	G	125	VAL
1	G	126	VAL
1	G	130	ILE
1	G	131	GLN
1	G	140	ASP
1	G	164	THR
1	G	169	LYS
1	G	170	CYS
1	G	182	LEU
1	G	193	GLN
1	G	200	GLN
1	G	202	THR
1	G	203	HIS
1	G	205	CYS
1	G	210	THR
1	G	212	LEU
1	G	226	THR
1	G	234	GLN
1	G	238	VAL
1	G	252	LEU
1	G	272	ASN
1	G	276	LEU
2	H	502	SER
2	H	512	SER
1	I	1	LEU
1	I	8	THR

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Mol	Chain	Res	Type
1	I	19	LEU
1	I	21	GLN
1	I	29	VAL
1	I	34	GLU
1	I	38	LEU
1	I	49	GLU
1	I	53	ARG
1	I	54	THR
1	I	55	LEU
1	I	58	ARG
1	I	59	THR
1	I	69	VAL
1	I	70	VAL
1	I	73	LEU
1	I	77	ASN
1	I	107	ARG
1	I	111	GLN
1	I	114	GLN
1	I	116	ARG
1	I	117	SER
1	I	123	LEU
1	I	125	VAL
1	I	126	VAL
1	I	131	GLN
1	I	144	LEU
1	I	150	LEU
1	I	161	ASN
1	I	175	LYS
1	I	182	LEU
1	I	190	ASN
1	I	193	GLN
1	I	202	THR
1	I	203	HIS
1	I	206	SER
1	I	207	SER
1	I	210	THR
1	I	216	ARG
1	I	224	VAL
1	I	243	THR
1	I	252	LEU
1	I	257	SER
1	I	261	ILE

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Mol	Chain	Res	Type
1	I	263	VAL
1	I	267	THR
1	I	268	LYS
2	J	513	LYS
1	K	1	LEU
1	K	8	THR
1	K	9	ASN
1	K	19	LEU
1	K	25	ARG
1	K	31	LEU
1	K	36	GLU
1	K	40	LEU
1	K	54	THR
1	K	55	LEU
1	K	58	ARG
1	K	63	ILE
1	K	66	LEU
1	K	70	VAL
1	K	106	GLU
1	K	113	LEU
1	K	116	ARG
1	K	123	LEU
1	K	125	VAL
1	K	126	VAL
1	K	163	ASP
1	K	169	LYS
1	K	176	CYS
1	K	182	LEU
1	K	187	LEU
1	K	189	GLN
1	K	193	GLN
1	K	206	SER
1	K	212	LEU
1	K	235	SER
1	K	239	ARG
1	K	243	THR
1	K	258	MET
1	K	268	LYS
2	L	502	SER
2	L	503	ASP
1	M	9	ASN
1	M	13	ARG

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Mol	Chain	Res	Type
1	M	25	ARG
1	M	29	VAL
1	M	37	GLU
1	M	38	LEU
1	M	40	LEU
1	M	53	ARG
1	M	55	LEU
1	M	59	THR
1	M	69	VAL
1	M	70	VAL
1	M	91	ARG
1	M	102	ASP
1	M	103	MET
1	M	114	GLN
1	M	123	LEU
1	M	125	VAL
1	M	126	VAL
1	M	150	LEU
1	M	169	LYS
1	M	170	CYS
1	M	184	LEU
1	M	185	GLU
1	M	187	LEU
1	M	192	ARG
1	M	193	GLN
1	M	198	LYS
1	M	201	SER
1	M	213	ILE
1	M	232	LYS
1	M	234	GLN
1	M	235	SER
1	M	252	LEU
1	M	261	ILE
1	M	263	VAL
1	M	268	LYS
1	M	272	ASN
1	O	1	LEU
1	O	13	ARG
1	O	15	GLU
1	O	31	LEU
1	O	36	GLU
1	O	40	LEU

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Mol	Chain	Res	Type
1	O	56	SER
1	O	63	ILE
1	O	67	THR
1	O	70	VAL
1	O	77	ASN
1	O	102	ASP
1	O	104	SER
1	O	114	GLN
1	O	116	ARG
1	O	125	VAL
1	O	126	VAL
1	O	176	CYS
1	O	182	LEU
1	O	185	GLU
1	O	187	LEU
1	O	192	ARG
1	O	206	SER
1	O	208	GLU
1	O	216	ARG
1	O	230	GLU
1	O	234	GLN
1	O	252	LEU
1	O	261	ILE
1	O	271	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	47	HIS
1	A	78	GLN
1	A	111	GLN
1	A	143	HIS
1	A	157	ASN
1	A	160	HIS
1	A	203	HIS
1	A	272	ASN
1	C	9	ASN
1	C	78	GLN
1	C	111	GLN
1	C	121	GLN
1	C	157	ASN

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Mol	Chain	Res	Type
1	C	186	ASN
1	C	193	GLN
1	C	200	GLN
1	C	260	HIS
1	C	272	ASN
1	E	121	GLN
1	E	128	HIS
1	E	157	ASN
1	E	233	ASN
1	E	249	HIS
1	E	251	HIS
1	E	259	ASN
1	G	9	ASN
1	G	21	GLN
1	G	77	ASN
1	G	78	GLN
1	G	111	GLN
1	G	121	GLN
1	G	131	GLN
1	G	157	ASN
1	G	160	HIS
1	G	200	GLN
1	G	251	HIS
1	G	272	ASN
1	I	77	ASN
1	I	114	GLN
1	I	121	GLN
1	I	157	ASN
1	I	161	ASN
1	I	190	ASN
1	I	193	GLN
1	I	203	HIS
1	I	259	ASN
1	I	273	HIS
1	K	9	ASN
1	K	21	GLN
1	K	47	HIS
1	K	114	GLN
1	K	121	GLN
1	K	128	HIS
1	K	157	ASN
1	K	160	HIS

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Mol	Chain	Res	Type
1	K	186	ASN
1	K	190	ASN
1	K	193	GLN
1	K	221	GLN
1	K	251	HIS
1	M	9	ASN
1	M	21	GLN
1	M	80	ASN
1	M	121	GLN
1	M	128	HIS
1	M	131	GLN
1	M	157	ASN
1	M	259	ASN
1	M	272	ASN
1	O	21	GLN
1	O	77	ASN
1	O	121	GLN
1	O	157	ASN
1	O	160	HIS
1	O	189	GLN
1	O	190	ASN
1	O	203	HIS
1	O	272	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ALC	D	504	2	9,11,12	0.58	0	10,13,15	1.60	2 (20%)
2	ALC	N	504	2	9,11,12	0.51	0	10,13,15	2.09	4 (40%)
2	ALC	P	504	2	9,11,12	0.58	0	10,13,15	1.05	1 (10%)
2	ALC	J	504	2	9,11,12	0.53	0	10,13,15	2.17	5 (50%)
2	ALC	L	504	2	9,11,12	0.61	0	10,13,15	1.13	1 (10%)
2	ALC	F	504	2	9,11,12	0.49	0	10,13,15	1.33	1 (10%)
2	ALC	H	504	2	9,11,12	0.58	0	10,13,15	1.98	3 (30%)
2	ALC	B	504	2	9,11,12	0.47	0	10,13,15	1.81	3 (30%)

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	ALC	D	504	2	-	0/5/14/16	0/1/1/1
2	ALC	N	504	2	-	0/5/14/16	0/1/1/1
2	ALC	P	504	2	-	0/5/14/16	0/1/1/1
2	ALC	J	504	2	-	0/5/14/16	0/1/1/1
2	ALC	L	504	2	-	0/5/14/16	0/1/1/1
2	ALC	F	504	2	-	2/5/14/16	0/1/1/1
2	ALC	H	504	2	-	0/5/14/16	0/1/1/1
2	ALC	B	504	2	-	4/5/14/16	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	504	ALC	CB-CG-CD1	-4.56	101.82	111.73
2	J	504	ALC	CB-CG-CD1	-3.61	103.90	111.73
2	N	504	ALC	CB-CG-CD1	-3.48	104.18	111.73
2	J	504	ALC	CD1-CG-CD2	3.45	117.76	109.33
2	B	504	ALC	CG-CB-CA	3.32	118.98	114.52
2	N	504	ALC	CD1-CG-CD2	3.13	116.99	109.33
2	B	504	ALC	CB-CG-CD2	-3.04	105.13	111.73
2	D	504	ALC	CB-CG-CD1	-2.99	105.24	111.73
2	N	504	ALC	CE2-CD2-CG	2.91	117.66	112.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	504	ALC	CB-CA-N	-2.72	104.27	110.32
2	J	504	ALC	CE1-CD1-CG	2.70	117.26	112.15
2	N	504	ALC	CE1-CD1-CG	2.63	117.13	112.15
2	D	504	ALC	CE2-CD2-CG	2.60	117.07	112.15
2	F	504	ALC	CB-CA-N	-2.53	104.70	110.32
2	B	504	ALC	CB-CA-N	-2.34	105.12	110.32
2	H	504	ALC	CB-CG-CD2	-2.32	106.69	111.73
2	P	504	ALC	CB-CG-CD1	-2.13	107.11	111.73
2	J	504	ALC	CZ-CE2-CD2	-2.09	107.16	111.42
2	H	504	ALC	CB-CA-N	-2.08	105.69	110.32
2	J	504	ALC	CB-CG-CD2	-2.02	107.34	111.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	504	ALC	O-C-CA-CB
2	F	504	ALC	C-CA-CB-CG
2	B	504	ALC	CA-CB-CG-CD2
2	B	504	ALC	CA-CB-CG-CD1
2	B	504	ALC	C-CA-CB-CG
2	B	504	ALC	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	504	ALC	1	0
2	L	504	ALC	1	0
2	B	504	ALC	2	0

5.5 Carbohydrates (i)

52 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	$\#\|Z\|>2$
3	NAG	Q	1	1,3	14,14,15	0.57	0	17,19,21	1.36	3 (17%)
3	NAG	Q	2	3	14,14,15	0.61	0	17,19,21	1.74	3 (17%)
3	FUC	Q	3	3	10,10,11	0.66	0	14,14,16	1.16	1 (7%)
4	NAG	R	1	1,4	14,14,15	0.54	0	17,19,21	1.57	2 (11%)
4	FUC	R	2	4	10,10,11	0.58	0	14,14,16	0.79	0
3	NAG	S	1	1,3	14,14,15	0.52	0	17,19,21	2.41	4 (23%)
3	NAG	S	2	3	14,14,15	0.67	0	17,19,21	1.51	3 (17%)
3	FUC	S	3	3	10,10,11	0.63	0	14,14,16	0.99	0
3	NAG	T	1	1,3	14,14,15	0.58	0	17,19,21	1.71	4 (23%)
3	NAG	T	2	3	14,14,15	0.55	0	17,19,21	1.41	1 (5%)
3	FUC	T	3	3	10,10,11	0.71	0	14,14,16	1.52	2 (14%)
4	NAG	U	1	1,4	14,14,15	0.57	0	17,19,21	1.93	4 (23%)
4	FUC	U	2	4	10,10,11	0.88	0	14,14,16	1.94	4 (28%)
4	NAG	V	1	1,4	14,14,15	0.53	0	17,19,21	1.81	3 (17%)
4	FUC	V	2	4	10,10,11	0.57	0	14,14,16	1.17	1 (7%)
5	NAG	W	1	1,5	14,14,15	0.66	0	17,19,21	1.04	1 (5%)
5	NAG	W	2	5	14,14,15	0.58	0	17,19,21	1.27	2 (11%)
4	NAG	X	1	1,4	14,14,15	0.56	0	17,19,21	1.57	2 (11%)
4	FUC	X	2	4	10,10,11	0.67	0	14,14,16	1.51	2 (14%)
4	NAG	Y	1	1,4	14,14,15	0.43	0	17,19,21	1.61	2 (11%)
4	FUC	Y	2	4	10,10,11	0.76	0	14,14,16	1.77	2 (14%)
6	NAG	Z	1	1,6	14,14,15	0.46	0	17,19,21	1.08	1 (5%)
6	NAG	Z	2	6	14,14,15	0.61	0	17,19,21	1.10	0
6	BMA	Z	3	6	11,11,12	0.49	0	15,15,17	2.99	6 (40%)
6	MAN	Z	4	6	11,11,12	0.64	0	15,15,17	2.21	4 (26%)
6	MAN	Z	5	6	11,11,12	0.74	0	15,15,17	1.26	2 (13%)
4	NAG	a	1	1,4	14,14,15	0.47	0	17,19,21	1.68	1 (5%)
4	FUC	a	2	4	10,10,11	0.60	0	14,14,16	1.14	1 (7%)
3	NAG	b	1	1,3	14,14,15	0.61	0	17,19,21	1.62	4 (23%)
3	NAG	b	2	3	14,14,15	0.62	0	17,19,21	2.50	3 (17%)
3	FUC	b	3	3	10,10,11	0.62	0	14,14,16	0.91	0
6	NAG	c	1	1,6	14,14,15	0.65	0	17,19,21	1.70	4 (23%)
6	NAG	c	2	6	14,14,15	0.69	0	17,19,21	1.30	2 (11%)
6	BMA	c	3	6	11,11,12	0.94	1 (9%)	15,15,17	1.87	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MAN	c	4	6	11,11,12	0.74	0	15,15,17	2.14	4 (26%)
6	MAN	c	5	6	11,11,12	0.70	0	15,15,17	1.40	3 (20%)
4	NAG	d	1	1,4	14,14,15	0.41	0	17,19,21	1.90	6 (35%)
4	FUC	d	2	4	10,10,11	0.68	0	14,14,16	1.00	1 (7%)
6	NAG	e	1	1,6	14,14,15	0.61	0	17,19,21	1.63	1 (5%)
6	NAG	e	2	6	14,14,15	0.61	0	17,19,21	1.15	1 (5%)
6	BMA	e	3	6	11,11,12	0.58	0	15,15,17	1.95	3 (20%)
6	MAN	e	4	6	11,11,12	0.78	0	15,15,17	2.88	6 (40%)
6	MAN	e	5	6	11,11,12	0.65	0	15,15,17	1.38	2 (13%)
5	NAG	f	1	1,5	14,14,15	0.66	0	17,19,21	1.29	1 (5%)
5	NAG	f	2	5	14,14,15	0.53	0	17,19,21	1.72	3 (17%)
4	NAG	g	1	1,4	14,14,15	0.53	0	17,19,21	1.33	3 (17%)
4	FUC	g	2	4	10,10,11	0.69	0	14,14,16	1.42	3 (21%)
6	NAG	h	1	1,6	14,14,15	0.66	0	17,19,21	1.78	4 (23%)
6	NAG	h	2	6	14,14,15	0.54	0	17,19,21	0.86	0
6	BMA	h	3	6	11,11,12	0.95	1 (9%)	15,15,17	1.69	3 (20%)
6	MAN	h	4	6	11,11,12	0.77	0	15,15,17	1.73	3 (20%)
6	MAN	h	5	6	11,11,12	0.64	0	15,15,17	1.97	2 (13%)

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
3	NAG	Q	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	6/6/23/26	0/1/1/1
3	FUC	Q	3	3	2/2/4/5	-	0/1/1/1
4	NAG	R	1	1,4	-	4/6/23/26	0/1/1/1
4	FUC	R	2	4	2/2/4/5	-	0/1/1/1
3	NAG	S	1	1,3	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	S	2	3	-	3/6/23/26	0/1/1/1
3	FUC	S	3	3	2/2/4/5	-	0/1/1/1
3	NAG	T	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	T	2	3	-	4/6/23/26	0/1/1/1
3	FUC	T	3	3	2/2/4/5	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	U	1	1,4	-	4/6/23/26	0/1/1/1
4	FUC	U	2	4	2/2/4/5	-	0/1/1/1
4	NAG	V	1	1,4	-	2/6/23/26	0/1/1/1
4	FUC	V	2	4	2/2/4/5	-	0/1/1/1
5	NAG	W	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	W	2	5	-	3/6/23/26	0/1/1/1
4	NAG	X	1	1,4	1/1/5/7	4/6/23/26	0/1/1/1
4	FUC	X	2	4	2/2/4/5	-	0/1/1/1
4	NAG	Y	1	1,4	-	4/6/23/26	0/1/1/1
4	FUC	Y	2	4	2/2/4/5	-	0/1/1/1
6	NAG	Z	1	1,6	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	4/6/23/26	0/1/1/1
6	BMA	Z	3	6	-	2/2/19/22	0/1/1/1
6	MAN	Z	4	6	-	2/2/19/22	0/1/1/1
6	MAN	Z	5	6	-	2/2/19/22	1/1/1/1
4	NAG	a	1	1,4	-	5/6/23/26	0/1/1/1
4	FUC	a	2	4	2/2/4/5	-	0/1/1/1
3	NAG	b	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	b	2	3	-	4/6/23/26	0/1/1/1
3	FUC	b	3	3	2/2/4/5	-	0/1/1/1
6	NAG	c	1	1,6	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	c	2	6	-	4/6/23/26	0/1/1/1
6	BMA	c	3	6	-	0/2/19/22	0/1/1/1
6	MAN	c	4	6	-	2/2/19/22	0/1/1/1
6	MAN	c	5	6	-	0/2/19/22	0/1/1/1
4	NAG	d	1	1,4	-	4/6/23/26	0/1/1/1
4	FUC	d	2	4	2/2/4/5	-	0/1/1/1
6	NAG	e	1	1,6	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	e	2	6	-	0/6/23/26	0/1/1/1
6	BMA	e	3	6	-	0/2/19/22	0/1/1/1
6	MAN	e	4	6	-	2/2/19/22	1/1/1/1
6	MAN	e	5	6	-	1/2/19/22	0/1/1/1
5	NAG	f	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	f	2	5	-	3/6/23/26	0/1/1/1
4	NAG	g	1	1,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUC	g	2	4	2/2/4/5	-	0/1/1/1
6	NAG	h	1	1,6	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	h	2	6	-	2/6/23/26	0/1/1/1
6	BMA	h	3	6	-	2/2/19/22	0/1/1/1
6	MAN	h	4	6	-	1/2/19/22	0/1/1/1
6	MAN	h	5	6	-	2/2/19/22	1/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	h	3	BMA	O5-C1	-2.43	1.39	1.43
6	c	3	BMA	O5-C1	-2.27	1.40	1.43

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Z	3	BMA	C1-O5-C5	8.86	124.20	112.19
3	b	2	NAG	C1-O5-C5	8.50	123.71	112.19
6	e	4	MAN	C1-C2-C3	-7.69	100.22	109.67
3	S	1	NAG	C1-O5-C5	7.62	122.51	112.19
6	Z	4	MAN	C1-C2-C3	-6.59	101.56	109.67
6	c	4	MAN	C1-C2-C3	-5.90	102.42	109.67
6	e	1	NAG	C1-O5-C5	5.71	119.94	112.19
3	Q	2	NAG	C1-O5-C5	5.66	119.86	112.19
4	a	1	NAG	C1-O5-C5	5.57	119.74	112.19
6	h	5	MAN	O5-C5-C6	5.24	115.41	107.20
6	c	3	BMA	C1-C2-C3	5.05	115.87	109.67
3	T	2	NAG	C1-O5-C5	5.02	119.00	112.19
5	f	2	NAG	C1-O5-C5	5.02	119.00	112.19
4	Y	2	FUC	C1-C2-C3	4.86	115.64	109.67
3	S	1	NAG	C4-C3-C2	4.76	117.99	111.02
6	e	3	BMA	C1-C2-C3	4.65	115.39	109.67
6	e	4	MAN	O2-C2-C1	4.65	118.67	109.15
4	V	1	NAG	O5-C5-C6	4.64	114.48	107.20
4	R	1	NAG	C1-O5-C5	4.57	118.39	112.19
6	h	4	MAN	C1-C2-C3	-4.51	104.12	109.67
4	U	1	NAG	C1-O5-C5	4.49	118.28	112.19
6	h	3	BMA	C1-C2-C3	4.37	115.04	109.67
4	X	1	NAG	C1-O5-C5	4.31	118.04	112.19
4	U	2	FUC	O5-C5-C4	4.17	117.00	109.52
3	T	3	FUC	C1-C2-C3	4.03	114.62	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	h	5	MAN	C1-O5-C5	4.03	117.65	112.19
4	d	1	NAG	C1-O5-C5	3.98	117.59	112.19
4	U	2	FUC	C3-C4-C5	3.90	115.85	109.77
4	U	1	NAG	O5-C5-C6	3.83	113.21	107.20
6	e	4	MAN	C1-O5-C5	-3.82	107.02	112.19
4	Y	1	NAG	C1-O5-C5	3.80	117.34	112.19
4	V	1	NAG	C1-O5-C5	3.77	117.31	112.19
6	c	1	NAG	O5-C5-C6	3.77	113.11	107.20
4	Y	1	NAG	C4-C3-C2	-3.74	105.54	111.02
3	b	1	NAG	O4-C4-C5	3.70	118.48	109.30
3	S	2	NAG	C4-C3-C2	3.69	116.43	111.02
6	e	3	BMA	C1-O5-C5	3.65	117.14	112.19
4	U	1	NAG	C3-C4-C5	3.55	116.57	110.24
6	Z	4	MAN	O2-C2-C1	3.54	116.40	109.15
6	Z	3	BMA	C1-C2-C3	3.47	113.93	109.67
6	c	2	NAG	O5-C5-C6	3.45	112.62	107.20
3	T	1	NAG	C4-C3-C2	3.44	116.06	111.02
6	h	1	NAG	C1-O5-C5	3.41	116.81	112.19
6	Z	3	BMA	O3-C3-C2	-3.38	103.51	109.99
6	c	3	BMA	O3-C3-C2	-3.37	103.54	109.99
6	h	1	NAG	C4-C3-C2	3.36	115.94	111.02
6	e	2	NAG	C1-O5-C5	3.34	116.72	112.19
6	Z	1	NAG	C1-O5-C5	3.33	116.70	112.19
5	W	2	NAG	C2-N2-C7	3.31	127.61	122.90
6	c	1	NAG	C1-O5-C5	3.30	116.67	112.19
5	f	1	NAG	C1-O5-C5	3.29	116.65	112.19
3	T	1	NAG	O5-C1-C2	-3.28	106.10	111.29
6	e	4	MAN	O5-C5-C6	3.26	112.32	107.20
6	e	5	MAN	C1-O5-C5	3.26	116.61	112.19
6	Z	3	BMA	C3-C4-C5	3.24	116.02	110.24
4	X	2	FUC	C1-C2-C3	-3.17	105.77	109.67
6	e	3	BMA	O3-C3-C2	-3.16	103.94	109.99
6	h	1	NAG	C2-N2-C7	-3.16	118.41	122.90
4	d	1	NAG	C4-C3-C2	-3.14	106.41	111.02
6	c	4	MAN	O5-C5-C6	3.13	112.11	107.20
4	g	2	FUC	C3-C4-C5	3.09	114.58	109.77
3	S	2	NAG	C1-O5-C5	3.09	116.37	112.19
4	X	1	NAG	O5-C5-C6	3.08	112.03	107.20
4	d	1	NAG	C2-N2-C7	-3.06	118.55	122.90
5	W	2	NAG	C1-O5-C5	3.05	116.32	112.19
6	c	5	MAN	O5-C5-C6	3.03	111.95	107.20
6	h	4	MAN	C3-C4-C5	2.99	115.57	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	b	2	NAG	C3-C4-C5	2.97	115.53	110.24
6	Z	3	BMA	O5-C5-C4	2.87	117.81	110.83
5	f	2	NAG	C4-C3-C2	2.85	115.20	111.02
4	Y	2	FUC	C2-C3-C4	2.81	115.75	110.89
3	Q	2	NAG	O5-C1-C2	2.75	115.63	111.29
3	b	1	NAG	O5-C5-C6	2.74	111.51	107.20
3	b	2	NAG	O5-C5-C4	2.69	117.38	110.83
3	b	1	NAG	C1-O5-C5	2.67	115.80	112.19
4	d	2	FUC	C1-O5-C5	2.65	118.78	112.78
3	S	2	NAG	O5-C1-C2	2.65	115.47	111.29
4	X	2	FUC	O5-C1-C2	-2.64	106.69	110.77
4	d	1	NAG	O5-C5-C6	2.64	111.34	107.20
4	V	1	NAG	C6-C5-C4	-2.63	106.84	113.00
3	Q	3	FUC	C3-C4-C5	2.63	113.87	109.77
4	V	2	FUC	C1-C2-C3	-2.63	106.44	109.67
6	h	4	MAN	O5-C1-C2	-2.62	106.72	110.77
3	T	1	NAG	C1-O5-C5	2.61	115.72	112.19
6	h	3	BMA	O5-C1-C2	-2.53	106.87	110.77
4	U	2	FUC	O5-C1-C2	-2.52	106.88	110.77
6	c	3	BMA	C3-C4-C5	2.52	114.73	110.24
3	Q	1	NAG	C4-C3-C2	2.51	114.69	111.02
4	d	1	NAG	O5-C1-C2	-2.51	107.33	111.29
4	d	1	NAG	C1-C2-N2	2.50	114.75	110.49
4	g	1	NAG	O5-C1-C2	-2.48	107.37	111.29
3	S	1	NAG	O5-C1-C2	2.47	115.19	111.29
6	Z	3	BMA	O5-C1-C2	2.45	114.56	110.77
4	U	1	NAG	C4-C3-C2	2.45	114.61	111.02
6	c	4	MAN	C3-C4-C5	2.44	114.60	110.24
6	Z	5	MAN	O2-C2-C1	2.43	114.13	109.15
5	f	2	NAG	C3-C4-C5	2.43	114.57	110.24
6	c	4	MAN	O2-C2-C1	2.40	114.07	109.15
6	e	4	MAN	C2-C3-C4	-2.40	106.74	110.89
6	Z	4	MAN	O5-C5-C6	2.38	110.94	107.20
6	c	5	MAN	O3-C3-C4	-2.35	104.91	110.35
3	T	3	FUC	C2-C3-C4	2.29	114.86	110.89
4	g	1	NAG	C2-N2-C7	-2.24	119.72	122.90
3	Q	1	NAG	C1-O5-C5	2.23	115.22	112.19
6	c	5	MAN	O6-C6-C5	-2.22	103.67	111.29
6	Z	5	MAN	O5-C5-C6	2.21	110.67	107.20
6	Z	4	MAN	C3-C4-C5	2.21	114.18	110.24
5	W	1	NAG	C1-O5-C5	2.20	115.18	112.19
6	c	2	NAG	O4-C4-C3	-2.20	105.26	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	e	5	MAN	C1-C2-C3	2.17	112.33	109.67
4	g	2	FUC	O5-C5-C6	2.14	111.92	107.33
3	Q	2	NAG	C4-C3-C2	2.13	114.14	111.02
3	T	1	NAG	C8-C7-N2	2.13	119.71	116.10
4	R	1	NAG	C2-N2-C7	-2.12	119.88	122.90
6	c	1	NAG	O7-C7-C8	-2.09	118.17	122.06
6	c	1	NAG	C8-C7-N2	2.09	119.63	116.10
3	Q	1	NAG	C8-C7-N2	2.08	119.63	116.10
3	b	1	NAG	O4-C4-C3	2.08	115.16	110.35
4	g	2	FUC	C1-C2-C3	-2.07	107.12	109.67
6	h	1	NAG	C1-C2-N2	2.06	114.01	110.49
3	S	1	NAG	O5-C5-C4	2.05	115.82	110.83
4	U	2	FUC	C2-C3-C4	2.05	114.44	110.89
4	a	2	FUC	O5-C5-C6	2.05	111.73	107.33
6	h	3	BMA	O3-C3-C4	-2.03	105.65	110.35
6	e	4	MAN	O5-C5-C4	-2.02	105.91	110.83
4	g	1	NAG	C3-C4-C5	-2.01	106.65	110.24

All (30) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	g	2	FUC	C5
4	g	2	FUC	C1
6	e	1	NAG	C1
4	X	1	NAG	C1
4	d	2	FUC	C5
4	d	2	FUC	C1
6	h	1	NAG	C1
4	U	2	FUC	C5
4	U	2	FUC	C1
3	b	3	FUC	C5
3	b	3	FUC	C1
6	c	1	NAG	C1
3	T	3	FUC	C5
3	T	3	FUC	C1
4	Y	2	FUC	C5
4	Y	2	FUC	C1
3	S	1	NAG	C1
4	R	2	FUC	C5
4	R	2	FUC	C1
6	Z	1	NAG	C1
3	Q	3	FUC	C5

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Mol	Chain	Res	Type	Atom
3	Q	3	FUC	C1
3	S	3	FUC	C5
3	S	3	FUC	C1
4	a	2	FUC	C5
4	a	2	FUC	C1
4	X	2	FUC	C5
4	X	2	FUC	C1
4	V	2	FUC	C5
4	V	2	FUC	C1

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	U	1	NAG	C8-C7-N2-C2
4	U	1	NAG	O7-C7-N2-C2
4	R	1	NAG	C8-C7-N2-C2
4	R	1	NAG	O7-C7-N2-C2
3	T	1	NAG	C8-C7-N2-C2
3	T	1	NAG	O7-C7-N2-C2
6	e	1	NAG	C8-C7-N2-C2
6	e	1	NAG	O7-C7-N2-C2
5	f	1	NAG	C8-C7-N2-C2
5	f	1	NAG	O7-C7-N2-C2
4	X	1	NAG	C8-C7-N2-C2
4	X	1	NAG	O7-C7-N2-C2
5	W	1	NAG	C8-C7-N2-C2
5	W	1	NAG	O7-C7-N2-C2
5	W	2	NAG	C3-C2-N2-C7
5	W	2	NAG	C8-C7-N2-C2
5	W	2	NAG	O7-C7-N2-C2
6	h	1	NAG	C8-C7-N2-C2
6	h	1	NAG	O7-C7-N2-C2
6	c	1	NAG	C8-C7-N2-C2
4	a	1	NAG	C3-C2-N2-C7
4	a	1	NAG	C8-C7-N2-C2
4	a	1	NAG	O7-C7-N2-C2
3	b	2	NAG	C8-C7-N2-C2
3	b	2	NAG	O7-C7-N2-C2
3	T	2	NAG	C8-C7-N2-C2
3	T	2	NAG	O7-C7-N2-C2
3	S	1	NAG	C8-C7-N2-C2
3	S	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	b	1	NAG	C8-C7-N2-C2
3	b	1	NAG	O7-C7-N2-C2
3	S	2	NAG	C8-C7-N2-C2
3	S	2	NAG	O7-C7-N2-C2
3	Q	1	NAG	C8-C7-N2-C2
3	Q	1	NAG	O7-C7-N2-C2
4	g	1	NAG	C8-C7-N2-C2
4	g	1	NAG	O7-C7-N2-C2
4	Y	1	NAG	C8-C7-N2-C2
4	Y	1	NAG	O7-C7-N2-C2
3	Q	2	NAG	C8-C7-N2-C2
3	Q	2	NAG	O7-C7-N2-C2
4	a	1	NAG	C4-C5-C6-O6
6	c	1	NAG	O7-C7-N2-C2
4	R	1	NAG	O5-C5-C6-O6
6	c	2	NAG	O5-C5-C6-O6
6	e	1	NAG	C4-C5-C6-O6
6	c	1	NAG	O5-C5-C6-O6
6	e	4	MAN	O5-C5-C6-O6
6	Z	3	BMA	O5-C5-C6-O6
5	f	2	NAG	C8-C7-N2-C2
6	Z	1	NAG	C8-C7-N2-C2
4	V	1	NAG	O5-C5-C6-O6
3	b	1	NAG	O5-C5-C6-O6
4	d	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
6	c	2	NAG	C4-C5-C6-O6
6	Z	4	MAN	O5-C5-C6-O6
6	c	4	MAN	O5-C5-C6-O6
6	e	4	MAN	C4-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
6	Z	4	MAN	C4-C5-C6-O6
4	a	1	NAG	O5-C5-C6-O6
6	Z	5	MAN	O5-C5-C6-O6
6	h	1	NAG	O5-C5-C6-O6
5	f	2	NAG	O7-C7-N2-C2
4	d	1	NAG	C8-C7-N2-C2
6	Z	1	NAG	O7-C7-N2-C2
6	e	1	NAG	O5-C5-C6-O6
3	b	1	NAG	C4-C5-C6-O6
4	d	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	V	1	NAG	C4-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
6	c	1	NAG	C4-C5-C6-O6
6	Z	2	NAG	C8-C7-N2-C2
6	Z	2	NAG	O7-C7-N2-C2
4	d	1	NAG	O7-C7-N2-C2
6	c	2	NAG	C8-C7-N2-C2
6	c	2	NAG	O7-C7-N2-C2
6	h	1	NAG	C4-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
6	Z	1	NAG	O5-C5-C6-O6
6	Z	5	MAN	C4-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	b	2	NAG	O5-C5-C6-O6
6	h	5	MAN	C4-C5-C6-O6
6	h	2	NAG	O5-C5-C6-O6
6	h	3	BMA	O5-C5-C6-O6
6	h	3	BMA	C4-C5-C6-O6
6	h	5	MAN	O5-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
6	Z	3	BMA	C4-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
3	b	2	NAG	C4-C5-C6-O6
3	Q	2	NAG	C1-C2-N2-C7
3	S	2	NAG	O5-C5-C6-O6
5	f	2	NAG	O5-C5-C6-O6
6	h	4	MAN	O5-C5-C6-O6
6	c	4	MAN	C4-C5-C6-O6
6	e	5	MAN	C4-C5-C6-O6
6	Z	2	NAG	C4-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
6	Z	1	NAG	C4-C5-C6-O6
4	U	1	NAG	C3-C2-N2-C7
6	Z	2	NAG	O5-C5-C6-O6
6	h	2	NAG	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	W	1	NAG	C4-C5-C6-O6
3	Q	2	NAG	C3-C2-N2-C7

All (3) ring outliers are listed below:

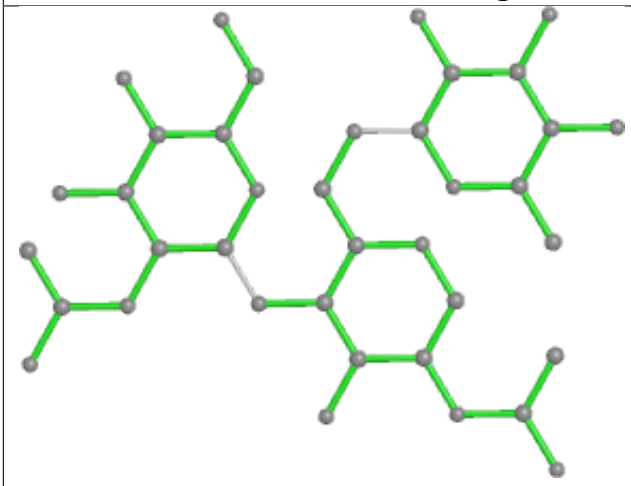
Mol	Chain	Res	Type	Atoms
6	h	5	MAN	C1-C2-C3-C4-C5-O5
6	e	4	MAN	C1-C2-C3-C4-C5-O5
6	Z	5	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 4 short contacts:

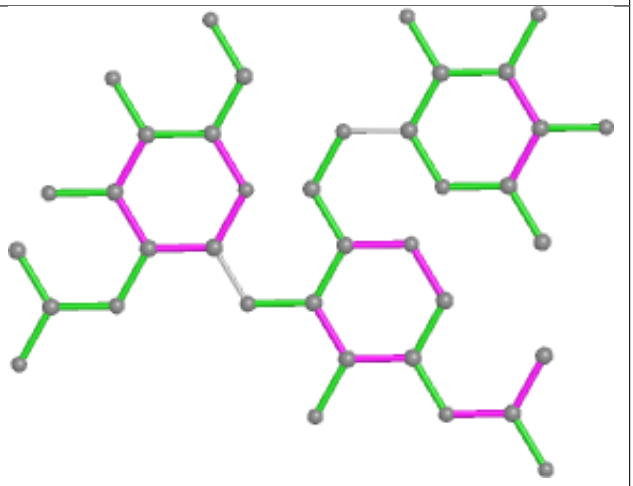
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	U	1	NAG	1	0
5	W	1	NAG	2	0
5	W	2	NAG	1	0
4	Y	1	NAG	1	0

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

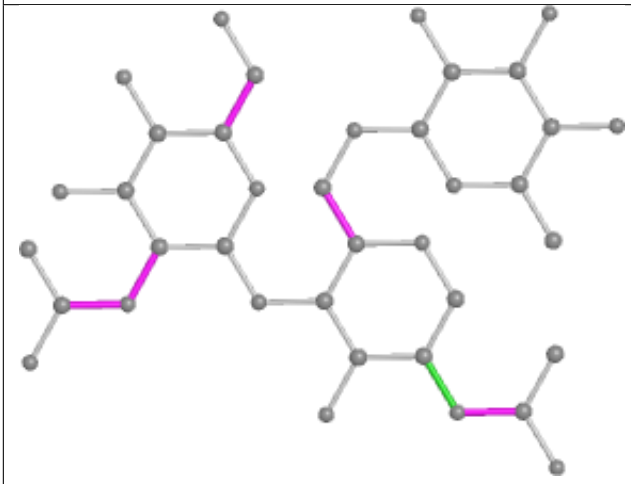
Oligosaccharide Chain Q



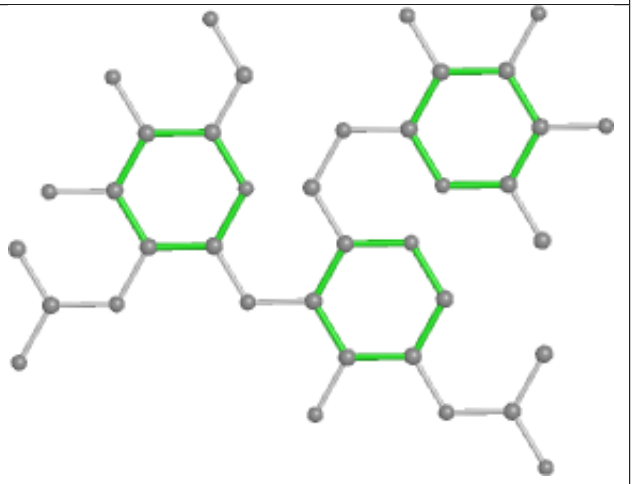
Bond lengths



Bond angles

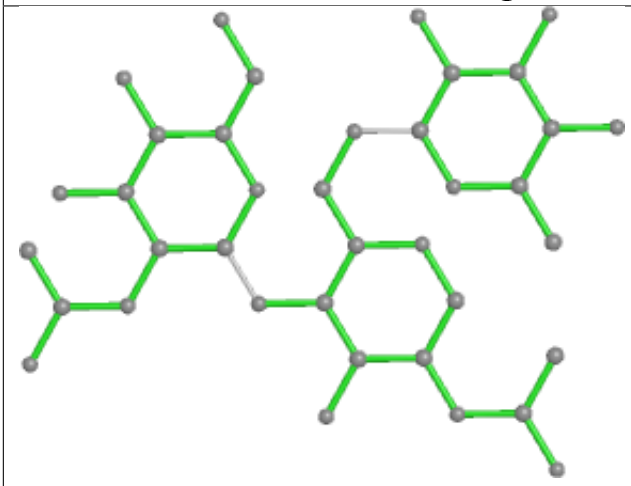


Torsions

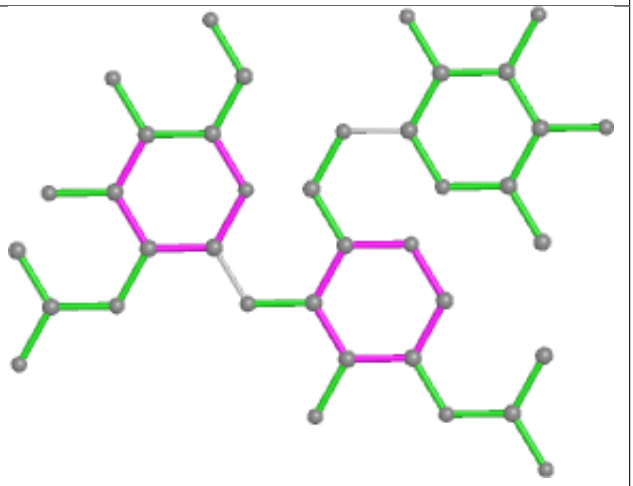


Rings

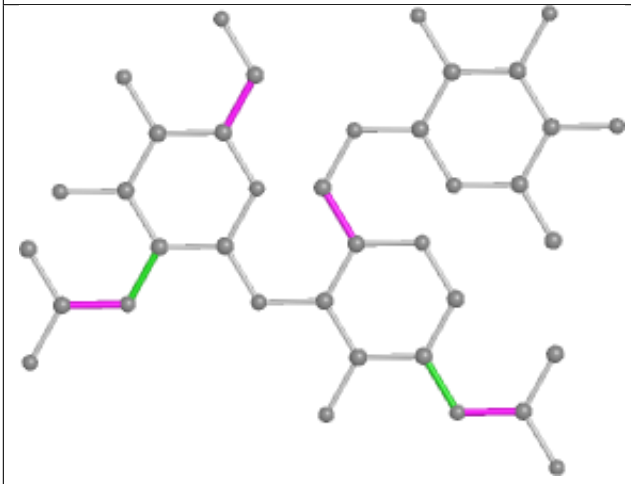
Oligosaccharide Chain S



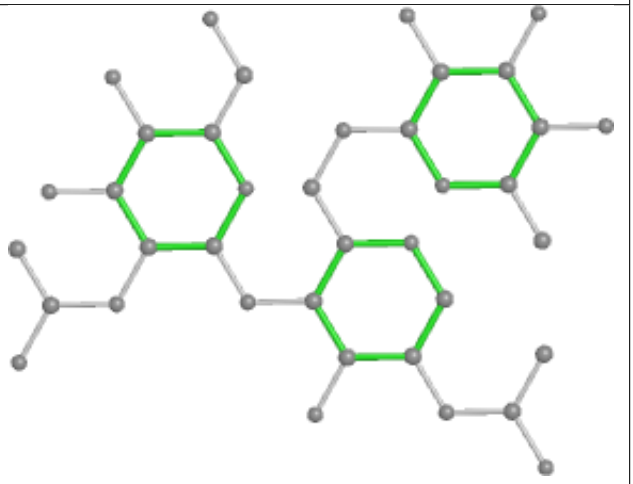
Bond lengths



Bond angles

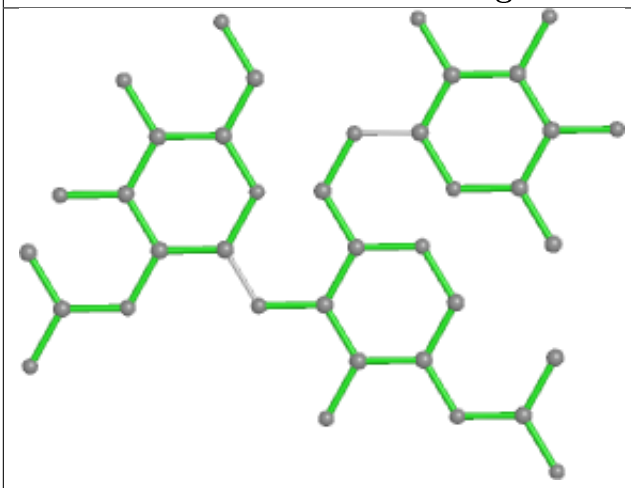


Torsions

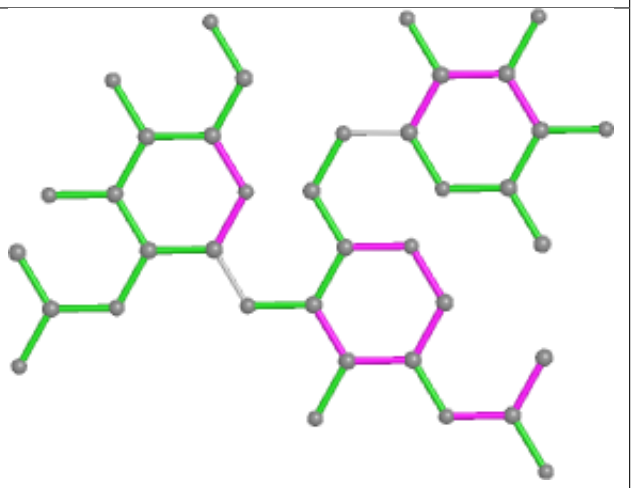


Rings

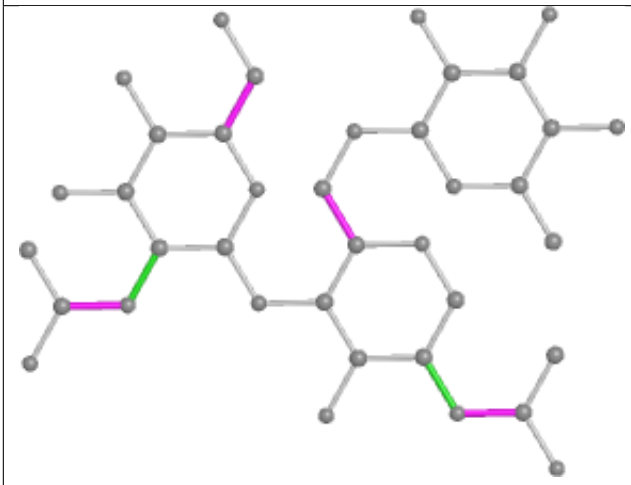
Oligosaccharide Chain T



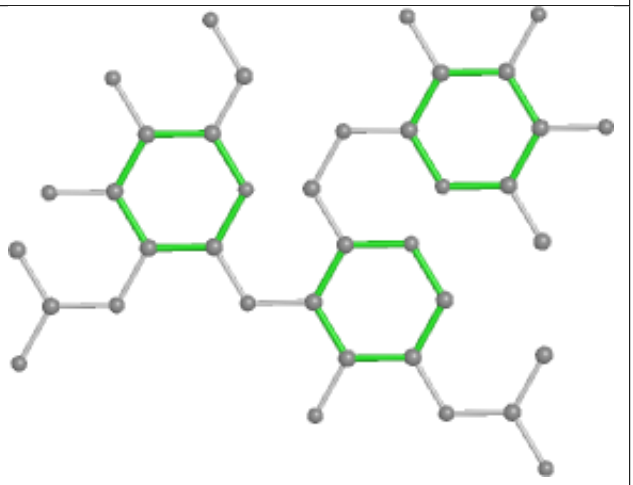
Bond lengths



Bond angles

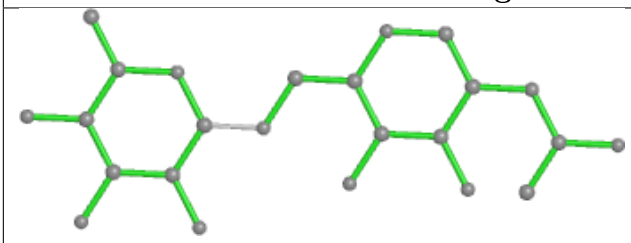


Torsions

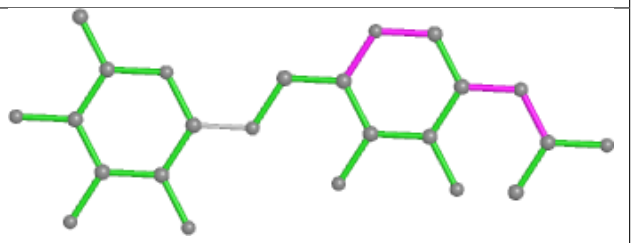


Rings

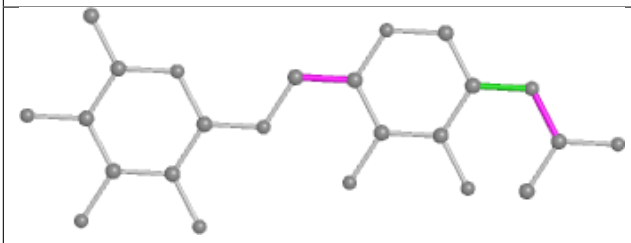
Oligosaccharide Chain R



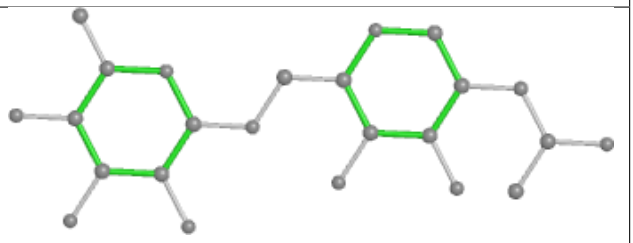
Bond lengths



Bond angles

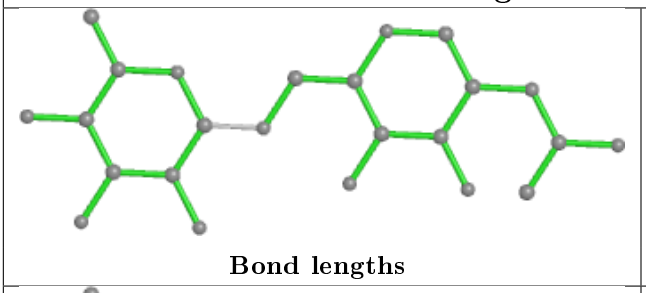


Torsions

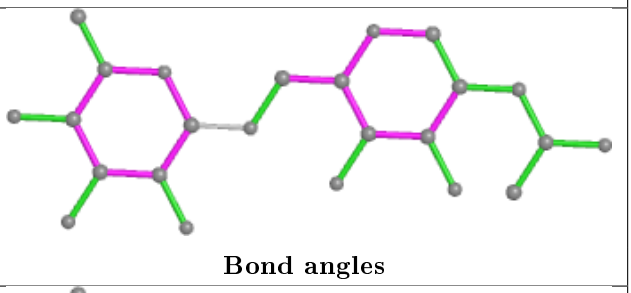


Rings

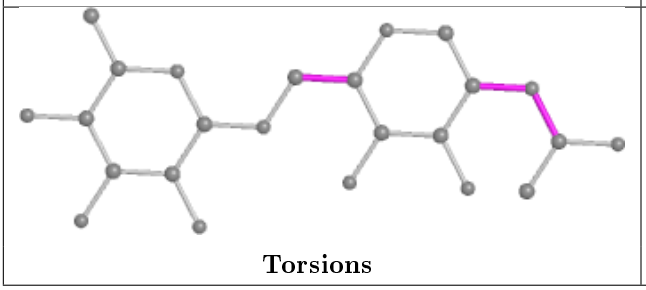
Oligosaccharide Chain U



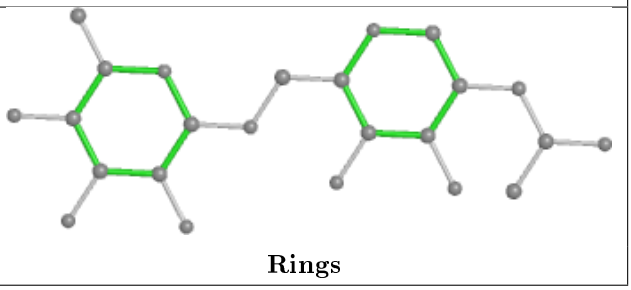
Bond lengths



Bond angles

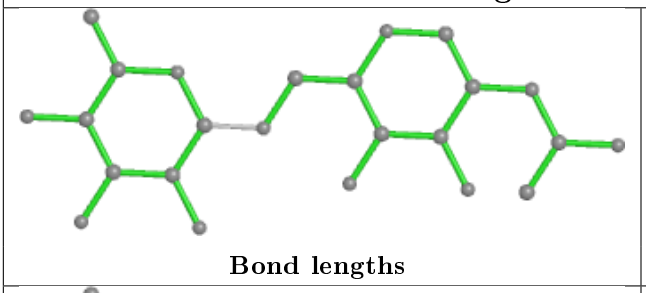


Torsions

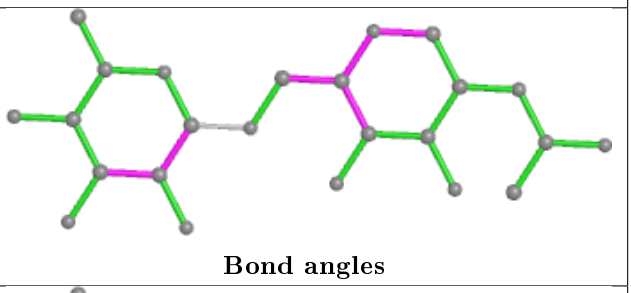


Rings

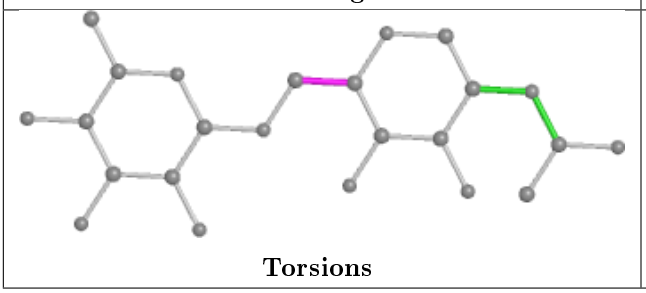
Oligosaccharide Chain V



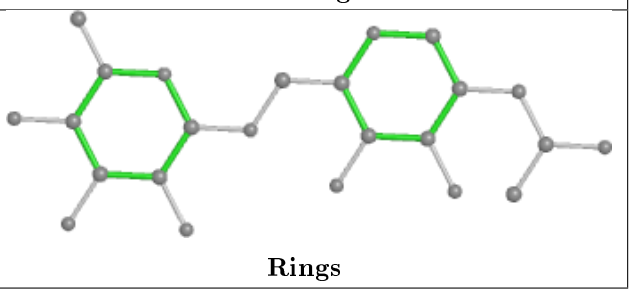
Bond lengths



Bond angles

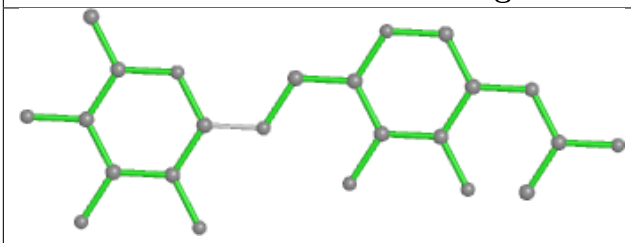


Torsions

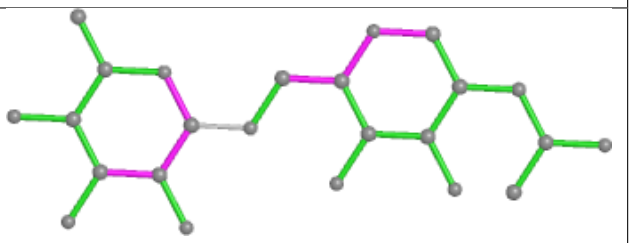


Rings

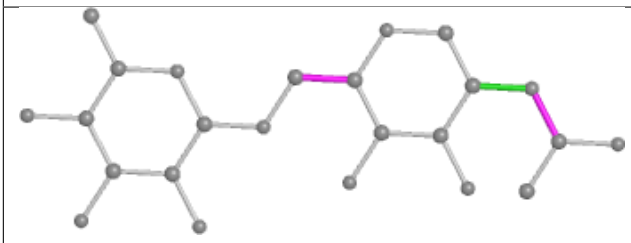
Oligosaccharide Chain X



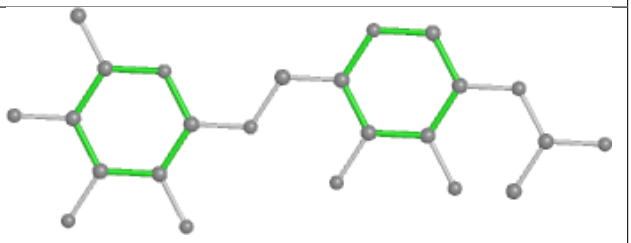
Bond lengths



Bond angles

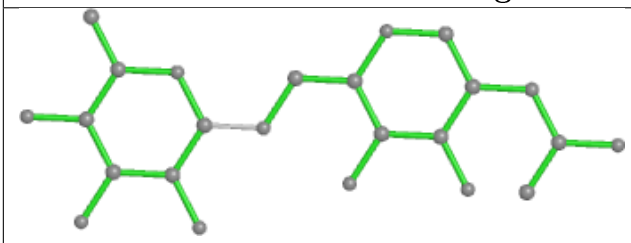


Torsions

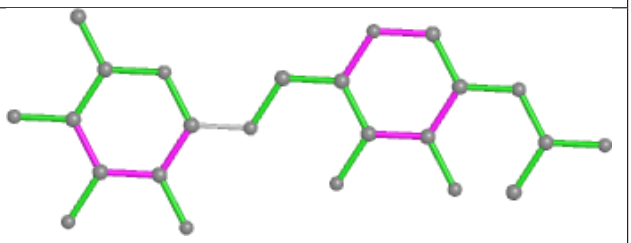


Rings

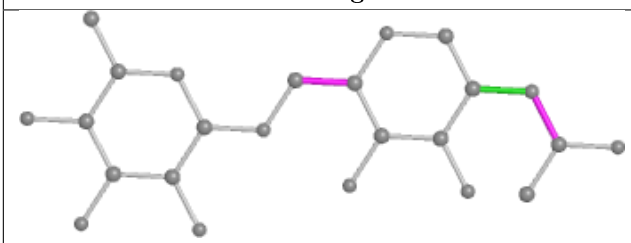
Oligosaccharide Chain Y



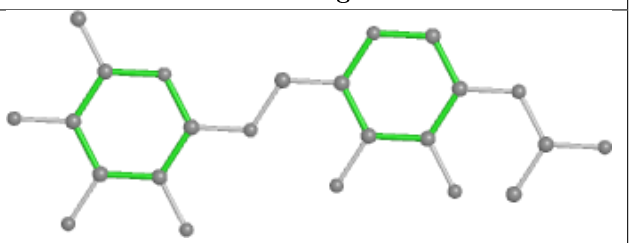
Bond lengths



Bond angles

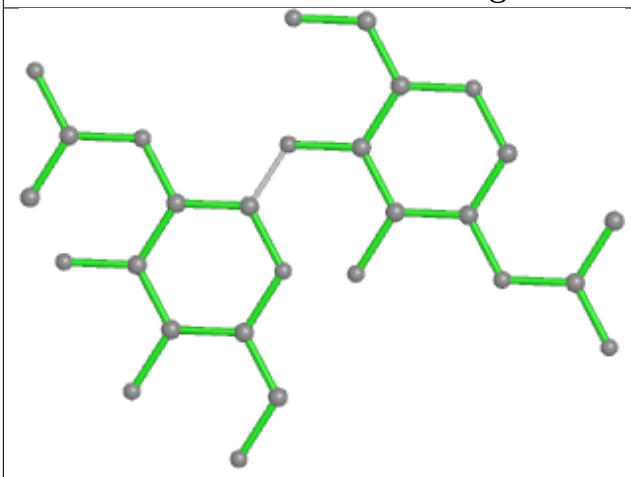


Torsions

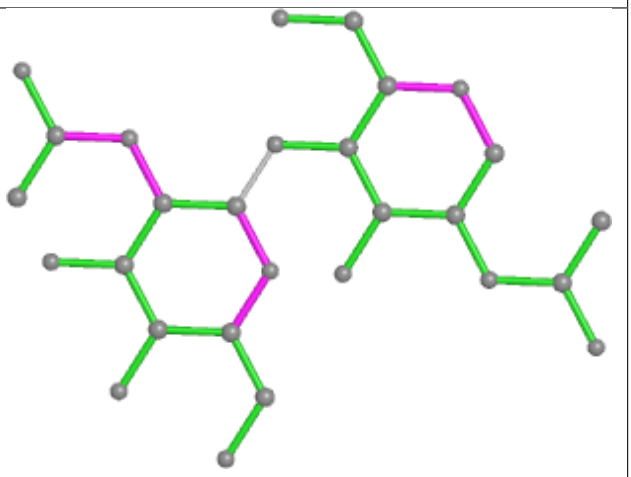


Rings

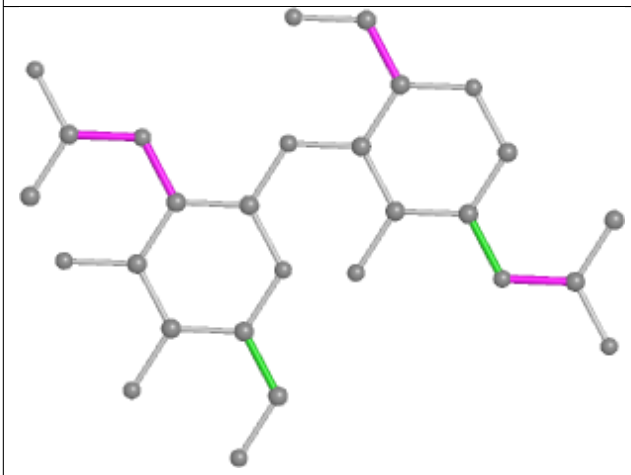
Oligosaccharide Chain W



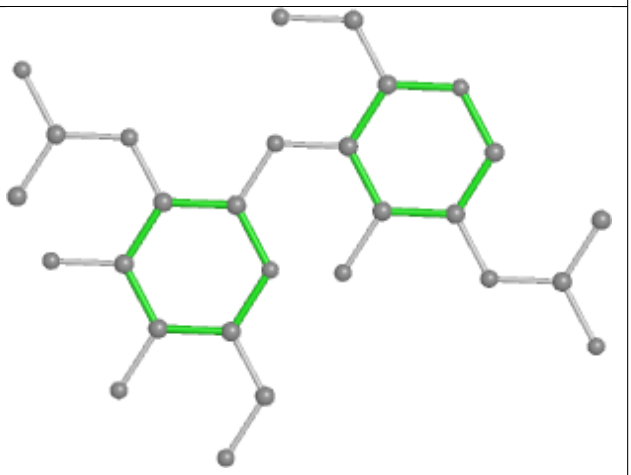
Bond lengths



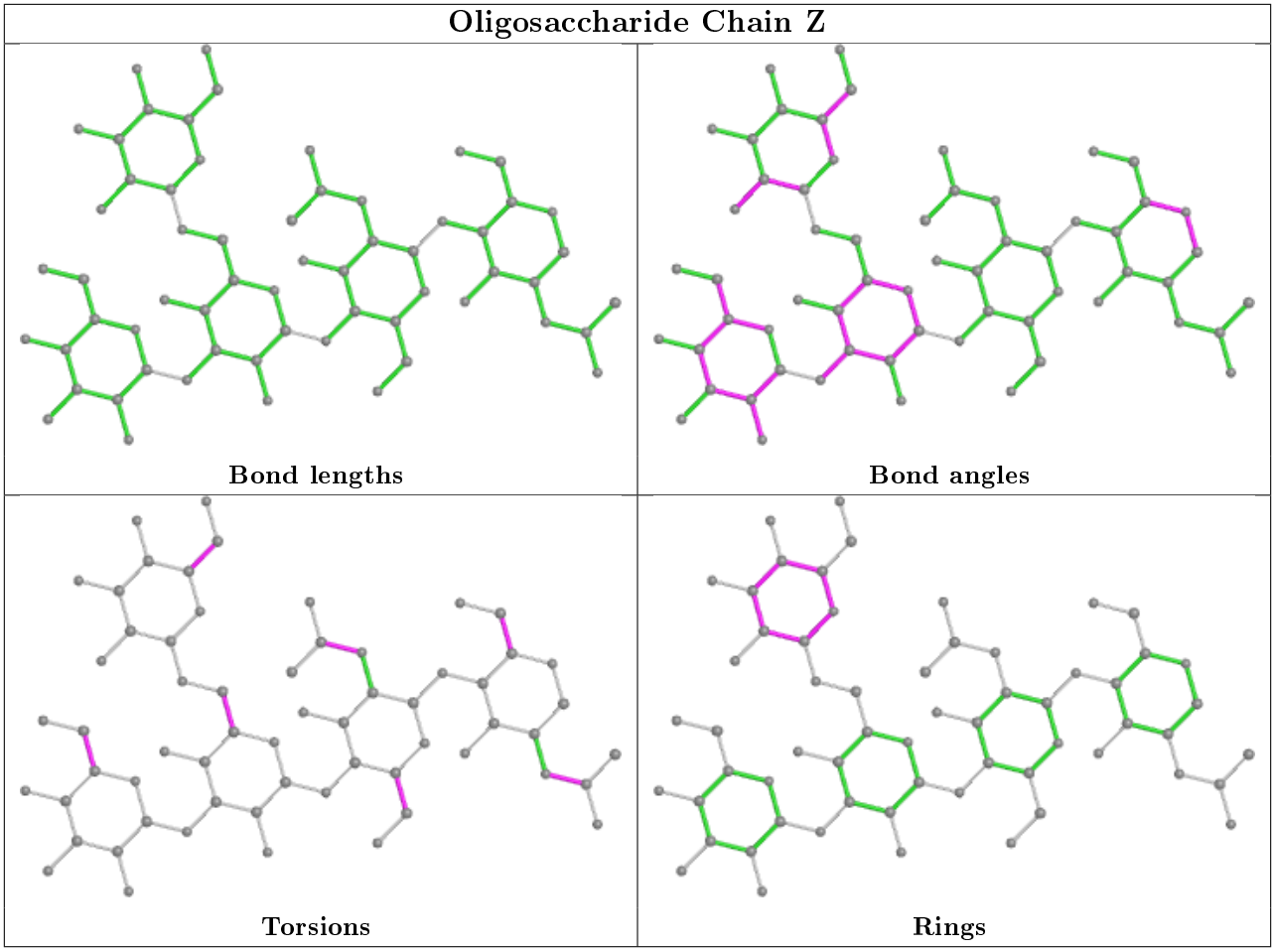
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

32 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	$\#\|Z\| > 2$
7	NAG	C	321	1	14,14,15	0.62	0	17,19,21	0.96	1 (5%)
7	NAG	K	322	1	14,14,15	0.82	0	17,19,21	1.34	2 (11%)
8	SO4	E	820	-	4,4,4	0.19	0	6,6,6	0.12	0
8	SO4	G	802	-	4,4,4	0.16	0	6,6,6	0.32	0
8	SO4	K	803	-	4,4,4	0.17	0	6,6,6	0.14	0
8	SO4	A	813	-	4,4,4	0.11	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	SO4	O	812	-	4,4,4	0.19	0	6,6,6	0.20	0
8	SO4	G	808	-	4,4,4	0.14	0	6,6,6	0.26	0
7	NAG	C	316	1	14,14,15	0.44	0	17,19,21	1.19	1 (5%)
7	NAG	A	317	1	14,14,15	0.47	0	17,19,21	1.73	3 (17%)
8	SO4	I	804	-	4,4,4	0.16	0	6,6,6	0.26	0
8	SO4	M	819	-	4,4,4	0.17	0	6,6,6	0.07	0
7	NAG	A	321	1	14,14,15	0.66	0	17,19,21	2.15	5 (29%)
8	SO4	I	821	-	4,4,4	0.16	0	6,6,6	0.14	0
8	SO4	C	806	-	4,4,4	0.13	0	6,6,6	0.30	0
7	NAG	M	331	1	14,14,15	0.40	0	17,19,21	1.57	1 (5%)
8	SO4	I	809	-	4,4,4	0.18	0	6,6,6	0.11	0
8	SO4	C	818	-	4,4,4	0.11	0	6,6,6	0.19	0
7	NAG	I	321	1	14,14,15	0.68	0	17,19,21	1.12	1 (5%)
8	SO4	C	814	-	4,4,4	0.16	0	6,6,6	0.42	0
7	NAG	E	317	1	14,14,15	0.57	0	17,19,21	1.45	2 (11%)
7	NAG	K	331	1	14,14,15	0.53	0	17,19,21	1.65	3 (17%)
8	SO4	E	815	-	4,4,4	0.19	0	6,6,6	0.60	0
8	SO4	K	810	-	4,4,4	0.17	0	6,6,6	0.11	0
7	NAG	G	321	1	14,14,15	0.68	0	17,19,21	1.24	2 (11%)
8	SO4	G	817	-	4,4,4	0.13	0	6,6,6	0.24	0
7	NAG	O	321	1	14,14,15	0.70	0	17,19,21	0.91	1 (5%)
8	SO4	E	807	-	4,4,4	0.14	0	6,6,6	0.16	0
8	SO4	M	811	-	4,4,4	0.17	0	6,6,6	0.28	0
8	SO4	A	805	-	4,4,4	0.13	0	6,6,6	0.10	0
8	SO4	A	801	-	4,4,4	0.20	0	6,6,6	0.35	0
8	SO4	G	816	-	4,4,4	0.16	0	6,6,6	0.58	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
7	NAG	I	321	1	-	2/6/23/26	0/1/1/1
7	NAG	C	321	1	1/1/5/7	5/6/23/26	0/1/1/1
7	NAG	A	317	1	1/1/5/7	3/6/23/26	0/1/1/1
7	NAG	K	322	1	-	5/6/23/26	0/1/1/1
7	NAG	O	321	1	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	E	317	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	321	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	K	331	1	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	C	316	1	1/1/5/7	5/6/23/26	0/1/1/1
7	NAG	G	321	1	-	5/6/23/26	0/1/1/1
7	NAG	M	331	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	321	NAG	C1-O5-C5	6.53	121.03	112.19
7	M	331	NAG	C1-O5-C5	5.78	120.02	112.19
7	A	317	NAG	C1-O5-C5	5.26	119.32	112.19
7	E	317	NAG	C1-O5-C5	3.77	117.30	112.19
7	K	331	NAG	C1-O5-C5	3.72	117.23	112.19
7	K	322	NAG	C2-N2-C7	3.22	127.48	122.90
7	G	321	NAG	C3-C4-C5	3.04	115.66	110.24
7	K	331	NAG	C4-C3-C2	2.99	115.40	111.02
7	K	322	NAG	C4-C3-C2	2.78	115.09	111.02
7	A	317	NAG	C3-C4-C5	2.77	115.19	110.24
7	K	331	NAG	C3-C4-C5	2.70	115.05	110.24
7	A	317	NAG	O5-C5-C6	2.63	111.33	107.20
7	C	316	NAG	C1-O5-C5	2.58	115.69	112.19
7	O	321	NAG	C4-C3-C2	2.47	114.63	111.02
7	A	321	NAG	C1-C2-N2	2.39	114.57	110.49
7	A	321	NAG	C8-C7-N2	2.38	120.12	116.10
7	G	321	NAG	C4-C3-C2	2.32	114.42	111.02
7	A	321	NAG	C4-C3-C2	-2.31	107.63	111.02
7	A	321	NAG	O5-C5-C6	2.27	110.75	107.20
7	E	317	NAG	O5-C5-C6	2.26	110.74	107.20
7	C	321	NAG	C2-N2-C7	2.24	126.09	122.90
7	I	321	NAG	O5-C5-C6	2.12	110.52	107.20

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	C	321	NAG	C1
7	C	316	NAG	C1
7	A	317	NAG	C1
7	A	321	NAG	C1
7	K	331	NAG	C1

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Mol	Chain	Res	Type	Atom
7	O	321	NAG	C1

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	321	NAG	C8-C7-N2-C2
7	C	321	NAG	O7-C7-N2-C2
7	K	322	NAG	C3-C2-N2-C7
7	K	322	NAG	C8-C7-N2-C2
7	K	322	NAG	O7-C7-N2-C2
7	C	316	NAG	C8-C7-N2-C2
7	C	316	NAG	O7-C7-N2-C2
7	A	321	NAG	C8-C7-N2-C2
7	A	321	NAG	O7-C7-N2-C2
7	M	331	NAG	C8-C7-N2-C2
7	M	331	NAG	O7-C7-N2-C2
7	I	321	NAG	C8-C7-N2-C2
7	I	321	NAG	O7-C7-N2-C2
7	E	317	NAG	C8-C7-N2-C2
7	E	317	NAG	O7-C7-N2-C2
7	G	321	NAG	C3-C2-N2-C7
7	G	321	NAG	C8-C7-N2-C2
7	G	321	NAG	O7-C7-N2-C2
7	O	321	NAG	C8-C7-N2-C2
7	O	321	NAG	O7-C7-N2-C2
7	A	317	NAG	C8-C7-N2-C2
7	A	317	NAG	O7-C7-N2-C2
7	C	321	NAG	C4-C5-C6-O6
7	A	321	NAG	O5-C5-C6-O6
7	C	316	NAG	O5-C5-C6-O6
7	K	322	NAG	C4-C5-C6-O6
7	E	317	NAG	O5-C5-C6-O6
7	G	321	NAG	C4-C5-C6-O6
7	C	321	NAG	O5-C5-C6-O6
7	M	331	NAG	O5-C5-C6-O6
7	G	321	NAG	O5-C5-C6-O6
7	C	316	NAG	C4-C5-C6-O6
7	A	321	NAG	C4-C5-C6-O6
7	E	317	NAG	C4-C5-C6-O6
7	M	331	NAG	C4-C5-C6-O6
7	K	322	NAG	O5-C5-C6-O6
7	A	317	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	C	321	NAG	C1-C2-N2-C7
7	C	316	NAG	C1-C2-N2-C7

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	K	803	SO4	1	0
8	I	804	SO4	1	0
8	C	818	SO4	1	0
8	K	810	SO4	2	0
8	G	817	SO4	1	0
8	M	811	SO4	1	0
8	A	801	SO4	1	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, 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	268/313 (85%)	0.96	35 (13%) 3 2	45, 57, 69, 98	0
1	C	259/313 (82%)	0.85	34 (13%) 3 2	48, 58, 66, 76	0
1	E	262/313 (83%)	0.80	30 (11%) 4 4	46, 56, 64, 72	0
1	G	258/313 (82%)	0.73	25 (9%) 7 6	46, 57, 67, 69	0
1	I	264/313 (84%)	0.94	44 (16%) 1 1	44, 58, 69, 89	0
1	K	257/313 (82%)	0.88	32 (12%) 3 3	45, 58, 67, 78	0
1	M	263/313 (84%)	0.84	30 (11%) 5 4	43, 57, 66, 83	0
1	O	258/313 (82%)	0.93	31 (12%) 4 3	47, 58, 68, 87	0
2	B	10/13 (76%)	0.87	1 (10%) 7 5	53, 60, 69, 71	0
2	D	10/13 (76%)	1.08	1 (10%) 7 5	50, 57, 64, 66	0
2	F	10/13 (76%)	1.19	2 (20%) 1 0	51, 63, 71, 71	0
2	H	10/13 (76%)	0.98	1 (10%) 7 5	52, 56, 65, 69	0
2	J	10/13 (76%)	1.28	2 (20%) 1 0	47, 54, 64, 70	0
2	L	10/13 (76%)	1.07	2 (20%) 1 0	50, 56, 72, 75	0
2	N	10/13 (76%)	1.13	1 (10%) 7 5	49, 55, 66, 71	0
2	P	10/13 (76%)	1.06	2 (20%) 1 0	52, 58, 72, 74	0
All	All	2169/2608 (83%)	0.88	273 (12%) 3 3	43, 57, 67, 98	0

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	VAL	9.8
1	E	231	PRO	8.7
1	A	138	PRO	8.3
1	A	279	GLN	7.9
1	I	275	ASP	7.9

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Mol	Chain	Res	Type	RSRZ
1	I	274	PRO	7.5
1	O	233	ASN	7.2
1	O	231	PRO	6.5
1	A	277	ASP	6.4
1	K	231	PRO	6.1
1	K	208	GLU	5.8
1	C	80	ASN	5.8
1	A	231	PRO	5.8
1	O	208	GLU	5.7
1	I	138	PRO	5.7
1	M	90	SER	5.6
1	C	139	LYS	5.5
1	G	107	ARG	5.5
1	I	82	GLY	5.4
1	G	202	THR	5.4
1	C	202	THR	5.2
1	I	19	LEU	5.2
1	A	131	GLN	5.2
1	A	276	LEU	5.2
1	O	202	THR	5.2
1	E	89	ARG	5.1
1	A	232	LYS	5.1
1	M	107	ARG	5.0
1	G	132	GLU	5.0
1	O	92	TYR	4.9
1	K	233	ASN	4.9
1	O	267	THR	4.9
1	I	33	GLU	4.9
1	K	102	ASP	4.8
1	C	102	ASP	4.7
1	I	107	ARG	4.7
1	M	19	LEU	4.7
1	M	106	GLU	4.7
1	M	277	ASP	4.7
1	M	89	ARG	4.6
1	K	230	GLU	4.6
1	C	203	HIS	4.6
1	A	102	ASP	4.6
1	A	137	ARG	4.6
1	I	110	HIS	4.6
1	K	203	HIS	4.5
1	A	107	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	131	GLN	4.5
1	A	202	THR	4.5
1	I	118	PRO	4.4
1	M	109	ARG	4.3
1	C	138	PRO	4.3
1	I	84	ALA	4.3
1	K	207	SER	4.3
1	O	204	GLY	4.3
1	M	92	TYR	4.2
1	C	231	PRO	4.2
1	C	107	ARG	4.1
1	K	202	THR	4.1
1	O	232	LYS	4.1
1	C	91	ARG	4.1
1	E	232	LYS	4.1
1	O	276	LEU	4.1
1	A	259	ASN	4.1
1	K	90	SER	4.1
1	K	229	HIS	4.0
1	C	274	PRO	4.0
1	G	110	HIS	4.0
1	C	230	GLU	4.0
1	A	90	SER	3.9
1	K	232	LYS	3.9
1	I	273	HIS	3.9
1	I	92	TYR	3.9
1	M	102	ASP	3.8
1	O	107	ARG	3.8
1	I	103	MET	3.8
1	E	107	ARG	3.8
1	I	85	VAL	3.8
1	A	234	GLN	3.8
1	O	106	GLU	3.7
1	I	83	ARG	3.7
1	M	91	ARG	3.7
1	I	137	ARG	3.6
1	I	81	SER	3.6
1	M	35	GLY	3.6
1	K	260	HIS	3.6
1	A	208	GLU	3.6
1	E	233	ASN	3.6
1	K	234	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	501	LYS	3.6
1	K	92	TYR	3.6
1	E	123	LEU	3.6
1	C	207	SER	3.6
1	K	110	HIS	3.5
1	M	232	LYS	3.5
1	O	275	ASP	3.5
1	C	106	GLU	3.5
1	E	102	ASP	3.5
1	O	260	HIS	3.5
1	G	102	ASP	3.5
1	E	106	GLU	3.5
1	K	139	LYS	3.5
1	E	90	SER	3.5
1	E	49	GLU	3.4
1	A	236	TYR	3.4
1	G	208	GLU	3.4
1	E	158	GLY	3.4
1	K	107	ARG	3.3
2	H	501	LYS	3.3
1	G	19	LEU	3.3
1	O	49	GLU	3.3
1	I	108	GLY	3.3
1	C	275	ASP	3.3
1	E	48	SER	3.3
1	K	235	SER	3.3
1	A	233	ASN	3.2
1	C	130	ILE	3.2
1	O	234	GLN	3.2
1	C	211	PHE	3.2
1	O	102	ASP	3.2
1	G	203	HIS	3.1
1	K	146	GLY	3.1
1	I	209	GLU	3.1
1	C	206	SER	3.1
1	C	209	GLU	3.1
1	G	106	GLU	3.1
1	E	168	LEU	3.1
1	E	242	ALA	3.1
1	I	146	GLY	3.1
1	A	81	SER	3.1
1	M	276	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	92	TYR	3.0
1	C	61	LEU	3.0
1	M	61	LEU	3.0
1	A	229	HIS	3.0
1	I	233	ASN	3.0
1	C	101	SER	3.0
1	I	139	LYS	3.0
1	G	131	GLN	2.9
1	K	118	PRO	2.9
1	I	102	ASP	2.9
1	G	229	HIS	2.9
1	M	108	GLY	2.9
1	M	146	GLY	2.9
1	C	208	GLU	2.9
1	C	109	ARG	2.9
1	A	103	MET	2.9
1	C	131	GLN	2.8
1	E	34	GLU	2.8
1	C	110	HIS	2.8
1	O	235	SER	2.8
1	A	130	ILE	2.8
1	I	61	LEU	2.8
1	I	232	LYS	2.8
1	M	148	GLY	2.8
1	M	88	SER	2.8
1	C	193	GLN	2.8
1	C	146	GLY	2.8
1	I	34	GLU	2.8
1	A	79	GLY	2.8
1	I	106	GLU	2.7
1	C	108	GLY	2.7
1	A	260	HIS	2.7
1	K	262	ASP	2.7
1	E	229	HIS	2.7
1	G	146	GLY	2.7
1	E	146	GLY	2.7
1	E	208	GLU	2.7
1	C	103	MET	2.7
1	G	234	GLN	2.7
2	J	501	LYS	2.6
1	K	48	SER	2.6
1	O	48	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	148	GLY	2.6
1	M	202	THR	2.6
1	O	230	GLU	2.6
1	K	259	ASN	2.6
1	M	47	HIS	2.6
1	G	139	LYS	2.6
1	K	106	GLU	2.6
1	E	230	GLU	2.6
1	E	203	HIS	2.6
1	O	271	CYS	2.6
1	G	230	GLU	2.6
2	P	501	LYS	2.6
1	A	230	GLU	2.5
1	M	34	GLU	2.5
1	C	19	LEU	2.5
1	K	240	GLY	2.5
1	E	140	ASP	2.5
1	M	81	SER	2.5
1	C	262	ASP	2.5
1	K	49	GLU	2.5
1	A	147	CYS	2.5
1	A	106	GLU	2.5
1	G	147	CYS	2.5
1	A	235	SER	2.5
1	A	140	ASP	2.5
1	G	231	PRO	2.4
2	N	509	LEU	2.4
1	G	109	ARG	2.4
1	G	232	LYS	2.4
1	I	207	SER	2.4
1	O	207	SER	2.4
1	A	92	TYR	2.4
1	C	140	ASP	2.4
1	O	229	HIS	2.4
1	E	157	ASN	2.4
2	B	501	LYS	2.4
1	I	131	GLN	2.4
1	A	274	PRO	2.3
1	G	101	SER	2.3
1	I	148	GLY	2.3
1	I	172	ASN	2.3
1	M	147	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	118	PRO	2.3
2	P	502	SER	2.3
1	M	125	VAL	2.3
1	G	240	GLY	2.3
1	K	204	GLY	2.3
2	L	502	SER	2.3
1	G	140	ASP	2.3
1	O	146	GLY	2.3
1	I	55	LEU	2.3
1	E	159	PHE	2.3
1	O	268	LYS	2.3
1	K	108	GLY	2.3
1	O	168	LEU	2.3
1	O	266	CYS	2.3
1	O	79	GLY	2.2
1	I	36	GLU	2.2
1	I	267	THR	2.2
1	E	278	VAL	2.2
1	A	211	PHE	2.2
1	E	234	GLN	2.2
1	K	111	GLN	2.2
1	G	211	PHE	2.2
1	I	80	ASN	2.2
1	O	56	SER	2.2
2	J	509	LEU	2.2
1	I	18	ALA	2.2
1	M	208	GLU	2.2
2	L	501	LYS	2.2
1	G	204	GLY	2.2
1	C	233	ASN	2.2
1	E	139	LYS	2.2
1	M	110	HIS	2.2
1	M	158	GLY	2.2
1	K	56	SER	2.1
2	F	501	LYS	2.1
1	E	125	VAL	2.1
1	O	203	HIS	2.1
1	C	118	PRO	2.1
1	M	55	LEU	2.1
1	I	208	GLU	2.1
1	K	266	CYS	2.1
2	F	512	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	125	VAL	2.1
1	C	180	PRO	2.1
1	I	158	GLY	2.1
1	I	240	GLY	2.1
1	I	112	SER	2.1
1	A	109	ARG	2.1
1	O	259	ASN	2.1
1	O	118	PRO	2.1
1	A	82	GLY	2.1
1	M	233	ASN	2.0
1	A	146	GLY	2.0
1	I	67	THR	2.0
1	E	61	LEU	2.0
1	I	54	THR	2.0
1	K	103	MET	2.0
1	I	181	ILE	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
2	DLY	P	507	9/10	0.86	0.27	54,55,61,63	0
2	DLY	B	507	9/10	0.89	0.26	53,54,58,58	0
2	ALC	H	504	11/12	0.93	0.27	54,56,61,61	0
2	ALC	N	504	11/12	0.93	0.28	55,56,57,58	0
2	DLY	F	507	9/10	0.93	0.22	51,52,57,57	0
2	DLY	L	507	9/10	0.94	0.23	51,52,59,61	0
2	ALC	D	504	11/12	0.94	0.27	53,54,55,56	0
2	DLY	D	507	9/10	0.94	0.29	51,52,53,53	0
2	DSN	P	506	6/7	0.94	0.17	56,56,56,57	0
2	ALC	J	504	11/12	0.94	0.28	55,56,57,57	0
2	DLY	N	507	9/10	0.95	0.32	47,50,50,51	0
2	ALC	P	504	11/12	0.96	0.26	59,60,61,63	0
2	DLY	J	507	9/10	0.96	0.30	49,50,50,51	0
2	ALC	L	504	11/12	0.96	0.22	60,61,63,63	0
2	ALC	F	504	11/12	0.96	0.25	54,54,56,58	0
2	DSN	N	506	6/7	0.96	0.28	51,51,52,53	0
2	DSN	D	506	6/7	0.96	0.23	51,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ALC	B	504	11/12	0.96	0.25	56,57,58,60	0
2	DSN	F	506	6/7	0.97	0.22	49,50,50,50	0
2	DLY	H	507	9/10	0.97	0.21	50,50,51,51	0
2	DSN	B	506	6/7	0.97	0.16	52,54,54,54	0
2	DSN	J	506	6/7	0.97	0.27	52,52,52,54	0
2	DSN	H	506	6/7	0.97	0.24	48,50,50,50	0
2	DSN	L	506	6/7	0.98	0.16	53,54,54,55	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FUC	X	2	10/11	0.55	0.54	94,95,96,96	0
5	NAG	f	1	14/15	0.57	0.48	82,86,88,92	0
4	FUC	U	2	10/11	0.67	0.42	84,85,86,86	0
4	NAG	U	1	14/15	0.67	0.52	76,79,82,83	0
3	NAG	S	2	14/15	0.68	0.46	99,101,101,102	0
5	NAG	f	2	14/15	0.70	0.48	95,96,98,99	0
4	FUC	a	2	10/11	0.71	0.41	83,84,84,84	0
5	NAG	W	2	14/15	0.72	0.41	91,92,93,93	0
3	FUC	T	3	10/11	0.72	0.30	84,85,85,85	0
6	MAN	h	4	11/12	0.74	0.39	74,76,77,77	0
6	MAN	Z	4	11/12	0.74	0.31	73,75,77,77	0
4	NAG	X	1	14/15	0.74	0.44	80,84,89,92	0
3	NAG	Q	2	14/15	0.74	0.35	83,84,86,86	0
3	NAG	T	2	14/15	0.75	0.40	89,91,92,93	0
6	MAN	c	4	11/12	0.75	0.21	55,57,59,59	0
3	NAG	b	2	14/15	0.76	0.45	81,83,86,86	0
3	NAG	T	1	14/15	0.77	0.19	74,77,83,86	0
4	NAG	a	1	14/15	0.78	0.28	76,79,81,82	0
3	NAG	S	1	14/15	0.79	0.34	85,91,95,96	0
5	NAG	W	1	14/15	0.79	0.46	80,86,87,90	0
6	MAN	h	5	11/12	0.81	0.20	65,69,71,72	0
4	FUC	R	2	10/11	0.82	0.34	71,72,73,73	0
6	BMA	Z	3	11/12	0.83	0.16	64,66,68,71	0
6	MAN	e	4	11/12	0.83	0.29	54,58,62,63	0
4	FUC	d	2	10/11	0.83	0.33	66,68,69,69	0

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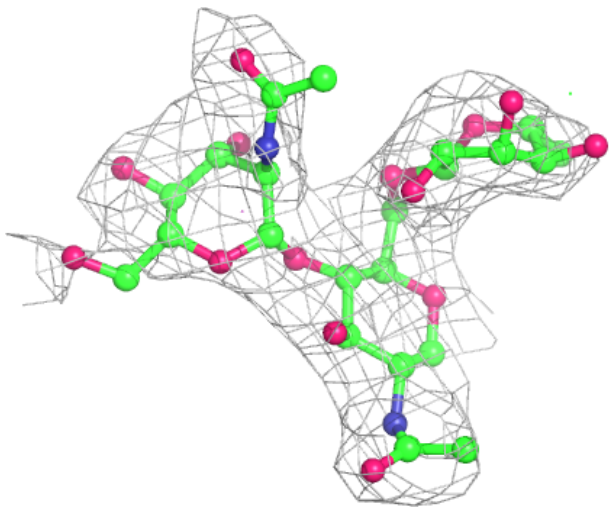
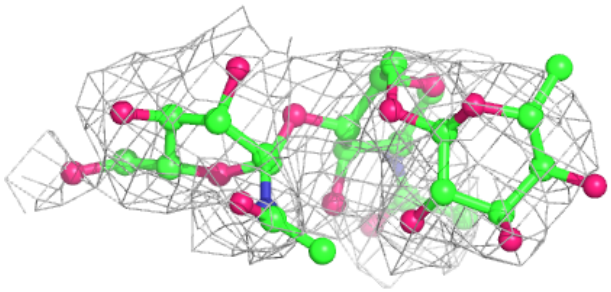
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MAN	Z	5	11/12	0.84	0.17	67,68,71,72	0
4	FUC	Y	2	10/11	0.85	0.23	73,75,76,76	0
3	FUC	S	3	10/11	0.85	0.47	96,97,97,98	0
4	NAG	g	1	14/15	0.86	0.21	63,65,67,70	0
4	NAG	d	1	14/15	0.87	0.26	57,59,61,64	0
4	FUC	V	2	10/11	0.87	0.34	71,73,74,75	0
3	NAG	b	1	14/15	0.88	0.17	68,72,74,78	0
6	NAG	h	2	14/15	0.88	0.24	66,69,71,71	0
6	NAG	h	1	14/15	0.88	0.21	61,65,67,67	0
4	FUC	g	2	10/11	0.90	0.35	71,72,73,73	0
6	BMA	h	3	11/12	0.90	0.29	70,71,72,73	0
4	NAG	Y	1	14/15	0.90	0.18	58,61,67,71	0
6	BMA	c	3	11/12	0.90	0.18	48,50,52,52	0
3	FUC	b	3	10/11	0.90	0.23	76,77,77,78	0
6	MAN	c	5	11/12	0.91	0.18	45,47,48,49	0
3	NAG	Q	1	14/15	0.92	0.17	68,73,79,80	0
6	BMA	e	3	11/12	0.92	0.17	47,49,51,54	0
6	NAG	Z	2	14/15	0.92	0.18	60,61,63,64	0
4	NAG	R	1	14/15	0.93	0.21	62,65,66,68	0
6	NAG	e	1	14/15	0.93	0.15	44,47,48,49	0
6	NAG	c	2	14/15	0.93	0.19	50,52,54,54	0
6	MAN	e	5	11/12	0.93	0.17	43,45,46,48	0
6	NAG	Z	1	14/15	0.93	0.16	57,58,61,63	0
3	FUC	Q	3	10/11	0.94	0.28	81,82,82,83	0
6	NAG	c	1	14/15	0.94	0.16	45,51,53,53	0
4	NAG	V	1	14/15	0.96	0.16	57,60,63,67	0
6	NAG	e	2	14/15	0.96	0.17	47,48,48,50	0

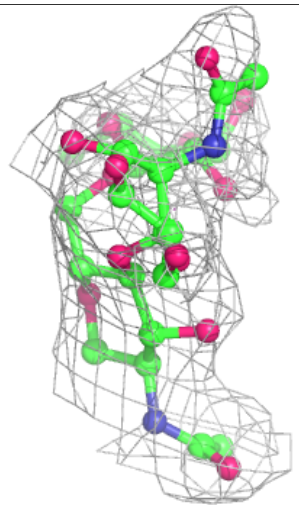
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain Q:

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

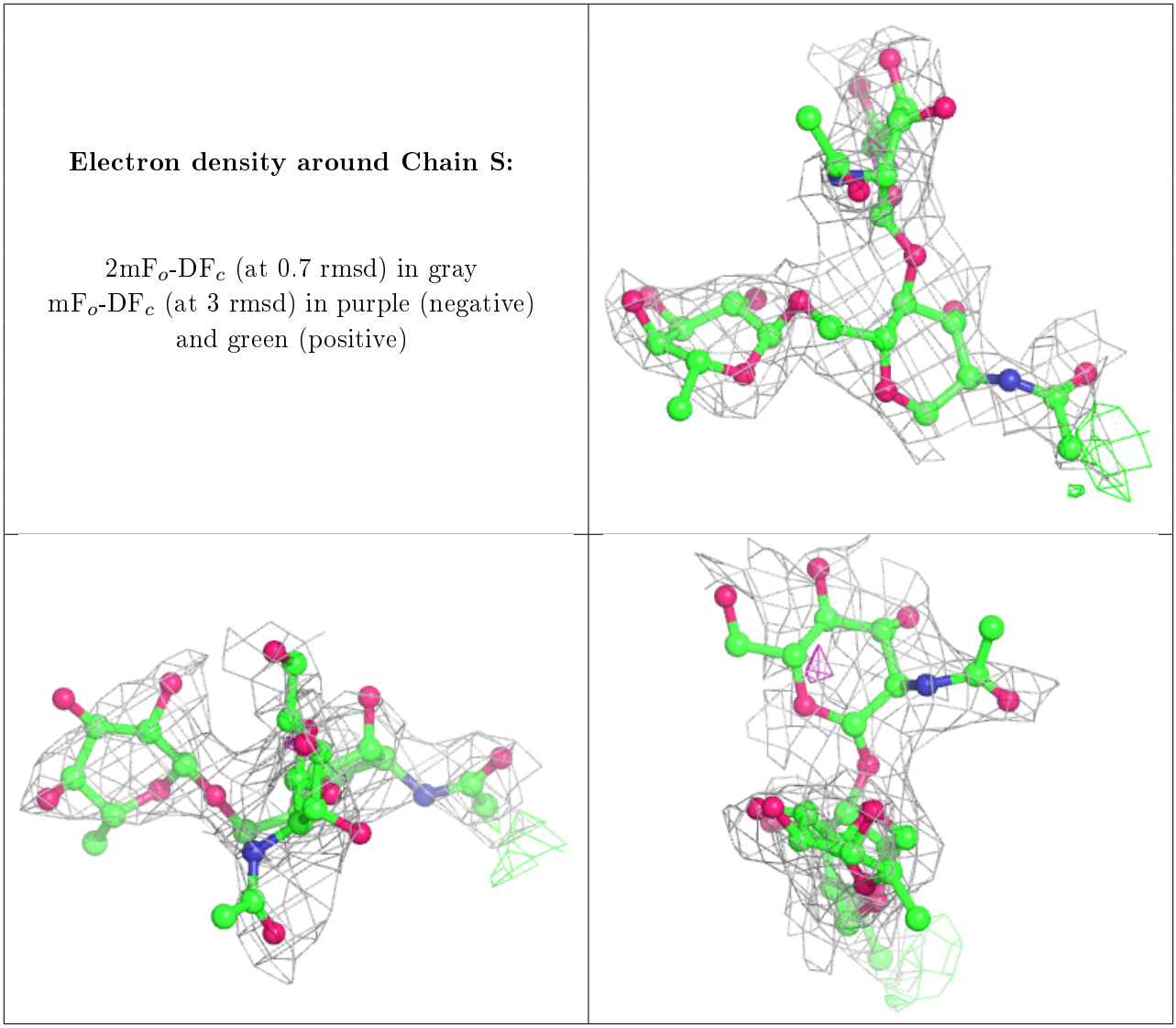






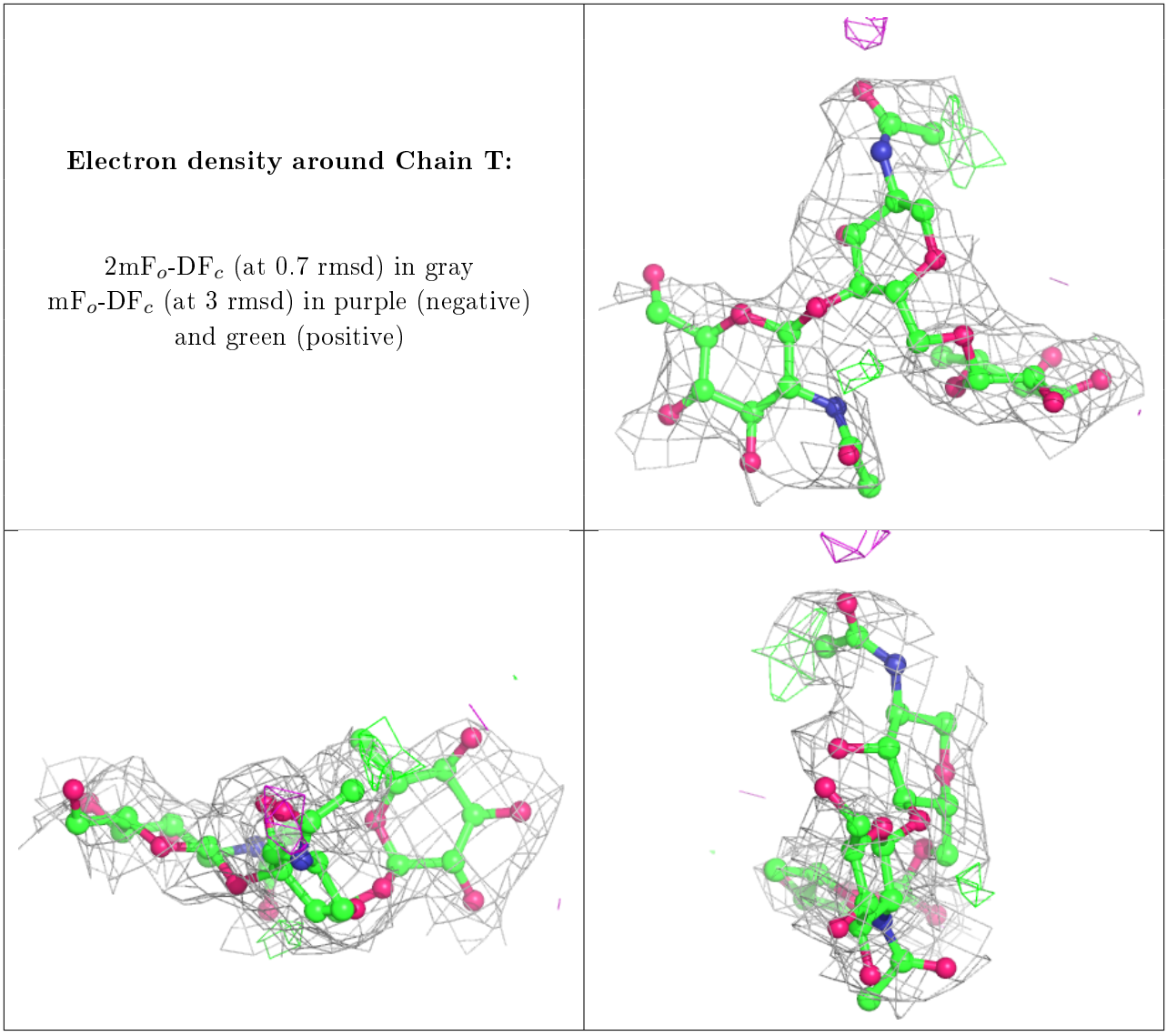
Electron density around Chain S:

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



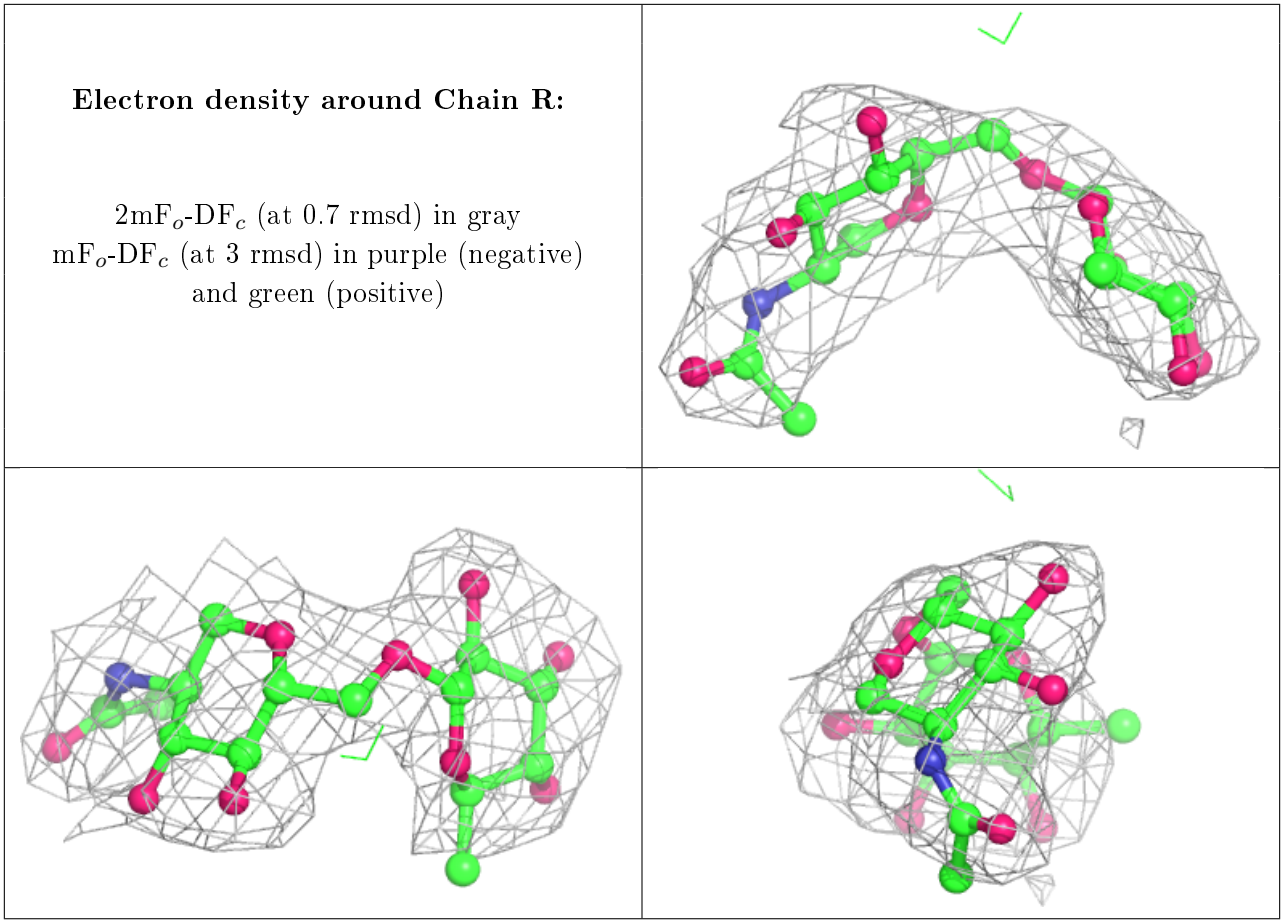
Electron density around Chain T:

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



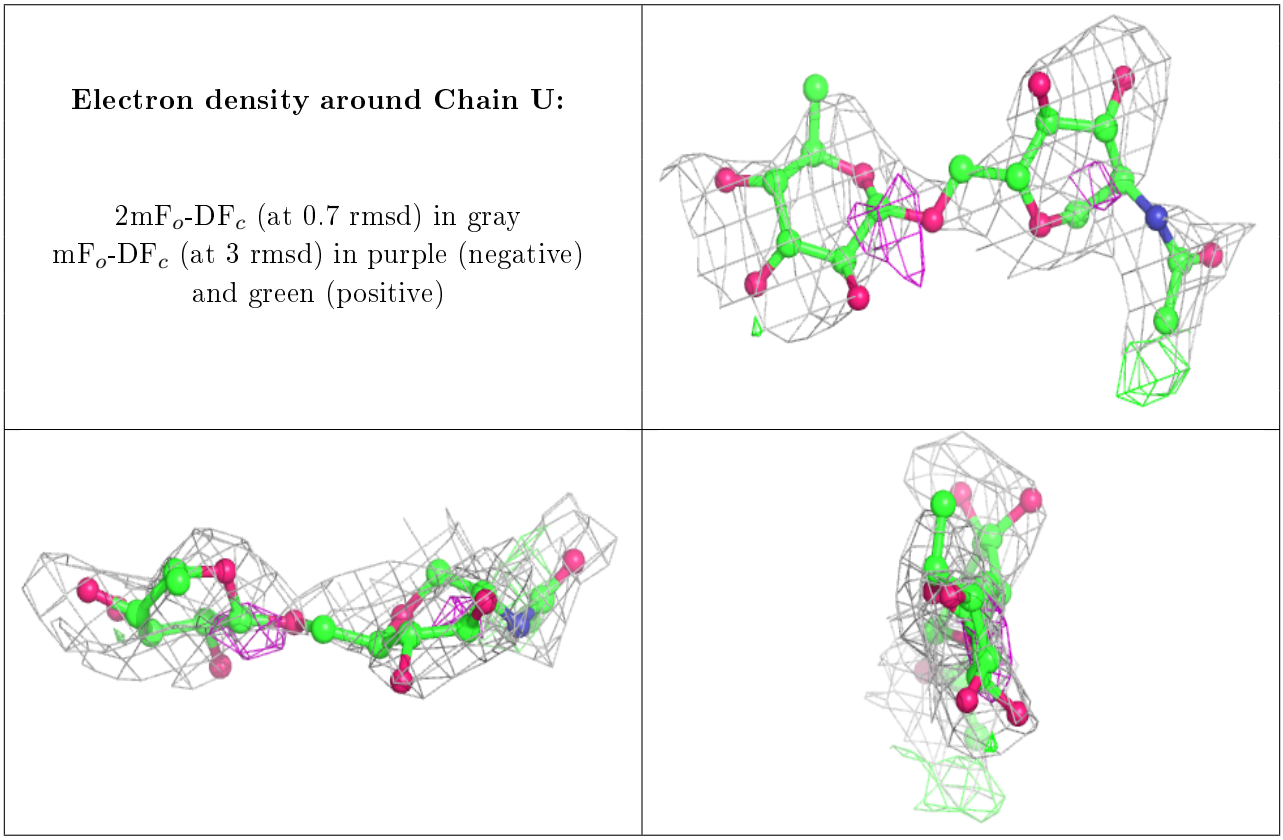
Electron density around Chain R:

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



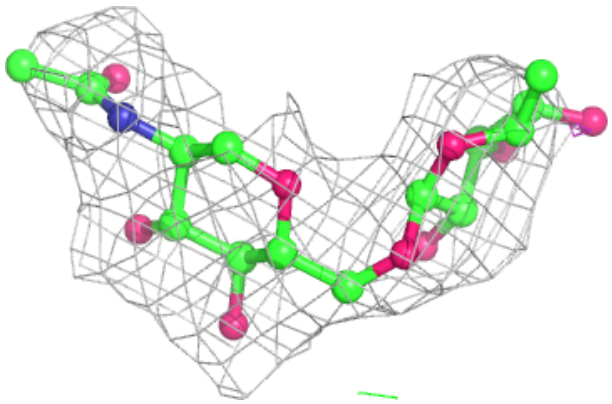
Electron density around Chain U:

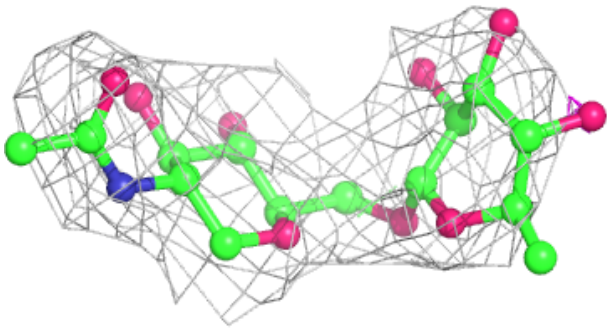
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

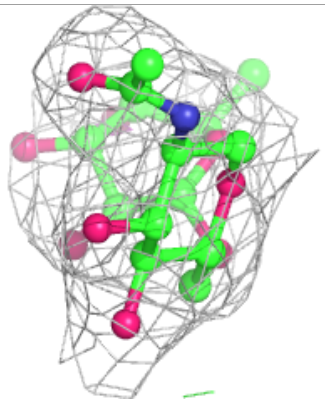


Electron density around Chain V:

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

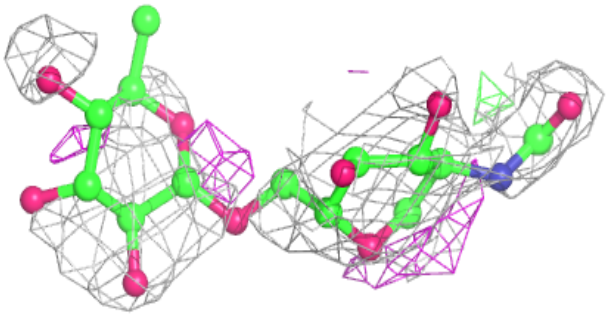


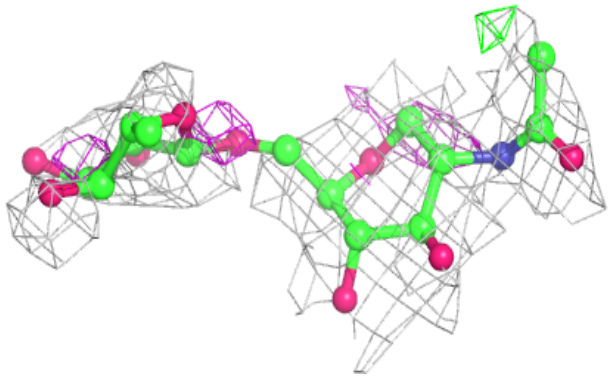


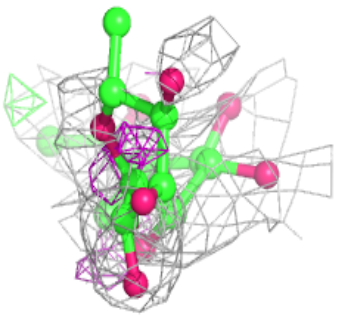


Electron density around Chain X:

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

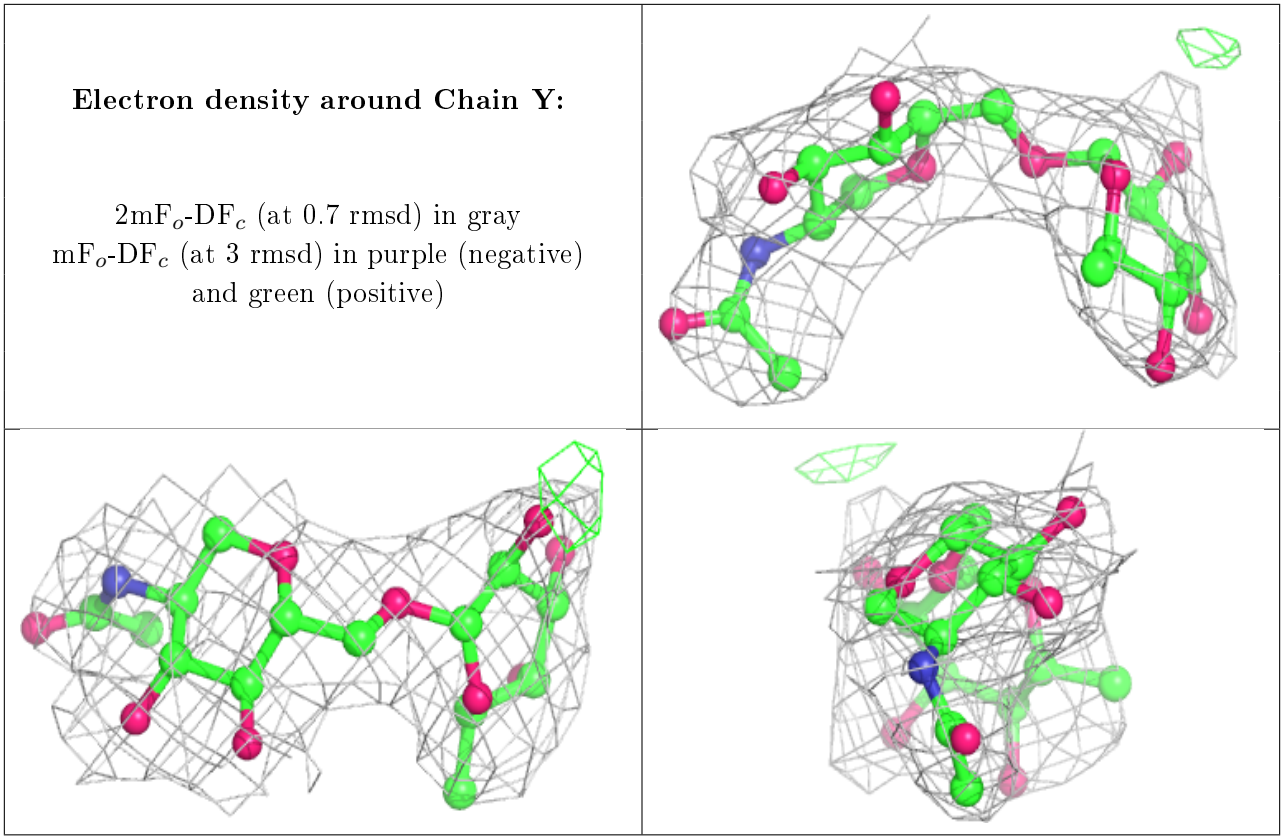






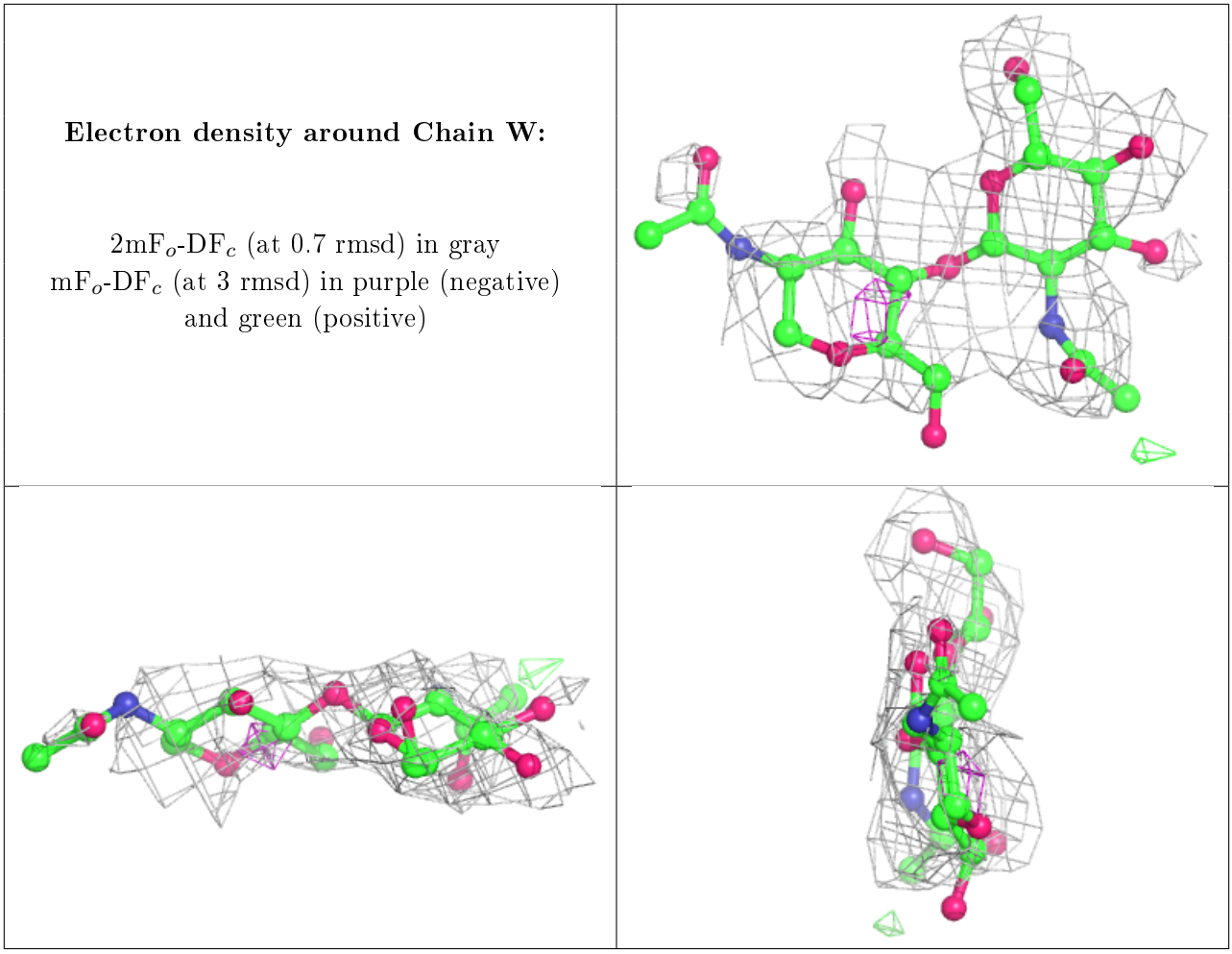
Electron density around Chain Y:

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



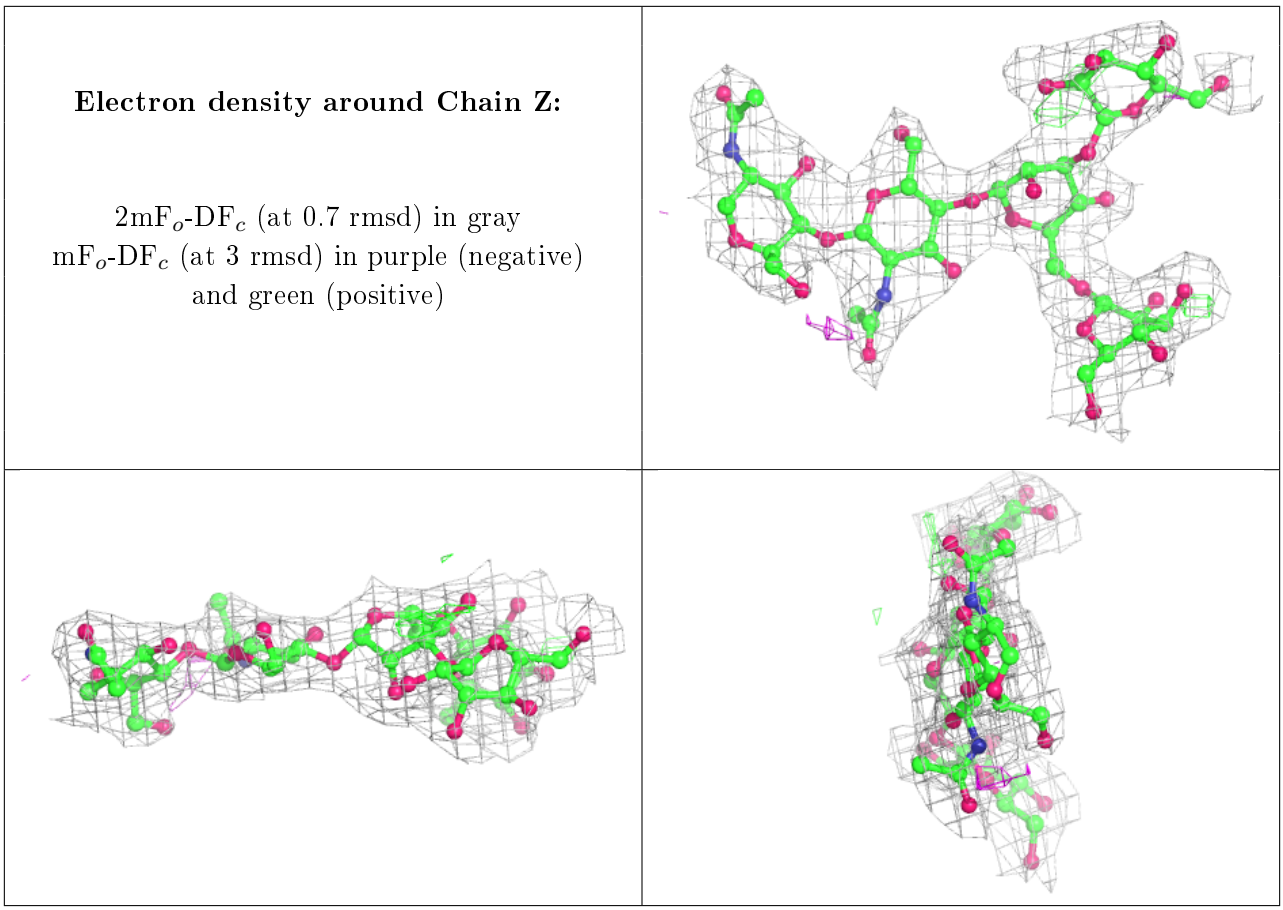
Electron density around Chain W:

$2mF_o$-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 Z:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	K	331	14/15	0.39	0.51	84,86,88,88	0
7	NAG	A	321	14/15	0.51	0.50	75,78,80,80	0
7	NAG	K	322	14/15	0.67	0.41	76,79,80,81	0
7	NAG	G	321	14/15	0.67	0.52	76,80,82,83	0
7	NAG	O	321	14/15	0.74	0.38	78,82,82,83	0
7	NAG	I	321	14/15	0.77	0.49	76,79,80,80	0
7	NAG	M	331	14/15	0.78	0.33	72,75,76,76	0
7	NAG	A	317	14/15	0.79	0.36	78,82,85,85	0
8	SO4	A	805	5/5	0.82	0.28	132,132,133,133	0
7	NAG	E	317	14/15	0.84	0.38	72,75,80,80	0
7	NAG	C	321	14/15	0.85	0.49	78,82,83,84	0
7	NAG	C	316	14/15	0.86	0.53	77,80,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	SO4	E	807	5/5	0.87	0.34	125,125,125,125	0
8	SO4	K	810	5/5	0.90	0.21	84,85,86,86	0
8	SO4	G	802	5/5	0.92	0.16	56,57,58,58	0
8	SO4	O	812	5/5	0.92	0.26	79,79,80,80	0
8	SO4	G	816	5/5	0.92	0.20	61,62,63,63	0
8	SO4	C	814	5/5	0.93	0.16	65,67,68,69	0
8	SO4	E	820	5/5	0.93	0.20	86,87,87,87	0
8	SO4	C	806	5/5	0.93	0.16	79,80,81,81	0
8	SO4	A	801	5/5	0.94	0.13	70,70,72,72	0
8	SO4	I	804	5/5	0.94	0.20	58,58,59,60	0
8	SO4	C	818	5/5	0.95	0.13	75,75,76,77	0
8	SO4	M	819	5/5	0.95	0.15	79,79,80,80	0
8	SO4	K	803	5/5	0.96	0.12	61,61,61,62	0
8	SO4	E	815	5/5	0.96	0.11	56,57,58,58	0
8	SO4	A	813	5/5	0.96	0.12	64,66,66,67	0
8	SO4	M	811	5/5	0.97	0.10	63,63,63,64	0
8	SO4	G	817	5/5	0.97	0.12	67,69,69,70	0
8	SO4	G	808	5/5	0.97	0.16	58,58,60,60	0
8	SO4	I	821	5/5	0.97	0.18	71,72,72,73	0
8	SO4	I	809	5/5	0.98	0.16	64,65,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.