



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:36 AM UTC

PDB ID : 5W08 / pdb_00005w08
Title : A/Texas/50/2012(H3N2) Influenza hemagglutinin in complex with K03.12 Fab
Authors : McCarthy, K.R.; Harrison, S.C.
Deposited on : 2017-05-30
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

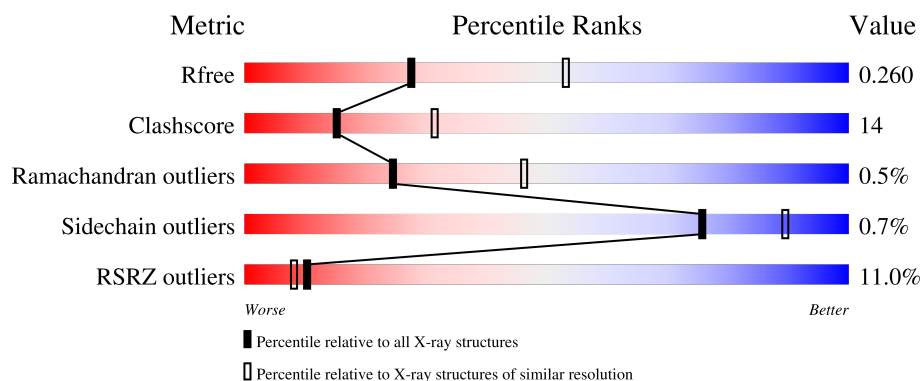
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	291	8% 71% 22% 7%
1	B	291	8% 74% 20% 6%
1	C	291	13% 67% 26% 7%
1	D	291	9% 73% 20% 6%
1	E	291	9% 73% 20% 6%

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Mol	Chain	Length	Quality of chain
1	F	291	
2	G	244	
2	I	244	
2	K	244	
2	M	244	
2	O	244	
2	Q	244	
3	H	214	
3	J	214	
3	L	214	
3	N	214	
3	P	214	
3	R	214	
4	S	2	
4	V	2	
4	W	2	
4	Y	2	
4	Z	2	
5	T	3	
5	U	3	
5	X	3	
5	a	3	
5	b	3	

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
5	NAG	T	1	-	-	X	-
6	NAG	A	406	-	-	X	-
6	NAG	D	405	-	-	X	-
6	NAG	D	406	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 34382 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2159	1362	383	404	10			
1	B	274	Total	C	N	O	S	0	0	0
			2171	1369	385	407	10			
1	C	272	Total	C	N	O	S	0	0	0
			2159	1362	383	404	10			
1	D	273	Total	C	N	O	S	0	0	0
			2166	1366	384	406	10			
1	E	273	Total	C	N	O	S	0	0	0
			2166	1366	384	406	10			
1	F	274	Total	C	N	O	S	0	0	0
			2171	1369	385	407	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	GLY	-	expression tag	UNP R4L1D1
A	321	ALA	-	expression tag	UNP R4L1D1
A	322	LEU	-	expression tag	UNP R4L1D1
A	323	GLU	-	expression tag	UNP R4L1D1
A	324	VAL	-	expression tag	UNP R4L1D1
A	325	LEU	-	expression tag	UNP R4L1D1
A	326	PHE	-	expression tag	UNP R4L1D1
A	327	GLN	-	expression tag	UNP R4L1D1
B	320	GLY	-	expression tag	UNP R4L1D1
B	321	ALA	-	expression tag	UNP R4L1D1
B	322	LEU	-	expression tag	UNP R4L1D1
B	323	GLU	-	expression tag	UNP R4L1D1
B	324	VAL	-	expression tag	UNP R4L1D1
B	325	LEU	-	expression tag	UNP R4L1D1
B	326	PHE	-	expression tag	UNP R4L1D1
B	327	GLN	-	expression tag	UNP R4L1D1
C	320	GLY	-	expression tag	UNP R4L1D1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	321	ALA	-	expression tag	UNP R4L1D1
C	322	LEU	-	expression tag	UNP R4L1D1
C	323	GLU	-	expression tag	UNP R4L1D1
C	324	VAL	-	expression tag	UNP R4L1D1
C	325	LEU	-	expression tag	UNP R4L1D1
C	326	PHE	-	expression tag	UNP R4L1D1
C	327	GLN	-	expression tag	UNP R4L1D1
D	320	GLY	-	expression tag	UNP R4L1D1
D	321	ALA	-	expression tag	UNP R4L1D1
D	322	LEU	-	expression tag	UNP R4L1D1
D	323	GLU	-	expression tag	UNP R4L1D1
D	324	VAL	-	expression tag	UNP R4L1D1
D	325	LEU	-	expression tag	UNP R4L1D1
D	326	PHE	-	expression tag	UNP R4L1D1
D	327	GLN	-	expression tag	UNP R4L1D1
E	320	GLY	-	expression tag	UNP R4L1D1
E	321	ALA	-	expression tag	UNP R4L1D1
E	322	LEU	-	expression tag	UNP R4L1D1
E	323	GLU	-	expression tag	UNP R4L1D1
E	324	VAL	-	expression tag	UNP R4L1D1
E	325	LEU	-	expression tag	UNP R4L1D1
E	326	PHE	-	expression tag	UNP R4L1D1
E	327	GLN	-	expression tag	UNP R4L1D1
F	320	GLY	-	expression tag	UNP R4L1D1
F	321	ALA	-	expression tag	UNP R4L1D1
F	322	LEU	-	expression tag	UNP R4L1D1
F	323	GLU	-	expression tag	UNP R4L1D1
F	324	VAL	-	expression tag	UNP R4L1D1
F	325	LEU	-	expression tag	UNP R4L1D1
F	326	PHE	-	expression tag	UNP R4L1D1
F	327	GLN	-	expression tag	UNP R4L1D1

- Molecule 2 is a protein called K03.12 antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	236	Total	C	N	O	S	0	0	0
			1790	1132	300	349	9			
2	I	238	Total	C	N	O	S	0	0	0
			1807	1142	303	353	9			
2	K	235	Total	C	N	O	S	0	0	0
			1784	1129	299	348	8			
2	M	235	Total	C	N	O	S	0	0	0
			1784	1129	299	348	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	235	Total	C	N	O	S	0	0	0
			1784	1129	299	348	8			
2	Q	235	Total	C	N	O	S	0	0	0
			1784	1129	299	348	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	239	HIS	-	expression tag	UNP S6C4S0
G	240	HIS	-	expression tag	UNP S6C4S0
G	241	HIS	-	expression tag	UNP S6C4S0
G	242	HIS	-	expression tag	UNP S6C4S0
G	243	HIS	-	expression tag	UNP S6C4S0
G	244	HIS	-	expression tag	UNP S6C4S0
I	239	HIS	-	expression tag	UNP S6C4S0
I	240	HIS	-	expression tag	UNP S6C4S0
I	241	HIS	-	expression tag	UNP S6C4S0
I	242	HIS	-	expression tag	UNP S6C4S0
I	243	HIS	-	expression tag	UNP S6C4S0
I	244	HIS	-	expression tag	UNP S6C4S0
K	239	HIS	-	expression tag	UNP S6C4S0
K	240	HIS	-	expression tag	UNP S6C4S0
K	241	HIS	-	expression tag	UNP S6C4S0
K	242	HIS	-	expression tag	UNP S6C4S0
K	243	HIS	-	expression tag	UNP S6C4S0
K	244	HIS	-	expression tag	UNP S6C4S0
M	239	HIS	-	expression tag	UNP S6C4S0
M	240	HIS	-	expression tag	UNP S6C4S0
M	241	HIS	-	expression tag	UNP S6C4S0
M	242	HIS	-	expression tag	UNP S6C4S0
M	243	HIS	-	expression tag	UNP S6C4S0
M	244	HIS	-	expression tag	UNP S6C4S0
O	239	HIS	-	expression tag	UNP S6C4S0
O	240	HIS	-	expression tag	UNP S6C4S0
O	241	HIS	-	expression tag	UNP S6C4S0
O	242	HIS	-	expression tag	UNP S6C4S0
O	243	HIS	-	expression tag	UNP S6C4S0
O	244	HIS	-	expression tag	UNP S6C4S0
Q	239	HIS	-	expression tag	UNP S6C4S0
Q	240	HIS	-	expression tag	UNP S6C4S0
Q	241	HIS	-	expression tag	UNP S6C4S0
Q	242	HIS	-	expression tag	UNP S6C4S0

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	243	HIS	-	expression tag	UNP S6C4S0
Q	244	HIS	-	expression tag	UNP S6C4S0

- Molecule 3 is a protein called K03.12 antibody light chain.

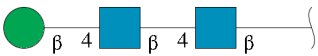
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	212	Total	C	N	O	S	0	0	0
			1561	973	258	325	5			
3	J	213	Total	C	N	O	S	0	0	0
			1568	978	259	326	5			
3	L	211	Total	C	N	O	S	0	0	0
			1555	970	257	324	4			
3	N	212	Total	C	N	O	S	0	0	0
			1562	975	258	325	4			
3	P	212	Total	C	N	O	S	0	0	0
			1562	975	258	325	4			
3	R	212	Total	C	N	O	S	0	0	0
			1562	975	258	325	4			

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



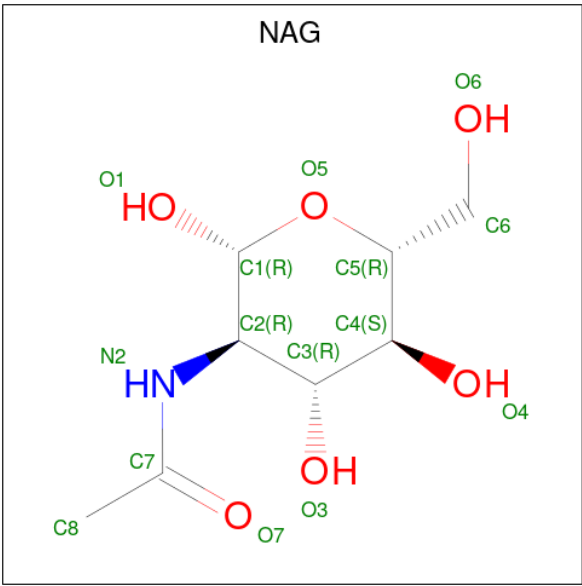
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called 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
5	T	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	U	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	X	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	a	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	b	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



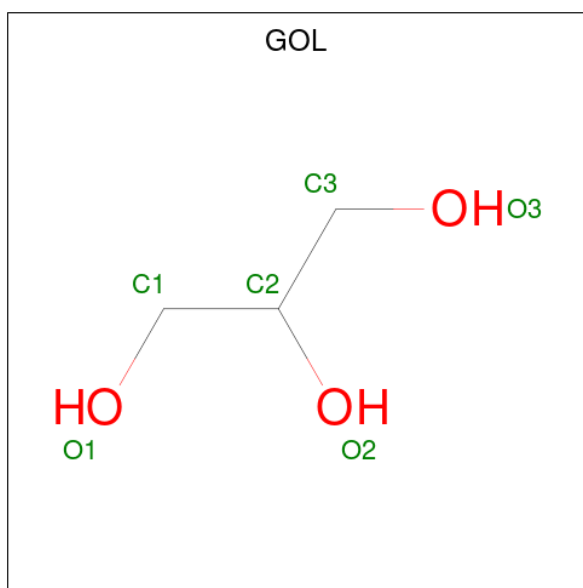
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

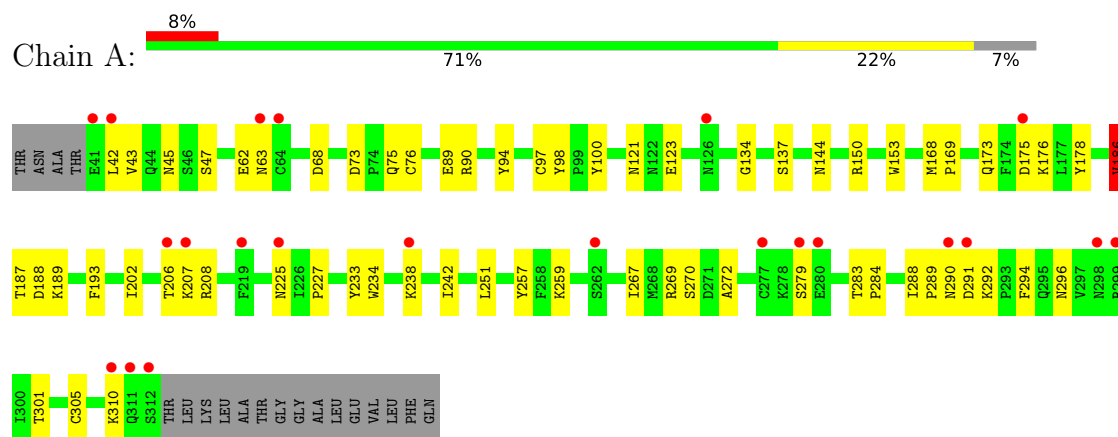
- Molecule 8 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	58	Total	O		0	0
			58	58			
8	B	79	Total	O		0	0
			79	79			
8	C	48	Total	O		0	0
			48	48			
8	D	49	Total	O		0	0
			49	49			
8	E	46	Total	O		0	0
			46	46			
8	F	37	Total	O		0	0
			37	37			
8	G	45	Total	O		0	0
			45	45			
8	H	41	Total	O		0	0
			41	41			
8	I	55	Total	O		0	0
			55	55			
8	J	43	Total	O		0	0
			43	43			
8	K	29	Total	O		0	0
			29	29			
8	L	23	Total	O		0	0
			23	23			
8	M	28	Total	O		0	0
			28	28			
8	N	40	Total	O		0	0
			40	40			
8	O	30	Total	O		0	0
			30	30			
8	P	22	Total	O		0	0
			22	22			
8	Q	24	Total	O		0	0
			24	24			
8	R	25	Total	O		0	0
			25	25			

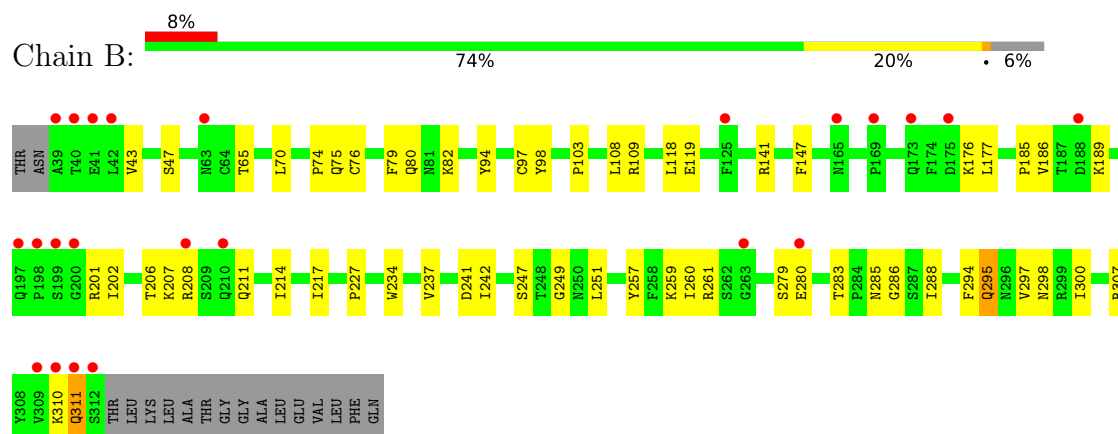
3 Residue-property plots [i](#)

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.

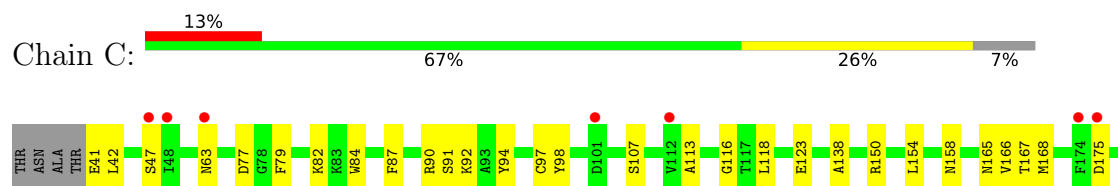
• Molecule 1: Hemagglutinin HA1

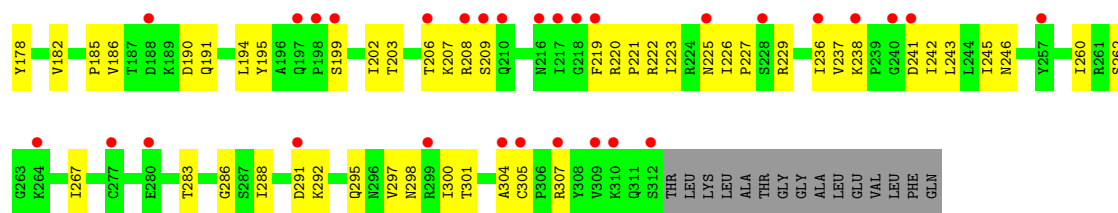


• Molecule 1: Hemagglutinin HA1

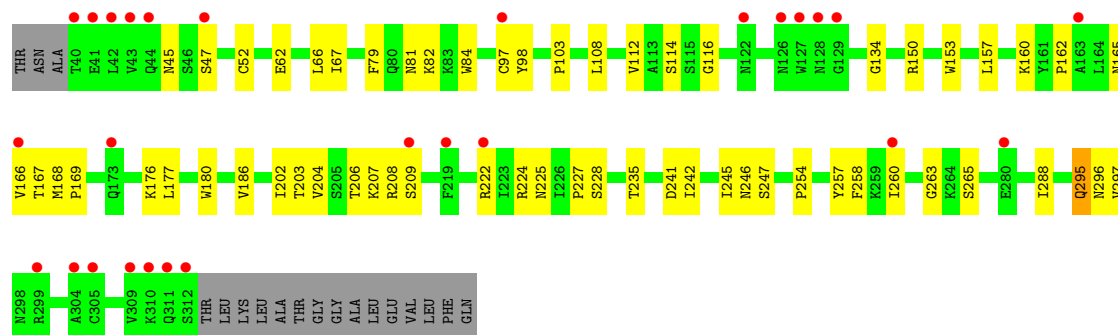
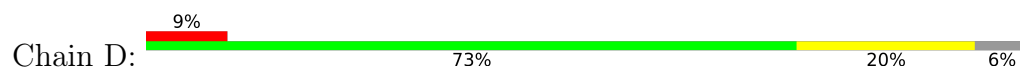


• Molecule 1: Hemagglutinin HA1

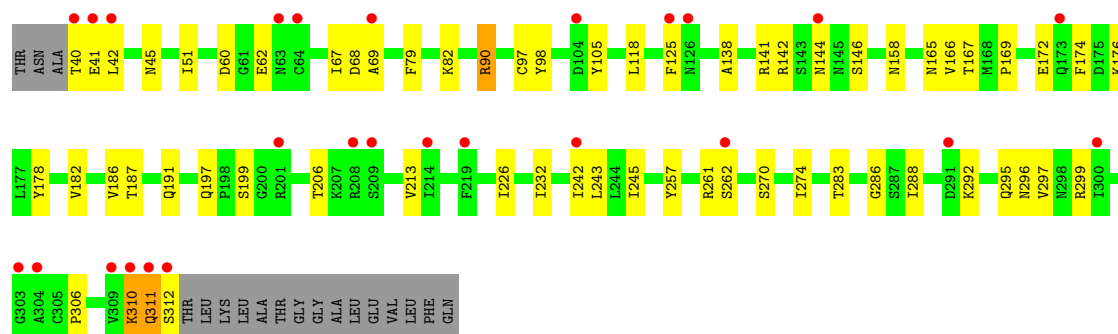
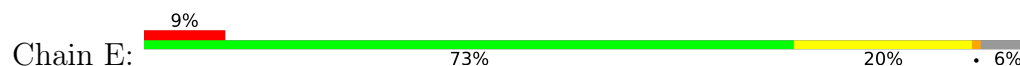




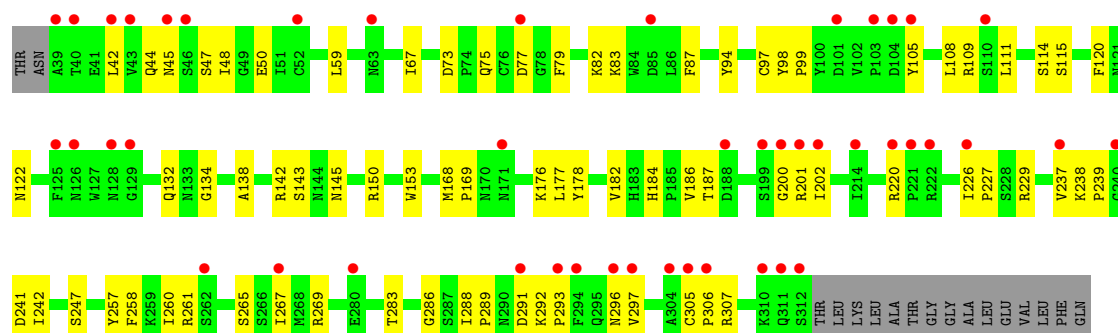
● Molecule 1: Hemagglutinin HA1



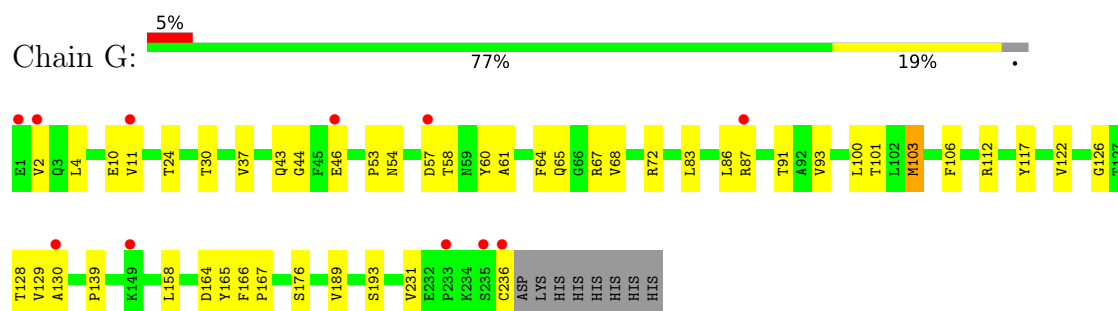
● Molecule 1: Hemagglutinin HA1



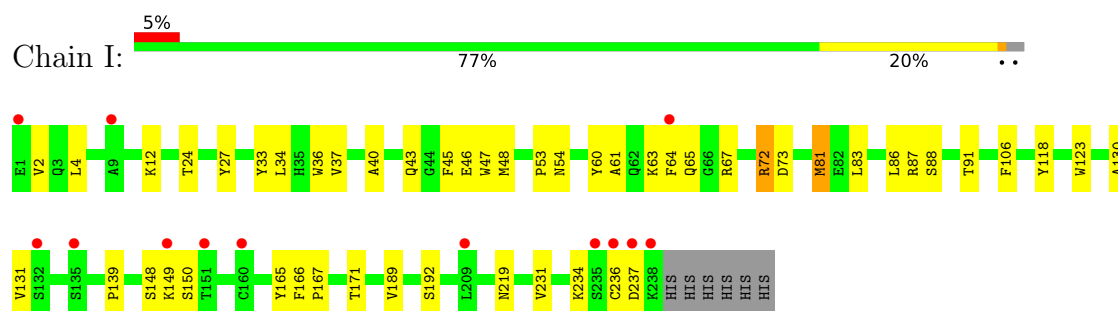
● Molecule 1: Hemagglutinin HA1



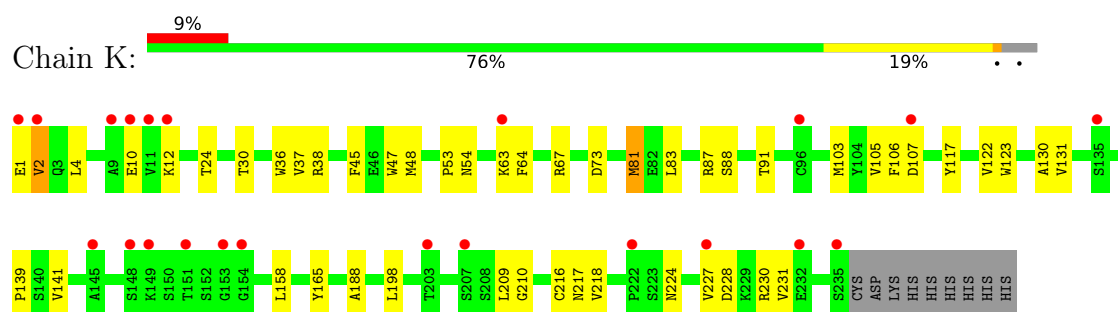
- Molecule 2: K03.12 antibody heavy chain



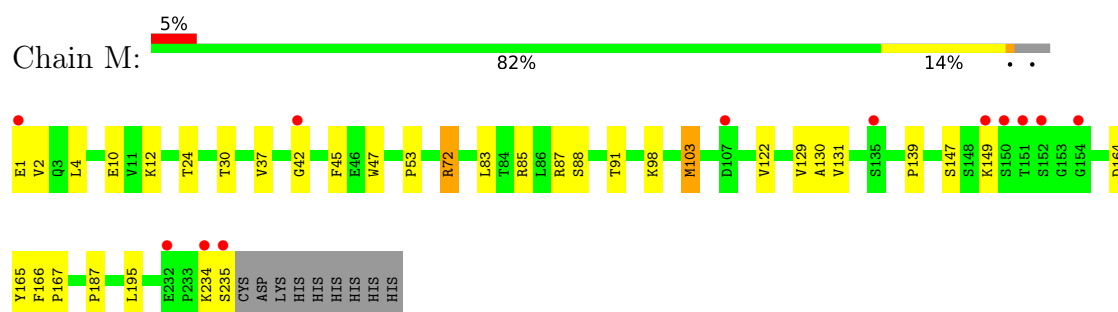
- Molecule 2: K03.12 antibody heavy chain



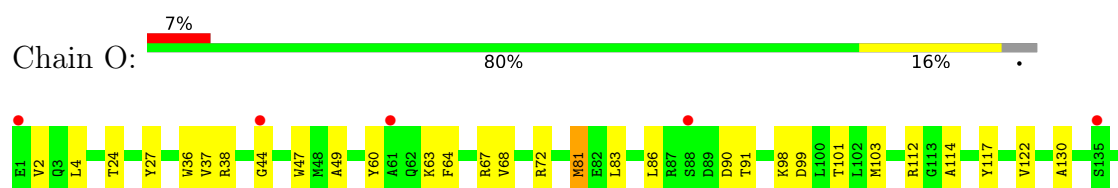
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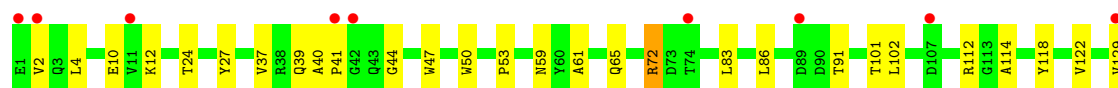
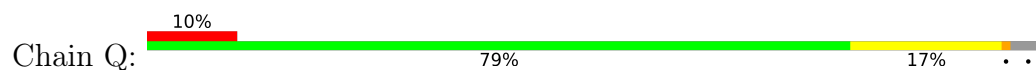


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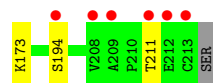
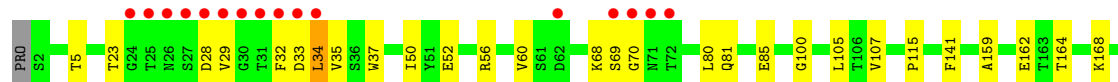
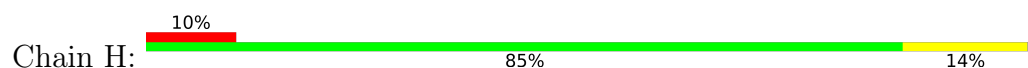




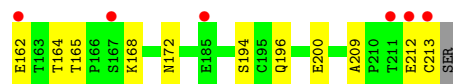
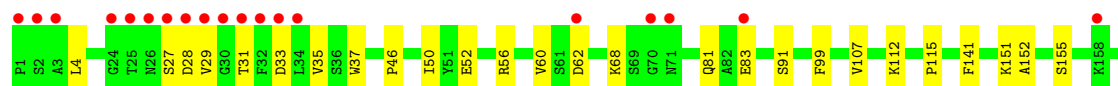
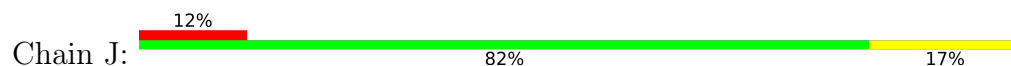
- Molecule 2: K03.12 antibody heavy chain



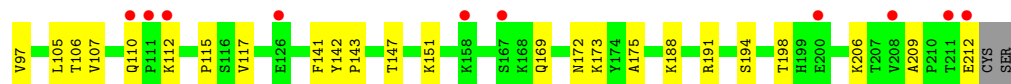
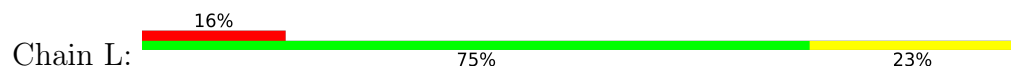
- Molecule 3: K03.12 antibody light chain



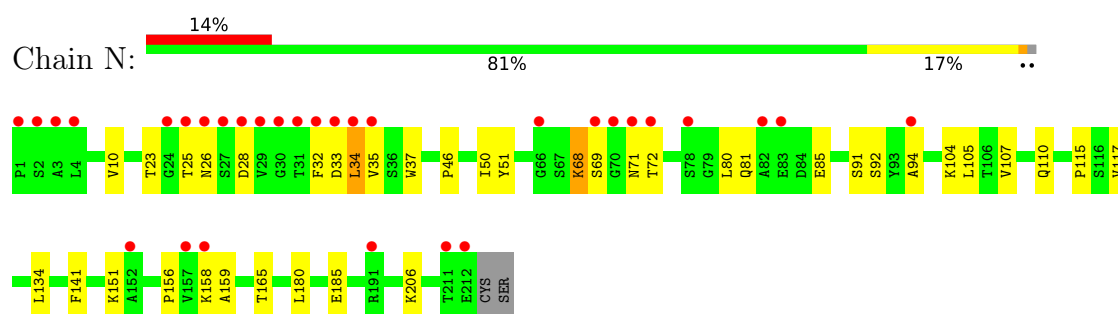
- Molecule 3: K03.12 antibody light chain



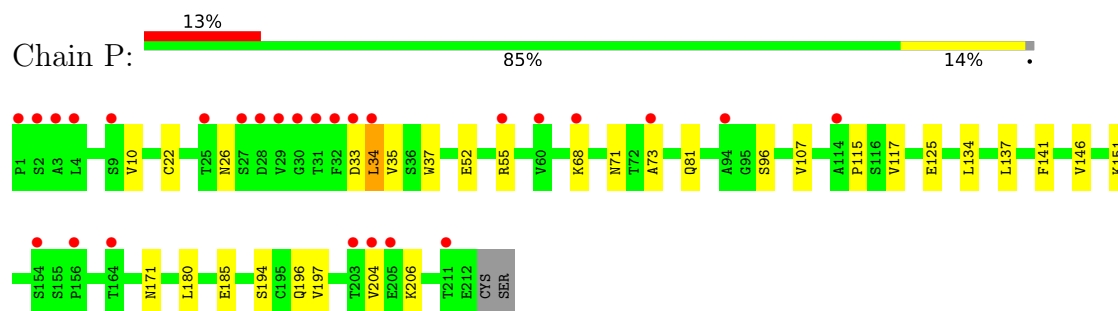
- Molecule 3: K03.12 antibody light chain



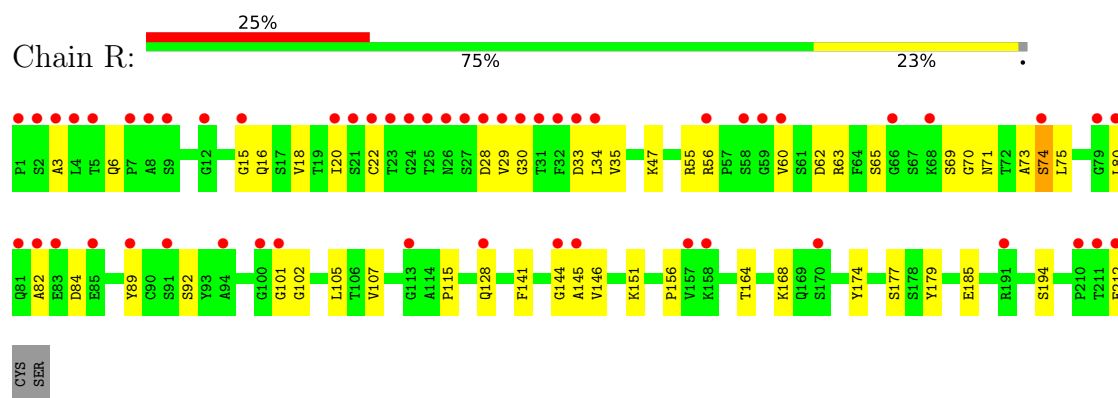
- Molecule 3: K03.12 antibody light chain



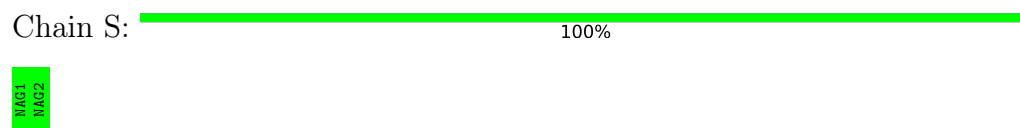
- Molecule 3: K03.12 antibody light chain



- Molecule 3: K03.12 antibody light chain



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



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



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

Chain W:  50% 50%

MAG1
MAG2

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

Chain Y:  50% 50%

MAG1
MAG2

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

Chain Z:  50% 50%

MAG1
MAG2

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

Chain T:  67% 33%

MAG1
MAG2
BMA3

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

Chain U:  33% 67%

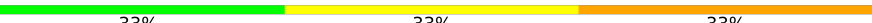
MAG1
MAG2
BMA3

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

Chain X:  100%

MAG1
MAG2
BMA3

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

Chain a:  33% 33% 33%



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

Chain b:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.80Å 325.12Å 156.99Å 90.00° 97.63° 90.00°	Depositor
Resolution (Å)	49.41 – 2.60 49.41 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.41-2.60) 99.2 (49.41-2.60)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.240 , 0.262 0.238 , 0.260	Depositor DCC
R_{free} test set	9069 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	34382	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, GOL

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	0.37	1/2213 (0.0%)	0.44	1/3006 (0.0%)
1	B	0.12	0/2225	0.38	0/3023
1	C	0.28	0/2213	0.45	0/3006
1	D	0.13	0/2220	0.38	0/3016
1	E	0.17	0/2220	0.42	0/3016
1	F	0.16	0/2225	0.44	0/3023
2	G	0.15	0/1837	0.39	0/2506
2	I	0.16	0/1854	0.38	0/2528
2	K	0.13	0/1831	0.36	0/2498
2	M	0.14	0/1831	0.40	0/2498
2	O	0.12	0/1831	0.37	0/2498
2	Q	0.12	0/1831	0.37	0/2498
3	H	0.32	0/1597	0.42	0/2178
3	J	0.15	0/1605	0.42	0/2189
3	L	0.22	0/1591	0.50	0/2170
3	N	0.15	0/1599	0.41	0/2181
3	P	0.15	0/1599	0.41	0/2181
3	R	0.20	0/1599	0.48	0/2181
All	All	0.20	1/33921 (0.0%)	0.41	1/46196 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	ASP	C-O	-5.66	1.16	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	VAL	CB-CA-C	-5.10	105.33	112.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2159	0	2106	77	0
1	B	2171	0	2118	58	0
1	C	2159	0	2105	85	0
1	D	2166	0	2112	48	0
1	E	2166	0	2113	68	0
1	F	2171	0	2117	82	0
2	G	1790	0	1735	34	0
2	I	1807	0	1752	46	0
2	K	1784	0	1731	46	0
2	M	1784	0	1731	29	0
2	O	1784	0	1731	32	0
2	Q	1784	0	1731	36	0
3	H	1561	0	1505	30	0
3	J	1568	0	1515	38	0
3	L	1555	0	1501	52	0
3	N	1562	0	1511	42	0
3	P	1562	0	1511	28	0
3	R	1562	0	1511	49	0
4	S	28	0	25	0	0
4	V	28	0	25	0	0
4	W	28	0	25	5	0
4	Y	28	0	25	1	0
4	Z	28	0	25	3	0
5	T	39	0	34	21	0
5	U	39	0	34	7	0
5	X	39	0	34	2	0
5	a	39	0	34	1	0
5	b	39	0	34	0	0
6	A	42	0	39	17	0
6	B	14	0	13	1	0
6	C	42	0	39	1	0
6	D	42	0	39	15	0
6	E	42	0	39	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	42	0	39	1	0
7	I	6	0	8	0	0
8	A	58	0	0	30	0
8	B	79	0	0	35	0
8	C	48	0	0	25	0
8	D	49	0	0	12	0
8	E	46	0	0	34	0
8	F	37	0	0	29	0
8	G	45	0	0	11	1
8	H	41	0	0	13	1
8	I	55	0	0	12	0
8	J	43	0	0	15	0
8	K	29	0	0	22	0
8	L	23	0	0	21	0
8	M	28	0	0	11	0
8	N	40	0	0	14	0
8	O	30	0	0	8	0
8	P	22	0	0	10	0
8	Q	24	0	0	13	0
8	R	25	0	0	12	0
All	All	34382	0	32647	902	1

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 14.

All (902) 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:A:63:ASN:HD21	5:T:1:NAG:C2	1.17	1.52
1:A:144:ASN:HD21	6:A:406:NAG:C1	1.21	1.49
1:C:220:ARG:CB	1:C:229:ARG:HH12	1.31	1.44
1:A:63:ASN:HD21	5:T:1:NAG:C1	1.41	1.32
1:A:144:ASN:ND2	6:A:406:NAG:C1	1.91	1.28
1:A:63:ASN:ND2	5:T:1:NAG:C2	1.95	1.27
1:B:201:ARG:HG3	8:B:505:HOH:O	1.16	1.26
1:A:290:ASN:HB2	8:A:501:HOH:O	1.27	1.25
3:L:172:ASN:CA	8:L:301:HOH:O	1.82	1.24
1:C:90:ARG:HB3	8:C:506:HOH:O	1.32	1.24
1:C:220:ARG:CB	1:C:229:ARG:NH1	1.99	1.23
1:F:283:THR:HG22	1:F:286:GLY:O	1.35	1.23
1:F:201:ARG:HA	8:F:506:HOH:O	1.41	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1:GLU:HA	8:K:304:HOH:O	1.05	1.20
2:O:101:THR:CB	8:O:301:HOH:O	1.88	1.19
1:A:63:ASN:ND2	5:T:1:NAG:H2	1.57	1.16
2:I:150:SER:HB3	8:I:404:HOH:O	1.46	1.16
1:B:207:LYS:C	8:B:502:HOH:O	1.89	1.16
1:C:220:ARG:HB3	1:C:229:ARG:NH1	1.54	1.15
3:R:145:ALA:C	8:R:303:HOH:O	1.88	1.15
3:J:33:ASP:OD2	3:J:68:LYS:HD2	1.43	1.14
2:K:10:GLU:N	8:K:302:HOH:O	1.81	1.13
2:K:10:GLU:CA	8:K:302:HOH:O	1.95	1.12
2:O:37:VAL:HG12	2:O:47:TRP:HA	1.31	1.12
3:R:145:ALA:N	8:R:303:HOH:O	1.82	1.12
3:N:91:SER:CB	8:N:303:HOH:O	1.94	1.11
1:A:225:ASN:C	8:A:503:HOH:O	1.91	1.10
3:J:33:ASP:OD2	3:J:68:LYS:CD	2.00	1.09
2:G:176:SER:C	8:G:303:HOH:O	1.93	1.08
3:L:172:ASN:CB	8:L:301:HOH:O	1.96	1.06
1:A:63:ASN:ND2	5:T:1:NAG:C1	2.14	1.06
2:O:101:THR:HB	8:O:301:HOH:O	1.47	1.05
1:C:219:PHE:N	8:C:503:HOH:O	1.80	1.04
3:L:25:THR:HG23	8:L:317:HOH:O	1.57	1.03
1:C:199:SER:O	8:C:502:HOH:O	1.73	1.03
3:L:172:ASN:C	8:L:301:HOH:O	1.98	1.02
1:A:290:ASN:CA	8:A:501:HOH:O	2.03	1.02
1:B:207:LYS:CA	8:B:502:HOH:O	2.06	1.02
1:F:142:ARG:N	8:F:505:HOH:O	1.90	1.02
1:B:202:ILE:N	8:B:505:HOH:O	1.91	1.02
3:N:158:LYS:N	8:N:301:HOH:O	1.83	1.01
1:C:220:ARG:HB3	1:C:229:ARG:HH12	0.88	1.01
2:K:224:ASN:ND2	8:K:303:HOH:O	1.82	1.01
2:K:216:CYS:C	8:K:301:HOH:O	2.04	1.01
1:A:290:ASN:C	8:A:501:HOH:O	2.04	1.00
1:E:242:ILE:HB	8:E:502:HOH:O	1.62	0.99
3:R:146:VAL:HG23	8:R:303:HOH:O	1.62	0.99
1:A:144:ASN:ND2	6:A:406:NAG:N2	2.09	0.99
1:F:201:ARG:CA	8:F:506:HOH:O	2.03	0.98
3:H:52:GLU:OE2	8:H:301:HOH:O	1.81	0.98
1:C:91:SER:N	8:C:506:HOH:O	1.94	0.98
3:P:125:GLU:CD	8:P:305:HOH:O	2.04	0.98
2:K:216:CYS:O	8:K:301:HOH:O	1.80	0.97
1:A:279:SER:O	8:A:502:HOH:O	1.82	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:10:GLU:CB	8:K:302:HOH:O	2.11	0.97
1:F:132:GLN:O	8:F:501:HOH:O	1.81	0.97
2:I:33:TYR:OH	8:I:401:HOH:O	1.81	0.97
1:D:166:VAL:O	8:D:501:HOH:O	1.83	0.97
3:L:48:LEU:O	8:L:302:HOH:O	1.82	0.96
1:C:220:ARG:HB2	1:C:229:ARG:HH12	1.26	0.96
1:A:290:ASN:O	8:A:501:HOH:O	1.81	0.96
1:B:206:THR:O	8:B:502:HOH:O	1.85	0.95
1:D:224:ARG:NH1	8:D:503:HOH:O	2.00	0.95
1:F:77:ASP:OD1	8:F:503:HOH:O	1.84	0.95
3:L:188:LYS:NZ	8:L:307:HOH:O	2.00	0.94
3:R:47:LYS:NZ	8:R:301:HOH:O	1.80	0.94
1:D:103:PRO:O	8:D:502:HOH:O	1.83	0.94
1:F:145:ASN:O	8:F:502:HOH:O	1.83	0.94
3:L:172:ASN:HB3	8:L:301:HOH:O	1.58	0.94
1:B:279:SER:O	8:B:501:HOH:O	1.84	0.94
1:E:172:GLU:OE1	8:E:501:HOH:O	1.84	0.94
1:A:144:ASN:HD22	6:A:406:NAG:HN2	1.00	0.94
1:A:63:ASN:HD21	5:T:1:NAG:H2	1.15	0.93
1:A:225:ASN:O	8:A:503:HOH:O	1.85	0.93
1:A:175:ASP:OD2	1:A:238:LYS:NZ	2.01	0.93
6:D:406:NAG:C8	6:D:406:NAG:H5	1.97	0.93
1:E:174:PHE:CE2	8:E:501:HOH:O	2.20	0.93
3:L:172:ASN:O	8:L:301:HOH:O	1.80	0.93
1:C:206:THR:HG23	1:C:208:ARG:H	1.32	0.93
3:L:5:THR:O	8:L:303:HOH:O	1.85	0.93
3:J:99:PHE:CE1	8:J:303:HOH:O	2.22	0.93
3:P:204:VAL:O	8:P:301:HOH:O	1.86	0.92
1:C:220:ARG:HB2	1:C:229:ARG:NH1	1.82	0.91
3:N:92:SER:N	8:N:303:HOH:O	2.02	0.91
1:A:144:ASN:ND2	6:A:406:NAG:HN2	1.67	0.91
2:I:149:LYS:C	8:I:404:HOH:O	2.12	0.91
1:F:283:THR:CG2	1:F:286:GLY:O	2.18	0.91
2:M:85:ARG:HA	8:M:303:HOH:O	1.70	0.91
8:A:514:HOH:O	5:T:1:NAG:H5	1.69	0.91
3:N:25:THR:HG22	3:N:26:ASN:H	1.35	0.91
1:F:108:LEU:O	8:F:504:HOH:O	1.89	0.91
2:K:1:GLU:OE1	8:K:304:HOH:O	1.87	0.91
2:M:85:ARG:N	8:M:303:HOH:O	1.99	0.90
2:M:149:LYS:O	8:M:301:HOH:O	1.90	0.90
3:J:112:LYS:O	8:J:301:HOH:O	1.89	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:THR:CB	8:E:510:HOH:O	2.21	0.89
2:O:99:ASP:OD1	8:O:301:HOH:O	1.88	0.89
2:G:44:GLY:O	8:G:301:HOH:O	1.89	0.89
1:D:165:ASN:HD22	4:Z:1:NAG:H61	1.35	0.88
1:E:242:ILE:O	8:E:502:HOH:O	1.91	0.88
2:Q:39:GLN:OE1	8:Q:301:HOH:O	1.91	0.88
8:B:504:HOH:O	4:W:2:NAG:O3	1.91	0.88
2:K:103:MET:O	8:K:305:HOH:O	1.92	0.88
1:C:219:PHE:HB2	8:C:503:HOH:O	1.73	0.88
1:E:283:THR:HB	8:E:510:HOH:O	1.74	0.87
1:F:111:LEU:HB3	8:F:504:HOH:O	1.74	0.87
2:M:85:ARG:CA	8:M:303:HOH:O	2.20	0.87
3:H:32:PHE:HB3	3:H:34:LEU:HD13	1.54	0.87
1:C:191:GLN:NE2	1:C:195:TYR:HD2	1.72	0.86
1:C:219:PHE:CB	8:C:503:HOH:O	2.23	0.86
1:F:200:GLY:O	8:F:506:HOH:O	1.93	0.86
2:G:100:LEU:O	8:G:302:HOH:O	1.91	0.86
3:H:162:GLU:OE2	8:H:302:HOH:O	1.92	0.86
3:R:101:GLY:O	8:R:305:HOH:O	1.91	0.86
3:R:6:GLN:HE22	3:R:102:GLY:N	1.73	0.86
1:E:172:GLU:HB3	8:E:501:HOH:O	1.76	0.85
1:A:233:TYR:HA	8:A:507:HOH:O	1.76	0.85
3:H:211:THR:CB	8:H:304:HOH:O	2.22	0.85
1:A:123:GLU:OE2	8:A:506:HOH:O	1.94	0.85
2:G:176:SER:O	8:G:303:HOH:O	1.92	0.85
1:E:242:ILE:O	8:E:504:HOH:O	1.94	0.84
1:E:199:SER:OG	8:E:503:HOH:O	1.94	0.84
1:E:243:LEU:HA	8:E:504:HOH:O	1.77	0.84
2:I:150:SER:CB	8:I:404:HOH:O	2.14	0.84
2:I:150:SER:N	8:I:404:HOH:O	2.10	0.84
3:L:32:PHE:O	8:L:304:HOH:O	1.95	0.84
1:A:234:TRP:N	8:A:507:HOH:O	1.98	0.84
1:C:118:LEU:O	8:C:505:HOH:O	1.94	0.83
3:L:34:LEU:O	8:L:305:HOH:O	1.96	0.83
1:A:144:ASN:ND2	6:A:406:NAG:C2	2.42	0.82
1:F:176:LYS:HB2	1:F:237:VAL:CG2	2.09	0.82
1:A:144:ASN:HD21	6:A:406:NAG:C2	1.93	0.81
1:E:144:ASN:ND2	6:E:405:NAG:O7	2.13	0.81
8:B:515:HOH:O	5:U:2:NAG:H4	1.79	0.81
1:C:41:GLU:HG2	1:C:42:LEU:H	1.43	0.81
2:I:83:LEU:HD23	2:I:86:LEU:CD2	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:406:NAG:H5	6:D:406:NAG:H82	1.62	0.80
3:L:175:ALA:O	8:L:306:HOH:O	1.99	0.80
3:N:104:LYS:NZ	8:N:306:HOH:O	2.14	0.80
3:P:52:GLU:OE1	8:P:303:HOH:O	2.00	0.80
1:F:292:LYS:C	8:F:510:HOH:O	2.24	0.80
2:K:10:GLU:OE1	2:K:12:LYS:NZ	2.15	0.80
2:O:44:GLY:O	8:O:302:HOH:O	1.99	0.80
1:B:202:ILE:CD1	1:B:247:SER:HB2	2.11	0.79
1:E:90:ARG:NH1	1:E:270:SER:O	2.14	0.79
1:B:201:ARG:CA	8:B:505:HOH:O	2.31	0.79
1:F:186:VAL:HG21	1:F:227:PRO:HG2	1.62	0.79
2:G:164:ASP:OD2	8:G:304:HOH:O	1.99	0.79
3:N:91:SER:C	8:N:303:HOH:O	2.23	0.79
1:B:285:ASN:OD1	8:B:508:HOH:O	1.98	0.79
3:J:91:SER:CB	8:J:303:HOH:O	2.30	0.79
1:A:150:ARG:HH12	6:A:407:NAG:H5	1.48	0.79
2:G:67:ARG:CZ	2:G:87:ARG:HH12	1.94	0.79
3:R:101:GLY:C	8:R:305:HOH:O	2.26	0.79
1:F:114:SER:O	8:F:507:HOH:O	2.01	0.79
3:J:99:PHE:CZ	8:J:303:HOH:O	2.36	0.79
2:K:10:GLU:HB2	8:K:302:HOH:O	1.76	0.79
1:A:63:ASN:ND2	5:T:1:NAG:N2	2.29	0.78
1:C:90:ARG:C	8:C:506:HOH:O	2.24	0.78
3:N:91:SER:OG	8:N:303:HOH:O	1.91	0.78
1:B:208:ARG:N	8:B:502:HOH:O	2.09	0.78
1:B:109:ARG:NH1	8:B:510:HOH:O	2.05	0.78
3:N:25:THR:HG22	3:N:26:ASN:N	1.97	0.78
1:C:191:GLN:NE2	1:C:195:TYR:CD2	2.52	0.77
2:M:42:GLY:N	8:M:302:HOH:O	1.95	0.77
3:P:196:GLN:OE1	8:P:304:HOH:O	2.02	0.77
2:Q:40:ALA:C	8:Q:304:HOH:O	2.26	0.77
1:F:293:PRO:N	8:F:510:HOH:O	2.18	0.77
6:A:406:NAG:C6	8:A:513:HOH:O	2.33	0.77
1:A:47:SER:HB3	1:A:288:ILE:HG22	1.66	0.77
1:D:66:LEU:HD21	1:D:112:VAL:HG13	1.67	0.77
3:J:155:SER:CB	8:J:304:HOH:O	2.32	0.77
2:Q:118:TYR:O	8:Q:302:HOH:O	2.01	0.77
3:L:5:THR:N	8:L:303:HOH:O	2.07	0.76
1:F:142:ARG:CA	8:F:505:HOH:O	2.32	0.76
2:I:27:TYR:O	8:I:402:HOH:O	2.03	0.76
3:R:28:ASP:O	3:R:30:GLY:N	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:TYR:CA	8:A:507:HOH:O	2.33	0.76
3:H:33:ASP:HB3	3:H:68:LYS:HZ3	1.50	0.76
1:C:77:ASP:OD2	8:C:507:HOH:O	2.01	0.76
1:E:262:SER:O	8:E:505:HOH:O	2.04	0.75
3:L:89:TYR:OH	8:L:308:HOH:O	2.03	0.75
1:A:206:THR:HG23	1:A:208:ARG:H	1.51	0.75
3:R:151:LYS:NZ	3:R:156:PRO:HG3	2.02	0.75
1:C:90:ARG:CB	8:C:506:HOH:O	2.07	0.74
3:R:145:ALA:CA	8:R:303:HOH:O	2.17	0.74
1:B:103:PRO:O	8:B:509:HOH:O	2.04	0.74
3:J:91:SER:OG	8:J:303:HOH:O	2.03	0.74
1:F:108:LEU:HA	8:F:504:HOH:O	1.86	0.74
1:F:201:ARG:CB	8:F:506:HOH:O	2.33	0.74
1:A:137:SER:OG	8:A:508:HOH:O	2.05	0.74
1:C:123:GLU:OE1	8:C:508:HOH:O	2.04	0.74
1:E:69:ALA:O	8:E:507:HOH:O	2.06	0.74
5:T:1:NAG:O7	5:T:1:NAG:O3	2.06	0.74
1:D:180:TRP:HE1	1:D:235:THR:HG23	1.52	0.74
1:E:68:ASP:OD2	8:E:506:HOH:O	2.05	0.74
5:U:1:NAG:O7	5:U:1:NAG:O3	2.06	0.73
3:L:209:ALA:HB3	3:L:212:GLU:OE2	1.87	0.73
1:F:115:SER:O	8:F:508:HOH:O	2.05	0.73
3:R:80:LEU:HD21	3:R:107:VAL:HG22	1.68	0.73
8:A:509:HOH:O	5:T:1:NAG:O5	2.06	0.73
2:O:101:THR:N	8:O:301:HOH:O	2.02	0.73
2:K:73:ASP:OD1	8:K:306:HOH:O	2.06	0.73
8:B:504:HOH:O	4:W:2:NAG:C3	2.36	0.73
3:H:211:THR:OG1	8:H:304:HOH:O	2.05	0.73
1:B:201:ARG:CG	8:B:505:HOH:O	1.93	0.72
1:F:120:PHE:HE2	1:F:122:ASN:OD1	1.71	0.72
3:J:151:LYS:HE2	8:J:324:HOH:O	1.89	0.72
2:K:217:ASN:CA	8:K:301:HOH:O	2.37	0.72
1:D:186:VAL:HG21	1:D:227:PRO:HG2	1.69	0.72
3:N:91:SER:HB2	8:N:303:HOH:O	1.70	0.72
3:P:125:GLU:OE2	8:P:305:HOH:O	2.04	0.72
1:A:121:ASN:HA	6:A:407:NAG:H82	1.70	0.72
2:I:83:LEU:HD23	2:I:86:LEU:HD21	1.71	0.72
1:D:263:GLY:O	8:D:504:HOH:O	2.07	0.72
1:E:158:ASN:OD1	8:E:508:HOH:O	2.07	0.72
2:M:147:SER:O	8:M:301:HOH:O	2.07	0.71
2:K:217:ASN:HA	8:K:301:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ARG:NH2	1:B:147:PHE:O	2.23	0.71
1:E:242:ILE:CA	8:E:502:HOH:O	2.37	0.71
6:A:408:NAG:O4	8:A:510:HOH:O	2.07	0.71
2:M:42:GLY:CA	8:M:302:HOH:O	2.32	0.71
1:B:211:GLN:NE2	8:B:516:HOH:O	2.24	0.71
3:L:32:PHE:HB3	3:L:34:LEU:HD13	1.71	0.71
2:M:187:PRO:O	8:M:304:HOH:O	2.07	0.71
1:A:186:VAL:HG11	1:A:227:PRO:HG2	1.72	0.70
3:J:52:GLU:OE2	8:J:305:HOH:O	2.09	0.70
1:B:119:GLU:OE1	1:B:261:ARG:NH1	2.23	0.70
3:J:91:SER:HB2	8:J:303:HOH:O	1.89	0.70
3:J:155:SER:N	8:J:304:HOH:O	2.08	0.70
3:R:20:ILE:O	3:R:74:SER:HA	1.91	0.70
2:I:192:SER:OG	8:I:403:HOH:O	2.09	0.70
2:Q:102:LEU:N	8:Q:305:HOH:O	2.22	0.70
2:I:150:SER:CA	8:I:404:HOH:O	2.38	0.69
1:B:118:LEU:O	8:B:511:HOH:O	2.09	0.69
2:Q:41:PRO:N	8:Q:304:HOH:O	2.26	0.69
8:D:505:HOH:O	4:Y:2:NAG:O5	2.08	0.69
3:N:51:TYR:OH	8:N:305:HOH:O	2.10	0.69
1:B:202:ILE:HD13	1:B:247:SER:HB2	1.74	0.69
1:E:62:GLU:O	8:E:509:HOH:O	2.09	0.69
3:H:100:GLY:O	8:H:305:HOH:O	2.09	0.69
2:I:83:LEU:CD2	2:I:86:LEU:CD2	2.71	0.69
6:D:405:NAG:H3	6:D:405:NAG:H82	1.74	0.69
2:G:43:GLN:O	8:G:306:HOH:O	2.10	0.69
1:C:150:ARG:O	8:C:509:HOH:O	2.11	0.68
1:F:305:CYS:O	8:F:509:HOH:O	2.11	0.68
2:G:93:VAL:HG22	2:G:128:THR:HG22	1.73	0.68
1:F:201:ARG:HB2	8:F:506:HOH:O	1.92	0.68
6:A:407:NAG:O7	8:A:512:HOH:O	2.12	0.68
1:C:203:THR:HG22	1:C:246:ASN:HB2	1.75	0.68
6:D:406:NAG:H82	6:D:406:NAG:C1	2.24	0.68
2:G:60:TYR:HB2	2:G:65:GLN:HG2	1.76	0.68
3:H:5:THR:O	8:H:307:HOH:O	2.10	0.68
1:B:207:LYS:HA	8:B:502:HOH:O	1.80	0.68
1:F:44:GLN:NE2	8:F:511:HOH:O	2.23	0.67
2:Q:72:ARG:NH1	8:Q:308:HOH:O	2.26	0.67
1:A:187:THR:OG1	8:A:504:HOH:O	1.93	0.67
6:A:406:NAG:O6	8:A:513:HOH:O	2.13	0.67
3:L:172:ASN:HA	8:L:301:HOH:O	1.68	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:THR:OG1	8:E:510:HOH:O	2.10	0.67
1:F:168:MET:HE3	1:F:169:PRO:HD2	1.77	0.67
1:E:60:ASP:OD1	1:E:90:ARG:NE	2.27	0.67
1:E:242:ILE:CB	8:E:502:HOH:O	2.32	0.67
2:O:72:ARG:NH1	8:O:304:HOH:O	2.28	0.67
3:R:6:GLN:NE2	3:R:102:GLY:N	2.43	0.67
1:D:52:CYS:O	8:D:507:HOH:O	2.12	0.67
6:D:406:NAG:H5	6:D:406:NAG:H83	1.77	0.66
1:E:206:THR:HG22	8:E:504:HOH:O	1.96	0.66
3:H:211:THR:HB	8:H:304:HOH:O	1.87	0.66
1:C:288:ILE:HG21	1:C:297:VAL:HG21	1.77	0.66
2:G:67:ARG:CZ	2:G:87:ARG:NH1	2.58	0.66
3:J:200:GLU:OE2	8:J:306:HOH:O	2.13	0.66
2:I:118:TYR:O	8:I:405:HOH:O	2.14	0.66
2:Q:2:VAL:CG1	2:Q:122:VAL:HG21	2.25	0.66
1:F:288:ILE:HG21	1:F:297:VAL:HG21	1.77	0.66
1:F:42:LEU:HD23	1:F:42:LEU:O	1.95	0.66
1:B:65:THR:HG23	8:B:518:HOH:O	1.95	0.65
3:R:151:LYS:HZ3	3:R:156:PRO:HG3	1.60	0.65
1:A:62:GLU:HG2	5:T:1:NAG:C8	2.27	0.65
2:Q:101:THR:O	8:Q:303:HOH:O	2.13	0.65
1:B:202:ILE:HD12	1:B:251:LEU:HB2	1.79	0.65
2:I:73:ASP:OD1	8:I:406:HOH:O	2.14	0.65
2:M:88:SER:HA	2:M:131:VAL:HG13	1.78	0.65
3:H:33:ASP:HB3	3:H:68:LYS:NZ	2.12	0.65
1:E:199:SER:CB	8:E:503:HOH:O	2.43	0.65
1:B:70:LEU:O	8:B:512:HOH:O	2.14	0.65
2:G:103:MET:HE3	2:G:112:ARG:HB3	1.78	0.65
3:J:155:SER:HB2	8:J:304:HOH:O	1.95	0.65
8:A:514:HOH:O	5:T:1:NAG:O6	2.13	0.64
1:C:63:ASN:OD1	1:C:92:LYS:HG3	1.97	0.64
1:C:154:LEU:O	8:C:512:HOH:O	2.15	0.64
8:Q:301:HOH:O	3:R:89:TYR:OH	2.14	0.64
1:A:290:ASN:CB	8:A:501:HOH:O	1.89	0.64
2:K:1:GLU:CA	8:K:304:HOH:O	1.88	0.64
1:A:168:MET:HE3	1:A:169:PRO:HD2	1.78	0.64
1:B:177:LEU:HB2	1:B:260:ILE:HD11	1.79	0.64
3:R:71:ASN:O	3:R:71:ASN:ND2	2.31	0.64
1:C:90:ARG:CA	8:C:506:HOH:O	2.38	0.64
2:K:30:THR:HA	2:K:53:PRO:HB2	1.78	0.64
3:L:209:ALA:HB3	3:L:212:GLU:CD	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:125:GLU:OE1	8:P:305:HOH:O	2.08	0.64
3:L:106:THR:HG21	3:L:143:PRO:HB3	1.81	0.63
1:A:63:ASN:HD22	5:T:1:NAG:H2	1.57	0.63
8:B:515:HOH:O	5:U:2:NAG:C5	2.46	0.63
1:B:185:PRO:HG2	1:B:217:ILE:HG12	1.80	0.63
1:E:167:THR:HG23	1:E:242:ILE:HG21	1.80	0.63
3:R:22:CYS:HB3	3:R:73:ALA:HB3	1.80	0.63
3:R:174:TYR:HE2	8:R:310:HOH:O	1.81	0.63
1:A:63:ASN:CG	5:T:1:NAG:C1	2.71	0.63
1:F:176:LYS:HB2	1:F:237:VAL:HG23	1.79	0.63
3:L:115:PRO:HB3	3:L:141:PHE:HB3	1.79	0.63
1:B:310:LYS:HB2	8:B:507:HOH:O	1.97	0.62
6:A:406:NAG:H61	8:A:513:HOH:O	1.95	0.62
1:F:186:VAL:HG12	1:F:187:THR:HG23	1.82	0.62
1:A:42:LEU:HA	1:A:292:LYS:HD2	1.81	0.62
1:A:150:ARG:NH1	6:A:407:NAG:H5	2.14	0.62
2:O:165:TYR:CE1	2:O:170:VAL:HG23	2.34	0.62
2:G:176:SER:CA	8:G:303:HOH:O	2.36	0.62
3:J:29:VAL:O	3:J:33:ASP:OD1	2.17	0.62
1:A:62:GLU:HG2	5:T:1:NAG:H83	1.81	0.62
4:Z:1:NAG:O7	4:Z:1:NAG:O3	2.18	0.62
3:P:151:LYS:HB2	3:P:194:SER:HB2	1.82	0.61
1:C:207:LYS:NZ	1:C:241:ASP:HA	2.13	0.61
1:D:245:ILE:N	8:D:501:HOH:O	2.29	0.61
1:A:144:ASN:CG	6:A:406:NAG:C1	2.71	0.61
6:C:406:NAG:O7	6:C:406:NAG:H3	1.99	0.61
3:J:56:ARG:HG2	3:J:60:VAL:HB	1.82	0.61
1:D:186:VAL:HG23	1:D:228:SER:OG	2.00	0.61
1:F:138:ALA:CB	1:F:226:ILE:CD1	2.79	0.61
2:I:87:ARG:O	2:I:131:VAL:HG11	2.00	0.61
3:N:10:VAL:HG23	3:N:105:LEU:HD13	1.83	0.61
2:M:87:ARG:O	2:M:131:VAL:HG11	2.01	0.61
1:B:80:GLN:O	8:B:514:HOH:O	2.16	0.61
8:B:515:HOH:O	5:U:2:NAG:C4	2.45	0.61
6:D:406:NAG:H82	6:D:406:NAG:C5	2.30	0.61
2:M:42:GLY:HA2	8:M:302:HOH:O	1.98	0.61
1:F:120:PHE:CE2	1:F:122:ASN:OD1	2.53	0.61
3:J:152:ALA:O	8:J:304:HOH:O	2.16	0.61
3:J:33:ASP:CG	3:J:68:LYS:CD	2.74	0.60
1:F:114:SER:C	8:F:507:HOH:O	2.43	0.60
2:G:193:SER:OG	8:G:305:HOH:O	2.04	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:6:GLN:HE22	3:R:102:GLY:C	2.09	0.60
1:E:165:ASN:HD22	6:E:406:NAG:H61	1.66	0.60
1:D:66:LEU:CD2	1:D:112:VAL:HG13	2.32	0.60
1:E:166:VAL:HG12	1:E:245:ILE:HB	1.84	0.60
3:N:185:GLU:OE1	3:N:185:GLU:N	2.33	0.60
3:H:159:ALA:O	8:H:308:HOH:O	2.16	0.60
3:L:169:GLN:N	8:L:311:HOH:O	2.34	0.60
3:N:10:VAL:HG23	3:N:105:LEU:CD1	2.31	0.60
2:Q:91:THR:HG23	2:Q:130:ALA:HA	1.83	0.60
1:F:177:LEU:HB2	1:F:260:ILE:HD11	1.83	0.60
2:G:83:LEU:HD23	2:G:86:LEU:CD2	2.31	0.59
2:O:2:VAL:HG12	2:O:122:VAL:HG11	1.84	0.59
2:Q:37:VAL:HG22	2:Q:47:TRP:HA	1.84	0.59
1:A:62:GLU:HB3	5:T:1:NAG:H82	1.85	0.59
1:D:165:ASN:ND2	4:Z:1:NAG:H61	2.13	0.59
6:F:406:NAG:O7	6:F:406:NAG:O3	2.19	0.59
2:G:2:VAL:HG12	2:G:122:VAL:HG11	1.82	0.59
1:E:242:ILE:C	8:E:502:HOH:O	2.38	0.59
3:P:134:LEU:HD12	3:P:180:LEU:HD23	1.84	0.59
1:A:207:LYS:HZ2	1:A:242:ILE:HD12	1.68	0.59
1:C:220:ARG:CG	1:C:229:ARG:NH1	2.66	0.59
2:G:101:THR:O	8:G:307:HOH:O	2.17	0.59
3:H:211:THR:N	8:H:304:HOH:O	2.34	0.59
3:P:71:ASN:O	3:P:71:ASN:ND2	2.34	0.59
2:Q:234:LYS:NZ	3:R:212:GLU:OE2	2.28	0.59
2:I:189:VAL:HG21	3:J:162:GLU:HG3	1.85	0.59
1:D:62:GLU:O	8:D:508:HOH:O	2.17	0.59
1:F:306:PRO:HA	8:F:509:HOH:O	2.02	0.59
3:J:33:ASP:OD2	3:J:68:LYS:CE	2.51	0.59
2:Q:53:PRO:HA	2:Q:72:ARG:HD2	1.83	0.59
1:C:47:SER:HB2	1:C:288:ILE:HG22	1.85	0.58
3:P:185:GLU:OE1	3:P:185:GLU:N	2.33	0.58
2:Q:2:VAL:HG11	2:Q:122:VAL:HG21	1.85	0.58
6:D:405:NAG:H3	6:D:405:NAG:C8	2.29	0.58
1:F:138:ALA:CB	1:F:226:ILE:HD12	2.34	0.58
8:K:311:HOH:O	3:L:44:LYS:C	2.46	0.58
3:L:110:GLN:OE1	3:L:173:LYS:NZ	2.21	0.58
3:N:32:PHE:HB3	3:N:34:LEU:HD13	1.86	0.58
1:B:283:THR:OG1	1:B:286:GLY:O	2.19	0.57
2:Q:2:VAL:HG23	2:Q:27:TYR:CD1	2.38	0.57
1:E:206:THR:HA	8:E:504:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:SER:OG	1:D:208:ARG:O	2.22	0.57
3:L:209:ALA:HB3	3:L:212:GLU:OE1	2.03	0.57
1:B:202:ILE:HD11	1:B:249:GLY:O	2.04	0.57
1:E:232:ILE:O	8:E:511:HOH:O	2.18	0.57
2:K:217:ASN:N	8:K:301:HOH:O	2.30	0.57
3:R:6:GLN:HE22	3:R:102:GLY:H	1.47	0.57
3:R:56:ARG:CZ	3:R:62:ASP:HA	2.33	0.57
2:I:53:PRO:O	2:I:72:ARG:NH1	2.37	0.57
3:N:33:ASP:O	3:N:35:VAL:N	2.29	0.57
3:N:71:ASN:O	3:N:71:ASN:ND2	2.36	0.57
1:B:201:ARG:HA	8:B:505:HOH:O	2.01	0.57
2:I:231:VAL:O	8:I:407:HOH:O	2.17	0.57
3:R:185:GLU:OE1	3:R:185:GLU:N	2.35	0.57
2:O:229:LYS:NZ	3:P:125:GLU:OE2	2.37	0.57
1:C:223:ILE:HD13	1:C:229:ARG:HH21	1.70	0.57
3:L:18:VAL:HG21	3:L:105:LEU:HD11	1.85	0.57
3:R:164:THR:HG22	3:R:177:SER:H	1.69	0.57
1:E:142:ARG:NH1	8:E:515:HOH:O	2.36	0.57
3:P:37:TRP:NE1	8:P:302:HOH:O	1.94	0.57
1:A:45:ASN:HA	1:A:296:ASN:OD1	2.05	0.56
1:D:206:THR:HG23	1:D:208:ARG:H	1.70	0.56
1:A:291:ASP:OD2	8:A:516:HOH:O	2.18	0.56
1:C:219:PHE:CD2	8:C:503:HOH:O	2.52	0.56
1:C:219:PHE:HD2	8:C:503:HOH:O	1.88	0.56
1:F:138:ALA:HB2	1:F:226:ILE:CD1	2.35	0.56
2:K:131:VAL:HG13	2:K:131:VAL:O	2.05	0.56
3:J:81:GLN:O	3:J:107:VAL:HG21	2.05	0.56
2:O:91:THR:HG23	2:O:130:ALA:HA	1.88	0.56
2:K:88:SER:HA	2:K:131:VAL:HG13	1.86	0.56
1:D:81:ASN:HD21	6:D:405:NAG:C8	2.18	0.56
3:H:81:GLN:O	3:H:107:VAL:HG21	2.06	0.56
3:R:28:ASP:C	3:R:30:GLY:H	2.11	0.56
1:A:234:TRP:NE1	8:A:505:HOH:O	1.94	0.56
1:B:206:THR:C	8:B:502:HOH:O	2.37	0.56
2:K:10:GLU:C	8:K:302:HOH:O	2.32	0.56
6:D:405:NAG:O4	6:D:405:NAG:O7	2.24	0.56
1:D:81:ASN:HD21	6:D:405:NAG:C7	2.19	0.56
3:J:33:ASP:CG	3:J:68:LYS:HD2	2.25	0.55
3:N:110:GLN:NE2	8:N:304:HOH:O	1.97	0.55
1:A:289:PRO:HB3	1:C:199:SER:HB3	1.87	0.55
1:C:206:THR:HG23	1:C:208:ARG:N	2.12	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:115:PRO:HB3	3:R:141:PHE:HB3	1.87	0.55
6:A:408:NAG:O7	8:A:517:HOH:O	2.18	0.55
3:H:56:ARG:HG2	3:H:60:VAL:HB	1.88	0.55
2:I:131:VAL:O	2:I:131:VAL:HG13	2.05	0.55
2:K:91:THR:HG23	2:K:130:ALA:HA	1.87	0.55
3:L:151:LYS:HB2	3:L:194:SER:HB2	1.87	0.55
1:C:87:PHE:HB3	1:C:267:ILE:HD12	1.88	0.55
2:O:83:LEU:HD23	2:O:86:LEU:CD2	2.37	0.55
1:C:222:ARG:HH21	1:C:225:ASN:CG	2.15	0.55
1:E:174:PHE:CZ	8:E:501:HOH:O	2.52	0.55
3:H:33:ASP:C	3:H:35:VAL:H	2.13	0.55
1:F:238:LYS:HG3	1:F:239:PRO:HD2	1.88	0.55
2:I:148:SER:OG	3:J:213:CYS:HB3	2.07	0.55
3:L:85:GLU:HG3	3:L:105:LEU:O	2.07	0.55
1:A:269:ARG:NE	8:A:515:HOH:O	2.16	0.55
2:Q:44:GLY:HA2	3:R:89:TYR:HE2	1.72	0.55
1:A:43:VAL:HG22	1:A:294:PHE:HB2	1.88	0.55
2:I:2:VAL:HG13	2:I:27:TYR:CD1	2.42	0.55
2:M:2:VAL:HG12	2:M:122:VAL:HG11	1.89	0.55
3:H:173:LYS:NZ	8:H:309:HOH:O	2.16	0.54
2:I:91:THR:HG23	2:I:130:ALA:HA	1.90	0.54
1:A:259:LYS:NZ	1:A:259:LYS:HB3	2.22	0.54
2:Q:2:VAL:HG23	2:Q:27:TYR:HD1	1.73	0.54
1:C:42:LEU:O	1:C:292:LYS:HB3	2.07	0.54
1:B:311:GLN:N	8:B:507:HOH:O	1.93	0.54
1:E:242:ILE:N	8:E:502:HOH:O	2.37	0.54
1:A:227:PRO:HD3	8:A:503:HOH:O	2.06	0.54
1:C:94:TYR:HE1	5:X:1:NAG:HN2	1.55	0.54
1:D:168:MET:HE3	1:D:169:PRO:HD2	1.90	0.54
1:E:97:CYS:SG	1:E:98:TYR:N	2.79	0.54
1:E:299:ARG:NH2	8:E:516:HOH:O	2.37	0.54
2:M:131:VAL:HG13	2:M:131:VAL:O	2.07	0.54
1:F:176:LYS:HB2	1:F:237:VAL:HG22	1.88	0.54
3:H:28:ASP:OD2	3:H:29:VAL:HG13	2.08	0.54
1:A:207:LYS:NZ	1:A:242:ILE:HD12	2.23	0.53
1:C:237:VAL:HG21	1:C:243:LEU:HB2	1.90	0.53
1:C:283:THR:HG22	1:C:301:THR:HG22	1.88	0.53
1:F:241:ASP:OD1	1:F:242:ILE:N	2.40	0.53
3:J:151:LYS:HB2	3:J:194:SER:HB2	1.89	0.53
1:B:74:PRO:HB3	1:B:141:ARG:HB2	1.89	0.53
1:E:45:ASN:HA	1:E:296:ASN:OD1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:168:LYS:HA	3:R:174:TYR:HD1	1.74	0.53
1:E:67:ILE:HG13	1:E:105:TYR:HE1	1.73	0.53
1:E:288:ILE:HG21	1:E:297:VAL:HG21	1.90	0.53
1:F:108:LEU:CA	8:F:504:HOH:O	2.52	0.53
1:C:283:THR:OG1	1:C:286:GLY:O	2.22	0.53
1:D:47:SER:HB3	1:D:288:ILE:HG22	1.89	0.53
3:N:32:PHE:HB3	3:N:34:LEU:CD1	2.39	0.53
1:A:173:GLN:NE2	1:F:307:ARG:NH1	2.57	0.53
1:B:186:VAL:HG21	1:B:227:PRO:HG2	1.91	0.53
2:K:218:VAL:HB	2:K:227:VAL:HG22	1.91	0.53
3:P:146:VAL:CG2	3:P:197:VAL:HG13	2.39	0.53
1:B:241:ASP:OD1	1:B:242:ILE:N	2.38	0.52
1:E:169:PRO:HB3	1:E:242:ILE:HD12	1.91	0.52
3:R:128:GLN:NE2	8:R:304:HOH:O	1.88	0.52
1:C:291:ASP:N	8:C:521:HOH:O	2.41	0.52
3:N:159:ALA:N	8:N:301:HOH:O	2.03	0.52
3:P:115:PRO:HB3	3:P:141:PHE:HB3	1.91	0.52
1:C:221:PRO:O	1:C:229:ARG:NH2	2.42	0.52
2:G:139:PRO:HB3	2:G:165:TYR:HB3	1.91	0.52
3:L:82:ALA:HA	3:L:107:VAL:HG11	1.90	0.52
1:F:138:ALA:CB	1:F:226:ILE:HD11	2.40	0.52
1:A:68:ASP:OD1	1:A:100:TYR:OH	2.21	0.52
1:C:186:VAL:HG21	1:C:227:PRO:HG2	1.90	0.52
1:E:158:ASN:ND2	3:P:52:GLU:OE1	2.35	0.52
3:H:85:GLU:CD	8:H:316:HOH:O	2.53	0.52
2:K:228:ASP:HA	8:K:301:HOH:O	2.08	0.52
2:M:87:ARG:HD2	8:M:311:HOH:O	2.10	0.52
3:N:134:LEU:HD12	3:N:180:LEU:HD23	1.92	0.52
3:P:117:VAL:O	3:P:206:LYS:NZ	2.43	0.52
1:E:42:LEU:HA	1:E:292:LYS:HD2	1.92	0.52
3:N:33:ASP:C	3:N:35:VAL:H	2.16	0.52
1:E:182:VAL:HG11	1:E:213:VAL:HG11	1.92	0.52
1:F:87:PHE:HB3	1:F:267:ILE:HD12	1.92	0.52
3:P:33:ASP:C	3:P:35:VAL:H	2.18	0.52
1:C:175:ASP:OD2	1:C:238:LYS:NZ	2.41	0.52
2:K:117:TYR:O	3:L:34:LEU:HD23	2.10	0.52
2:K:218:VAL:HB	2:K:227:VAL:CG2	2.40	0.52
3:P:52:GLU:HB3	3:P:55:ARG:HH21	1.73	0.52
3:R:6:GLN:HE22	3:R:102:GLY:CA	2.22	0.52
1:B:202:ILE:CD1	1:B:251:LEU:HB2	2.38	0.52
1:A:189:LYS:O	1:A:193:PHE:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:406:NAG:C8	6:D:406:NAG:C1	2.85	0.51
1:E:40:THR:OG1	1:E:41:GLU:N	2.44	0.51
2:K:87:ARG:O	2:K:131:VAL:HG11	2.10	0.51
1:F:306:PRO:C	8:F:509:HOH:O	2.53	0.51
3:H:194:SER:OG	8:H:310:HOH:O	2.19	0.51
2:I:36:TRP:HB3	2:I:48:MET:HE3	1.91	0.51
1:C:207:LYS:HZ1	1:C:241:ASP:HA	1.75	0.51
1:A:283:THR:HG22	1:A:301:THR:HG22	1.92	0.51
1:C:182:VAL:HG22	1:C:202:ILE:HD12	1.92	0.51
3:J:168:LYS:HD3	3:J:172:ASN:OD1	2.09	0.51
1:E:310:LYS:O	1:E:311:GLN:HG3	2.11	0.51
2:M:4:LEU:HD22	2:M:24:THR:HG22	1.93	0.51
3:P:22:CYS:HB3	3:P:73:ALA:HB3	1.92	0.51
2:Q:41:PRO:C	8:Q:304:HOH:O	2.54	0.51
2:G:57:ASP:OD1	2:G:58:THR:N	2.44	0.51
2:M:37:VAL:HG22	2:M:47:TRP:HA	1.92	0.51
1:F:138:ALA:HB2	1:F:226:ILE:HD11	1.91	0.51
1:F:109:ARG:HH12	1:F:269:ARG:NE	2.08	0.51
1:D:177:LEU:HB2	1:D:260:ILE:HD11	1.92	0.51
2:Q:40:ALA:CB	8:Q:304:HOH:O	2.59	0.51
1:C:138:ALA:HB2	1:C:226:ILE:CD1	2.40	0.50
2:Q:4:LEU:HD22	2:Q:24:THR:HG22	1.93	0.50
3:L:23:THR:O	8:L:303:HOH:O	2.19	0.50
2:Q:139:PRO:HB3	2:Q:165:TYR:HB3	1.92	0.50
1:D:204:VAL:HG13	1:D:245:ILE:HG12	1.92	0.50
1:F:59:LEU:HD22	1:F:87:PHE:CE2	2.47	0.50
1:D:222:ARG:NH1	1:D:227:PRO:HD3	2.26	0.50
3:N:151:LYS:NZ	3:N:156:PRO:HG3	2.27	0.50
2:K:158:LEU:HB2	2:K:231:VAL:HG11	1.93	0.50
3:L:56:ARG:CZ	3:L:62:ASP:HA	2.42	0.50
2:M:1:GLU:O	2:M:1:GLU:HG2	2.11	0.50
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.92	0.50
1:E:199:SER:HB3	8:E:503:HOH:O	2.10	0.50
3:L:58:SER:O	8:L:310:HOH:O	2.20	0.50
8:B:503:HOH:O	4:W:2:NAG:C4	2.49	0.50
1:D:97:CYS:SG	1:D:98:TYR:N	2.83	0.50
1:D:168:MET:HE3	1:D:168:MET:HA	1.94	0.50
2:K:37:VAL:HG21	2:K:123:TRP:CZ3	2.46	0.50
3:L:30:GLY:HA3	3:L:71:ASN:HA	1.94	0.50
1:C:283:THR:CB	8:C:513:HOH:O	2.60	0.50
8:A:509:HOH:O	5:T:1:NAG:C5	2.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:PHE:HA	1:B:82:LYS:HD2	1.95	0.49
1:E:118:LEU:O	8:E:512:HOH:O	2.19	0.49
1:E:167:THR:HG23	1:E:242:ILE:CG2	2.42	0.49
1:F:97:CYS:SG	1:F:98:TYR:N	2.80	0.49
3:L:29:VAL:HG23	3:L:35:VAL:HG21	1.92	0.49
1:B:47:SER:HB3	1:B:288:ILE:HG22	1.93	0.49
1:B:259:LYS:NZ	1:B:259:LYS:HB3	2.27	0.49
3:H:37:TRP:HB2	3:H:50:ILE:HB	1.93	0.49
2:K:210:GLY:HA2	8:K:307:HOH:O	2.11	0.49
8:B:515:HOH:O	5:U:2:NAG:O5	2.20	0.49
5:a:1:NAG:O7	5:a:1:NAG:H3	2.11	0.49
1:E:125:PHE:O	8:E:513:HOH:O	2.20	0.49
2:K:10:GLU:O	8:K:302:HOH:O	2.20	0.49
2:Q:41:PRO:O	8:Q:304:HOH:O	2.19	0.49
1:B:43:VAL:HG22	1:B:294:PHE:HB2	1.94	0.49
1:E:283:THR:OG1	1:E:286:GLY:O	2.28	0.49
2:I:189:VAL:HB	3:J:164:THR:HG22	1.93	0.49
2:K:139:PRO:HB3	2:K:165:TYR:HB3	1.94	0.49
2:M:139:PRO:HB3	2:M:165:TYR:HB3	1.94	0.49
5:T:1:NAG:HO3	5:T:1:NAG:C7	2.18	0.49
5:U:1:NAG:HO3	5:U:1:NAG:C7	2.17	0.49
1:C:203:THR:CG2	1:C:246:ASN:HB2	2.42	0.49
1:F:261:ARG:HB2	8:F:508:HOH:O	2.12	0.49
1:A:301:THR:HB	1:A:305:CYS:SG	2.53	0.49
3:R:179:TYR:O	8:R:306:HOH:O	2.19	0.49
1:C:79:PHE:HA	1:C:82:LYS:HD2	1.95	0.49
1:E:261:ARG:NH1	8:E:521:HOH:O	2.45	0.49
1:F:306:PRO:CA	8:F:509:HOH:O	2.59	0.49
1:A:97:CYS:SG	1:A:98:TYR:N	2.84	0.48
1:D:241:ASP:OD1	1:D:242:ILE:N	2.43	0.48
3:R:15:GLY:N	3:R:80:LEU:O	2.37	0.48
1:F:201:ARG:O	1:F:247:SER:HA	2.12	0.48
8:Q:301:HOH:O	3:R:89:TYR:CE2	2.66	0.48
3:N:117:VAL:O	3:N:206:LYS:NZ	2.46	0.48
2:O:37:VAL:HG12	2:O:47:TRP:CA	2.23	0.48
2:O:67:ARG:NH2	2:O:90:ASP:OD2	2.45	0.48
3:N:23:THR:HG22	3:N:72:THR:HG23	1.95	0.48
1:C:301:THR:HB	1:C:305:CYS:SG	2.54	0.48
2:Q:40:ALA:HB1	8:Q:304:HOH:O	2.13	0.48
1:C:138:ALA:HB2	1:C:226:ILE:HD11	1.95	0.48
1:F:109:ARG:HH12	1:F:269:ARG:HE	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:62:ASP:CG	8:J:302:HOH:O	2.56	0.48
3:P:81:GLN:O	3:P:107:VAL:HG21	2.13	0.48
1:B:295:GLN:HG2	1:B:297:VAL:H	1.79	0.48
1:C:97:CYS:SG	1:C:98:TYR:N	2.84	0.48
2:I:4:LEU:HD22	2:I:24:THR:HG22	1.95	0.48
2:I:12:LYS:O	2:I:131:VAL:HA	2.14	0.48
3:R:18:VAL:HG21	3:R:105:LEU:HD11	1.95	0.48
1:C:92:LYS:HG2	8:C:506:HOH:O	2.12	0.48
1:E:299:ARG:NE	8:E:516:HOH:O	2.44	0.48
2:O:83:LEU:HD23	2:O:86:LEU:HD21	1.95	0.48
1:B:214:ILE:O	1:B:214:ILE:HG13	2.12	0.48
2:K:209:LEU:O	8:K:307:HOH:O	2.20	0.48
3:R:6:GLN:NE2	3:R:102:GLY:H	2.09	0.48
6:D:406:NAG:O6	8:D:506:HOH:O	2.20	0.47
2:G:126:GLY:O	8:G:308:HOH:O	2.20	0.47
2:G:189:VAL:HB	3:H:164:THR:HG22	1.95	0.47
2:O:201:VAL:HG21	3:P:137:LEU:HD13	1.95	0.47
2:Q:234:LYS:HG2	2:Q:235:SER:H	1.79	0.47
1:D:108:LEU:O	1:D:112:VAL:HG12	2.14	0.47
3:J:27:SER:HA	3:J:31:THR:OG1	2.14	0.47
2:K:47:TRP:CG	3:L:97:VAL:HB	2.48	0.47
2:Q:12:LYS:O	2:Q:131:VAL:HA	2.15	0.47
3:R:56:ARG:HD3	3:R:60:VAL:O	2.14	0.47
3:R:151:LYS:HZ2	3:R:156:PRO:HG3	1.74	0.47
2:G:10:GLU:HB2	2:G:129:VAL:HG12	1.95	0.47
1:D:84:TRP:CE2	1:D:116:GLY:HA2	2.49	0.47
1:F:47:SER:HB3	1:F:288:ILE:HG22	1.96	0.47
2:I:46:GLU:OE2	2:I:63:LYS:HE2	2.14	0.47
2:I:139:PRO:HB3	2:I:165:TYR:HB3	1.97	0.47
2:M:234:LYS:HG2	2:M:235:SER:N	2.29	0.47
1:B:176:LYS:HD3	1:B:257:TYR:CD1	2.50	0.47
1:D:79:PHE:HA	1:D:82:LYS:HD2	1.96	0.47
1:F:75:GLN:NE2	1:F:94:TYR:O	2.43	0.47
2:G:4:LEU:HD22	2:G:24:THR:HG22	1.97	0.47
3:R:6:GLN:NE2	3:R:102:GLY:C	2.73	0.47
1:B:97:CYS:SG	1:B:98:TYR:N	2.84	0.47
1:B:280:GLU:HG3	1:B:280:GLU:O	2.14	0.47
1:D:134:GLY:HA3	1:D:153:TRP:HB3	1.97	0.47
1:D:202:ILE:HD13	1:D:247:SER:HB2	1.96	0.47
1:D:254:PRO:O	8:D:509:HOH:O	2.20	0.47
1:F:79:PHE:HA	1:F:82:LYS:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:SER:HA	1:F:265:SER:O	2.15	0.47
2:I:171:THR:OG1	2:I:219:ASN:HB3	2.15	0.47
2:K:36:TRP:HB3	2:K:48:MET:HE3	1.95	0.47
2:Q:10:GLU:HB2	2:Q:129:VAL:HG23	1.97	0.47
1:D:206:THR:OG1	1:D:207:LYS:N	2.48	0.47
3:N:25:THR:CG2	3:N:26:ASN:N	2.68	0.47
8:A:514:HOH:O	5:T:1:NAG:C5	2.44	0.47
1:F:176:LYS:HD3	1:F:257:TYR:CD1	2.50	0.47
3:H:23:THR:N	8:H:307:HOH:O	2.47	0.47
2:I:60:TYR:HB2	2:I:65:GLN:HG2	1.96	0.47
3:J:33:ASP:OD2	3:J:68:LYS:HD3	2.08	0.47
2:K:141:VAL:HG21	2:K:227:VAL:HG21	1.96	0.47
1:C:304:ALA:N	8:C:520:HOH:O	2.39	0.47
3:L:191:ARG:O	3:L:209:ALA:HB1	2.15	0.47
1:E:295:GLN:HB3	1:E:306:PRO:HG2	1.96	0.46
2:O:4:LEU:HD22	2:O:24:THR:HG22	1.96	0.46
2:O:101:THR:OG1	8:O:301:HOH:O	2.14	0.46
2:O:229:LYS:NZ	8:P:305:HOH:O	2.47	0.46
3:P:33:ASP:O	3:P:35:VAL:N	2.41	0.46
1:E:167:THR:CG2	1:E:242:ILE:HG21	2.45	0.46
2:I:47:TRP:O	8:I:408:HOH:O	2.20	0.46
2:O:64:PHE:O	2:O:68:VAL:HG12	2.15	0.46
1:C:166:VAL:HG12	1:C:245:ILE:HB	1.97	0.46
1:D:203:THR:CG2	1:D:246:ASN:HB2	2.45	0.46
1:D:206:THR:HG23	1:D:209:SER:H	1.80	0.46
3:N:165:THR:O	8:N:307:HOH:O	2.21	0.46
1:E:165:ASN:ND2	6:E:406:NAG:H61	2.31	0.46
1:F:108:LEU:HD12	8:F:504:HOH:O	2.15	0.46
2:O:117:TYR:O	3:P:34:LEU:HD23	2.14	0.46
1:B:189:LYS:NZ	8:B:529:HOH:O	2.48	0.46
1:A:42:LEU:O	1:A:292:LYS:HB3	2.16	0.46
1:F:138:ALA:HB3	1:F:226:ILE:CD1	2.44	0.46
1:E:176:LYS:HD3	1:E:257:TYR:CD1	2.50	0.46
3:R:82:ALA:C	3:R:84:ASP:H	2.24	0.46
1:C:185:PRO:HG3	1:C:191:GLN:OE1	2.15	0.46
1:F:291:ASP:HA	8:F:513:HOH:O	2.15	0.46
2:I:54:ASN:ND2	2:I:106:PHE:HE1	2.14	0.46
2:M:91:THR:HG23	2:M:130:ALA:HA	1.97	0.46
3:L:24:GLY:C	8:L:317:HOH:O	2.58	0.46
1:C:292:LYS:H	1:C:292:LYS:HD2	1.81	0.45
2:I:48:MET:HG2	2:I:64:PHE:CE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:209:ALA:CB	3:L:212:GLU:OE2	2.62	0.45
2:Q:50:TRP:NE1	2:Q:59:ASN:HD22	2.15	0.45
3:R:89:TYR:HA	8:R:309:HOH:O	2.15	0.45
1:A:63:ASN:OD1	5:T:1:NAG:C1	2.64	0.45
1:A:175:ASP:CG	1:A:238:LYS:NZ	2.71	0.45
1:B:176:LYS:HB2	1:B:237:VAL:HG22	1.98	0.45
2:G:117:TYR:O	3:H:34:LEU:HD23	2.17	0.45
2:G:158:LEU:HB2	2:G:231:VAL:HG11	1.98	0.45
3:J:4:LEU:HD21	3:J:28:ASP:OD2	2.17	0.45
2:M:45:PHE:CZ	3:N:46:PRO:HG3	2.51	0.45
3:R:35:VAL:HG22	3:R:92:SER:OG	2.16	0.45
6:D:405:NAG:O3	6:D:405:NAG:H62	2.16	0.45
1:D:295:GLN:OE1	1:D:297:VAL:N	2.50	0.45
1:E:262:SER:N	8:E:505:HOH:O	2.36	0.45
1:F:109:ARG:NH1	1:F:269:ARG:NH2	2.65	0.45
2:I:67:ARG:NH2	2:I:83:LEU:HD11	2.30	0.45
3:J:165:THR:HG22	8:J:328:HOH:O	2.17	0.45
3:N:69:SER:HA	8:N:313:HOH:O	2.16	0.45
3:R:55:ARG:NH2	8:R:311:HOH:O	2.49	0.45
1:B:141:ARG:HD3	8:B:520:HOH:O	2.16	0.45
1:F:182:VAL:HG22	1:F:202:ILE:HD13	1.98	0.45
2:G:91:THR:HG23	2:G:130:ALA:HA	1.99	0.45
3:H:115:PRO:HB3	3:H:141:PHE:HB3	1.98	0.45
1:F:83:LYS:NZ	1:F:83:LYS:HB2	2.31	0.45
2:M:30:THR:HA	2:M:53:PRO:HB2	1.99	0.45
1:F:99:PRO:HB2	1:F:229:ARG:HD3	1.98	0.45
1:F:178:TYR:HE2	1:F:237:VAL:HG21	1.82	0.45
2:O:158:LEU:HB2	2:O:231:VAL:HG11	1.98	0.45
3:P:52:GLU:OE2	3:P:55:ARG:NH2	2.49	0.45
2:Q:2:VAL:CG2	2:Q:27:TYR:CD1	2.99	0.45
1:C:158:ASN:ND2	3:L:52:GLU:OE2	2.35	0.45
1:C:168:MET:HG2	8:C:508:HOH:O	2.17	0.45
2:Q:166:PHE:HA	2:Q:167:PRO:HA	1.78	0.45
8:B:515:HOH:O	5:U:2:NAG:C6	2.65	0.45
2:G:30:THR:HA	2:G:53:PRO:HB2	1.99	0.45
2:K:45:PHE:CZ	3:L:46:PRO:HG3	2.52	0.45
1:D:81:ASN:ND2	6:D:405:NAG:C8	2.80	0.45
3:H:69:SER:OG	3:H:70:GLY:N	2.45	0.45
2:I:83:LEU:CD2	2:I:86:LEU:HD23	2.47	0.45
2:I:37:VAL:HG21	2:I:123:TRP:CZ3	2.52	0.44
2:I:61:ALA:O	2:I:65:GLN:HG3	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:212:GLU:OE1	3:L:212:GLU:N	2.49	0.44
2:Q:112:ARG:NH1	2:Q:114:ALA:O	2.49	0.44
1:A:175:ASP:CG	1:A:238:LYS:HZ3	2.20	0.44
1:B:298:ASN:OD1	1:B:300:ILE:N	2.47	0.44
1:C:167:THR:HG23	1:C:242:ILE:HG21	2.00	0.44
2:K:1:GLU:C	8:K:304:HOH:O	2.40	0.44
5:X:2:NAG:H3	5:X:3:BMA:O2	2.17	0.44
1:C:236:ILE:HD12	1:C:260:ILE:HD11	1.98	0.44
1:F:176:LYS:HD3	1:F:257:TYR:CG	2.52	0.44
3:J:115:PRO:HB3	3:J:141:PHE:HB3	1.99	0.44
3:H:85:GLU:HG3	3:H:105:LEU:O	2.16	0.44
2:I:45:PHE:CZ	3:J:46:PRO:HG3	2.52	0.44
3:L:85:GLU:HG3	3:L:106:THR:HA	1.99	0.44
2:O:49:ALA:HB2	2:O:60:TYR:HA	1.99	0.44
1:A:75:GLN:NE2	1:A:94:TYR:O	2.44	0.44
1:E:176:LYS:HD3	1:E:257:TYR:CG	2.52	0.44
3:H:168:LYS:HB3	3:H:168:LYS:HE3	1.73	0.44
2:I:81:MET:HE3	2:I:81:MET:HB3	1.79	0.44
1:C:165:ASN:OD1	1:C:165:ASN:O	2.35	0.44
1:F:67:ILE:HG13	1:F:105:TYR:CE1	2.52	0.44
3:N:81:GLN:O	3:N:107:VAL:HG21	2.17	0.44
3:P:96:SER:HA	8:P:312:HOH:O	2.16	0.44
1:B:206:THR:HG21	1:B:237:VAL:HG12	1.98	0.44
1:C:207:LYS:HZ3	1:C:241:ASP:HA	1.80	0.44
3:P:71:ASN:HD22	3:P:71:ASN:C	2.26	0.44
8:B:503:HOH:O	4:W:2:NAG:C5	2.66	0.44
1:F:59:LEU:HD21	1:F:79:PHE:CD1	2.53	0.44
1:F:150:ARG:HG2	1:F:258:PHE:CZ	2.52	0.44
3:L:5:THR:C	8:L:303:HOH:O	2.51	0.44
2:I:40:ALA:HB3	2:I:43:GLN:HG3	1.99	0.44
3:J:33:ASP:CG	3:J:68:LYS:HD3	2.41	0.44
2:K:2:VAL:HG12	2:K:122:VAL:HG11	2.00	0.44
2:M:103:MET:HE3	2:M:103:MET:HB3	1.81	0.44
2:O:101:THR:CA	8:O:301:HOH:O	2.29	0.44
2:Q:151:THR:HG22	2:Q:152:SER:H	1.83	0.44
1:D:45:ASN:HA	1:D:296:ASN:OD1	2.17	0.43
6:E:406:NAG:O6	6:E:406:NAG:O4	2.26	0.43
1:F:150:ARG:HG2	1:F:258:PHE:HZ	1.82	0.43
2:M:12:LYS:O	2:M:131:VAL:HA	2.18	0.43
3:H:80:LEU:HG	3:H:107:VAL:HG22	2.00	0.43
2:K:188:ALA:HA	2:K:198:LEU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:37:TRP:HB2	3:L:50:ILE:HB	1.99	0.43
2:M:164:ASP:HB3	2:M:195:LEU:HD13	1.99	0.43
2:O:112:ARG:NH1	2:O:114:ALA:O	2.47	0.43
1:A:176:LYS:HD3	1:A:257:TYR:CG	2.52	0.43
1:D:167:THR:HG23	1:D:242:ILE:CG2	2.48	0.43
1:E:67:ILE:HG13	1:E:105:TYR:CE1	2.53	0.43
1:F:45:ASN:HA	1:F:296:ASN:OD1	2.19	0.43
1:F:67:ILE:HG13	1:F:105:TYR:HE1	1.83	0.43
3:R:65:SER:O	3:R:75:LEU:HD12	2.17	0.43
1:A:176:LYS:HD3	1:A:257:TYR:CD1	2.53	0.43
1:D:160:LYS:HD3	1:D:162:PRO:HD3	2.00	0.43
2:K:48:MET:HG2	2:K:64:PHE:CE2	2.53	0.43
2:M:147:SER:HB3	8:M:301:HOH:O	2.19	0.43
2:O:81:MET:HE3	2:O:81:MET:HB3	1.76	0.43
1:C:206:THR:CG2	1:C:209:SER:H	2.30	0.43
1:D:150:ARG:HG3	1:D:258:PHE:HZ	1.83	0.43
1:D:157:LEU:HD11	2:Q:118:TYR:CZ	2.54	0.43
2:M:10:GLU:HB2	2:M:129:VAL:HG23	2.00	0.43
3:N:85:GLU:HG3	3:N:105:LEU:O	2.18	0.43
1:A:270:SER:HB2	1:A:284:PRO:HA	2.01	0.43
1:F:134:GLY:HA3	1:F:153:TRP:HB3	2.00	0.43
2:I:36:TRP:CE3	2:I:81:MET:HE2	2.54	0.43
1:E:141:ARG:NH1	1:E:146:SER:OG	2.52	0.43
1:C:283:THR:HB	8:C:513:HOH:O	2.18	0.43
1:F:143:SER:N	8:F:505:HOH:O	2.48	0.43
2:Q:155:THR:HB	2:Q:203:THR:HG22	2.01	0.43
1:E:311:GLN:HB3	1:E:312:SER:H	1.59	0.43
1:F:48:ILE:HG13	1:F:50:GLU:H	1.83	0.43
2:Q:83:LEU:HD23	2:Q:86:LEU:HD23	2.00	0.43
1:A:90:ARG:NH2	1:A:272:ALA:O	2.51	0.43
1:C:237:VAL:HA	8:C:504:HOH:O	2.18	0.43
6:D:406:NAG:O4	8:D:506:HOH:O	2.11	0.43
1:E:42:LEU:O	1:E:292:LYS:HB3	2.18	0.43
3:H:33:ASP:CB	3:H:68:LYS:NZ	2.80	0.43
2:K:4:LEU:HD22	2:K:24:THR:HG22	2.01	0.43
6:B:408:NAG:H83	6:B:408:NAG:O4	2.18	0.42
2:G:176:SER:HA	8:G:303:HOH:O	2.08	0.42
2:M:53:PRO:O	2:M:72:ARG:NH1	2.52	0.42
3:N:28:ASP:HB3	3:N:94:ALA:HB2	2.01	0.42
3:R:16:GLN:O	3:R:80:LEU:N	2.46	0.42
1:A:173:GLN:CD	1:F:307:ARG:NH1	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:ASP:OD2	2:K:107:ASP:HB2	2.19	0.42
1:C:298:ASN:OD1	1:C:300:ILE:N	2.51	0.42
1:B:295:GLN:HE21	1:B:295:GLN:HB3	1.58	0.42
1:C:283:THR:CG2	1:C:301:THR:HG22	2.49	0.42
1:F:168:MET:HE3	1:F:168:MET:HA	2.01	0.42
2:G:83:LEU:CD2	2:G:86:LEU:CD2	2.97	0.42
3:L:191:ARG:O	3:L:191:ARG:NH1	2.52	0.42
3:N:10:VAL:HG23	3:N:105:LEU:HD12	2.01	0.42
1:E:138:ALA:HB2	1:E:226:ILE:HD13	2.01	0.42
3:N:68:LYS:HE3	8:N:331:HOH:O	2.19	0.42
2:G:54:ASN:ND2	2:G:106:PHE:HE1	2.17	0.42
3:L:23:THR:N	8:L:303:HOH:O	2.45	0.42
2:M:166:PHE:HA	2:M:167:PRO:HA	1.78	0.42
1:B:75:GLN:NE2	1:B:94:TYR:O	2.48	0.42
1:B:310:LYS:CA	8:B:507:HOH:O	2.67	0.42
1:C:194:LEU:CD1	2:K:105:VAL:HG11	2.50	0.42
2:O:27:TYR:CZ	2:O:98:LYS:HD2	2.55	0.42
2:Q:61:ALA:O	2:Q:65:GLN:N	2.53	0.42
1:A:75:GLN:HG3	1:A:76:CYS:SG	2.59	0.42
1:B:108:LEU:HB2	1:B:234:TRP:CZ3	2.55	0.42
1:D:114:SER:HA	1:D:265:SER:O	2.19	0.42
1:E:283:THR:C	8:E:510:HOH:O	2.63	0.42
1:F:109:ARG:HE	1:F:267:ILE:HG12	1.85	0.42
2:G:61:ALA:O	2:G:65:GLN:HG3	2.20	0.42
3:L:142:TYR:HB2	3:L:173:LYS:HG2	2.01	0.42
2:O:36:TRP:CE3	2:O:81:MET:HE2	2.55	0.42
3:P:197:VAL:HB	8:P:301:HOH:O	2.20	0.42
1:C:178:TYR:CD2	1:C:243:LEU:HD22	2.55	0.42
1:F:44:GLN:CD	1:F:289:PRO:HG2	2.44	0.42
2:K:54:ASN:ND2	2:K:106:PHE:HE1	2.18	0.42
2:I:236:CYS:SG	2:I:237:ASP:N	2.93	0.42
3:L:11:SER:HA	3:L:106:THR:O	2.19	0.42
1:B:75:GLN:HG3	1:B:76:CYS:SG	2.60	0.42
1:C:295:GLN:N	1:C:307:ARG:O	2.52	0.42
1:D:202:ILE:HD11	1:D:245:ILE:HG23	2.02	0.42
1:E:51:ILE:HB	1:E:274:ILE:HD13	2.01	0.42
1:E:178:TYR:CD2	1:E:243:LEU:HD22	2.55	0.42
2:O:213:THR:HG22	2:O:230:ARG:HH12	1.85	0.42
3:R:144:GLY:CA	3:R:174:TYR:HD2	2.33	0.42
5:T:1:NAG:C2	5:T:1:NAG:C6	2.94	0.42
1:C:295:GLN:HG3	1:C:307:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:37:VAL:HG23	2:G:46:GLU:C	2.45	0.41
3:N:33:ASP:C	3:N:35:VAL:N	2.76	0.41
3:N:80:LEU:HG	3:N:107:VAL:HG22	2.02	0.41
2:Q:161:LEU:HG	2:Q:163:LYS:HG3	2.02	0.41
3:R:144:GLY:HA3	3:R:174:TYR:CD2	2.54	0.41
1:A:168:MET:HE3	1:A:168:MET:HA	2.01	0.41
1:B:176:LYS:HD3	1:B:257:TYR:CG	2.55	0.41
1:D:67:ILE:HG12	8:D:524:HOH:O	2.19	0.41
1:E:186:VAL:HG22	1:E:187:THR:HG23	2.02	0.41
3:J:37:TRP:HB2	3:J:50:ILE:HB	2.02	0.41
2:K:38:ARG:HH21	2:K:63:LYS:NZ	2.19	0.41
2:O:165:TYR:CE1	2:O:170:VAL:CG2	3.01	0.41
1:B:202:ILE:HD12	1:B:247:SER:HB2	1.99	0.41
1:C:262:SER:HA	8:C:515:HOH:O	2.20	0.41
1:F:307:ARG:N	8:F:509:HOH:O	2.52	0.41
2:I:88:SER:HA	2:I:131:VAL:HG13	2.02	0.41
1:A:202:ILE:HD11	1:A:251:LEU:HA	2.01	0.41
8:B:504:HOH:O	4:W:2:NAG:H2	2.20	0.41
1:C:241:ASP:OD1	1:C:242:ILE:N	2.52	0.41
1:D:222:ARG:HB3	1:D:225:ASN:HA	2.03	0.41
2:Q:2:VAL:HG13	2:Q:122:VAL:HG21	2.00	0.41
1:E:42:LEU:HA	1:E:42:LEU:HD23	1.88	0.41
1:E:191:GLN:HG3	1:E:197:GLN:O	2.21	0.41
1:F:73:ASP:OD1	1:F:75:GLN:HG2	2.20	0.41
2:G:166:PHE:HA	2:G:167:PRO:HA	1.80	0.41
3:L:23:THR:HG22	3:L:72:THR:HG23	2.02	0.41
3:N:10:VAL:CG2	3:N:105:LEU:HD13	2.49	0.41
1:C:41:GLU:HG2	1:C:42:LEU:N	2.24	0.41
1:C:113:ALA:HB1	1:C:267:ILE:HB	2.02	0.41
2:I:148:SER:HB2	2:I:237:ASP:HB3	2.02	0.41
3:L:117:VAL:O	3:L:206:LYS:NZ	2.53	0.41
3:N:46:PRO:O	8:N:308:HOH:O	2.22	0.41
1:C:84:TRP:CE2	1:C:116:GLY:HA2	2.56	0.41
1:E:79:PHE:HA	1:E:82:LYS:HD2	2.01	0.41
2:I:83:LEU:HG	2:I:86:LEU:HD23	2.03	0.41
1:A:73:ASP:OD1	1:A:75:GLN:HG2	2.20	0.41
2:I:166:PHE:HA	2:I:167:PRO:HA	1.83	0.41
1:B:176:LYS:HB2	1:B:237:VAL:CG2	2.51	0.41
1:C:90:ARG:HB3	1:C:92:LYS:HG2	2.03	0.41
2:G:64:PHE:O	2:G:68:VAL:HG12	2.21	0.41
3:H:33:ASP:O	3:H:35:VAL:N	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:29:VAL:HG23	3:L:35:VAL:CG2	2.51	0.41
3:N:151:LYS:HZ2	3:N:156:PRO:HG3	1.85	0.41
3:R:151:LYS:HB2	3:R:194:SER:HB3	2.03	0.41
1:A:206:THR:HG23	1:A:208:ARG:N	2.28	0.41
1:D:176:LYS:HD3	1:D:257:TYR:CD1	2.56	0.41
3:J:35:VAL:HA	3:J:91:SER:O	2.20	0.41
2:K:81:MET:HE3	2:K:81:MET:HB3	1.74	0.41
3:L:147:THR:OG1	3:L:198:THR:HB	2.21	0.41
2:O:162:VAL:HG11	2:O:170:VAL:HG11	2.03	0.41
3:R:164:THR:CG2	3:R:177:SER:H	2.33	0.41
1:C:77:ASP:CG	8:C:507:HOH:O	2.57	0.40
1:D:180:TRP:HB3	1:D:254:PRO:HD3	2.02	0.40
3:N:151:LYS:HD3	3:N:156:PRO:HA	2.03	0.40
3:P:146:VAL:HG21	3:P:197:VAL:HG13	2.02	0.40
1:A:89:GLU:HG3	1:A:267:ILE:HD11	2.02	0.40
1:A:178:TYR:HA	8:A:526:HOH:O	2.21	0.40
1:C:206:THR:HG22	1:C:209:SER:H	1.86	0.40
2:O:38:ARG:NH2	2:O:63:LYS:NZ	2.68	0.40
3:J:209:ALA:O	3:J:212:GLU:HG3	2.21	0.40
3:N:25:THR:CG2	3:N:26:ASN:H	2.10	0.40
3:N:115:PRO:HB3	3:N:141:PHE:HB3	2.04	0.40
1:B:207:LYS:NZ	1:B:241:ASP:HA	2.35	0.40
2:G:11:VAL:HG23	2:G:11:VAL:O	2.22	0.40
2:I:34:LEU:HD23	2:I:34:LEU:HA	1.93	0.40
3:J:151:LYS:HD2	3:J:196:GLN:NE2	2.37	0.40
3:R:33:ASP:C	3:R:35:VAL:H	2.30	0.40
1:F:184:HIS:HB3	1:F:220:ARG:HH22	1.86	0.40
3:N:37:TRP:HB2	3:N:50:ILE:HB	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:334:HOH:O	8:H:338:HOH:O[1_455]	1.91	0.29

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	270/291 (93%)	255 (94%)	14 (5%)	1 (0%)	30	51
1	B	272/291 (94%)	259 (95%)	12 (4%)	1 (0%)	30	51
1	C	270/291 (93%)	257 (95%)	13 (5%)	0	100	100
1	D	271/291 (93%)	258 (95%)	13 (5%)	0	100	100
1	E	271/291 (93%)	256 (94%)	13 (5%)	2 (1%)	18	38
1	F	272/291 (94%)	257 (94%)	15 (6%)	0	100	100
2	G	234/244 (96%)	228 (97%)	6 (3%)	0	100	100
2	I	236/244 (97%)	228 (97%)	8 (3%)	0	100	100
2	K	233/244 (96%)	227 (97%)	5 (2%)	1 (0%)	30	51
2	M	233/244 (96%)	227 (97%)	6 (3%)	0	100	100
2	O	233/244 (96%)	227 (97%)	6 (3%)	0	100	100
2	Q	233/244 (96%)	225 (97%)	6 (3%)	2 (1%)	14	30
3	H	210/214 (98%)	199 (95%)	10 (5%)	1 (0%)	24	46
3	J	211/214 (99%)	196 (93%)	14 (7%)	1 (0%)	24	46
3	L	209/214 (98%)	194 (93%)	11 (5%)	4 (2%)	6	13
3	N	210/214 (98%)	194 (92%)	15 (7%)	1 (0%)	24	46
3	P	210/214 (98%)	197 (94%)	11 (5%)	2 (1%)	12	28
3	R	210/214 (98%)	188 (90%)	16 (8%)	6 (3%)	3	6
All	All	4288/4494 (95%)	4072 (95%)	194 (4%)	22 (0%)	24	46

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	LYS
3	H	34	LEU
3	L	26	ASN
3	N	34	LEU

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Mol	Chain	Res	Type
2	Q	154	GLY
3	R	29	VAL
1	E	310	LYS
1	E	311	GLN
3	P	34	LEU
2	Q	234	LYS
3	R	3	ALA
3	R	74	SER
3	R	69	SER
2	K	2	VAL
3	L	71	ASN
3	R	34	LEU
3	R	70	GLY
3	J	83	GLU
3	L	83	GLU
3	L	112	LYS
1	B	311	GLN
3	P	26	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	244/258 (95%)	243 (100%)	1 (0%)	84	93
1	B	245/258 (95%)	243 (99%)	2 (1%)	73	88
1	C	244/258 (95%)	244 (100%)	0	100	100
1	D	245/258 (95%)	244 (100%)	1 (0%)	84	93
1	E	245/258 (95%)	244 (100%)	1 (0%)	84	93
1	F	245/258 (95%)	245 (100%)	0	100	100
2	G	197/205 (96%)	194 (98%)	3 (2%)	57	80
2	I	199/205 (97%)	196 (98%)	3 (2%)	57	80
2	K	196/205 (96%)	192 (98%)	4 (2%)	48	74
2	M	196/205 (96%)	192 (98%)	4 (2%)	48	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	196/205 (96%)	194 (99%)	2 (1%)	68	86
2	Q	196/205 (96%)	195 (100%)	1 (0%)	81	92
3	H	176/178 (99%)	176 (100%)	0	100	100
3	J	177/178 (99%)	177 (100%)	0	100	100
3	L	175/178 (98%)	175 (100%)	0	100	100
3	N	176/178 (99%)	175 (99%)	1 (1%)	78	91
3	P	176/178 (99%)	173 (98%)	3 (2%)	53	78
3	R	176/178 (99%)	175 (99%)	1 (1%)	78	91
All	All	3704/3846 (96%)	3677 (99%)	27 (1%)	76	89

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	VAL
1	B	295	GLN
1	B	307	ARG
1	D	295	GLN
1	E	90	ARG
2	G	72	ARG
2	G	103	MET
2	G	236	CYS
2	I	72	ARG
2	I	81	MET
2	I	234	LYS
2	K	67	ARG
2	K	81	MET
2	K	83	LEU
2	K	230	ARG
2	M	72	ARG
2	M	83	LEU
2	M	98	LYS
2	M	103	MET
3	N	68	LYS
2	O	81	MET
2	O	103	MET
3	P	10	VAL
3	P	68	LYS
3	P	171	ASN
2	Q	72	ARG

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Mol	Chain	Res	Type
3	R	63	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	144	ASN
1	B	56	HIS
1	C	80	GLN
1	C	165	ASN
1	D	81	ASN
1	D	211	GLN
1	E	80	GLN
1	E	173	GLN
1	F	56	HIS
2	G	59	ASN
3	J	196	GLN
2	K	59	ASN
3	L	196	GLN
2	M	59	ASN
3	N	110	GLN
2	O	191	GLN
3	P	39	GLN
3	P	130	ASN
2	Q	39	GLN
2	Q	59	ASN
3	R	6	GLN
3	R	40	GLN
3	R	71	ASN
3	R	110	GLN
3	R	169	GLN
3	R	172	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

25 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	S	1	1,4	14,14,15	0.29	0	17,19,21	0.56	0
4	NAG	S	2	4	14,14,15	0.28	0	17,19,21	0.57	0
5	NAG	T	1	5	14,14,15	0.31	0	17,19,21	0.50	0
5	NAG	T	2	5	14,14,15	0.29	0	17,19,21	0.57	0
5	BMA	T	3	5	11,11,12	0.27	0	15,15,17	0.53	0
5	NAG	U	1	1,5	14,14,15	0.30	0	17,19,21	0.55	0
5	NAG	U	2	5	14,14,15	0.30	0	17,19,21	0.57	0
5	BMA	U	3	5	11,11,12	0.25	0	15,15,17	0.52	0
4	NAG	V	1	1,4	14,14,15	0.90	1 (7%)	17,19,21	1.33	1 (5%)
4	NAG	V	2	4	14,14,15	0.42	0	17,19,21	0.56	0
4	NAG	W	1	1,4	14,14,15	0.34	0	17,19,21	0.44	0
4	NAG	W	2	4	14,14,15	0.51	0	17,19,21	0.45	0
5	NAG	X	1	1,5	14,14,15	0.36	0	17,19,21	0.67	1 (5%)
5	NAG	X	2	5	14,14,15	0.45	0	17,19,21	0.98	2 (11%)
5	BMA	X	3	5	11,11,12	0.88	1 (9%)	15,15,17	0.79	0
4	NAG	Y	1	1,4	14,14,15	0.39	0	17,19,21	0.52	0
4	NAG	Y	2	4	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	Z	1	1,4	14,14,15	0.45	0	17,19,21	0.65	1 (5%)
4	NAG	Z	2	4	14,14,15	0.29	0	17,19,21	0.35	0
5	NAG	a	1	1,5	14,14,15	0.40	0	17,19,21	0.81	1 (5%)
5	NAG	a	2	5	14,14,15	0.43	0	17,19,21	0.91	0
5	BMA	a	3	5	11,11,12	0.31	0	15,15,17	1.01	2 (13%)
5	NAG	b	1	1,5	14,14,15	0.41	0	17,19,21	0.53	0
5	NAG	b	2	5	14,14,15	0.31	0	17,19,21	0.42	0
5	BMA	b	3	5	11,11,12	0.69	0	15,15,17	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	S	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	3/6/23/26	0/1/1/1
5	NAG	T	1	5	-	3/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	BMA	T	3	5	-	2/2/19/22	0/1/1/1
5	NAG	U	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	U	2	5	-	4/6/23/26	0/1/1/1
5	BMA	U	3	5	-	2/2/19/22	0/1/1/1
4	NAG	V	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
4	NAG	W	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	1/6/23/26	0/1/1/1
5	NAG	X	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	X	2	5	-	3/6/23/26	0/1/1/1
5	BMA	X	3	5	-	2/2/19/22	0/1/1/1
4	NAG	Y	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	1/6/23/26	0/1/1/1
4	NAG	Z	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	1/6/23/26	0/1/1/1
5	NAG	a	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	a	2	5	-	0/6/23/26	0/1/1/1
5	BMA	a	3	5	-	0/2/19/22	0/1/1/1
5	NAG	b	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	1/6/23/26	0/1/1/1
5	BMA	b	3	5	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	1	NAG	O5-C1	3.21	1.49	1.43
5	X	3	BMA	C1-C2	2.43	1.58	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	1	NAG	C1-O5-C5	5.30	119.30	112.19
5	X	2	NAG	C2-N2-C7	2.66	126.46	122.90
5	X	1	NAG	C1-O5-C5	2.19	115.12	112.19
5	a	3	BMA	C3-C4-C5	2.17	114.17	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	2	NAG	C1-C2-N2	2.06	113.68	110.43
5	a	1	NAG	O5-C1-C2	-2.06	108.11	111.29
5	a	3	BMA	C1-O5-C5	-2.04	109.46	112.19
4	Z	1	NAG	C2-N2-C7	2.00	125.58	122.90

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	S	2	NAG	C8-C7-N2-C2
4	S	2	NAG	O7-C7-N2-C2
5	X	2	NAG	C1-C2-N2-C7
5	T	2	NAG	C8-C7-N2-C2
5	T	2	NAG	O7-C7-N2-C2
5	T	1	NAG	O5-C5-C6-O6
5	T	3	BMA	O5-C5-C6-O6
5	T	3	BMA	C4-C5-C6-O6
5	X	3	BMA	O5-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
5	X	2	NAG	O5-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
5	b	3	BMA	O5-C5-C6-O6
5	X	3	BMA	C4-C5-C6-O6
5	X	2	NAG	C4-C5-C6-O6
5	b	3	BMA	C4-C5-C6-O6
5	U	2	NAG	C4-C5-C6-O6
5	U	3	BMA	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
4	Z	1	NAG	C3-C2-N2-C7
5	a	1	NAG	C3-C2-N2-C7
5	b	2	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
5	U	1	NAG	C1-C2-N2-C7
4	S	1	NAG	C8-C7-N2-C2
4	W	1	NAG	C4-C5-C6-O6
5	U	2	NAG	C8-C7-N2-C2
4	Z	2	NAG	C3-C2-N2-C7
5	T	1	NAG	C3-C2-N2-C7
5	U	1	NAG	C3-C2-N2-C7
4	S	1	NAG	O7-C7-N2-C2

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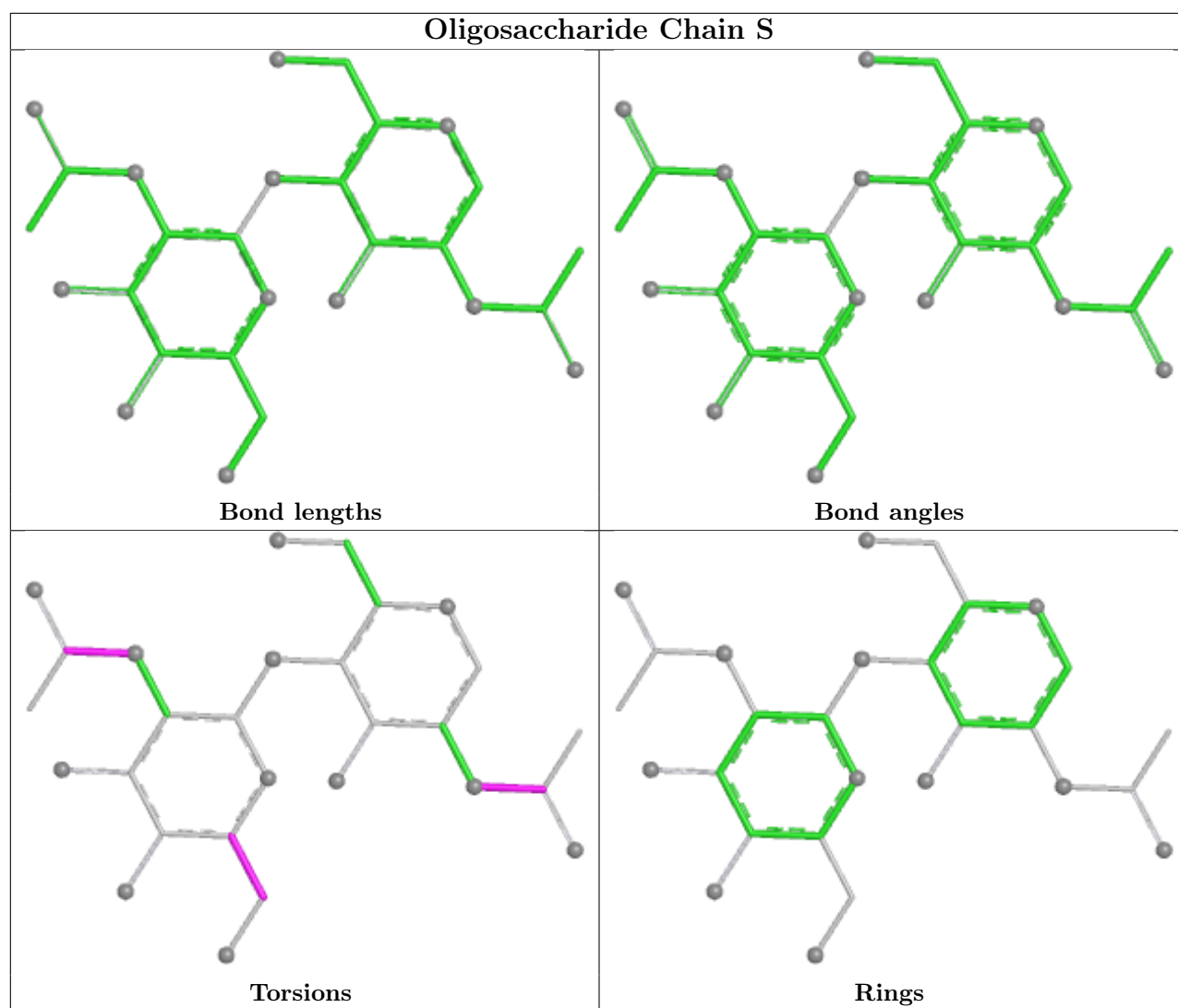
Mol	Chain	Res	Type	Atoms
4	W	2	NAG	O5-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
5	U	2	NAG	O7-C7-N2-C2
5	X	1	NAG	C3-C2-N2-C7
5	U	3	BMA	C4-C5-C6-O6
5	a	1	NAG	C4-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6

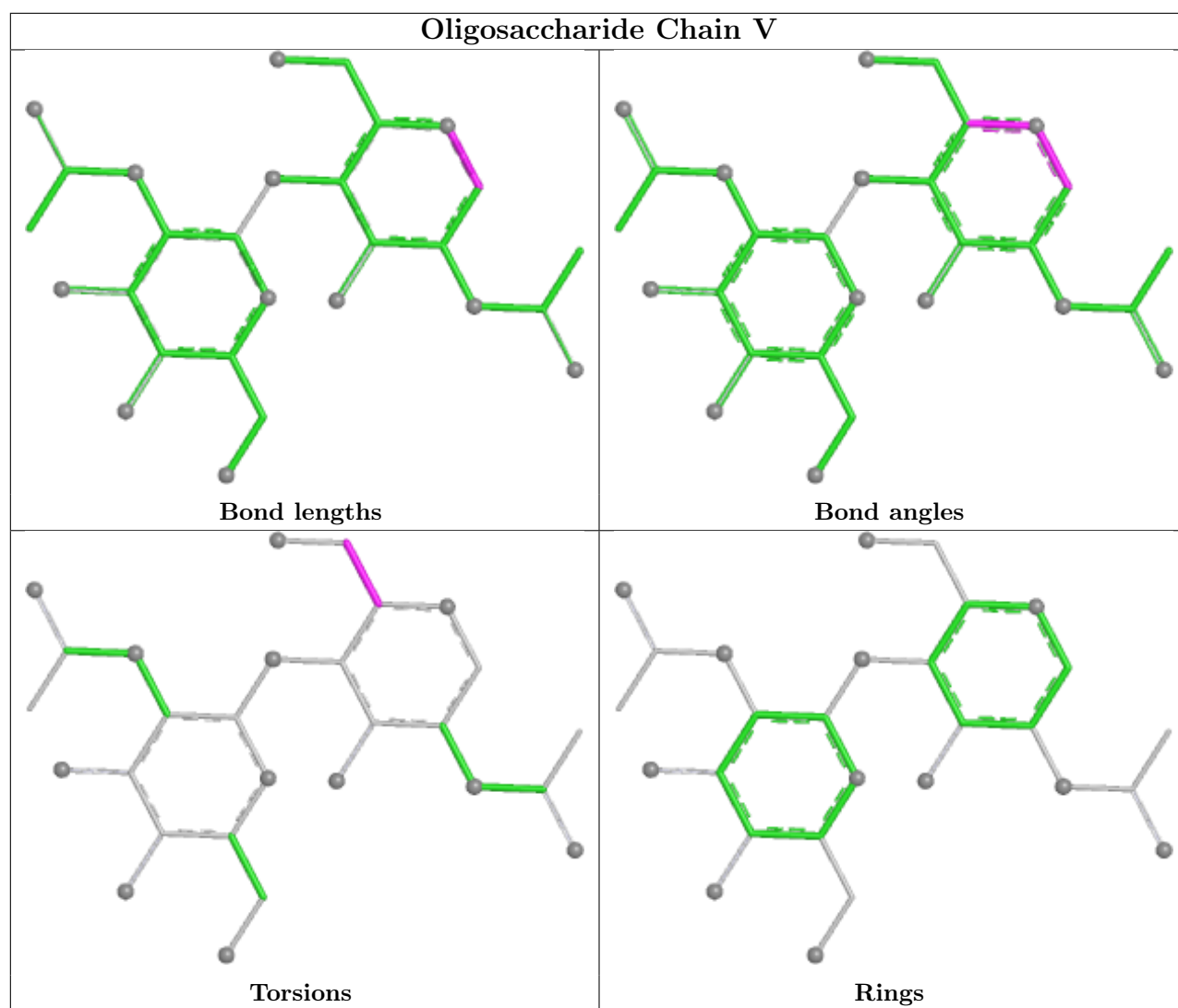
There are no ring outliers.

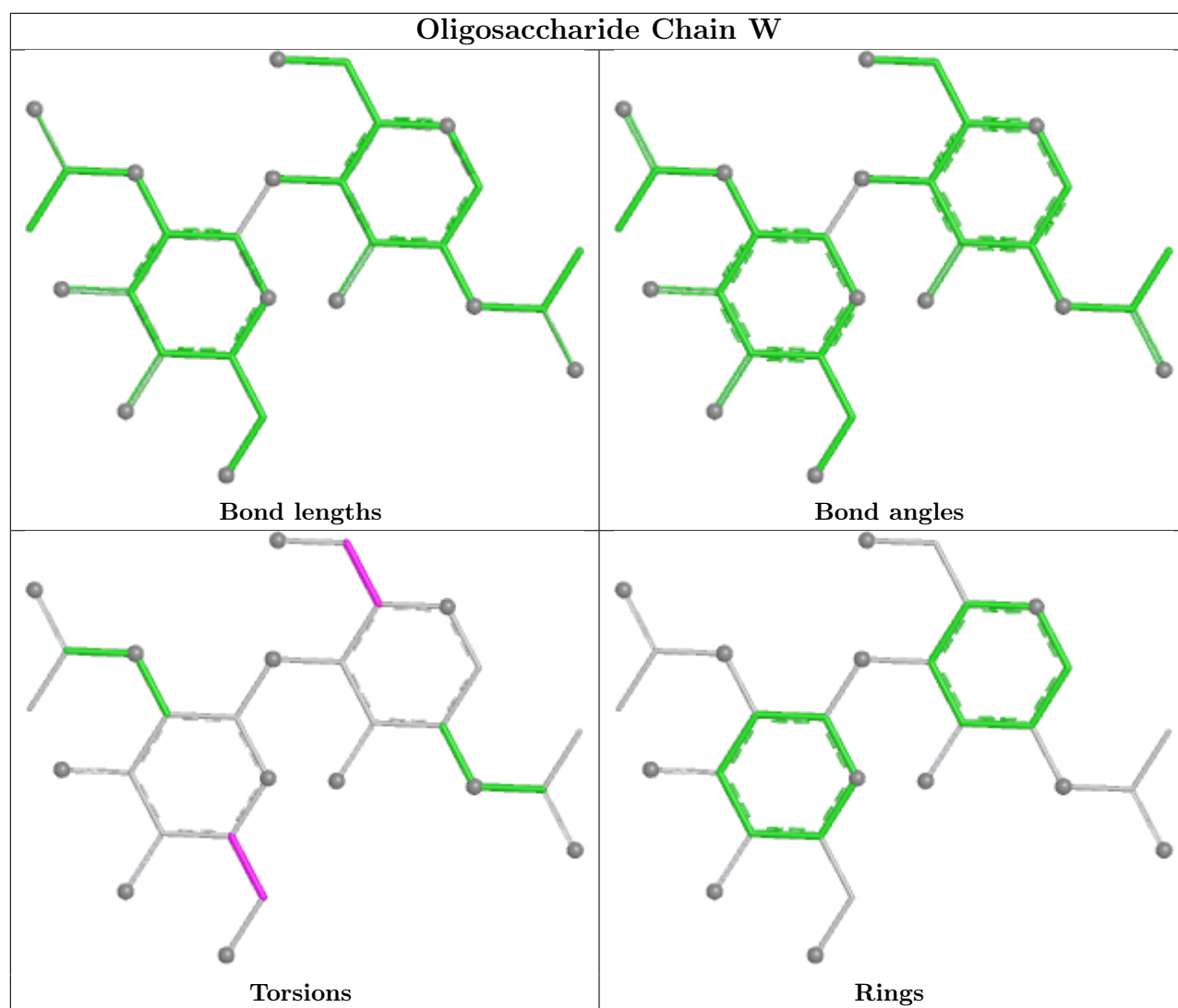
10 monomers are involved in 40 short contacts:

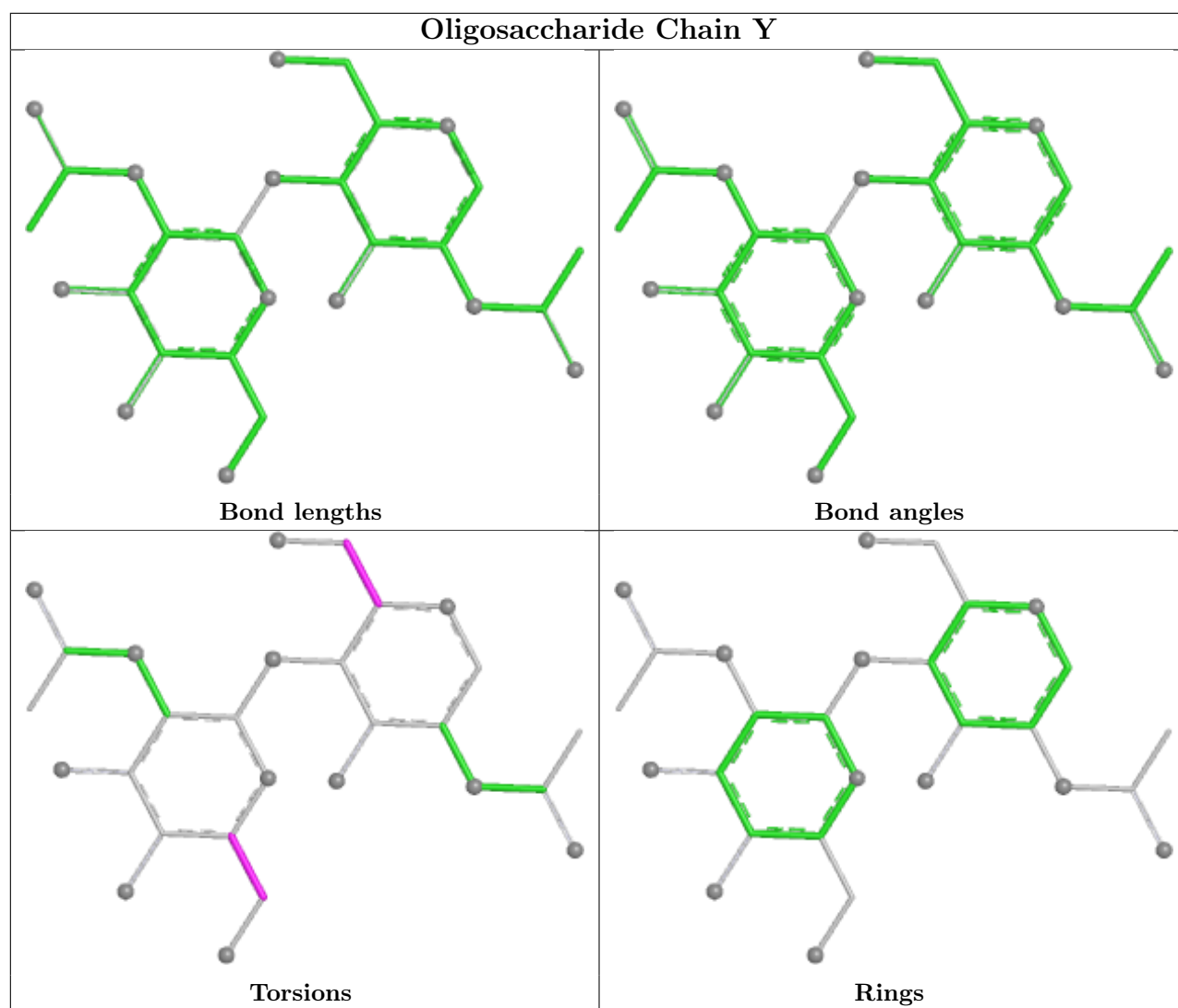
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	U	2	NAG	5	0
4	W	2	NAG	5	0
5	T	1	NAG	21	0
5	X	3	BMA	1	0
5	X	1	NAG	1	0
5	X	2	NAG	1	0
4	Y	2	NAG	1	0
5	a	1	NAG	1	0
4	Z	1	NAG	3	0
5	U	1	NAG	2	0

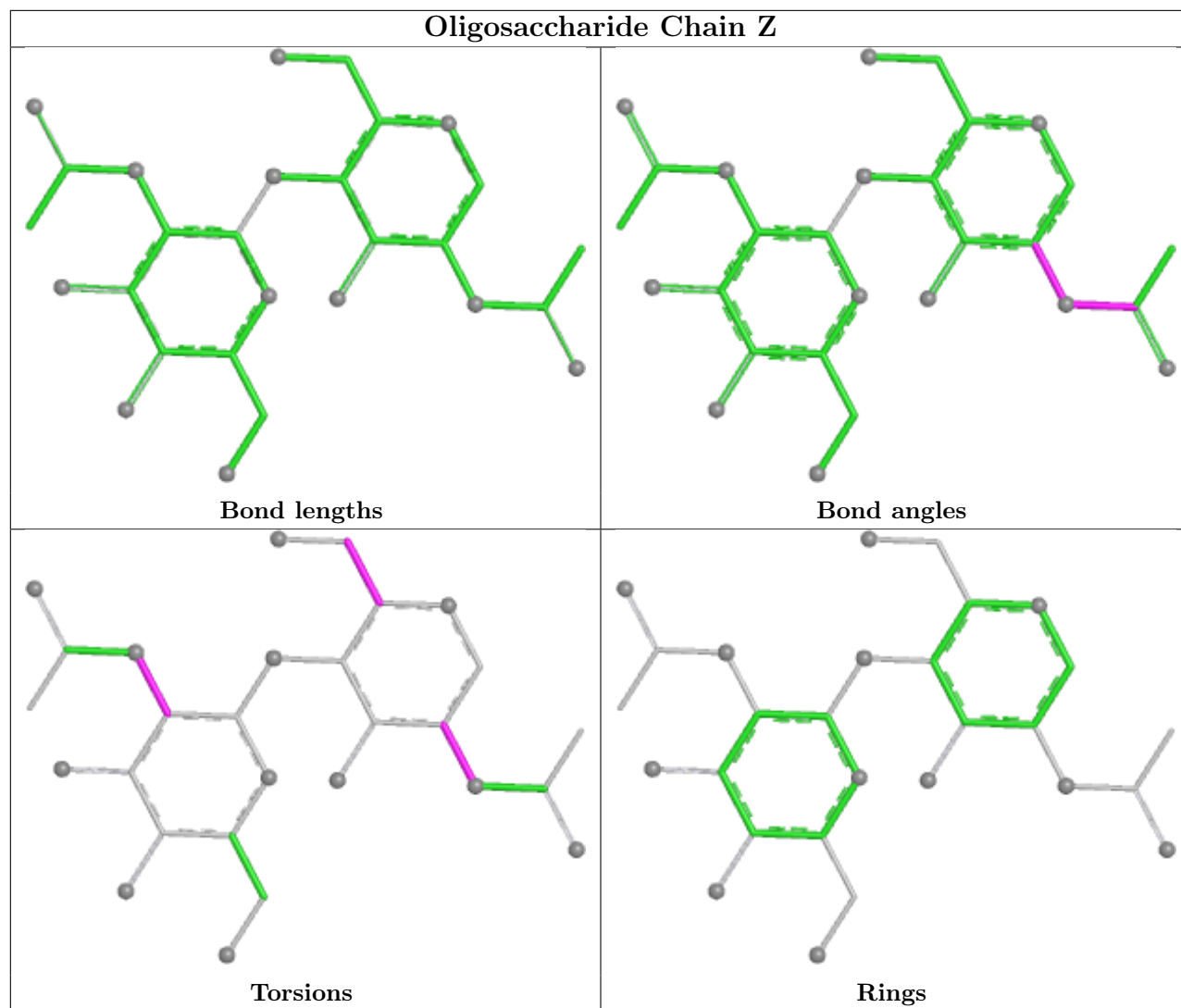
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

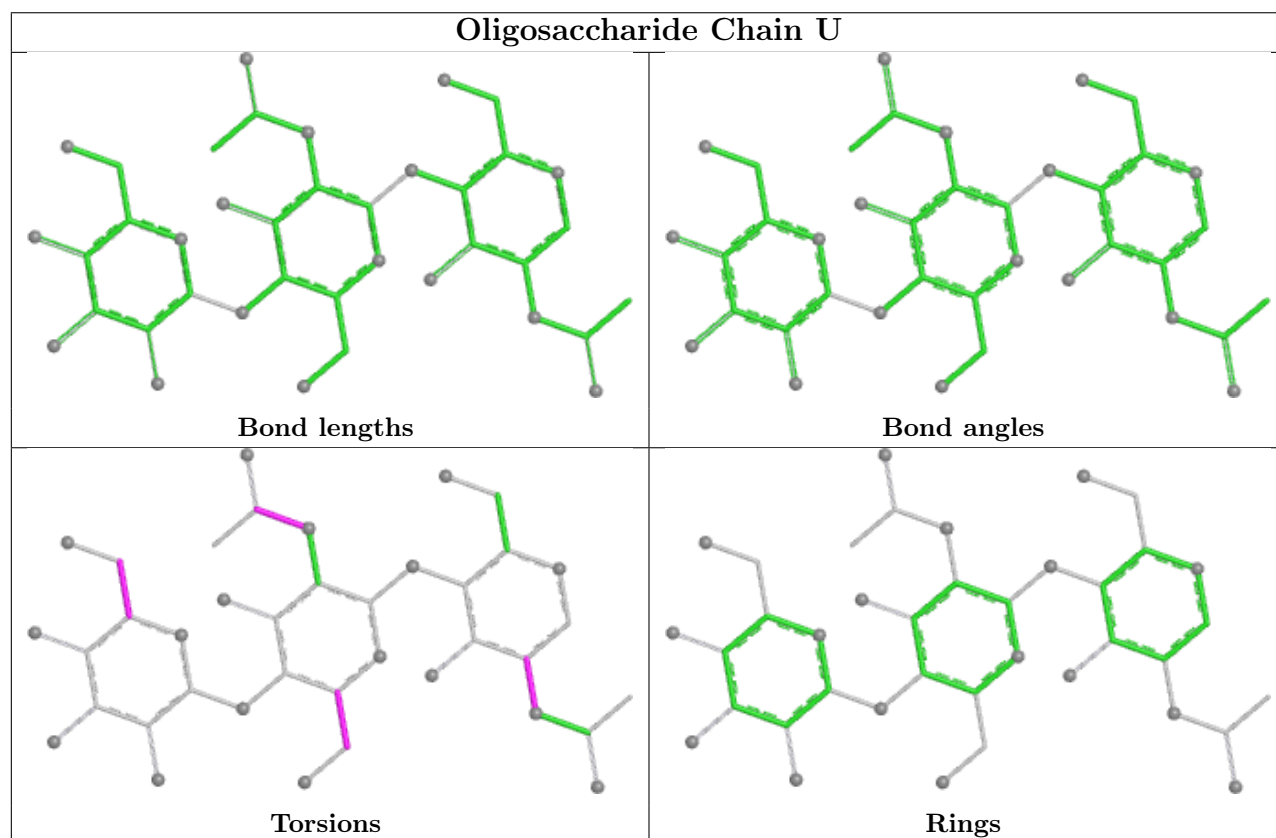
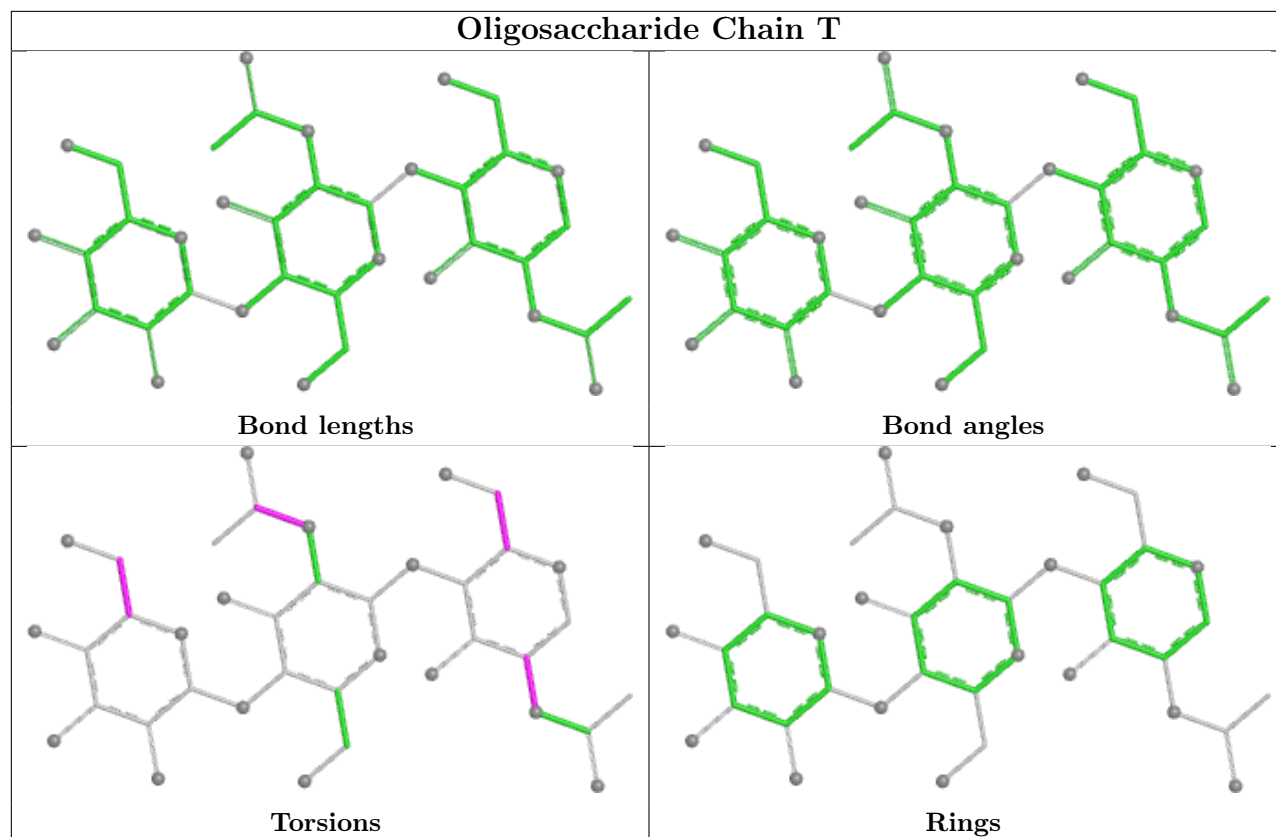


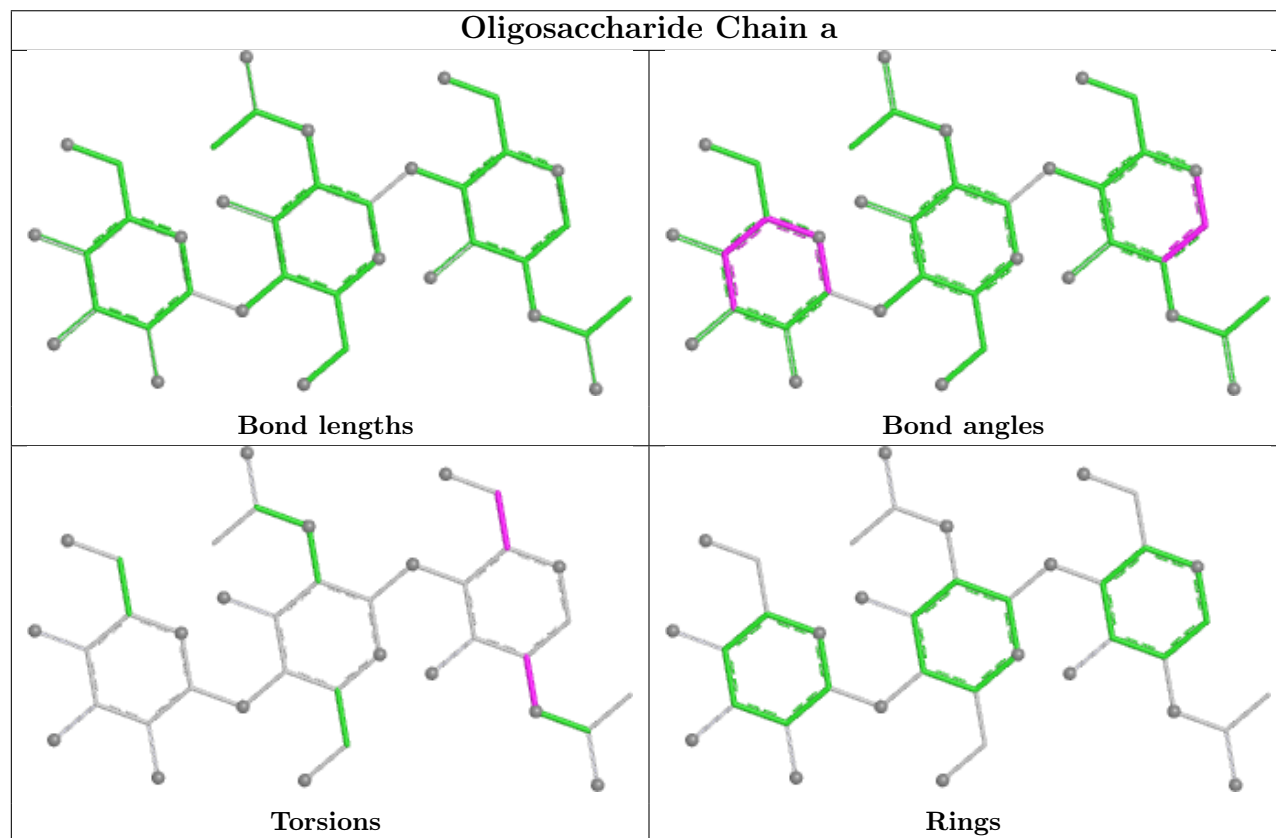
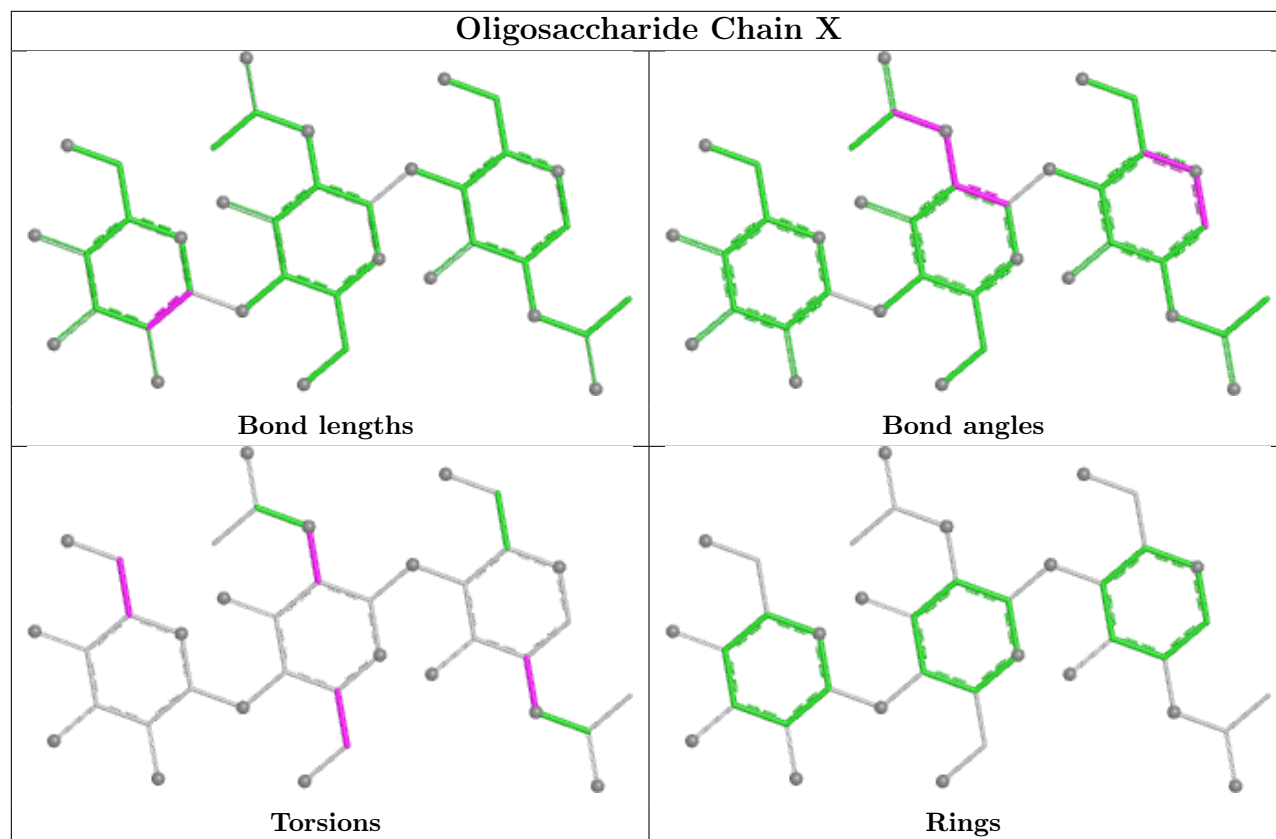


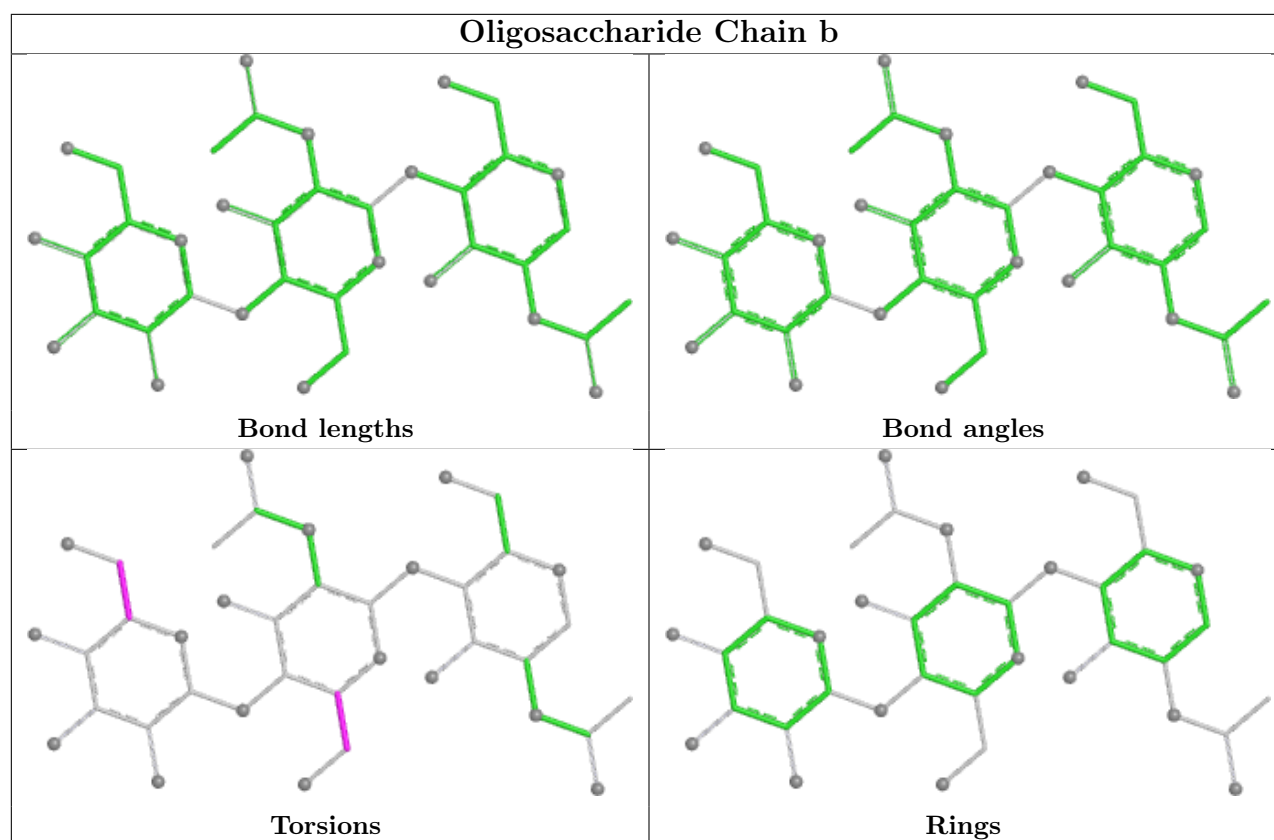












5.6 Ligand geometry [i](#)

17 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	GOL	I	301	-	5,5,5	0.38	0	5,5,5	0.37	0
6	NAG	A	408	1	14,14,15	0.38	0	17,19,21	0.70	0
6	NAG	E	405	1	14,14,15	0.88	1 (7%)	17,19,21	1.51	3 (17%)
6	NAG	F	405	1	14,14,15	0.42	0	17,19,21	1.42	1 (5%)
6	NAG	D	405	1	14,14,15	0.42	0	17,19,21	1.30	3 (17%)
6	NAG	D	406	1	14,14,15	0.23	0	17,19,21	1.02	1 (5%)
6	NAG	E	404	1	14,14,15	0.63	1 (7%)	17,19,21	0.44	0
6	NAG	F	404	1	14,14,15	0.35	0	17,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	C	401	1	14,14,15	0.31	0	17,19,21	0.44	0
6	NAG	D	407	1	14,14,15	0.36	0	17,19,21	0.85	0
6	NAG	B	408	1	14,14,15	1.22	2 (14%)	17,19,21	1.86	4 (23%)
6	NAG	A	407	1	14,14,15	0.32	0	17,19,21	0.62	0
6	NAG	C	406	1	14,14,15	0.33	0	17,19,21	0.58	0
6	NAG	F	406	1	14,14,15	0.35	0	17,19,21	0.68	0
6	NAG	E	406	1	14,14,15	0.28	0	17,19,21	0.78	1 (5%)
6	NAG	C	405	1	14,14,15	0.71	1 (7%)	17,19,21	0.66	0
6	NAG	A	406	-	14,14,15	0.28	0	17,19,21	0.57	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	GOL	I	301	-	-	2/4/4/4	-
6	NAG	A	408	1	-	4/6/23/26	0/1/1/1
6	NAG	E	405	1	-	3/6/23/26	0/1/1/1
6	NAG	F	405	1	-	2/6/23/26	0/1/1/1
6	NAG	D	405	1	-	4/6/23/26	0/1/1/1
6	NAG	D	406	1	-	4/6/23/26	0/1/1/1
6	NAG	E	404	1	-	0/6/23/26	0/1/1/1
6	NAG	F	404	1	-	2/6/23/26	0/1/1/1
6	NAG	C	401	1	-	0/6/23/26	0/1/1/1
6	NAG	D	407	1	-	5/6/23/26	0/1/1/1
6	NAG	B	408	1	-	5/6/23/26	0/1/1/1
6	NAG	A	407	1	-	1/6/23/26	0/1/1/1
6	NAG	C	406	1	-	2/6/23/26	0/1/1/1
6	NAG	F	406	1	-	2/6/23/26	0/1/1/1
6	NAG	E	406	1	-	4/6/23/26	0/1/1/1
6	NAG	C	405	1	-	0/6/23/26	0/1/1/1
6	NAG	A	406	-	-	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	408	NAG	O5-C1	-3.44	1.37	1.43
6	E	405	NAG	O5-C1	2.55	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	405	NAG	C1-C2	2.42	1.55	1.52
6	B	408	NAG	C1-C2	2.38	1.55	1.52
6	E	404	NAG	C1-C2	2.14	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	405	NAG	C1-O5-C5	5.24	119.21	112.19
6	B	408	NAG	C2-N2-C7	5.11	129.75	122.90
6	E	405	NAG	C2-N2-C7	4.44	128.85	122.90
6	E	405	NAG	C1-C2-N2	3.38	115.76	110.43
6	B	408	NAG	C4-C3-C2	3.25	115.79	111.02
6	B	408	NAG	C1-C2-N2	3.03	115.21	110.43
6	D	405	NAG	C1-O5-C5	2.90	116.08	112.19
6	D	405	NAG	O5-C1-C2	2.89	115.77	111.29
6	D	406	NAG	C1-C2-N2	-2.33	106.77	110.43
6	B	408	NAG	C1-O5-C5	-2.29	109.12	112.19
6	D	405	NAG	C2-N2-C7	-2.17	119.99	122.90
6	E	405	NAG	C1-O5-C5	2.13	115.03	112.19
6	E	406	NAG	C4-C3-C2	-2.07	107.98	111.02

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	408	NAG	O7-C7-N2-C2
6	C	406	NAG	C3-C2-N2-C7
6	D	405	NAG	C3-C2-N2-C7
6	D	405	NAG	C8-C7-N2-C2
6	D	405	NAG	O7-C7-N2-C2
6	D	406	NAG	C1-C2-N2-C7
6	D	406	NAG	C8-C7-N2-C2
6	D	406	NAG	O7-C7-N2-C2
6	E	405	NAG	C1-C2-N2-C7
7	I	301	GOL	O1-C1-C2-O2
6	A	408	NAG	C8-C7-N2-C2
6	F	405	NAG	O5-C5-C6-O6
6	E	405	NAG	C4-C5-C6-O6
6	F	405	NAG	C4-C5-C6-O6
6	E	406	NAG	O5-C5-C6-O6
6	E	405	NAG	O5-C5-C6-O6
6	B	408	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	B	408	NAG	O7-C7-N2-C2
6	D	407	NAG	C8-C7-N2-C2
6	F	404	NAG	C8-C7-N2-C2
6	F	404	NAG	O7-C7-N2-C2
6	B	408	NAG	O5-C5-C6-O6
6	D	407	NAG	O7-C7-N2-C2
6	C	406	NAG	O5-C5-C6-O6
6	B	408	NAG	C4-C5-C6-O6
7	I	301	GOL	O1-C1-C2-C3
6	A	407	NAG	O5-C5-C6-O6
6	F	406	NAG	O5-C5-C6-O6
6	D	405	NAG	O5-C5-C6-O6
6	D	406	NAG	O5-C5-C6-O6
6	B	408	NAG	C1-C2-N2-C7
6	E	406	NAG	C4-C5-C6-O6
6	D	407	NAG	C4-C5-C6-O6
6	A	406	NAG	C4-C5-C6-O6
6	A	408	NAG	C4-C5-C6-O6
6	D	407	NAG	C1-C2-N2-C7
6	D	407	NAG	C3-C2-N2-C7
6	F	406	NAG	C3-C2-N2-C7
6	A	408	NAG	O5-C5-C6-O6
6	E	406	NAG	C8-C7-N2-C2
6	E	406	NAG	O7-C7-N2-C2

There are no ring outliers.

10 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	408	NAG	2	0
6	E	405	NAG	1	0
6	D	405	NAG	7	0
6	D	406	NAG	8	0
6	B	408	NAG	1	0
6	A	407	NAG	4	0
6	C	406	NAG	1	0
6	F	406	NAG	1	0
6	E	406	NAG	3	0
6	A	406	NAG	11	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	272/291 (93%)	0.59	22 (8%) 18 14	23, 49, 83, 116	0
1	B	274/291 (94%)	0.51	23 (8%) 17 13	26, 45, 82, 134	0
1	C	272/291 (93%)	0.97	37 (13%) 7 5	28, 62, 97, 136	0
1	D	273/291 (93%)	0.84	27 (9%) 13 10	35, 57, 95, 156	0
1	E	273/291 (93%)	0.82	26 (9%) 14 10	29, 59, 96, 141	0
1	F	274/291 (94%)	1.23	46 (16%) 4 3	39, 73, 111, 206	0
2	G	236/244 (96%)	0.50	11 (4%) 36 30	26, 44, 72, 139	0
2	I	238/244 (97%)	0.44	13 (5%) 30 25	25, 44, 72, 156	0
2	K	235/244 (96%)	0.76	22 (9%) 14 11	35, 57, 85, 110	0
2	M	235/244 (96%)	0.47	12 (5%) 33 28	33, 49, 90, 158	0
2	O	235/244 (96%)	0.69	16 (6%) 23 19	34, 52, 87, 159	0
2	Q	235/244 (96%)	0.93	25 (10%) 11 9	41, 63, 108, 153	0
3	H	212/214 (99%)	0.70	22 (10%) 11 9	29, 47, 112, 200	0
3	J	213/214 (99%)	0.67	25 (11%) 9 7	22, 44, 121, 182	0
3	L	211/214 (98%)	1.18	35 (16%) 4 3	40, 66, 119, 156	0
3	N	212/214 (99%)	0.88	31 (14%) 6 4	33, 54, 133, 167	0
3	P	212/214 (99%)	0.95	27 (12%) 8 6	38, 62, 116, 160	0
3	R	212/214 (99%)	1.51	54 (25%) 1 1	45, 81, 143, 166	0
All	All	4324/4494 (96%)	0.81	474 (10%) 10 8	22, 56, 105, 206	0

All (474) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	29	VAL	6.8
3	J	1	PRO	6.6
3	R	82	ALA	6.6

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Mol	Chain	Res	Type	RSRZ
3	J	32	PHE	6.4
1	F	312	SER	6.3
1	B	39	ALA	6.3
3	H	29	VAL	6.3
3	N	34	LEU	6.2
3	N	32	PHE	6.1
3	N	1	PRO	5.8
3	H	32	PHE	5.5
3	N	27	SER	5.5
3	J	28	ASP	5.4
3	J	29	VAL	5.4
3	N	3	ALA	5.3
3	R	66	GLY	5.2
3	L	28	ASP	5.2
1	F	40	THR	5.2
3	L	212	GLU	5.1
2	I	238	LYS	5.1
1	F	77	ASP	5.0
1	B	312	SER	5.0
3	P	1	PRO	4.9
3	L	27	SER	4.9
3	H	27	SER	4.9
3	L	32	PHE	4.9
3	P	32	PHE	4.9
2	O	135	SER	4.8
3	R	29	VAL	4.8
3	R	8	ALA	4.6
3	P	3	ALA	4.6
3	H	213	CYS	4.6
1	D	312	SER	4.6
3	R	3	ALA	4.6
1	F	42	LEU	4.5
3	H	31	THR	4.5
3	R	7	PRO	4.5
3	H	28	ASP	4.5
3	H	33	ASP	4.5
3	L	34	LEU	4.5
3	J	31	THR	4.5
3	H	34	LEU	4.4
3	J	3	ALA	4.4
3	P	34	LEU	4.4
1	F	85	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
3	J	34	LEU	4.3
3	N	33	ASP	4.3
1	F	200	GLY	4.2
3	J	25	THR	4.2
3	R	5	THR	4.2
1	F	293	PRO	4.2
2	M	1	GLU	4.2
3	L	31	THR	4.2
3	P	31	THR	4.2
3	L	33	ASP	4.1
3	R	32	PHE	4.1
1	D	40	THR	4.1
1	B	310	LYS	4.1
1	A	42	LEU	4.1
3	N	35	VAL	4.1
3	J	211	THR	4.1
3	L	5	THR	4.0
3	P	33	ASP	4.0
2	G	236	CYS	4.0
1	F	294	PHE	4.0
3	J	213	CYS	3.9
3	N	82	ALA	3.9
3	N	31	THR	3.9
3	L	111	PRO	3.9
1	F	39	ALA	3.9
1	F	221	PRO	3.9
3	P	29	VAL	3.9
3	L	30	GLY	3.8
3	P	30	GLY	3.8
1	E	310	LYS	3.8
2	K	1	GLU	3.8
1	D	309	VAL	3.8
2	I	235	SER	3.8
1	F	304	ALA	3.8
3	J	24	GLY	3.8
3	N	25	THR	3.7
3	P	28	ASP	3.7
2	Q	152	SER	3.7
1	A	291	ASP	3.7
3	R	25	THR	3.7
3	J	2	SER	3.7
3	R	34	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	I	149	LYS	3.6
3	R	212	GLU	3.6
2	G	1	GLU	3.6
2	Q	1	GLU	3.6
2	O	149	LYS	3.6
3	L	25	THR	3.5
3	H	30	GLY	3.5
1	D	310	LYS	3.5
1	E	303	GLY	3.5
2	O	151	THR	3.5
3	L	158	LYS	3.5
2	K	9	ALA	3.5
1	A	175	ASP	3.4
1	D	126	ASN	3.4
3	N	28	ASP	3.4
1	E	219	PHE	3.4
2	M	235	SER	3.4
3	N	2	SER	3.4
2	Q	209	LEU	3.4
3	J	70	GLY	3.4
2	K	235	SER	3.3
2	M	152	SER	3.3
3	P	154	SER	3.3
1	E	40	THR	3.3
3	P	25	THR	3.3
3	R	1	PRO	3.3
1	D	128	ASN	3.3
3	H	24	GLY	3.3
3	J	30	GLY	3.3
3	N	30	GLY	3.3
3	R	145	ALA	3.3
1	C	312	SER	3.3
2	O	150	SER	3.3
1	C	216	ASN	3.3
3	N	29	VAL	3.3
2	I	236	CYS	3.3
1	A	312	SER	3.3
1	C	209	SER	3.3
3	R	91	SER	3.3
2	Q	2	VAL	3.2
1	C	63	ASN	3.2
1	E	291	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	299	ARG	3.2
2	Q	149	LYS	3.2
3	J	212	GLU	3.2
3	N	83	GLU	3.2
1	D	311	GLN	3.2
3	R	79	GLY	3.2
1	C	277	CYS	3.2
1	A	206	THR	3.2
1	B	40	THR	3.2
2	Q	150	SER	3.2
1	A	311	GLN	3.1
1	F	305	CYS	3.1
2	K	153	GLY	3.1
3	R	21	SER	3.1
1	F	201	ARG	3.1
3	R	33	ASP	3.1
3	R	211	THR	3.1
3	R	2	SER	3.1
2	K	10	GLU	3.1
1	D	129	GLY	3.1
3	J	158	LYS	3.1
1	A	299	ARG	3.1
2	K	135	SER	3.1
2	O	1	GLU	3.1
3	J	33	ASP	3.1
3	R	100	GLY	3.1
1	F	310	LYS	3.1
1	A	219	PHE	3.1
1	F	296	ASN	3.0
1	C	240	GLY	3.0
3	R	94	ALA	3.0
3	J	162	GLU	3.0
1	C	219	PHE	3.0
1	D	43	VAL	3.0
1	E	214	ILE	3.0
1	C	208	ARG	3.0
3	H	25	THR	3.0
1	A	63	ASN	2.9
1	F	129	GLY	2.9
2	Q	42	GLY	2.9
2	K	151	THR	2.9
2	O	178	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
2	G	2	VAL	2.9
1	A	310	LYS	2.9
3	L	2	SER	2.9
1	C	175	ASP	2.9
2	M	234	LYS	2.9
3	P	205	GLU	2.9
2	O	235	SER	2.9
1	C	305	CYS	2.9
1	C	112	VAL	2.9
1	D	166	VAL	2.9
1	F	43	VAL	2.9
2	M	107	ASP	2.8
1	B	309	VAL	2.8
1	F	125	PHE	2.8
3	N	212	GLU	2.8
1	C	307	ARG	2.8
3	R	58	SER	2.8
1	F	291	ASP	2.8
2	O	154	GLY	2.8
1	D	163	ALA	2.8
1	E	309	VAL	2.8
3	N	157	VAL	2.8
1	C	188	ASP	2.8
1	F	104	ASP	2.8
1	C	304	ALA	2.8
2	Q	74	THR	2.8
1	F	297	VAL	2.8
3	R	74	SER	2.8
1	B	263	GLY	2.8
2	Q	161	LEU	2.8
2	Q	179	LEU	2.8
3	R	31	THR	2.8
1	F	214	ILE	2.7
1	B	42	LEU	2.7
1	B	200	GLY	2.7
1	A	280	GLU	2.7
1	B	280	GLU	2.7
1	F	188	ASP	2.7
3	N	158	LYS	2.7
1	D	42	LEU	2.7
1	E	312	SER	2.7
2	I	135	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	Q	147	SER	2.7
2	I	1	GLU	2.7
2	Q	151	THR	2.7
3	L	208	VAL	2.7
3	P	211	THR	2.7
1	C	264	LYS	2.7
2	K	149	LYS	2.7
3	R	128	GLN	2.7
1	D	305	CYS	2.7
1	F	267	ILE	2.7
1	C	280	GLU	2.7
3	J	71	ASN	2.7
3	N	71	ASN	2.7
3	R	60	VAL	2.7
2	G	57	ASP	2.7
2	Q	107	ASP	2.7
1	F	311	GLN	2.7
3	L	93	TYR	2.7
3	R	4	LEU	2.7
1	A	126	ASN	2.7
1	F	262	SER	2.7
2	G	235	SER	2.7
1	D	219	PHE	2.7
2	I	64	PHE	2.7
3	L	82	ALA	2.7
3	N	211	THR	2.7
1	F	306	PRO	2.7
1	A	41	GLU	2.6
3	H	70	GLY	2.6
1	E	63	ASN	2.6
2	G	149	LYS	2.6
3	J	26	ASN	2.6
1	E	304	ALA	2.6
2	Q	159	GLY	2.6
1	B	63	ASN	2.6
1	C	206	THR	2.6
3	R	23	THR	2.6
1	C	291	ASP	2.6
1	F	202	ILE	2.6
2	I	209	LEU	2.6
2	Q	11	VAL	2.6
3	L	94	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
3	L	72	THR	2.6
2	I	237	ASP	2.6
1	D	299	ARG	2.6
3	R	158	LYS	2.6
1	F	63	ASN	2.6
3	L	73	ALA	2.6
2	M	135	SER	2.5
3	H	211	THR	2.5
3	R	24	GLY	2.5
2	Q	41	PRO	2.5
2	Q	178	ALA	2.5
1	A	290	ASN	2.5
1	A	298	ASN	2.5
3	H	71	ASN	2.5
3	H	194	SER	2.5
3	P	27	SER	2.5
2	G	87	ARG	2.5
3	P	68	LYS	2.5
1	F	237	VAL	2.5
1	B	311	GLN	2.5
3	L	3	ALA	2.5
1	A	225	ASN	2.5
3	N	69	SER	2.5
2	K	107	ASP	2.5
3	P	55	ARG	2.5
2	M	154	GLY	2.5
2	O	61	ALA	2.5
2	M	151	THR	2.5
1	A	279	SER	2.5
2	M	42	GLY	2.5
3	R	59	GLY	2.5
3	P	204	VAL	2.5
3	L	23	THR	2.4
1	F	110	SER	2.4
1	C	241	ASP	2.4
1	C	210	GLN	2.4
2	Q	234	LYS	2.4
3	N	152	ALA	2.4
3	J	27	SER	2.4
3	N	78	SER	2.4
1	F	52	CYS	2.4
3	J	62	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	169	PRO	2.4
1	A	207	LYS	2.4
2	G	11	VAL	2.4
3	H	209	ALA	2.4
3	P	4	LEU	2.4
2	O	232	GLU	2.4
2	G	233	PRO	2.4
2	M	149	LYS	2.4
1	E	125	PHE	2.4
2	K	203	THR	2.4
3	N	72	THR	2.4
3	J	185	GLU	2.4
3	L	67	SER	2.4
1	F	101	ASP	2.4
2	K	222	PRO	2.4
1	E	201	ARG	2.4
1	C	48	ILE	2.3
1	C	217	ILE	2.3
1	C	199	SER	2.3
1	C	238	LYS	2.3
2	Q	89	ASP	2.3
1	B	125	PHE	2.3
1	F	171	ASN	2.3
3	H	26	ASN	2.3
1	A	262	SER	2.3
3	P	2	SER	2.3
1	E	208	ARG	2.3
2	O	153	GLY	2.3
2	Q	154	GLY	2.3
3	R	30	GLY	2.3
3	R	113	GLY	2.3
3	L	22	CYS	2.3
3	L	112	LYS	2.3
3	R	85	GLU	2.3
1	B	188	ASP	2.3
1	C	198	PRO	2.3
1	C	197	GLN	2.3
2	Q	210	GLY	2.3
1	C	236	ILE	2.3
3	N	94	ALA	2.3
1	D	47	SER	2.3
1	F	199	SER	2.3

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Mol	Chain	Res	Type	RSRZ
3	L	56	ARG	2.3
3	R	28	ASP	2.3
2	K	96	CYS	2.2
2	O	160	CYS	2.2
2	Q	134	ALA	2.2
3	P	94	ALA	2.2
3	R	22	CYS	2.2
1	F	126	ASN	2.2
3	P	156	PRO	2.2
3	R	210	PRO	2.2
1	C	47	SER	2.2
1	C	101	ASP	2.2
1	E	104	ASP	2.2
2	K	148	SER	2.2
2	M	150	SER	2.2
1	F	240	GLY	2.2
1	C	309	VAL	2.2
2	K	11	VAL	2.2
2	O	209	LEU	2.2
1	D	97	CYS	2.2
3	P	203	THR	2.2
1	C	257	TYR	2.2
1	F	45	ASN	2.2
3	N	191	ARG	2.2
1	B	210	GLN	2.2
1	D	44	GLN	2.2
1	B	175	ASP	2.2
1	C	218	GLY	2.2
1	D	209	SER	2.2
1	E	262	SER	2.2
2	O	44	GLY	2.2
3	L	95	GLY	2.2
3	N	70	GLY	2.2
3	R	101	GLY	2.2
3	N	4	LEU	2.2
3	H	208	VAL	2.2
3	R	68	LYS	2.2
1	D	280	GLU	2.2
1	E	64	CYS	2.2
2	M	232	GLU	2.2
3	H	212	GLU	2.2
3	P	164	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	208	ARG	2.2
1	E	126	ASN	2.2
1	B	173	GLN	2.2
1	E	209	SER	2.2
2	K	12	LYS	2.2
3	R	15	GLY	2.2
3	J	167	SER	2.2
3	R	9	SER	2.2
2	I	9	ALA	2.2
3	P	73	ALA	2.2
1	E	41	GLU	2.2
3	J	83	GLU	2.2
3	H	72	THR	2.2
3	L	211	THR	2.2
2	I	160	CYS	2.2
1	F	105	TYR	2.2
3	L	26	ASN	2.2
3	R	89	TYR	2.2
1	B	197	GLN	2.2
1	A	238	LYS	2.2
1	C	310	LYS	2.2
1	E	42	LEU	2.2
3	N	66	GLY	2.2
2	I	132	SER	2.2
3	H	69	SER	2.2
3	L	167	SER	2.2
3	R	170	SER	2.2
1	A	64	CYS	2.1
1	E	173	GLN	2.1
1	F	128	ASN	2.1
3	L	110	GLN	2.1
3	N	26	ASN	2.1
3	R	26	ASN	2.1
3	R	81	GLN	2.1
1	B	199	SER	2.1
1	E	242	ILE	2.1
2	K	2	VAL	2.1
3	R	157	VAL	2.1
1	E	69	ALA	2.1
1	F	280	GLU	2.1
3	L	200	GLU	2.1
1	F	222	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
3	R	56	ARG	2.1
1	F	103	PRO	2.1
2	O	146	PRO	2.1
1	C	228	SER	2.1
2	Q	148	SER	2.1
2	K	232	GLU	2.1
3	L	126	GLU	2.1
2	I	151	THR	2.1
1	E	311	GLN	2.1
3	R	80	LEU	2.1
1	D	122	ASN	2.1
1	D	260	ILE	2.1
1	E	300	ILE	2.1
3	R	20	ILE	2.1
1	B	41	GLU	2.1
1	D	222	ARG	2.1
1	D	304	ALA	2.1
1	F	220	ARG	2.1
2	G	130	ALA	2.1
2	Q	206	SER	2.1
3	R	83	GLU	2.1
1	D	127	TRP	2.1
1	B	198	PRO	2.1
1	E	144	ASN	2.1
3	N	24	GLY	2.1
3	R	144	GLY	2.1
2	K	227	VAL	2.1
1	C	174	PHE	2.1
1	F	46	SER	2.0
2	K	145	ALA	2.0
3	L	83	GLU	2.0
2	K	207	SER	2.0
3	P	9	SER	2.0
1	B	165	ASN	2.0
1	C	225	ASN	2.0
1	F	226	ILE	2.0
2	K	154	GLY	2.0
1	A	277	CYS	2.0
3	L	35	VAL	2.0
1	D	41	GLU	2.0
2	G	46	GLU	2.0
3	H	62	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	K	63	LYS	2.0
3	P	114	ALA	2.0
2	O	88	SER	2.0
3	R	27	SER	2.0
1	D	173	GLN	2.0
3	R	12	GLY	2.0
2	Q	129	VAL	2.0
3	P	60	VAL	2.0
3	R	191	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

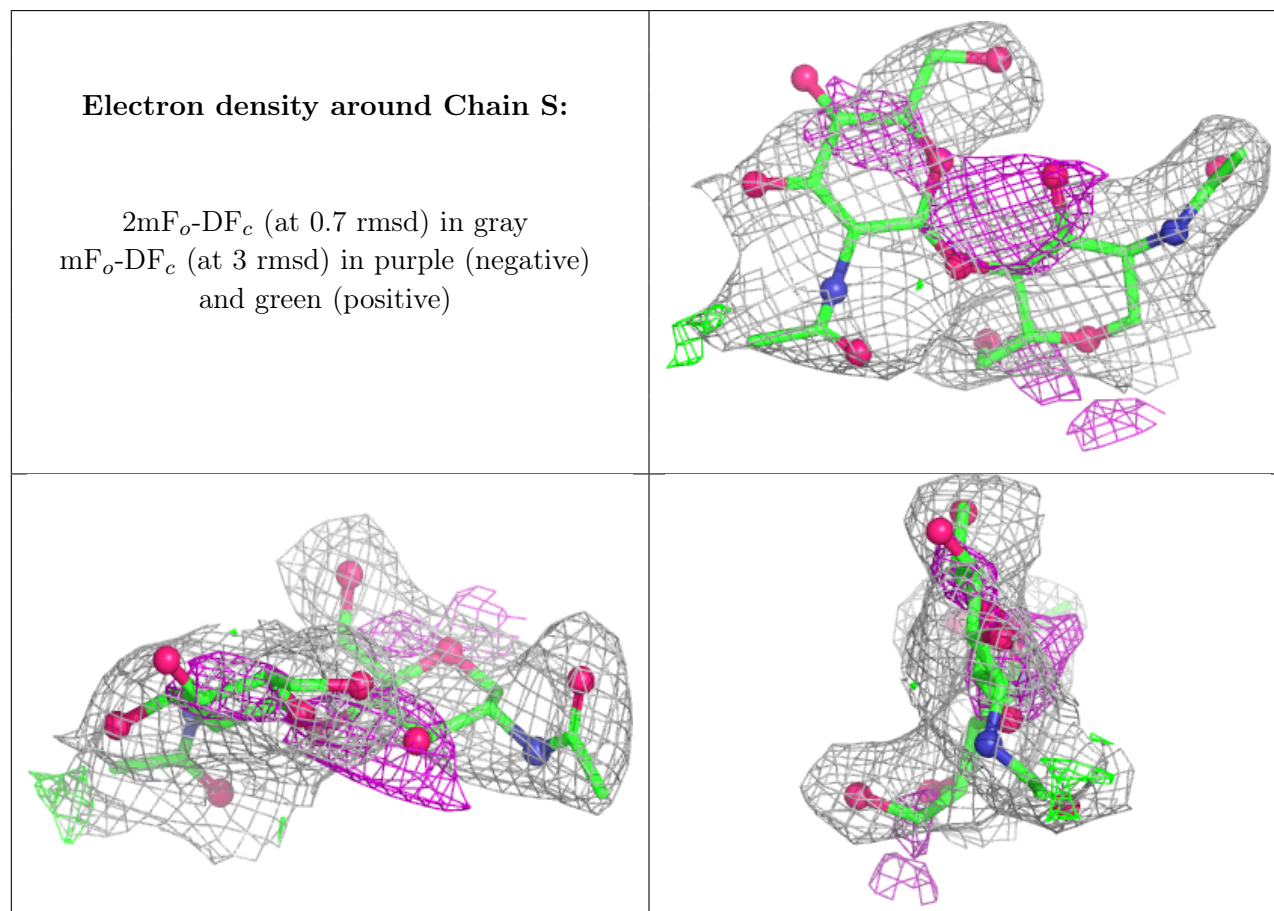
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	T	3	11/12	0.24	0.19	75,77,77,78	0
4	NAG	S	2	14/15	0.36	0.19	63,67,68,68	0
5	BMA	X	3	11/12	0.38	0.17	75,77,77,77	0
4	NAG	Z	2	14/15	0.41	0.19	69,71,72,73	0
5	BMA	U	3	11/12	0.46	0.16	71,73,74,74	0
5	NAG	X	2	14/15	0.52	0.16	65,70,71,73	0
4	NAG	Y	2	14/15	0.54	0.16	58,61,62,62	0
4	NAG	W	1	14/15	0.59	0.17	47,52,54,58	0
5	NAG	X	1	14/15	0.59	0.19	50,52,55,60	0
4	NAG	Z	1	14/15	0.61	0.15	58,64,65,67	0
5	NAG	U	2	14/15	0.64	0.15	60,64,66,68	0
5	NAG	T	2	14/15	0.65	0.16	63,68,70,73	0
4	NAG	W	2	14/15	0.66	0.15	61,65,66,66	0
5	NAG	U	1	14/15	0.72	0.15	46,47,50,55	0
4	NAG	S	1	14/15	0.78	0.13	44,49,53,58	0
4	NAG	V	2	14/15	0.79	0.14	54,57,58,59	0
4	NAG	V	1	14/15	0.81	0.12	38,44,46,51	0
4	NAG	Y	1	14/15	0.83	0.12	45,47,49,54	0
5	NAG	T	1	14/15	0.84	0.11	45,46,51,57	0

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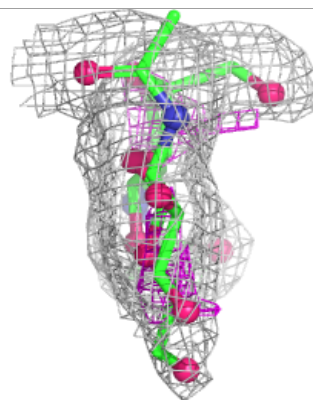
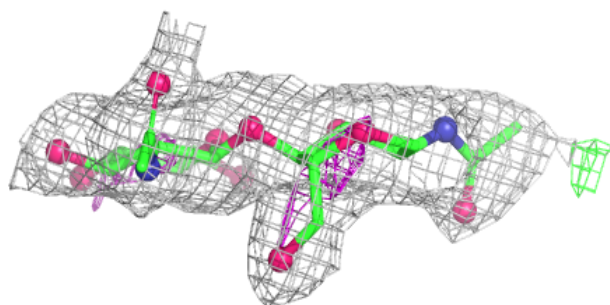
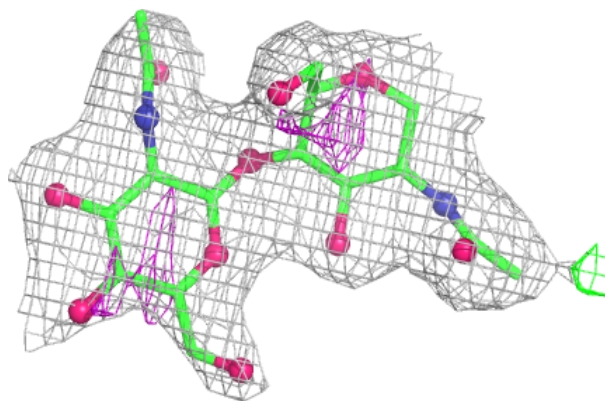
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	a	1	14/15	-	-	44,49,52,57	0
5	NAG	a	2	14/15	-	-	63,67,69,72	0
5	BMA	a	3	11/12	-	-	75,76,77,77	0
5	NAG	b	1	14/15	-	-	46,48,51,56	0
5	NAG	b	2	14/15	-	-	61,66,68,70	0
5	BMA	b	3	11/12	-	-	72,73,74,74	0

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.

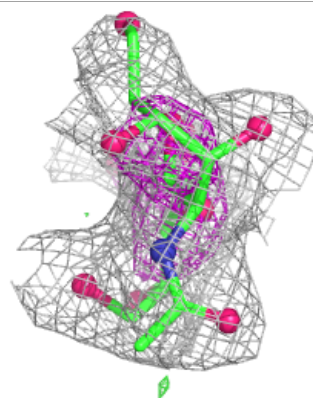
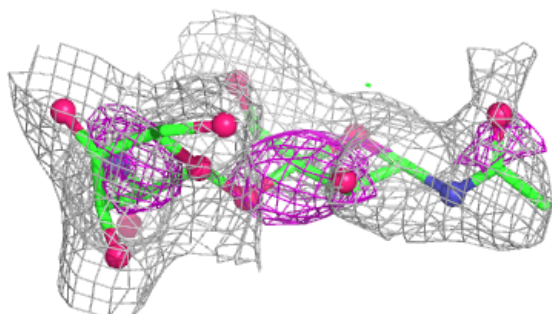
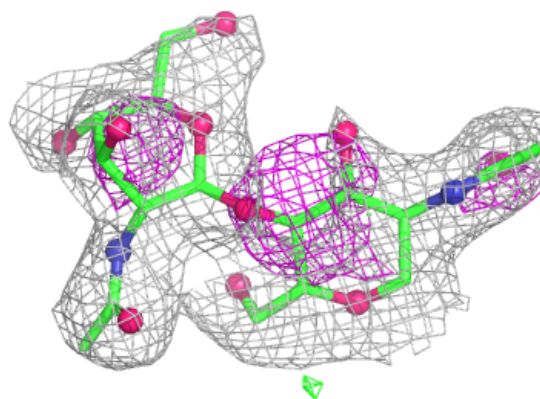


Electron density around Chain V:

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

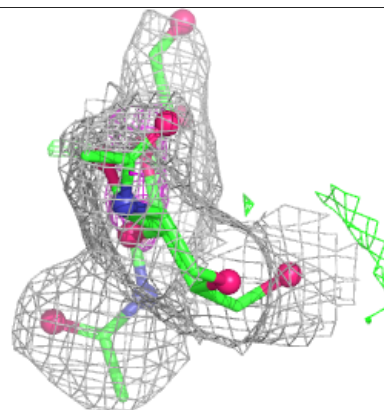
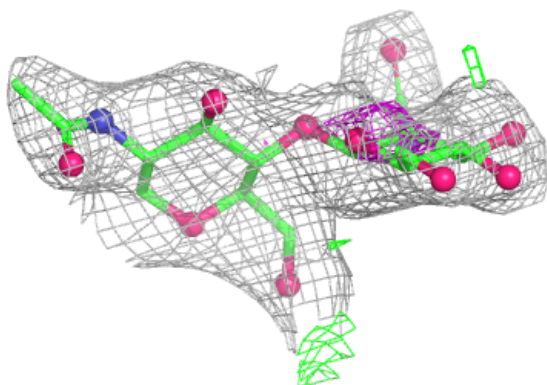
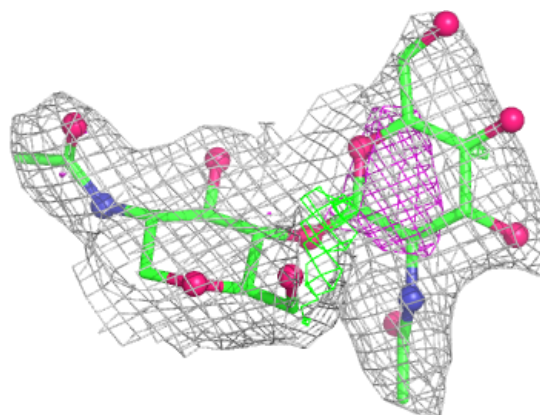
**Electron density around Chain W:**

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

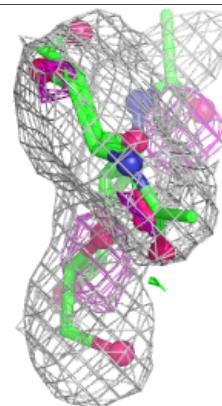
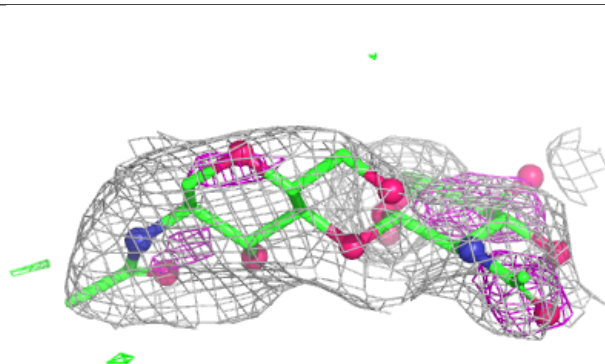
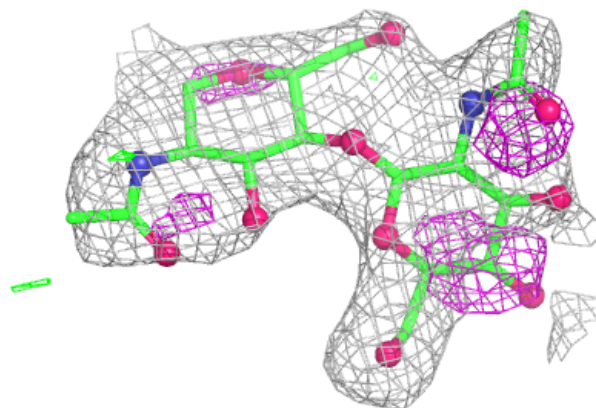


Electron density around Chain Y:

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

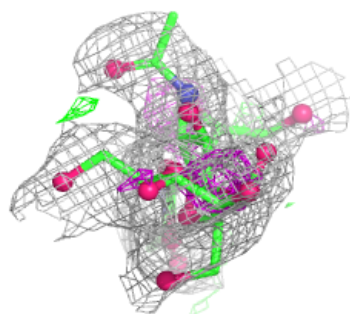
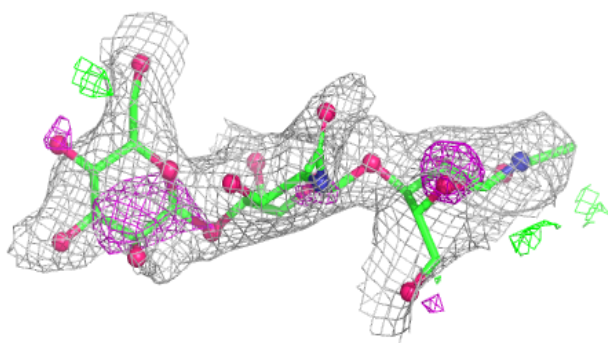
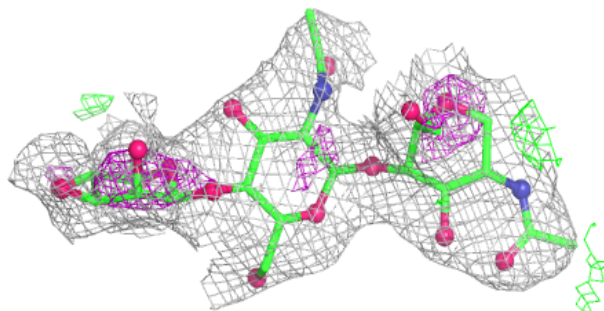
**Electron density around Chain Z:**

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

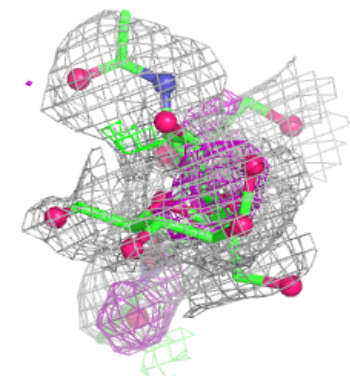
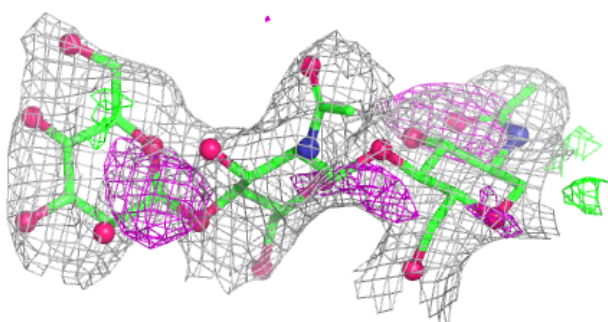
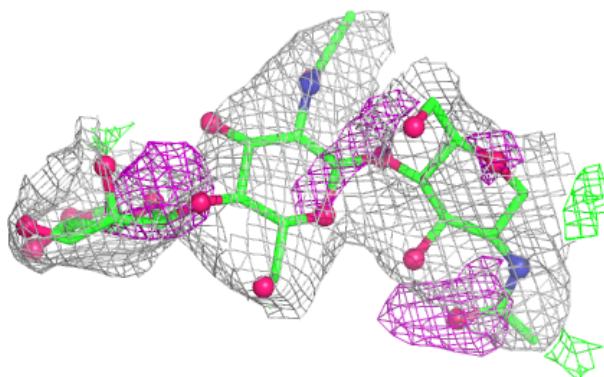


Electron density around Chain T:

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

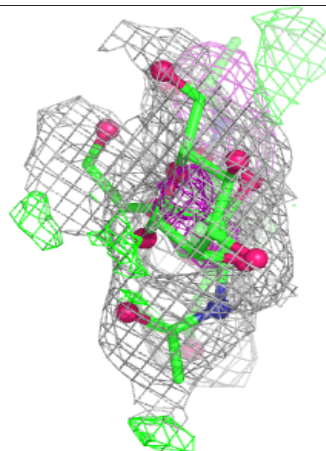
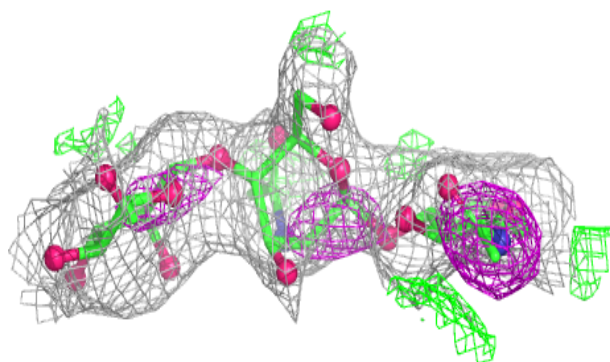
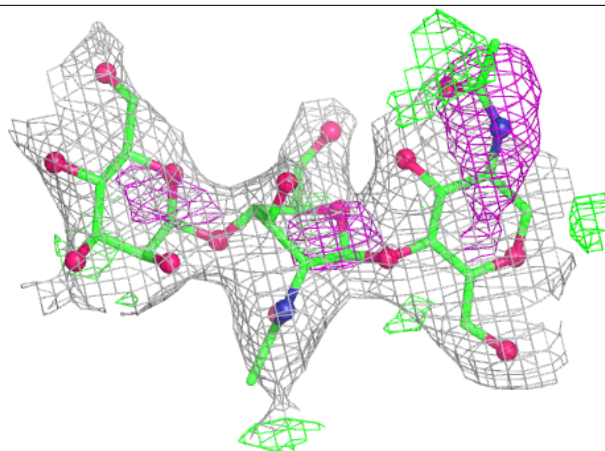
**Electron density around Chain U:**

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

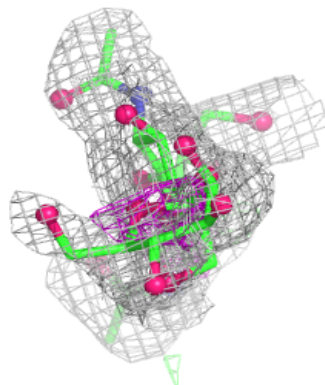
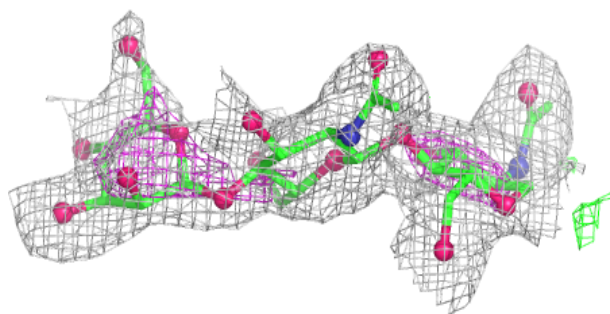
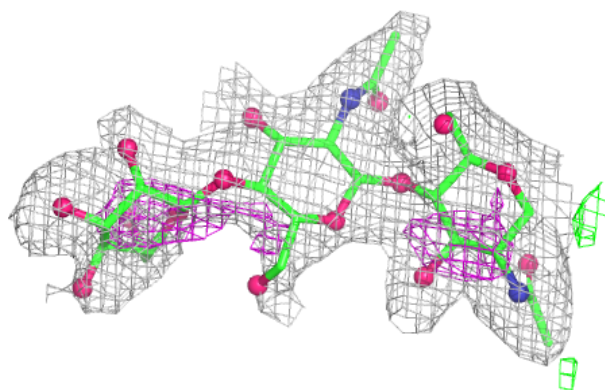


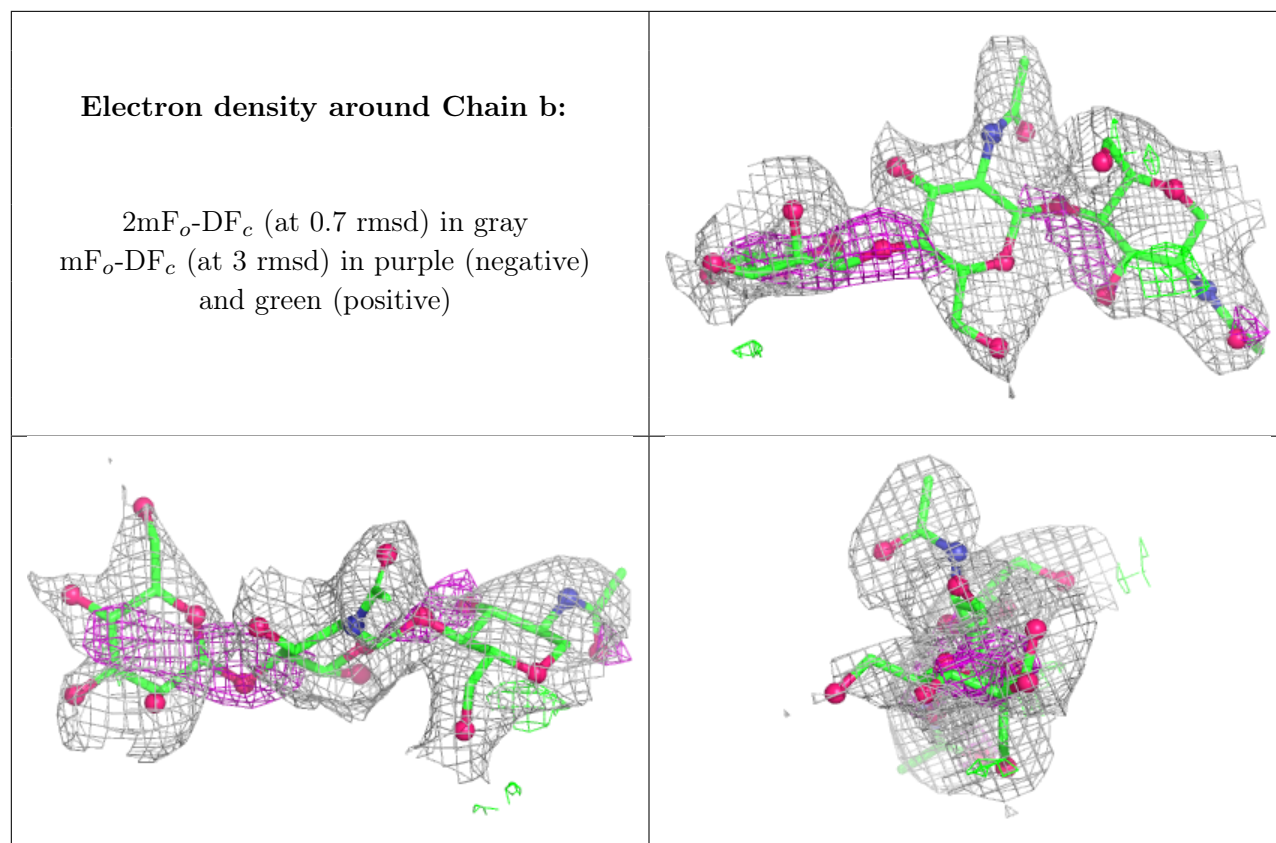
Electron density around Chain X:

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

**Electron density around Chain a:**

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	D	405	14/15	0.26	0.23	43,47,49,50	0
6	NAG	C	401	14/15	0.48	0.18	46,50,53,53	0
6	NAG	A	408	14/15	0.48	0.21	41,46,47,47	0
6	NAG	D	406	14/15	0.50	0.18	43,47,52,53	0
6	NAG	E	405	14/15	0.52	0.19	46,50,52,52	0
6	NAG	A	407	14/15	0.55	0.18	45,50,53,54	0
6	NAG	A	406	14/15	0.55	0.16	43,46,48,49	0
6	NAG	F	405	14/15	0.55	0.19	46,46,49,49	0
6	NAG	C	405	14/15	0.56	0.17	50,52,54,55	0
6	NAG	D	407	14/15	0.58	0.16	42,46,48,48	0
6	NAG	E	406	14/15	0.67	0.15	41,47,48,49	0
6	NAG	E	404	14/15	0.69	0.17	40,44,48,51	0
6	NAG	F	406	14/15	0.70	0.15	37,39,40,41	0
6	NAG	B	408	14/15	0.71	0.14	48,52,55,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	C	406	14/15	0.72	0.15	38,43,45,46	0
6	NAG	F	404	14/15	0.79	0.12	41,45,47,49	0
7	GOL	I	301	6/6	0.88	0.14	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.