



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:37 AM UTC

PDB ID : 4MHJ / pdb_00004mhj
Title : Crystal structure of Fab H5M9 in complex with influenza virus hemagglutinin from A/goose/Guangdong/1/96 (H5N1)
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2013-08-29
Resolution : 6.98 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:

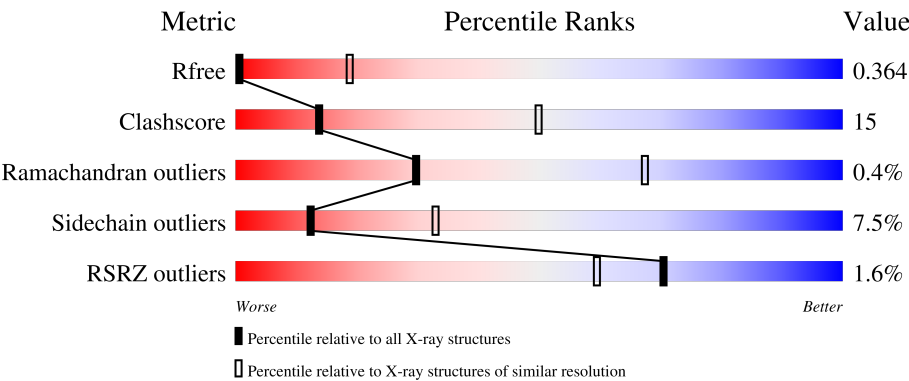
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 6.98 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	1166 (9.70-4.00)
Clashscore	190562	1007 (9.70-4.04)
Ramachandran outliers	187476	1053 (9.70-4.00)
Sidechain outliers	187428	1016 (9.70-4.00)
RSRZ outliers	180081	1159 (9.70-4.00)

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

Mol	Chain	Length	Quality of chain
1	A	334	2% 72% 23% ..
1	C	334	2% 72% 22% ..
1	G	334	3% 70% 24% ..
1	M	334	% 73% 22% ..
1	O	334	2% 70% 23% 5% ..

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Mol	Chain	Length	Quality of chain
1	S	334	
2	B	182	
2	D	182	
2	I	182	
2	N	182	
2	P	182	
2	U	182	
3	E	218	
3	J	218	
3	L	218	
3	Q	218	
3	V	218	
3	X	218	
4	F	222	
4	H	222	
4	K	222	
4	R	222	
4	T	222	
4	W	222	
5	Y	3	
5	d	3	
5	f	3	
6	Z	8	
7	a	2	
7	c	2	

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Mol	Chain	Length	Quality of chain
8	b	3	 67%33%
9	e	4	 25%75%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 43995 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2542	1603	440	484	15			
1	C	321	Total	C	N	O	S	0	0	0
			2533	1598	438	482	15			
1	G	321	Total	C	N	O	S	0	0	0
			2530	1594	439	482	15			
1	M	322	Total	C	N	O	S	0	0	0
			2542	1603	440	484	15			
1	O	318	Total	C	N	O	S	0	0	0
			2514	1587	435	477	15			
1	S	322	Total	C	N	O	S	0	0	0
			2542	1603	440	484	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q9Q0U6
A	8	ASP	-	expression tag	UNP Q9Q0U6
A	9	PRO	-	expression tag	UNP Q9Q0U6
A	10	GLY	-	expression tag	UNP Q9Q0U6
C	7	ALA	-	expression tag	UNP Q9Q0U6
C	8	ASP	-	expression tag	UNP Q9Q0U6
C	9	PRO	-	expression tag	UNP Q9Q0U6
C	10	GLY	-	expression tag	UNP Q9Q0U6
G	7	ALA	-	expression tag	UNP Q9Q0U6
G	8	ASP	-	expression tag	UNP Q9Q0U6
G	9	PRO	-	expression tag	UNP Q9Q0U6
G	10	GLY	-	expression tag	UNP Q9Q0U6
M	7	ALA	-	expression tag	UNP Q9Q0U6
M	8	ASP	-	expression tag	UNP Q9Q0U6
M	9	PRO	-	expression tag	UNP Q9Q0U6
M	10	GLY	-	expression tag	UNP Q9Q0U6
O	7	ALA	-	expression tag	UNP Q9Q0U6

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Chain	Residue	Modelled	Actual	Comment	Reference
O	8	ASP	-	expression tag	UNP Q9Q0U6
O	9	PRO	-	expression tag	UNP Q9Q0U6
O	10	GLY	-	expression tag	UNP Q9Q0U6
S	7	ALA	-	expression tag	UNP Q9Q0U6
S	8	ASP	-	expression tag	UNP Q9Q0U6
S	9	PRO	-	expression tag	UNP Q9Q0U6
S	10	GLY	-	expression tag	UNP Q9Q0U6

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1393	866	239	280	8			
2	D	172	Total	C	N	O	S	0	0	0
			1393	866	239	280	8			
2	N	169	Total	C	N	O	S	0	0	0
			1363	846	233	276	8			
2	P	172	Total	C	N	O	S	0	0	0
			1393	866	239	280	8			
2	I	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	U	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	176	SER	-	expression tag	UNP Q9Q0U6
B	177	GLY	-	expression tag	UNP Q9Q0U6
B	178	ARG	-	expression tag	UNP Q9Q0U6
B	179	LEU	-	expression tag	UNP Q9Q0U6
B	180	VAL	-	expression tag	UNP Q9Q0U6
B	181	PRO	-	expression tag	UNP Q9Q0U6
B	182	ARG	-	expression tag	UNP Q9Q0U6
D	176	SER	-	expression tag	UNP Q9Q0U6
D	177	GLY	-	expression tag	UNP Q9Q0U6
D	178	ARG	-	expression tag	UNP Q9Q0U6
D	179	LEU	-	expression tag	UNP Q9Q0U6
D	180	VAL	-	expression tag	UNP Q9Q0U6
D	181	PRO	-	expression tag	UNP Q9Q0U6
D	182	ARG	-	expression tag	UNP Q9Q0U6
N	176	SER	-	expression tag	UNP Q9Q0U6

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Chain	Residue	Modelled	Actual	Comment	Reference
N	177	GLY	-	expression tag	UNP Q9Q0U6
N	178	ARG	-	expression tag	UNP Q9Q0U6
N	179	LEU	-	expression tag	UNP Q9Q0U6
N	180	VAL	-	expression tag	UNP Q9Q0U6
N	181	PRO	-	expression tag	UNP Q9Q0U6
N	182	ARG	-	expression tag	UNP Q9Q0U6
P	176	SER	-	expression tag	UNP Q9Q0U6
P	177	GLY	-	expression tag	UNP Q9Q0U6
P	178	ARG	-	expression tag	UNP Q9Q0U6
P	179	LEU	-	expression tag	UNP Q9Q0U6
P	180	VAL	-	expression tag	UNP Q9Q0U6
P	181	PRO	-	expression tag	UNP Q9Q0U6
P	182	ARG	-	expression tag	UNP Q9Q0U6
I	176	SER	-	expression tag	UNP Q9Q0U6
I	177	GLY	-	expression tag	UNP Q9Q0U6
I	178	ARG	-	expression tag	UNP Q9Q0U6
I	179	LEU	-	expression tag	UNP Q9Q0U6
I	180	VAL	-	expression tag	UNP Q9Q0U6
I	181	PRO	-	expression tag	UNP Q9Q0U6
I	182	ARG	-	expression tag	UNP Q9Q0U6
U	176	SER	-	expression tag	UNP Q9Q0U6
U	177	GLY	-	expression tag	UNP Q9Q0U6
U	178	ARG	-	expression tag	UNP Q9Q0U6
U	179	LEU	-	expression tag	UNP Q9Q0U6
U	180	VAL	-	expression tag	UNP Q9Q0U6
U	181	PRO	-	expression tag	UNP Q9Q0U6
U	182	ARG	-	expression tag	UNP Q9Q0U6

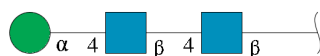
- Molecule 3 is a protein called H5M9 antibody, light chain (kappa).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	0	0
			1666	1032	289	339	6			
3	E	216	Total	C	N	O	S	0	0	0
			1672	1035	290	341	6			
3	J	211	Total	C	N	O	S	0	0	0
			1634	1015	280	333	6			
3	X	216	Total	C	N	O	S	0	0	0
			1672	1035	290	341	6			
3	Q	215	Total	C	N	O	S	0	0	0
			1665	1031	289	339	6			
3	V	214	Total	C	N	O	S	0	0	0
			1655	1026	285	338	6			

- Molecule 4 is a protein called H5M9 antibody, heavy chain (IgG1).

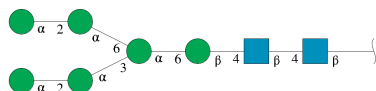
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	221	Total	C	N	O	S	0	0	0
			1675	1059	276	331	9			
4	F	221	Total	C	N	O	S	0	0	0
			1675	1059	276	331	9			
4	K	221	Total	C	N	O	S	0	0	0
			1674	1057	276	332	9			
4	T	220	Total	C	N	O	S	0	0	0
			1666	1054	274	329	9			
4	R	221	Total	C	N	O	S	0	0	0
			1675	1059	276	331	9			
4	W	221	Total	C	N	O	S	0	0	0
			1675	1059	276	331	9			

- Molecule 5 is an oligosaccharide called alpha-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	Y	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	d	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	f	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



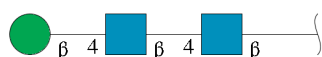
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	Z	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 7 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
7	a	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	c	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 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.



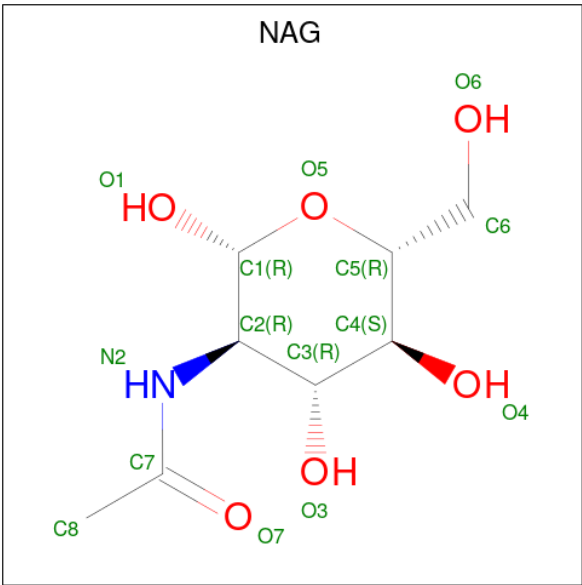
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	b	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
9	e	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

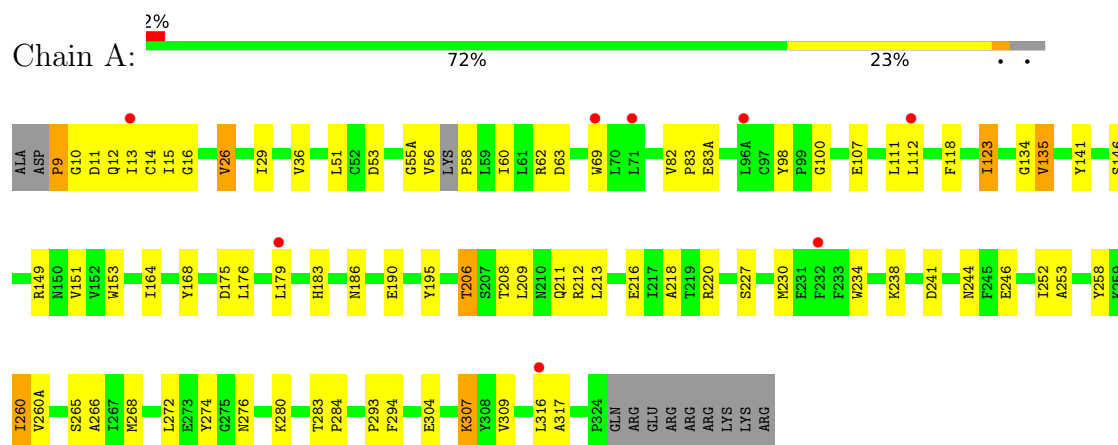


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	M	1	Total	C	N	O	0	0
			14	8	1	5		
10	O	1	Total	C	N	O	0	0
			14	8	1	5		
10	P	1	Total	C	N	O	0	0
			14	8	1	5		
10	S	1	Total	C	N	O	0	0
			14	8	1	5		

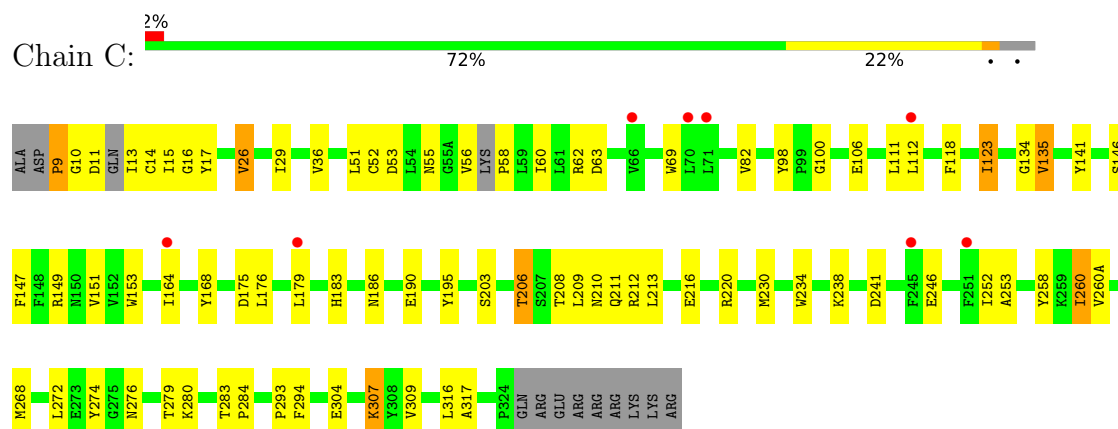
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

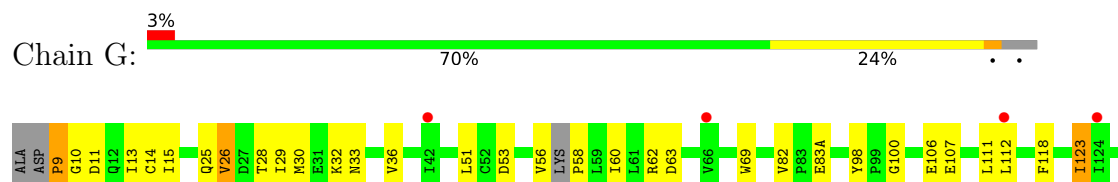
• Molecule 1: Hemagglutinin HA1 chain

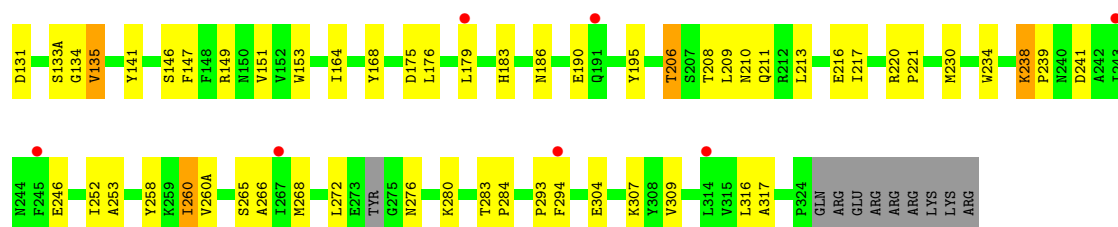


• Molecule 1: Hemagglutinin HA1 chain

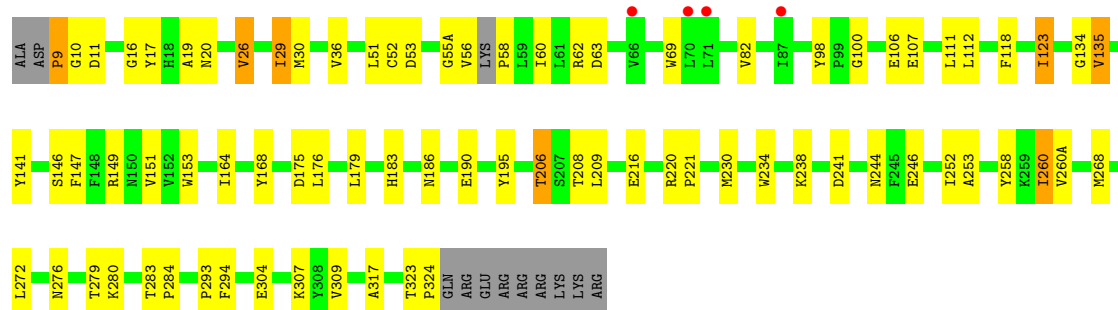
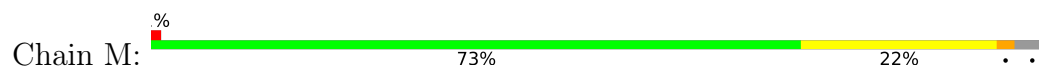


• Molecule 1: Hemagglutinin HA1 chain

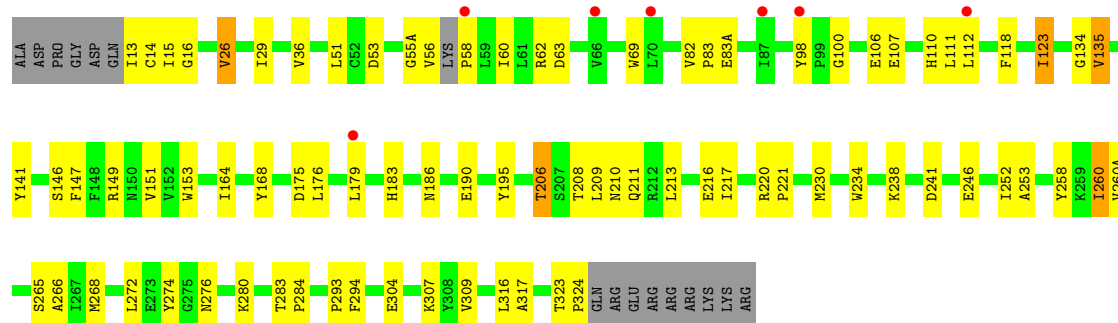




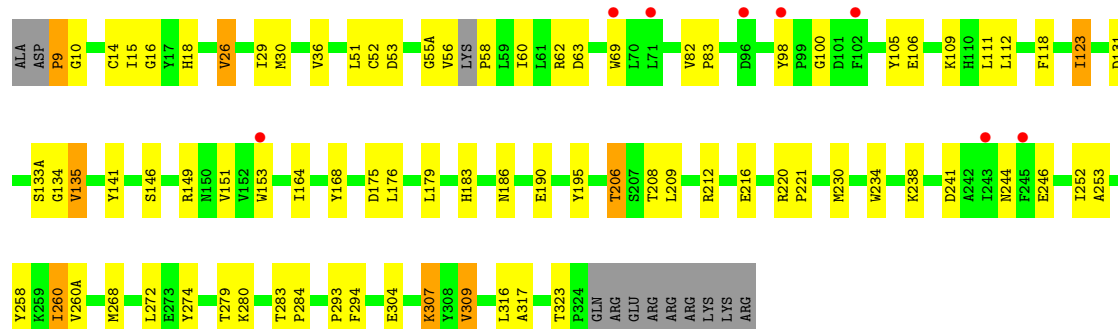
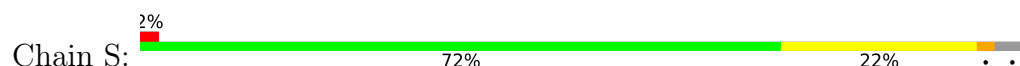
• Molecule 1: Hemagglutinin HA1 chain



• Molecule 1: Hemagglutinin HA1 chain

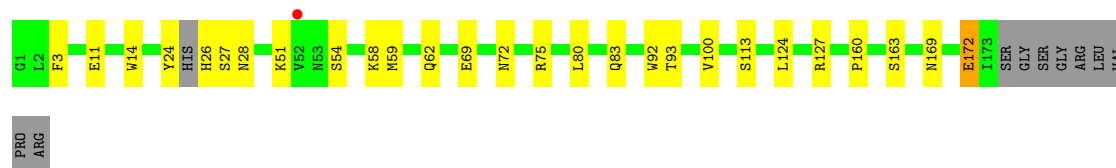


• Molecule 1: Hemagglutinin HA1 chain



- Molecule 2: Hemagglutinin HA2 chain

Chain B: 



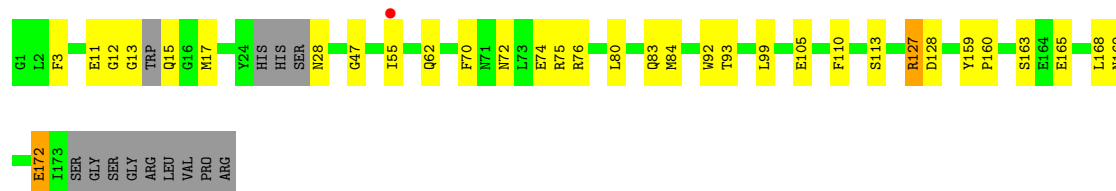
- Molecule 2: Hemagglutinin HA2 chain

Chain D: 



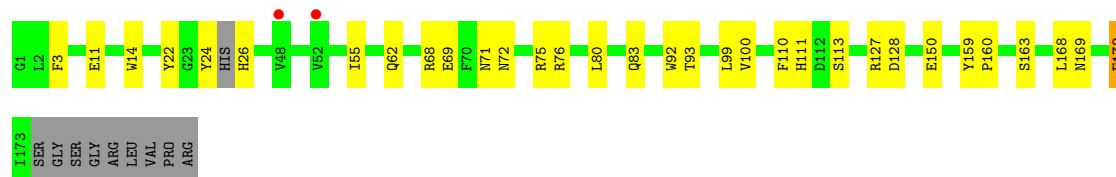
- Molecule 2: Hemagglutinin HA2 chain

Chain N: 



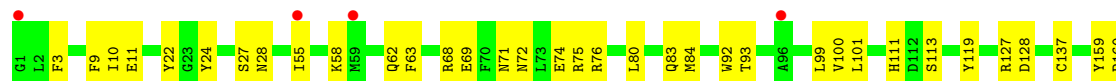
- Molecule 2: Hemagglutinin HA2 chain

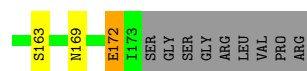
Chain P: 



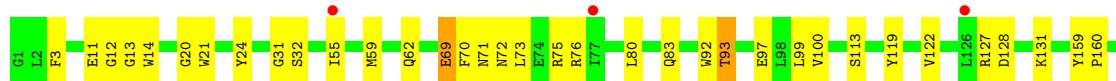
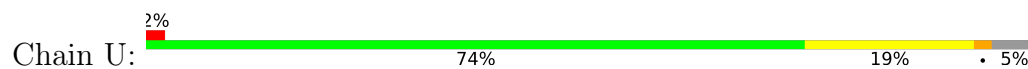
- Molecule 2: Hemagglutinin HA2 chain

Chain I: 

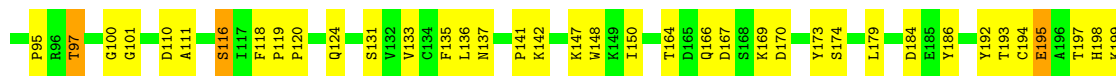




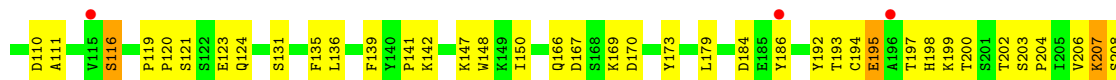
• Molecule 2: Hemagglutinin HA2 chain



• Molecule 3: H5M9 antibody, light chain (kappa)

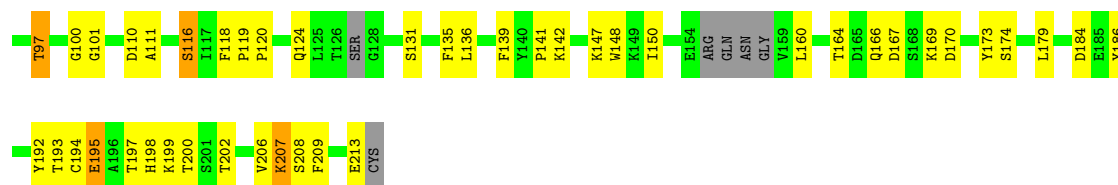


• Molecule 3: H5M9 antibody, light chain (kappa)

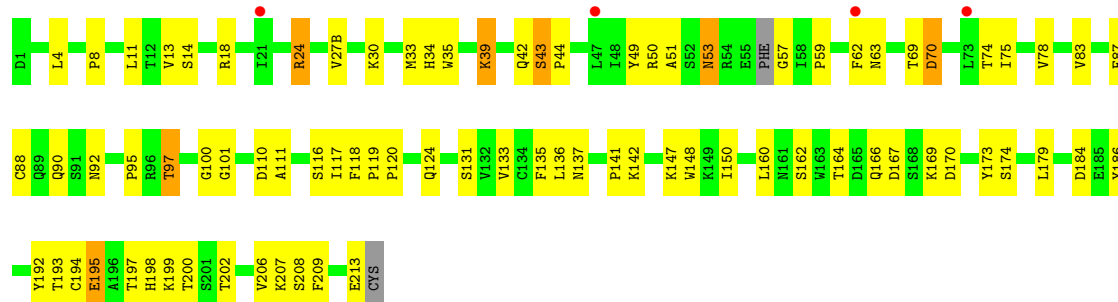


• Molecule 3: H5M9 antibody, light chain (kappa)

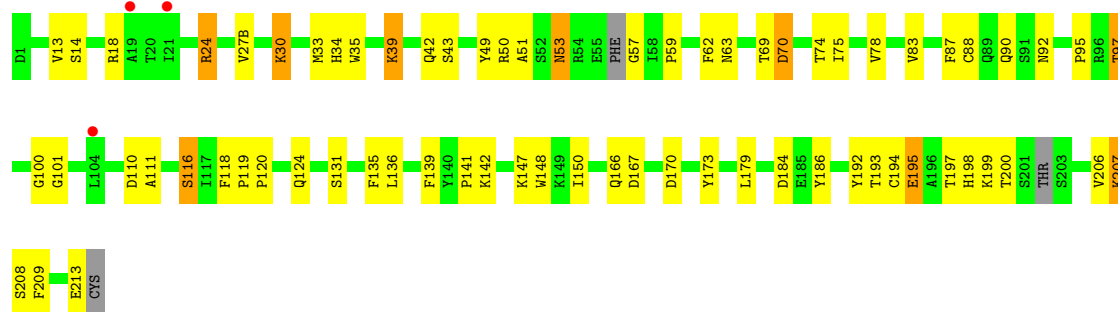




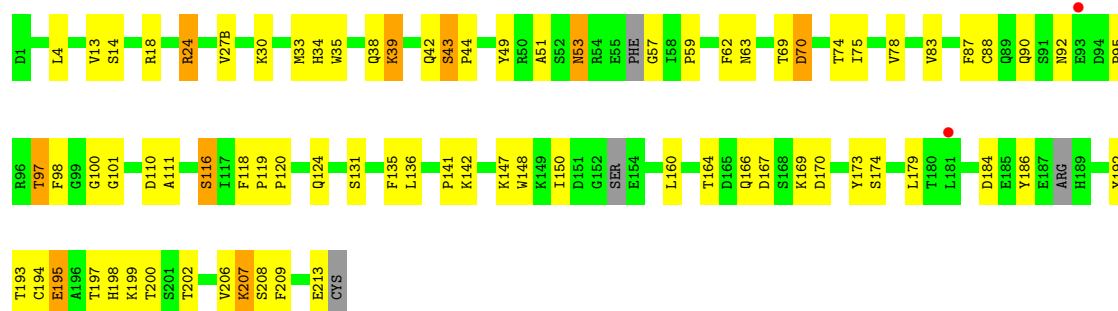
• Molecule 3: H5M9 antibody, light chain (kappa)



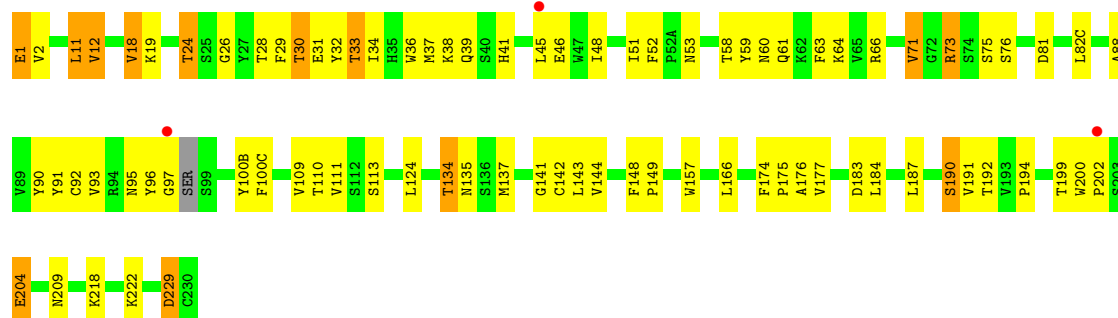
• Molecule 3: H5M9 antibody, light chain (kappa)



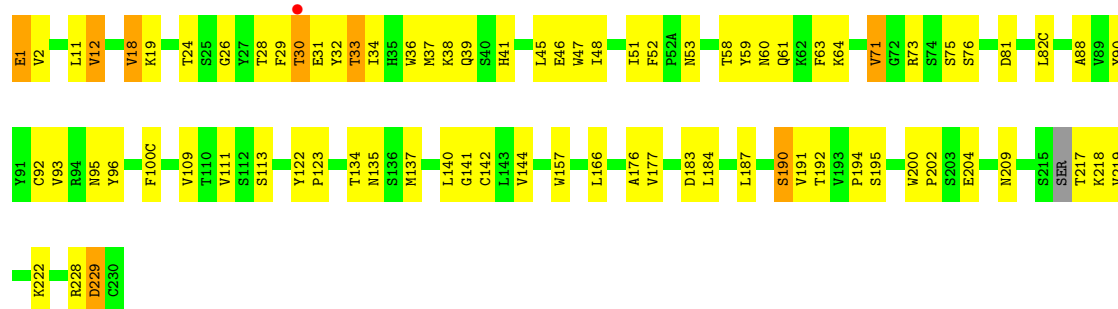
• Molecule 3: H5M9 antibody, light chain (kappa)



• Molecule 4: H5M9 antibody, heavy chain (IgG1)



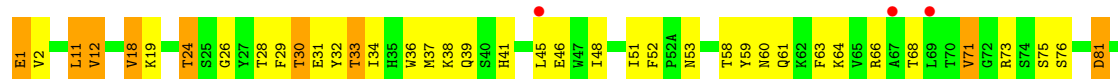
- Molecule 4: H5M9 antibody, heavy chain (IgG1)

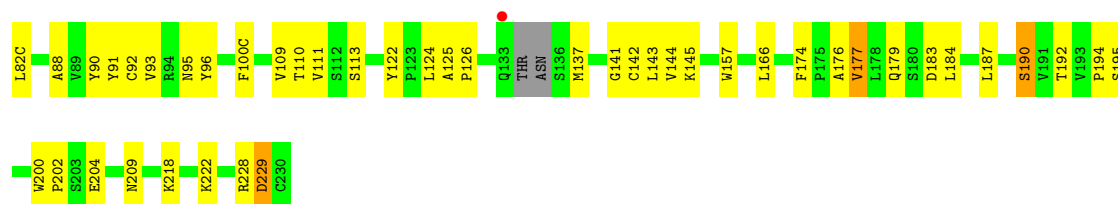


- Molecule 4: H5M9 antibody, heavy chain (IgG1)

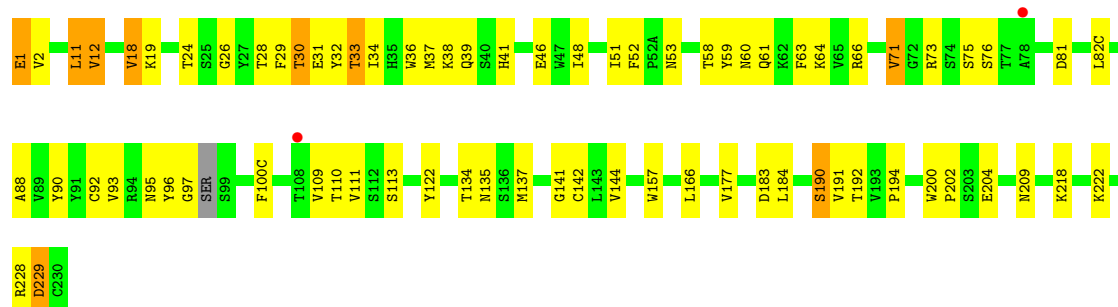


- Molecule 4: H5M9 antibody, heavy chain (IgG1)

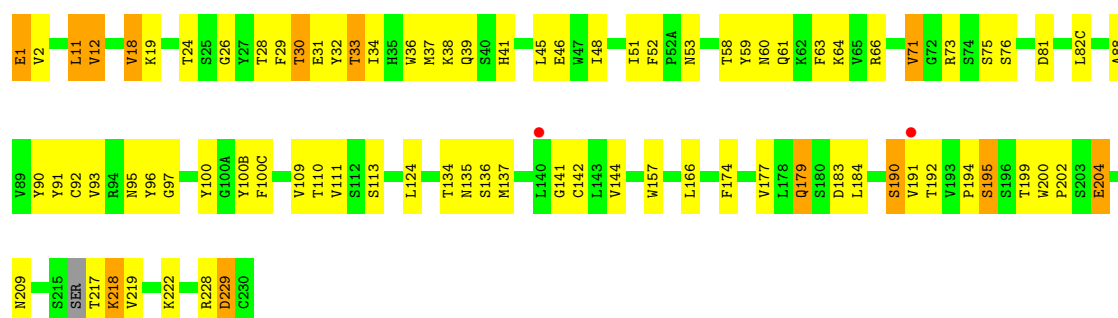




- Molecule 4: H5M9 antibody, heavy chain (IgG1)



- Molecule 4: H5M9 antibody, heavy chain (IgG1)



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



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

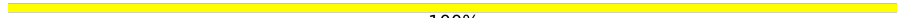


- Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  33% 67%

MAG1
MAG2
MAN3

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

Chain Z:  100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  100%

MAG1
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  100%

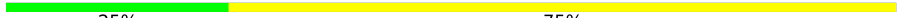
MAG1
MAG2

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  67% 33%

MAG1
MAG2
BMA3

- Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  25% 75%

MAG1
MAG2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	199.55Å 199.55Å 466.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.08 – 6.98 50.08 – 6.98	Depositor EDS
% Data completeness (in resolution range)	92.7 (50.08-6.98) 92.7 (50.08-6.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 6.68Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.377 , 0.387 0.368 , 0.364	Depositor DCC
R_{free} test set	843 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	375.9	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 309.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	43995	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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, MAN

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	0.61	0/2606	0.99	6/3542 (0.2%)
1	C	0.61	0/2596	0.99	6/3527 (0.2%)
1	G	0.61	0/2592	0.99	6/3521 (0.2%)
1	M	0.61	0/2606	0.99	6/3542 (0.2%)
1	O	0.60	0/2577	0.98	5/3503 (0.1%)
1	S	0.61	0/2606	0.99	6/3542 (0.2%)
2	B	0.62	0/1418	0.93	2/1906 (0.1%)
2	D	0.62	0/1418	0.93	2/1906 (0.1%)
2	I	0.62	0/1430	0.94	2/1924 (0.1%)
2	N	0.62	0/1384	0.94	2/1857 (0.1%)
2	P	0.62	0/1418	0.93	2/1906 (0.1%)
2	U	0.62	0/1430	0.94	2/1924 (0.1%)
3	E	0.75	0/1707	1.03	4/2313 (0.2%)
3	J	0.74	0/1667	1.02	4/2257 (0.2%)
3	L	0.75	0/1700	1.03	4/2301 (0.2%)
3	Q	0.75	0/1699	1.03	4/2300 (0.2%)
3	V	0.74	0/1688	1.03	4/2285 (0.2%)
3	X	0.75	0/1707	1.03	4/2313 (0.2%)
4	F	0.78	1/1720 (0.1%)	1.09	1/2350 (0.0%)
4	H	0.78	1/1720 (0.1%)	1.08	1/2350 (0.0%)
4	K	0.78	1/1718 (0.1%)	1.08	1/2345 (0.0%)
4	R	0.78	1/1720 (0.1%)	1.07	1/2350 (0.0%)
4	T	0.75	0/1711	1.08	1/2337 (0.0%)
4	W	0.78	1/1720 (0.1%)	1.09	1/2350 (0.0%)
All	All	0.68	5/44558 (0.0%)	1.01	77/60451 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	E	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	134	THR	CA-CB	6.53	1.62	1.53
4	W	134	THR	CA-CB	6.52	1.62	1.53
4	K	134	THR	CA-CB	6.51	1.62	1.53
4	R	134	THR	CA-CB	6.49	1.62	1.53
4	F	134	THR	CA-CB	6.47	1.62	1.53

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	PRO	CA-N-CD	-8.82	99.65	112.00
1	C	9	PRO	CA-N-CD	-8.82	99.66	112.00
1	G	9	PRO	CA-N-CD	-8.81	99.66	112.00
1	M	9	PRO	CA-N-CD	-8.80	99.68	112.00
1	S	9	PRO	CA-N-CD	-8.80	99.68	112.00
2	U	172	GLU	N-CA-C	-6.66	104.64	112.89
2	N	172	GLU	N-CA-C	-6.64	104.66	112.89
2	B	172	GLU	N-CA-C	-6.62	104.68	112.89
2	D	172	GLU	N-CA-C	-6.61	104.69	112.89
2	I	172	GLU	N-CA-C	-6.58	104.72	112.89
2	P	172	GLU	N-CA-C	-6.58	104.73	112.89
4	H	141	GLY	N-CA-C	6.48	120.56	111.10
4	W	141	GLY	N-CA-C	6.47	120.54	111.10
4	F	141	GLY	N-CA-C	6.46	120.53	111.10
4	R	141	GLY	N-CA-C	6.45	120.52	111.10
4	K	141	GLY	N-CA-C	6.43	120.48	111.10
4	T	141	GLY	N-CA-C	6.42	120.47	111.10
1	G	238	LYS	CA-C-N	6.27	127.68	119.84
1	G	238	LYS	C-N-CA	6.27	127.68	119.84
1	C	238	LYS	CA-C-N	6.27	127.68	119.84
1	C	238	LYS	C-N-CA	6.27	127.68	119.84
1	S	238	LYS	CA-C-N	6.27	127.67	119.84
1	S	238	LYS	C-N-CA	6.27	127.67	119.84
1	O	238	LYS	CA-C-N	6.23	127.63	119.84
1	O	238	LYS	C-N-CA	6.23	127.63	119.84
1	M	238	LYS	CA-C-N	6.23	127.63	119.84
1	M	238	LYS	C-N-CA	6.23	127.63	119.84
1	A	238	LYS	CA-C-N	6.21	127.61	119.84
1	A	238	LYS	C-N-CA	6.21	127.61	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	253	ALA	CA-C-N	-5.73	114.03	119.76
1	O	253	ALA	C-N-CA	-5.73	114.03	119.76
1	M	253	ALA	CA-C-N	-5.71	114.05	119.76
1	M	253	ALA	C-N-CA	-5.71	114.05	119.76
1	A	253	ALA	CA-C-N	-5.71	114.06	119.76
1	A	253	ALA	C-N-CA	-5.71	114.06	119.76
1	G	253	ALA	CA-C-N	-5.68	114.08	119.76
1	G	253	ALA	C-N-CA	-5.68	114.08	119.76
1	S	253	ALA	CA-C-N	-5.66	114.10	119.76
1	S	253	ALA	C-N-CA	-5.66	114.10	119.76
1	C	253	ALA	CA-C-N	-5.64	114.12	119.76
1	C	253	ALA	C-N-CA	-5.64	114.12	119.76
3	L	195	GLU	N-CA-C	5.58	117.83	108.23
3	Q	195	GLU	N-CA-C	5.58	117.83	108.23
3	E	195	GLU	N-CA-C	5.58	117.82	108.23
3	V	57	GLY	CA-C-N	-5.57	118.49	123.33
3	V	57	GLY	C-N-CA	-5.57	118.49	123.33
3	J	195	GLU	N-CA-C	5.56	117.79	108.23
3	V	195	GLU	N-CA-C	5.55	117.78	108.23
3	X	195	GLU	N-CA-C	5.54	117.75	108.23
2	B	127	ARG	CB-CA-C	-5.53	110.18	116.54
2	P	127	ARG	CB-CA-C	-5.53	110.18	116.54
3	Q	57	GLY	CA-C-N	-5.53	118.52	123.33
3	Q	57	GLY	C-N-CA	-5.53	118.52	123.33
3	L	57	GLY	CA-C-N	-5.53	118.52	123.33
3	L	57	GLY	C-N-CA	-5.53	118.52	123.33
3	J	57	GLY	CA-C-N	-5.52	118.53	123.33
3	J	57	GLY	C-N-CA	-5.52	118.53	123.33
2	D	127	ARG	CB-CA-C	-5.51	110.20	116.54
2	I	127	ARG	CB-CA-C	-5.51	110.20	116.54
3	X	57	GLY	CA-C-N	-5.50	118.55	123.33
3	X	57	GLY	C-N-CA	-5.50	118.55	123.33
3	E	57	GLY	CA-C-N	-5.49	118.55	123.33
3	E	57	GLY	C-N-CA	-5.49	118.55	123.33
2	U	127	ARG	CB-CA-C	-5.49	110.23	116.54
2	N	127	ARG	CB-CA-C	-5.48	110.23	116.54
3	X	100	GLY	N-CA-C	-5.48	106.16	112.73
3	V	100	GLY	N-CA-C	-5.44	106.20	112.73
3	Q	100	GLY	N-CA-C	-5.40	106.25	112.73
1	O	175	ASP	N-CA-C	-5.40	103.01	110.35
1	M	175	ASP	N-CA-C	-5.37	103.04	110.35
1	S	175	ASP	N-CA-C	-5.36	103.06	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	175	ASP	N-CA-C	-5.36	103.06	110.35
3	L	100	GLY	N-CA-C	-5.35	106.31	112.73
3	E	100	GLY	N-CA-C	-5.35	106.31	112.73
1	A	175	ASP	N-CA-C	-5.34	103.09	110.35
3	J	100	GLY	N-CA-C	-5.33	106.33	112.73
1	G	175	ASP	N-CA-C	-5.32	103.12	110.35

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	50	ARG	Sidechain

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	2542	0	2464	77	0
1	C	2533	0	2455	77	0
1	G	2530	0	2453	75	0
1	M	2542	0	2464	81	0
1	O	2514	0	2440	79	0
1	S	2542	0	2463	76	0
2	B	1393	0	1295	24	0
2	D	1393	0	1295	58	0
2	I	1403	0	1302	39	0
2	N	1363	0	1272	59	0
2	P	1393	0	1294	36	0
2	U	1403	0	1302	47	0
3	E	1672	0	1597	58	0
3	J	1634	0	1560	80	0
3	L	1666	0	1592	72	0
3	Q	1665	0	1589	59	0
3	V	1655	0	1577	78	0
3	X	1672	0	1597	78	0
4	F	1675	0	1626	62	0
4	H	1675	0	1626	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	1674	0	1625	80	0
4	R	1675	0	1626	60	0
4	T	1666	0	1618	80	0
4	W	1675	0	1626	102	0
5	Y	39	0	34	1	0
5	d	39	0	34	2	0
5	f	39	0	34	2	0
6	Z	94	0	79	0	0
7	a	28	0	25	1	0
7	c	28	0	25	1	0
8	b	39	0	34	3	0
9	e	50	0	43	0	0
10	A	14	0	13	0	0
10	C	14	0	13	0	0
10	M	14	0	13	0	0
10	O	14	0	13	0	0
10	P	14	0	13	2	0
10	S	14	0	13	0	0
All	All	43995	0	42144	1246	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (1246) 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)
4:H:31:GLU:HG3	4:H:32:TYR:CD1	1.57	1.40
4:K:31:GLU:HG3	4:K:32:TYR:CD1	1.57	1.39
4:W:31:GLU:HG3	4:W:32:TYR:CD1	1.57	1.39
3:V:164:THR:HG23	4:W:174:PHE:CD1	1.59	1.38
4:R:31:GLU:HG3	4:R:32:TYR:CD1	1.57	1.38
4:F:31:GLU:HG3	4:F:32:TYR:CD1	1.57	1.37
4:T:31:GLU:HG3	4:T:32:TYR:CD1	1.57	1.37
4:R:31:GLU:HG3	4:R:32:TYR:CE1	1.79	1.17
1:O:274:TYR:CE2	4:R:97:GLY:HA2	1.81	1.16
4:F:31:GLU:HG3	4:F:32:TYR:CE1	1.79	1.16
4:W:31:GLU:HG3	4:W:32:TYR:CE1	1.79	1.16
4:H:31:GLU:HG3	4:H:32:TYR:CE1	1.79	1.15
4:K:31:GLU:HG3	4:K:32:TYR:CE1	1.79	1.15
4:T:31:GLU:HG3	4:T:32:TYR:CE1	1.79	1.15
1:G:316:LEU:HD21	2:I:100:VAL:HG22	1.29	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:164:THR:HG23	4:K:174:PHE:CD1	1.83	1.12
3:V:43:SER:HB3	4:W:91:TYR:CE1	1.84	1.11
3:X:117:ILE:HG22	3:X:207:LYS:HG3	1.29	1.11
4:K:31:GLU:CD	4:K:32:TYR:CE1	2.32	1.08
4:W:31:GLU:CD	4:W:32:TYR:CE1	2.32	1.08
4:H:31:GLU:CD	4:H:32:TYR:CE1	2.32	1.08
4:F:31:GLU:CD	4:F:32:TYR:CE1	2.32	1.08
4:R:31:GLU:CD	4:R:32:TYR:CE1	2.32	1.08
4:T:31:GLU:CD	4:T:32:TYR:CE1	2.32	1.07
2:D:76:ARG:NH2	2:I:74:GLU:OE2	1.89	1.06
4:W:31:GLU:CG	4:W:32:TYR:CE1	2.39	1.05
4:T:31:GLU:CG	4:T:32:TYR:CE1	2.39	1.05
4:H:31:GLU:CG	4:H:32:TYR:CE1	2.39	1.05
4:R:31:GLU:CG	4:R:32:TYR:CE1	2.39	1.05
4:F:31:GLU:CG	4:F:32:TYR:CE1	2.39	1.04
4:K:31:GLU:CG	4:K:32:TYR:CE1	2.39	1.04
1:G:9:PRO:HD2	1:G:10:GLY:H	1.23	1.03
1:S:9:PRO:HD2	1:S:10:GLY:H	1.23	1.03
1:C:9:PRO:HD2	1:C:10:GLY:H	1.23	1.02
1:O:274:TYR:HE2	4:R:97:GLY:HA2	1.13	1.01
4:T:68:THR:HB	4:T:81:ASP:OD2	1.61	1.01
4:K:31:GLU:CG	4:K:32:TYR:CD1	2.44	1.00
4:F:31:GLU:CG	4:F:32:TYR:CD1	2.44	1.00
4:W:31:GLU:CG	4:W:32:TYR:CD1	2.44	1.00
1:M:9:PRO:HD2	1:M:10:GLY:H	1.23	1.00
4:R:31:GLU:CG	4:R:32:TYR:CD1	2.44	1.00
4:H:31:GLU:CG	4:H:32:TYR:CD1	2.44	1.00
4:T:31:GLU:CG	4:T:32:TYR:CD1	2.44	0.99
4:W:33:THR:HB	4:W:52:PHE:CD1	1.96	0.99
4:R:31:GLU:OE2	4:R:32:TYR:HE1	1.47	0.98
1:A:9:PRO:HD2	1:A:10:GLY:H	1.23	0.98
4:F:31:GLU:OE2	4:F:32:TYR:HE1	1.47	0.98
3:V:164:THR:CG2	4:W:174:PHE:CD1	2.46	0.97
4:K:31:GLU:OE2	4:K:32:TYR:HE1	1.47	0.97
4:W:31:GLU:OE2	4:W:32:TYR:HE1	1.47	0.97
4:T:31:GLU:OE2	4:T:32:TYR:HE1	1.46	0.97
1:G:316:LEU:CD2	2:I:100:VAL:HG22	1.94	0.97
4:H:31:GLU:OE2	4:H:32:TYR:HE1	1.47	0.97
2:D:167:ARG:HG2	2:D:170:ARG:NH2	1.80	0.96
1:O:274:TYR:OH	4:R:97:GLY:HA3	1.67	0.95
3:L:43:SER:HB3	4:H:91:TYR:CE1	2.01	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:168:LEU:HD12	2:N:169:ASN:N	1.81	0.94
3:Q:119:PRO:HB2	4:R:228:ARG:HH21	1.31	0.94
1:M:17:TYR:CE2	2:N:13:GLY:CA	2.50	0.94
2:N:76:ARG:HH12	2:P:68:ARG:HG2	1.32	0.93
1:M:17:TYR:CZ	2:N:12:GLY:C	2.47	0.93
1:S:274:TYR:HD2	4:W:31:GLU:O	1.51	0.93
1:M:276:ASN:ND2	4:T:52:PHE:CE1	2.38	0.92
3:V:164:THR:HG23	4:W:174:PHE:HD1	1.00	0.92
3:J:8:PRO:HB3	3:X:11:LEU:CD1	1.99	0.92
2:D:32:SER:O	4:W:217:THR:HG23	1.71	0.90
3:X:117:ILE:CG2	3:X:207:LYS:HG3	2.01	0.90
1:O:274:TYR:OH	4:R:97:GLY:CA	2.20	0.89
3:L:44:PRO:HG2	4:H:45:LEU:HD11	1.54	0.88
1:M:17:TYR:CE2	2:N:13:GLY:HA3	2.07	0.88
2:B:51:LYS:HE3	1:G:30:MET:HE2	1.54	0.88
2:D:167:ARG:HG2	2:D:170:ARG:HH21	1.36	0.88
3:J:164:THR:HG23	4:K:174:PHE:HD1	1.36	0.88
4:R:31:GLU:CD	4:R:32:TYR:HE1	1.78	0.86
4:W:31:GLU:CD	4:W:32:TYR:HE1	1.78	0.86
2:N:76:ARG:NH1	2:P:68:ARG:HG2	1.91	0.86
3:X:160:LEU:HD11	4:T:179:GLN:CD	2.01	0.86
1:M:9:PRO:HD2	1:M:10:GLY:N	1.91	0.85
1:G:9:PRO:HD2	1:G:10:GLY:N	1.91	0.85
1:S:9:PRO:HD2	1:S:10:GLY:N	1.91	0.85
3:V:174:SER:HB2	4:W:174:PHE:HE1	1.42	0.85
3:J:119:PRO:HB2	4:K:228:ARG:HH21	1.40	0.85
3:J:160:LEU:HD11	4:K:179:GLN:OE1	1.77	0.85
1:A:9:PRO:HD2	1:A:10:GLY:N	1.91	0.84
2:U:32:SER:O	4:F:217:THR:HA	1.76	0.84
1:C:11:ASP:OD1	2:D:28:ASN:HA	1.77	0.84
3:X:117:ILE:HG22	3:X:207:LYS:CG	2.08	0.84
3:V:43:SER:HB3	4:W:91:TYR:HE1	1.34	0.84
3:V:119:PRO:HB2	4:W:228:ARG:HH21	1.44	0.83
1:G:11:ASP:OD1	2:I:28:ASN:HA	1.78	0.83
1:G:276:ASN:O	4:K:98:SER:HB3	1.78	0.82
3:X:160:LEU:HD11	4:T:179:GLN:OE1	1.79	0.82
3:V:160:LEU:HD21	4:W:179:GLN:HE21	1.42	0.82
4:K:31:GLU:CD	4:K:32:TYR:HE1	1.78	0.82
1:A:83:PRO:CG	4:H:100(B):TYR:OH	2.28	0.82
3:J:43:SER:HB3	4:K:91:TYR:CE1	2.13	0.82
4:T:31:GLU:CD	4:T:32:TYR:HE1	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:PRO:HD2	1:C:10:GLY:N	1.91	0.82
3:X:118:PHE:CD2	4:T:124:LEU:HB3	2.14	0.82
1:M:17:TYR:OH	2:N:12:GLY:C	2.23	0.82
1:A:274:TYR:OH	4:H:97:GLY:HA3	1.80	0.81
2:N:165:GLU:HA	2:N:168:LEU:CD2	2.10	0.81
1:A:274:TYR:OH	4:H:97:GLY:CA	2.29	0.81
1:M:17:TYR:CZ	2:N:13:GLY:N	2.48	0.81
4:F:31:GLU:CD	4:F:32:TYR:HE1	1.78	0.81
1:G:106:GLU:CD	2:I:71:ASN:HB3	2.05	0.81
1:M:107:GLU:OE2	2:U:76:ARG:HG3	1.81	0.81
4:H:31:GLU:CD	4:H:32:TYR:HE1	1.78	0.80
1:C:11:ASP:CG	2:D:28:ASN:HA	2.06	0.80
1:G:25:GLN:OE1	1:G:33:ASN:OD1	1.99	0.80
3:V:44:PRO:HG2	4:W:45:LEU:HD11	1.62	0.80
1:O:274:TYR:CE2	4:R:97:GLY:CA	2.65	0.79
4:K:28:THR:O	4:K:31:GLU:HG2	1.83	0.79
1:S:105:TYR:CZ	1:S:109:LYS:HE3	2.16	0.79
2:N:76:ARG:HH11	2:N:76:ARG:HG2	1.44	0.79
1:M:276:ASN:HD21	4:T:31:GLU:C	1.91	0.79
4:F:28:THR:O	4:F:31:GLU:HG2	1.83	0.79
3:J:118:PHE:CD2	4:K:124:LEU:HB3	2.17	0.78
4:T:28:THR:O	4:T:31:GLU:HG2	1.83	0.78
1:S:83:PRO:CG	4:W:100(B):TYR:OH	2.32	0.78
4:R:28:THR:O	4:R:31:GLU:HG2	1.83	0.78
1:M:11:ASP:CG	2:N:28:ASN:HA	2.09	0.78
3:V:174:SER:HB2	4:W:174:PHE:CE1	2.18	0.78
3:J:8:PRO:HB3	3:X:11:LEU:HD11	1.64	0.78
1:M:118:PHE:HE1	1:M:260:ILE:HD13	1.49	0.78
4:W:28:THR:O	4:W:31:GLU:HG2	1.82	0.78
1:G:118:PHE:HE1	1:G:260:ILE:HD13	1.49	0.78
1:M:206:THR:HB	1:M:209:LEU:HB3	1.66	0.78
4:H:28:THR:O	4:H:31:GLU:HG2	1.83	0.78
1:G:206:THR:HB	1:G:209:LEU:HB3	1.66	0.77
1:S:15:ILE:HD11	2:U:122:VAL:HG21	1.66	0.77
1:G:206:THR:HG22	1:G:208:THR:H	1.50	0.77
1:G:316:LEU:HD23	2:I:100:VAL:HG13	1.65	0.77
1:A:206:THR:HG22	1:A:208:THR:H	1.50	0.77
3:J:120:PRO:HB3	3:J:131:SER:H	1.50	0.77
4:W:48:ILE:HA	4:W:63:PHE:HD2	1.49	0.77
1:C:15:ILE:C	2:D:14:TRP:CH2	2.63	0.77
1:M:206:THR:HG22	1:M:208:THR:H	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:118:PHE:HE1	1:O:260:ILE:HD13	1.49	0.77
1:A:206:THR:HB	1:A:209:LEU:HB3	1.66	0.77
4:H:48:ILE:HA	4:H:63:PHE:HD2	1.49	0.76
1:O:106:GLU:OE2	2:P:71:ASN:HB3	1.85	0.76
1:C:206:THR:HB	1:C:209:LEU:HB3	1.66	0.76
3:L:120:PRO:HB3	3:L:131:SER:H	1.50	0.76
3:Q:120:PRO:HB3	3:Q:131:SER:H	1.50	0.76
1:S:206:THR:HG22	1:S:208:THR:H	1.50	0.76
1:O:206:THR:HG22	1:O:208:THR:H	1.50	0.76
4:T:48:ILE:HA	4:T:63:PHE:HD2	1.50	0.76
4:F:48:ILE:HA	4:F:63:PHE:HD2	1.50	0.76
3:X:120:PRO:HB3	3:X:131:SER:H	1.50	0.76
4:R:48:ILE:HA	4:R:63:PHE:HD2	1.49	0.76
1:O:206:THR:HB	1:O:209:LEU:HB3	1.66	0.76
1:S:206:THR:HB	1:S:209:LEU:HB3	1.66	0.76
4:K:48:ILE:HA	4:K:63:PHE:HD2	1.49	0.76
1:O:316:LEU:HD21	2:P:100:VAL:HG22	1.69	0.75
1:S:118:PHE:HE1	1:S:260:ILE:HD13	1.49	0.75
1:A:11:ASP:OD1	2:B:28:ASN:HA	1.86	0.75
1:A:118:PHE:HE1	1:A:260:ILE:HD13	1.49	0.75
1:C:118:PHE:HE1	1:C:260:ILE:HD13	1.49	0.75
1:G:276:ASN:ND2	4:K:52:PHE:CE1	2.55	0.75
1:C:206:THR:HG22	1:C:208:THR:H	1.50	0.74
3:L:137:ASN:ND2	4:H:174:PHE:HZ	1.85	0.74
3:E:120:PRO:HB3	3:E:131:SER:H	1.50	0.74
3:V:120:PRO:HB3	3:V:131:SER:H	1.50	0.74
3:J:8:PRO:CB	3:X:11:LEU:HD12	2.17	0.74
4:W:33:THR:HB	4:W:52:PHE:CE1	2.21	0.74
1:O:216:GLU:O	1:O:220:ARG:NH2	2.21	0.74
1:C:16:GLY:N	2:D:14:TRP:CH2	2.56	0.74
1:M:216:GLU:O	1:M:220:ARG:NH2	2.21	0.73
1:G:276:ASN:O	4:K:98:SER:CB	2.36	0.73
1:A:56:VAL:HG21	3:L:30:LYS:NZ	2.03	0.73
2:D:76:ARG:NE	1:G:107:GLU:OE2	2.20	0.73
1:S:274:TYR:OH	4:W:97:GLY:HA2	1.88	0.73
2:N:74:GLU:OE2	2:U:76:ARG:NH2	2.21	0.73
1:G:216:GLU:O	1:G:220:ARG:NH2	2.21	0.73
1:O:13:ILE:HA	2:P:26:HIS:HA	1.70	0.73
3:J:8:PRO:CB	3:X:11:LEU:CD1	2.67	0.73
1:S:83:PRO:CB	4:W:100(B):TYR:OH	2.36	0.72
1:A:216:GLU:O	1:A:220:ARG:NH2	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:17:TYR:CE1	2:N:12:GLY:O	2.43	0.72
2:N:165:GLU:HA	2:N:168:LEU:HD21	1.70	0.72
1:O:15:ILE:C	2:P:14:TRP:CH2	2.67	0.72
1:S:216:GLU:O	1:S:220:ARG:NH2	2.21	0.72
1:C:216:GLU:O	1:C:220:ARG:NH2	2.21	0.72
1:C:220:ARG:NE	1:G:210:ASN:OD1	2.22	0.72
3:V:160:LEU:HD11	4:W:179:GLN:HG2	1.73	0.71
2:D:80:LEU:HD11	2:I:80:LEU:HD22	1.72	0.71
1:A:274:TYR:CE2	4:H:97:GLY:HA2	2.26	0.71
1:G:106:GLU:OE2	2:I:71:ASN:HB3	1.91	0.71
1:M:9:PRO:CD	1:M:10:GLY:H	2.02	0.71
1:S:106:GLU:CD	2:U:71:ASN:HB3	2.16	0.71
1:G:9:PRO:CD	1:G:10:GLY:H	2.02	0.70
1:S:307:LYS:HD3	2:U:59:MET:O	1.91	0.70
1:S:9:PRO:CD	1:S:10:GLY:H	2.02	0.70
1:S:55(A):GLY:HA2	4:W:100:TYR:HB2	1.74	0.70
1:S:106:GLU:OE2	2:U:71:ASN:HB3	1.91	0.70
1:O:274:TYR:CZ	4:R:97:GLY:CA	2.75	0.69
1:M:17:TYR:CD2	2:N:13:GLY:HA3	2.27	0.69
1:O:106:GLU:CD	2:P:71:ASN:HB3	2.17	0.69
1:C:118:PHE:CE1	1:C:260:ILE:HD13	2.28	0.69
1:C:9:PRO:CD	1:C:10:GLY:H	2.02	0.69
4:K:31:GLU:OE2	4:K:32:TYR:CE1	2.36	0.69
1:M:62:ARG:HG2	1:M:63:ASP:N	2.08	0.69
3:V:43:SER:HA	4:W:91:TYR:OH	1.93	0.69
4:T:31:GLU:OE2	4:T:32:TYR:CE1	2.36	0.69
1:O:118:PHE:CE1	1:O:260:ILE:HD13	2.28	0.68
1:C:62:ARG:HG2	1:C:63:ASP:N	2.08	0.68
1:S:118:PHE:CE1	1:S:260:ILE:HD13	2.28	0.68
1:S:274:TYR:OH	4:W:97:GLY:CA	2.40	0.68
4:W:33:THR:HB	4:W:52:PHE:HD1	1.54	0.68
2:P:150:GLU:HB2	10:P:2001:NAG:H62	1.74	0.68
3:V:98:PHE:CD1	4:W:45:LEU:O	2.46	0.68
1:A:62:ARG:HG2	1:A:63:ASP:N	2.08	0.68
1:G:118:PHE:CE1	1:G:260:ILE:HD13	2.28	0.68
1:G:62:ARG:HG2	1:G:63:ASP:N	2.08	0.68
1:O:56:VAL:HG21	3:Q:30:LYS:NZ	2.08	0.68
1:M:118:PHE:CE1	1:M:260:ILE:HD13	2.28	0.68
1:O:62:ARG:HG2	1:O:63:ASP:N	2.08	0.68
1:S:62:ARG:HG2	1:S:63:ASP:N	2.08	0.68
1:A:107:GLU:OE2	2:I:76:ARG:NE	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ARG:NH2	1:G:217:ILE:O	2.25	0.68
4:T:68:THR:CB	4:T:81:ASP:OD2	2.41	0.68
2:N:76:ARG:NH1	2:N:76:ARG:HG2	2.08	0.67
3:J:90:GLN:HE21	3:J:97:THR:CG2	2.08	0.67
3:X:90:GLN:HE21	3:X:97:THR:CG2	2.08	0.67
3:Q:90:GLN:HE21	3:Q:97:THR:CG2	2.08	0.67
1:A:118:PHE:CE1	1:A:260:ILE:HD13	2.28	0.67
3:E:90:GLN:HE21	3:E:97:THR:CG2	2.08	0.67
3:L:90:GLN:HE21	3:L:97:THR:CG2	2.08	0.67
3:V:90:GLN:HE21	3:V:97:THR:CG2	2.08	0.67
2:D:76:ARG:NH1	2:I:74:GLU:OE1	2.27	0.67
3:X:164:THR:HG23	4:T:174:PHE:CD1	2.30	0.67
1:A:83:PRO:HG3	4:H:100(B):TYR:OH	1.94	0.67
1:C:13:ILE:HA	2:D:26:HIS:HA	1.78	0.66
1:M:107:GLU:OE2	2:U:76:ARG:CG	2.43	0.66
1:M:17:TYR:CZ	2:N:13:GLY:CA	2.78	0.65
1:A:244:ASN:ND2	1:G:221:PRO:HD3	2.12	0.65
3:X:133:VAL:HG21	4:T:143:LEU:HD13	1.78	0.65
1:M:9:PRO:CD	1:M:10:GLY:N	2.59	0.65
1:M:17:TYR:OH	2:N:12:GLY:CA	2.44	0.65
2:N:168:LEU:HD12	2:N:168:LEU:C	2.20	0.65
1:S:274:TYR:CD2	4:W:31:GLU:O	2.42	0.65
1:A:216:GLU:HB3	1:C:212:ARG:HB3	1.79	0.65
1:M:276:ASN:ND2	4:T:52:PHE:HE1	1.94	0.65
1:O:16:GLY:N	2:P:14:TRP:CH2	2.64	0.65
3:J:44:PRO:HG2	4:K:45:LEU:HD11	1.79	0.65
1:C:9:PRO:CD	1:C:10:GLY:N	2.59	0.64
2:D:80:LEU:HD21	2:I:80:LEU:HD21	1.79	0.64
1:A:56:VAL:HG21	3:L:30:LYS:HZ2	1.61	0.64
1:G:123:ILE:HD11	1:G:168:TYR:CZ	2.33	0.64
1:M:123:ILE:HD11	1:M:168:TYR:CZ	2.33	0.64
4:K:12:VAL:HG21	4:K:82(C):LEU:HD13	1.80	0.64
1:A:123:ILE:HD11	1:A:168:TYR:CZ	2.33	0.64
4:W:12:VAL:HG21	4:W:82(C):LEU:HD13	1.80	0.64
4:T:12:VAL:HG21	4:T:82(C):LEU:HD13	1.80	0.64
1:S:123:ILE:HD11	1:S:168:TYR:CZ	2.33	0.64
3:E:63:ASN:HB3	3:E:74:THR:HB	1.80	0.64
1:A:9:PRO:CD	1:A:10:GLY:N	2.59	0.64
3:V:160:LEU:CD1	4:W:179:GLN:HG2	2.27	0.64
1:C:123:ILE:HD11	1:C:168:TYR:CZ	2.33	0.64
1:M:17:TYR:CD2	2:N:13:GLY:CA	2.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:12:VAL:HG21	4:H:82(C):LEU:HD13	1.80	0.63
1:C:316:LEU:HD21	2:D:100:VAL:HG22	1.79	0.63
3:J:43:SER:HB3	4:K:91:TYR:HE1	1.63	0.63
3:J:119:PRO:HB2	4:K:228:ARG:NH2	2.13	0.63
3:V:164:THR:CG2	4:W:174:PHE:HD1	1.94	0.63
1:A:218:ALA:HB2	1:C:203:SER:HB2	1.80	0.63
1:O:123:ILE:HD11	1:O:168:TYR:CZ	2.33	0.63
3:J:119:PRO:CB	4:K:228:ARG:HH21	2.11	0.63
4:W:18:VAL:HG22	4:W:82(C):LEU:HD11	1.81	0.63
1:G:9:PRO:CD	1:G:10:GLY:N	2.59	0.63
3:X:160:LEU:CD1	4:T:179:GLN:CD	2.70	0.63
4:F:18:VAL:HG22	4:F:82(C):LEU:HD11	1.81	0.63
4:R:18:VAL:HG22	4:R:82(C):LEU:HD11	1.81	0.63
1:A:12:GLN:O	2:B:27:SER:N	2.32	0.63
1:A:274:TYR:HE2	4:H:97:GLY:HA2	1.63	0.63
4:H:18:VAL:HG22	4:H:82(C):LEU:HD11	1.81	0.63
2:N:80:LEU:HD22	2:U:80:LEU:HD11	1.81	0.62
4:F:12:VAL:HG21	4:F:82(C):LEU:HD13	1.80	0.62
3:L:63:ASN:HB3	3:L:74:THR:HB	1.80	0.62
3:X:63:ASN:HB3	3:X:74:THR:HB	1.80	0.62
3:V:174:SER:CB	4:W:174:PHE:CE1	2.81	0.62
4:R:12:VAL:HG21	4:R:82(C):LEU:HD13	1.80	0.62
1:O:55(A):GLY:O	3:Q:50:ARG:NH2	2.33	0.62
3:Q:63:ASN:HB3	3:Q:74:THR:HB	1.80	0.62
4:T:18:VAL:HG22	4:T:82(C):LEU:HD11	1.81	0.62
1:S:9:PRO:CD	1:S:10:GLY:N	2.59	0.62
3:L:118:PHE:CD2	4:H:124:LEU:HB3	2.35	0.62
3:V:63:ASN:HB3	3:V:74:THR:HB	1.80	0.62
3:J:63:ASN:HB3	3:J:74:THR:HB	1.80	0.62
1:C:276:ASN:HD21	4:F:32:TYR:HA	1.64	0.62
3:Q:119:PRO:HB2	4:R:228:ARG:NH2	2.11	0.62
2:D:76:ARG:HH12	2:I:74:GLU:CD	2.08	0.62
1:S:323:THR:HG21	2:U:12:GLY:HA2	1.82	0.62
4:K:18:VAL:HG22	4:K:82(C):LEU:HD11	1.81	0.61
1:A:11:ASP:CG	2:B:28:ASN:HA	2.25	0.61
1:M:17:TYR:CE2	2:N:13:GLY:N	2.68	0.61
3:L:137:ASN:HD21	4:H:174:PHE:HZ	1.48	0.61
2:D:80:LEU:HD21	2:I:80:LEU:CD2	2.30	0.61
1:O:274:TYR:CZ	4:R:97:GLY:HA2	2.32	0.61
1:M:293:PRO:HG2	1:M:294:PHE:HD1	1.66	0.61
1:A:16:GLY:N	2:B:14:TRP:CH2	2.68	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:PRO:HG2	1:C:294:PHE:HD1	1.66	0.61
2:D:32:SER:O	4:W:217:THR:CG2	2.46	0.61
1:O:293:PRO:HG2	1:O:294:PHE:HD1	1.66	0.61
1:G:293:PRO:HG2	1:G:294:PHE:HD1	1.66	0.61
1:O:276:ASN:OD1	4:R:33:THR:HG22	1.99	0.61
3:L:174:SER:CB	4:H:174:PHE:HE1	2.14	0.61
4:K:200:TRP:CD1	4:K:202:PRO:HA	2.36	0.61
2:P:80:LEU:HD21	2:U:80:LEU:CD2	2.31	0.61
4:R:200:TRP:CD1	4:R:202:PRO:HA	2.36	0.61
4:W:48:ILE:HA	4:W:63:PHE:CD2	2.35	0.61
1:S:83:PRO:HB2	4:W:100(B):TYR:OH	2.00	0.60
1:G:83(A):GLU:H	3:J:49:TYR:HH	1.46	0.60
1:M:186:ASN:ND2	1:M:190:GLU:OE1	2.33	0.60
1:A:293:PRO:HG2	1:A:294:PHE:HD1	1.66	0.60
3:J:164:THR:CG2	4:K:174:PHE:CD1	2.74	0.60
3:J:174:SER:HB2	4:K:174:PHE:CE1	2.36	0.60
4:H:200:TRP:CD1	4:H:202:PRO:HA	2.36	0.60
1:O:83:PRO:HB3	3:Q:49:TYR:CE2	2.36	0.60
1:O:217:ILE:O	1:S:212:ARG:NH2	2.31	0.60
1:A:15:ILE:C	2:B:14:TRP:CH2	2.79	0.60
1:O:56:VAL:CG2	3:Q:30:LYS:NZ	2.64	0.60
4:K:48:ILE:HA	4:K:63:PHE:CD2	2.35	0.60
4:T:200:TRP:CD1	4:T:202:PRO:HA	2.36	0.60
1:A:268:MET:HG3	1:A:284:PRO:HG3	1.84	0.60
3:L:164:THR:HG23	4:H:174:PHE:HD1	1.66	0.60
4:T:48:ILE:HA	4:T:63:PHE:CD2	2.36	0.60
4:W:200:TRP:CD1	4:W:202:PRO:HA	2.36	0.60
3:L:164:THR:HG23	4:H:174:PHE:CD1	2.37	0.60
1:O:14:CYS:O	2:P:24:TYR:HA	2.02	0.60
1:C:268:MET:HG3	1:C:284:PRO:HG3	1.84	0.60
1:A:83(A):GLU:N	3:L:49:TYR:OH	2.28	0.59
3:X:44:PRO:HG2	4:T:45:LEU:HD11	1.84	0.59
3:X:124:GLN:HB2	4:T:122:TYR:CE1	2.37	0.59
1:S:268:MET:HG3	1:S:284:PRO:HG3	1.84	0.59
1:S:293:PRO:HG2	1:S:294:PHE:HD1	1.66	0.59
3:E:90:GLN:HE21	3:E:97:THR:HG23	1.68	0.59
3:Q:90:GLN:HE21	3:Q:97:THR:HG23	1.68	0.59
3:V:174:SER:CB	4:W:174:PHE:HE1	2.13	0.59
4:K:1:GLU:O	4:K:26:GLY:HA3	2.03	0.59
4:T:39:GLN:O	4:T:88:ALA:HB1	2.03	0.59
4:T:68:THR:HB	4:T:81:ASP:CG	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ASN:ND2	1:A:190:GLU:OE1	2.33	0.59
3:X:90:GLN:HE21	3:X:97:THR:HG23	1.68	0.59
4:K:19:LYS:NZ	4:K:81:ASP:HB2	2.18	0.59
1:G:268:MET:HG3	1:G:284:PRO:HG3	1.84	0.59
3:J:160:LEU:CD1	4:K:179:GLN:OE1	2.49	0.59
3:X:119:PRO:HB2	4:T:228:ARG:HH21	1.68	0.59
1:G:32:LYS:HG2	8:b:1:NAG:H81	1.85	0.59
3:E:123:GLU:OE1	4:F:123:PRO:CD	2.51	0.59
3:V:43:SER:CB	4:W:91:TYR:CE1	2.75	0.59
2:U:72:ASN:OD1	2:U:75:ARG:NH2	2.36	0.59
3:J:174:SER:HB2	4:K:174:PHE:HE1	1.68	0.59
4:R:39:GLN:O	4:R:88:ALA:HB1	2.03	0.59
4:W:1:GLU:O	4:W:26:GLY:HA3	2.02	0.59
4:R:19:LYS:NZ	4:R:81:ASP:HB2	2.18	0.59
1:O:83:PRO:HB3	3:Q:49:TYR:HE2	1.66	0.59
4:H:19:LYS:NZ	4:H:81:ASP:HB2	2.18	0.59
4:K:39:GLN:O	4:K:88:ALA:HB1	2.03	0.59
4:K:200:TRP:CG	4:K:202:PRO:HA	2.38	0.59
4:T:81:ASP:OD1	4:T:81:ASP:C	2.45	0.59
2:D:72:ASN:OD1	2:D:75:ARG:NH2	2.36	0.58
1:M:268:MET:HG3	1:M:284:PRO:HG3	1.84	0.58
2:N:72:ASN:OD1	2:N:75:ARG:NH2	2.36	0.58
1:O:268:MET:HG3	1:O:284:PRO:HG3	1.84	0.58
4:H:31:GLU:OE2	4:H:32:TYR:CE1	2.36	0.58
4:F:1:GLU:O	4:F:26:GLY:HA3	2.03	0.58
4:F:19:LYS:NZ	4:F:81:ASP:HB2	2.18	0.58
4:F:200:TRP:CD1	4:F:202:PRO:HA	2.36	0.58
4:R:1:GLU:O	4:R:26:GLY:HA3	2.02	0.58
4:W:31:GLU:OE2	4:W:32:TYR:CE1	2.36	0.58
3:V:164:THR:HG23	4:W:174:PHE:CE1	2.31	0.58
4:H:39:GLN:O	4:H:88:ALA:HB1	2.03	0.58
3:L:90:GLN:HE21	3:L:97:THR:HG23	1.68	0.58
4:W:19:LYS:NZ	4:W:81:ASP:HB2	2.18	0.58
4:W:200:TRP:CG	4:W:202:PRO:HA	2.38	0.58
2:P:72:ASN:OD1	2:P:75:ARG:NH2	2.36	0.58
3:J:90:GLN:HE21	3:J:97:THR:HG23	1.68	0.58
3:V:174:SER:HB3	4:W:174:PHE:CZ	2.39	0.58
2:I:72:ASN:OD1	2:I:75:ARG:NH2	2.36	0.58
4:H:200:TRP:CG	4:H:202:PRO:HA	2.39	0.58
4:F:39:GLN:O	4:F:88:ALA:HB1	2.03	0.58
1:M:107:GLU:OE1	2:U:75:ARG:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:124:GLN:HG3	4:R:122:TYR:CE2	2.39	0.58
4:H:1:GLU:O	4:H:26:GLY:HA3	2.02	0.58
4:R:200:TRP:CG	4:R:202:PRO:HA	2.38	0.58
3:V:90:GLN:HE21	3:V:97:THR:HG23	1.68	0.58
4:K:190:SER:O	4:K:190:SER:OG	2.22	0.58
4:R:48:ILE:HA	4:R:63:PHE:CD2	2.36	0.58
4:F:31:GLU:OE2	4:F:32:TYR:CE1	2.36	0.58
4:R:31:GLU:OE2	4:R:32:TYR:CE1	2.36	0.58
4:T:1:GLU:O	4:T:26:GLY:HA3	2.03	0.58
4:W:190:SER:O	4:W:190:SER:OG	2.22	0.58
1:A:9:PRO:CD	1:A:10:GLY:H	2.02	0.58
1:M:276:ASN:OD1	4:T:32:TYR:HA	2.02	0.58
3:V:118:PHE:CD2	4:W:124:LEU:HB3	2.39	0.58
3:V:135:PHE:CZ	4:W:124:LEU:HD13	2.39	0.58
1:A:316:LEU:HD21	2:B:100:VAL:HG22	1.86	0.57
1:C:62:ARG:HG2	1:C:63:ASP:H	1.70	0.57
2:D:33:GLY:HA2	4:W:217:THR:HA	1.85	0.57
1:G:186:ASN:ND2	1:G:190:GLU:OE1	2.33	0.57
4:T:200:TRP:CG	4:T:202:PRO:HA	2.38	0.57
4:W:39:GLN:O	4:W:88:ALA:HB1	2.03	0.57
1:M:11:ASP:CB	2:N:28:ASN:HA	2.34	0.57
4:F:48:ILE:HA	4:F:63:PHE:CD2	2.36	0.57
4:K:19:LYS:HZ1	4:K:81:ASP:HB2	1.69	0.57
1:S:307:LYS:NZ	2:U:59:MET:HB2	2.19	0.57
3:V:98:PHE:CD2	4:W:45:LEU:HB2	2.39	0.57
4:F:200:TRP:CG	4:F:202:PRO:HA	2.38	0.57
4:R:59:TYR:HD2	4:R:64:LYS:HD3	1.70	0.57
1:G:62:ARG:HG2	1:G:63:ASP:H	1.70	0.57
3:E:116:SER:HA	3:E:207:LYS:HD2	1.87	0.57
3:V:116:SER:HA	3:V:207:LYS:HD2	1.87	0.57
4:H:48:ILE:HA	4:H:63:PHE:CD2	2.36	0.57
1:O:186:ASN:ND2	1:O:190:GLU:OE1	2.33	0.57
3:L:43:SER:HB3	4:H:91:TYR:HE1	1.66	0.57
2:B:72:ASN:OD1	2:B:75:ARG:NH2	2.36	0.57
2:P:80:LEU:HD21	2:U:80:LEU:HD21	1.86	0.57
3:L:116:SER:HA	3:L:207:LYS:HD2	1.87	0.57
3:X:174:SER:CB	4:T:174:PHE:HE1	2.17	0.57
3:Q:116:SER:HA	3:Q:207:LYS:HD2	1.87	0.57
4:H:59:TYR:HD2	4:H:64:LYS:HD3	1.70	0.57
3:V:119:PRO:CB	4:W:228:ARG:HH21	2.16	0.56
1:A:83:PRO:HB3	3:L:49:TYR:HE2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:LEU:HD22	2:I:80:LEU:HD11	1.88	0.56
1:O:62:ARG:HG2	1:O:63:ASP:H	1.70	0.56
3:E:192:TYR:HB2	3:E:209:PHE:CE1	2.41	0.56
4:F:190:SER:O	4:F:190:SER:OG	2.21	0.56
1:A:83:PRO:HG2	4:H:100(B):TYR:OH	2.05	0.56
3:Q:192:TYR:HB2	3:Q:209:PHE:CE1	2.41	0.56
3:V:192:TYR:HB2	3:V:209:PHE:CE1	2.41	0.56
4:T:59:TYR:HD2	4:T:64:LYS:HD3	1.70	0.56
1:G:83(A):GLU:OE1	3:J:53:ASN:ND2	2.39	0.56
1:A:307:LYS:HD3	2:B:59:MET:O	2.06	0.56
2:D:33:GLY:CA	4:W:217:THR:HA	2.36	0.56
1:S:62:ARG:HG2	1:S:63:ASP:H	1.70	0.56
3:L:192:TYR:HB2	3:L:209:PHE:CE1	2.41	0.56
3:V:98:PHE:CE2	4:W:45:LEU:HB2	2.41	0.56
1:M:29:ILE:HD12	2:N:105:GLU:OE1	2.06	0.56
3:J:192:TYR:HB2	3:J:209:PHE:CE1	2.41	0.56
1:G:14:CYS:O	2:I:24:TYR:HA	2.06	0.56
1:M:62:ARG:HG2	1:M:63:ASP:H	1.70	0.56
3:J:116:SER:HA	3:J:207:LYS:HD2	1.87	0.56
1:A:293:PRO:HG2	1:A:294:PHE:CD1	2.42	0.55
1:C:293:PRO:HG2	1:C:294:PHE:CD1	2.41	0.55
3:L:110:ASP:OD2	3:L:199:LYS:HE2	2.07	0.55
4:W:59:TYR:HD2	4:W:64:LYS:HD3	1.70	0.55
1:M:293:PRO:HG2	1:M:294:PHE:CD1	2.42	0.55
1:S:186:ASN:ND2	1:S:190:GLU:OE1	2.33	0.55
1:S:293:PRO:HG2	1:S:294:PHE:CD1	2.41	0.55
3:L:174:SER:HB2	4:H:174:PHE:HE1	1.71	0.55
3:X:110:ASP:OD2	3:X:199:LYS:HE2	2.07	0.55
3:X:192:TYR:HB2	3:X:209:PHE:CE1	2.41	0.55
2:U:31:GLY:HA3	4:F:219:VAL:HG22	1.86	0.55
4:F:59:TYR:HD2	4:F:64:LYS:HD3	1.70	0.55
1:S:18:HIS:N	2:U:21:TRP:O	2.34	0.55
1:S:100:GLY:HA3	1:S:230:MET:O	2.07	0.55
3:E:110:ASP:OD2	3:E:199:LYS:HE2	2.07	0.55
1:G:293:PRO:HG2	1:G:294:PHE:CD1	2.41	0.55
3:V:119:PRO:HB2	4:W:228:ARG:NH2	2.17	0.55
4:K:59:TYR:HD2	4:K:64:LYS:HD3	1.70	0.55
1:S:105:TYR:OH	1:S:109:LYS:HE3	2.06	0.55
3:E:123:GLU:OE1	4:F:123:PRO:HD2	2.06	0.55
3:Q:110:ASP:OD2	3:Q:199:LYS:HE2	2.07	0.55
1:A:62:ARG:HG2	1:A:63:ASP:H	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:293:PRO:HG2	1:O:294:PHE:CD1	2.42	0.55
1:S:15:ILE:HG13	2:U:119:TYR:HA	1.89	0.55
1:C:100:GLY:HA3	1:C:230:MET:O	2.07	0.54
1:M:220:ARG:NH2	1:O:210:ASN:OD1	2.40	0.54
1:O:274:TYR:OH	4:R:97:GLY:C	2.50	0.54
3:V:110:ASP:OD2	3:V:199:LYS:HE2	2.07	0.54
1:M:69:TRP:HZ3	1:M:112:LEU:HD21	1.73	0.54
1:M:100:GLY:HA3	1:M:230:MET:O	2.07	0.54
1:C:16:GLY:N	2:D:14:TRP:CZ3	2.76	0.54
2:D:167:ARG:CG	2:D:170:ARG:HH21	2.14	0.54
1:G:69:TRP:HZ3	1:G:112:LEU:HD21	1.73	0.54
1:A:100:GLY:HA3	1:A:230:MET:O	2.07	0.54
1:A:183:HIS:HB2	1:A:252:ILE:HD11	1.90	0.54
1:C:186:ASN:ND2	1:C:190:GLU:OE1	2.33	0.54
1:O:183:HIS:HB2	1:O:252:ILE:HD11	1.90	0.54
1:O:100:GLY:HA3	1:O:230:MET:O	2.07	0.54
3:L:124:GLN:NE2	3:L:131:SER:OG	2.38	0.54
3:J:110:ASP:OD2	3:J:199:LYS:HE2	2.07	0.54
3:X:35:TRP:CZ3	3:X:88:CYS:HB3	2.43	0.54
1:G:100:GLY:HA3	1:G:230:MET:O	2.07	0.54
1:O:56:VAL:HG21	3:Q:30:LYS:HZ1	1.72	0.54
1:O:274:TYR:CZ	4:R:97:GLY:HA3	2.39	0.54
1:S:69:TRP:HZ3	1:S:112:LEU:HD21	1.73	0.54
3:J:49:TYR:CE1	3:J:53:ASN:HB2	2.43	0.54
3:X:164:THR:HG23	4:T:174:PHE:HD1	1.69	0.54
4:H:190:SER:O	4:H:190:SER:OG	2.22	0.54
1:A:51:LEU:HD13	1:A:272:LEU:HB2	1.90	0.54
3:X:160:LEU:CD1	4:T:179:GLN:OE1	2.52	0.54
1:C:183:HIS:HB2	1:C:252:ILE:HD11	1.90	0.54
1:S:51:LEU:HD13	1:S:272:LEU:HB2	1.90	0.54
1:M:183:HIS:HB2	1:M:252:ILE:HD11	1.90	0.53
3:Q:49:TYR:CE1	3:Q:53:ASN:HB2	2.43	0.53
3:V:124:GLN:NE2	3:V:131:SER:OG	2.38	0.53
1:C:69:TRP:HZ3	1:C:112:LEU:HD21	1.73	0.53
3:L:35:TRP:CZ3	3:L:88:CYS:HB3	2.43	0.53
3:E:35:TRP:CZ3	3:E:88:CYS:HB3	2.43	0.53
3:J:35:TRP:CZ3	3:J:88:CYS:HB3	2.43	0.53
3:X:193:THR:HG23	3:X:208:SER:HB3	1.90	0.53
3:Q:193:THR:HG23	3:Q:208:SER:HB3	1.90	0.53
3:V:164:THR:HG22	4:W:174:PHE:HA	1.89	0.53
3:V:193:THR:HG23	3:V:208:SER:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:LEU:HD13	1:G:272:LEU:HB2	1.90	0.53
3:L:49:TYR:CE1	3:L:53:ASN:HB2	2.43	0.53
3:E:49:TYR:CE1	3:E:53:ASN:HB2	2.43	0.53
3:X:137:ASN:ND2	4:T:174:PHE:HZ	2.06	0.53
3:X:193:THR:HG22	3:X:194:CYS:H	1.74	0.53
3:Q:35:TRP:CZ3	3:Q:88:CYS:HB3	2.43	0.53
3:Q:124:GLN:HB2	4:R:122:TYR:CD1	2.43	0.53
3:V:49:TYR:CE1	3:V:53:ASN:HB2	2.43	0.53
1:G:183:HIS:HB2	1:G:252:ILE:HD11	1.90	0.53
1:O:69:TRP:HZ3	1:O:112:LEU:HD21	1.72	0.53
3:X:174:SER:HB2	4:T:174:PHE:HE1	1.74	0.53
3:L:193:THR:HG22	3:L:194:CYS:H	1.74	0.53
3:J:174:SER:HB3	4:K:174:PHE:CZ	2.43	0.53
3:L:147:LYS:HE3	3:L:195:GLU:HB3	1.91	0.53
3:X:49:TYR:CE1	3:X:53:ASN:HB2	2.43	0.53
3:V:35:TRP:CZ3	3:V:88:CYS:HB3	2.43	0.53
1:A:26:VAL:HG11	1:A:317:ALA:HB2	1.91	0.53
1:C:276:ASN:ND2	4:F:52:PHE:CE1	2.76	0.53
3:L:141:PRO:HD2	3:L:198:HIS:HE1	1.74	0.53
1:O:26:VAL:HG11	1:O:317:ALA:HB2	1.91	0.53
3:J:141:PRO:HD2	3:J:198:HIS:HE1	1.74	0.53
1:G:26:VAL:HG11	1:G:317:ALA:HB2	1.91	0.53
1:M:26:VAL:HG11	1:M:317:ALA:HB2	1.91	0.53
1:S:26:VAL:HG11	1:S:317:ALA:HB2	1.91	0.53
3:X:147:LYS:HE3	3:X:195:GLU:HB3	1.91	0.53
4:R:33:THR:CG2	4:R:95:ASN:HD22	2.22	0.53
1:S:183:HIS:HB2	1:S:252:ILE:HD11	1.90	0.52
3:E:147:LYS:HE3	3:E:195:GLU:HB3	1.91	0.52
3:X:141:PRO:HD2	3:X:198:HIS:HE1	1.74	0.52
1:A:69:TRP:HZ3	1:A:112:LEU:HD21	1.73	0.52
3:E:141:PRO:HD2	3:E:198:HIS:HE1	1.74	0.52
3:J:124:GLN:NE2	3:J:131:SER:OG	2.38	0.52
3:V:174:SER:HB3	4:W:174:PHE:HZ	1.73	0.52
4:K:33:THR:CG2	4:K:95:ASN:HD22	2.22	0.52
1:C:14:CYS:C	2:D:14:TRP:HH2	2.17	0.52
1:C:26:VAL:HG11	1:C:317:ALA:HB2	1.91	0.52
1:M:244:ASN:ND2	1:S:221:PRO:HD3	2.23	0.52
3:X:124:GLN:HB2	4:T:122:TYR:CZ	2.44	0.52
2:D:80:LEU:HD11	2:I:80:LEU:CD2	2.38	0.52
1:O:51:LEU:HD13	1:O:272:LEU:HB2	1.90	0.52
2:P:160:PRO:HA	2:P:163:SER:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:193:THR:HG23	3:L:208:SER:HB3	1.90	0.52
3:E:193:THR:HG23	3:E:208:SER:HB3	1.91	0.52
3:J:174:SER:CB	4:K:174:PHE:CE1	2.92	0.52
4:W:33:THR:CG2	4:W:95:ASN:HD22	2.22	0.52
3:E:193:THR:HG22	3:E:194:CYS:H	1.74	0.52
4:R:38:LYS:HB2	4:R:90:TYR:CE1	2.45	0.52
1:C:51:LEU:HD13	1:C:272:LEU:HB2	1.90	0.52
3:Q:147:LYS:HE3	3:Q:195:GLU:HB3	1.91	0.52
3:Q:193:THR:HG22	3:Q:194:CYS:H	1.74	0.52
2:U:160:PRO:HA	2:U:163:SER:HB2	1.92	0.52
4:W:38:LYS:HB2	4:W:90:TYR:CE1	2.45	0.52
2:B:160:PRO:HA	2:B:163:SER:HB2	1.92	0.52
1:M:51:LEU:HD13	1:M:272:LEU:HB2	1.91	0.52
1:M:55(A):GLY:O	3:X:50:ARG:NH2	2.42	0.52
3:X:118:PHE:CB	4:T:124:LEU:HD22	2.40	0.52
3:V:147:LYS:HE3	3:V:195:GLU:HB3	1.91	0.52
4:H:33:THR:CG2	4:H:95:ASN:HD22	2.22	0.52
3:J:193:THR:HG23	3:J:208:SER:HB3	1.91	0.52
3:Q:141:PRO:HD2	3:Q:198:HIS:HE1	1.74	0.52
3:V:141:PRO:HD2	3:V:198:HIS:HE1	1.74	0.52
4:T:33:THR:CG2	4:T:95:ASN:HD22	2.23	0.52
4:T:38:LYS:HB2	4:T:90:TYR:CE1	2.45	0.52
1:S:16:GLY:HA3	2:U:14:TRP:CH2	2.44	0.52
4:F:38:LYS:HB2	4:F:90:TYR:CE1	2.45	0.52
2:D:160:PRO:HA	2:D:163:SER:HB2	1.92	0.52
1:O:56:VAL:HG21	3:Q:30:LYS:HZ2	1.73	0.52
1:O:316:LEU:HD23	2:P:100:VAL:HG13	1.92	0.52
1:S:309:VAL:HG22	2:U:93:THR:HA	1.92	0.52
4:K:38:LYS:HB2	4:K:90:TYR:CE1	2.45	0.52
2:B:124:LEU:HD13	2:I:9:PHE:HB2	1.91	0.51
3:J:193:THR:HG22	3:J:194:CYS:H	1.74	0.51
3:V:193:THR:HG22	3:V:194:CYS:H	1.74	0.51
2:D:32:SER:HB2	4:W:218:LYS:O	2.11	0.51
2:I:22:TYR:HH	2:I:111:HIS:HD1	1.55	0.51
1:O:16:GLY:N	2:P:14:TRP:CZ3	2.79	0.51
4:H:38:LYS:HB2	4:H:90:TYR:CE1	2.45	0.51
1:A:13:ILE:HA	2:B:26:HIS:HA	1.91	0.51
1:C:56:VAL:CG2	3:E:50:ARG:NH1	2.74	0.51
3:E:120:PRO:O	4:F:228:ARG:NH2	2.44	0.51
3:J:147:LYS:HE3	3:J:195:GLU:HB3	1.91	0.51
4:F:33:THR:CG2	4:F:95:ASN:HD22	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:106:GLU:HG2	2:U:70:PHE:CA	2.41	0.51
3:V:13:VAL:HG11	3:V:78:VAL:HG21	1.93	0.51
1:A:56:VAL:CG2	3:L:30:LYS:NZ	2.72	0.51
3:L:13:VAL:HG11	3:L:78:VAL:HG21	1.93	0.51
3:E:13:VAL:HG11	3:E:78:VAL:HG21	1.93	0.51
3:E:95:PRO:HA	4:F:47:TRP:CZ3	2.46	0.51
4:T:12:VAL:HG23	4:T:111:VAL:HG22	1.93	0.51
1:A:83:PRO:HB3	3:L:49:TYR:CE2	2.45	0.51
1:A:83(A):GLU:H	3:L:49:TYR:HH	1.55	0.51
1:G:11:ASP:HA	2:I:27:SER:O	2.11	0.51
2:N:168:LEU:CD1	2:N:169:ASN:N	2.67	0.51
3:E:98:PHE:CE1	4:F:37:MET:HE1	2.45	0.51
1:M:220:ARG:NE	1:O:210:ASN:OD1	2.44	0.51
2:I:160:PRO:HA	2:I:163:SER:HB2	1.92	0.51
3:J:174:SER:HB3	4:K:174:PHE:HZ	1.76	0.51
4:W:12:VAL:HG23	4:W:111:VAL:HG22	1.93	0.51
3:Q:13:VAL:HG11	3:Q:78:VAL:HG21	1.93	0.50
4:R:190:SER:O	4:R:190:SER:OG	2.22	0.50
3:X:13:VAL:HG11	3:X:78:VAL:HG21	1.93	0.50
2:N:165:GLU:O	2:N:168:LEU:HG	2.12	0.50
3:E:96:ARG:HB2	4:F:47:TRP:CG	2.47	0.50
3:E:148:TRP:CE3	3:E:179:LEU:HD13	2.47	0.50
1:M:17:TYR:CE1	2:N:12:GLY:C	2.90	0.50
1:O:221:PRO:HD3	1:S:244:ASN:ND2	2.27	0.50
2:P:22:TYR:HH	2:P:111:HIS:HD1	1.56	0.50
3:E:121:SER:HB2	4:F:123:PRO:O	2.12	0.50
3:J:13:VAL:HG11	3:J:78:VAL:HG21	1.93	0.50
4:F:19:LYS:HZ1	4:F:81:ASP:HB2	1.75	0.50
4:K:12:VAL:HG23	4:K:111:VAL:HG22	1.93	0.50
2:B:54:SER:OG	1:G:32:LYS:NZ	2.45	0.50
4:K:93:VAL:HG11	4:K:100(C):PHE:HB3	1.94	0.50
4:R:12:VAL:HG23	4:R:111:VAL:HG22	1.93	0.50
2:D:22:TYR:HH	2:D:111:HIS:HD1	1.58	0.50
1:G:58:PRO:O	4:K:96:TYR:OH	2.27	0.50
1:O:14:CYS:C	2:P:14:TRP:HH2	2.19	0.50
3:J:27(B):VAL:HG22	3:J:27(B):VAL:O	2.12	0.50
3:J:148:TRP:CE3	3:J:179:LEU:HD13	2.47	0.50
3:X:148:TRP:CE3	3:X:179:LEU:HD13	2.47	0.50
3:X:166:GLN:HB2	3:X:173:TYR:CE1	2.47	0.50
2:N:160:PRO:HA	2:N:163:SER:HB2	1.92	0.50
1:S:307:LYS:HZ2	2:U:59:MET:HB2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:148:TRP:CE3	3:L:179:LEU:HD13	2.47	0.50
3:Q:27(B):VAL:O	3:Q:27(B):VAL:HG22	2.12	0.50
1:M:107:GLU:OE2	2:U:76:ARG:NE	2.45	0.49
1:S:106:GLU:OE1	2:U:71:ASN:ND2	2.34	0.49
3:J:164:THR:HG23	4:K:174:PHE:CE1	2.44	0.49
3:V:27(B):VAL:O	3:V:27(B):VAL:HG22	2.12	0.49
3:V:166:GLN:HB2	3:V:173:TYR:CE1	2.48	0.49
4:R:93:VAL:HG11	4:R:100(C):PHE:HB3	1.94	0.49
3:L:27(B):VAL:O	3:L:27(B):VAL:HG22	2.12	0.49
3:Q:148:TRP:CE3	3:Q:179:LEU:HD13	2.47	0.49
3:V:148:TRP:CE3	3:V:179:LEU:HD13	2.47	0.49
4:W:93:VAL:HG11	4:W:100(C):PHE:HB3	1.94	0.49
1:C:17:TYR:O	2:D:14:TRP:N	2.36	0.49
1:G:98:TYR:CD1	1:G:230:MET:HG3	2.48	0.49
2:P:80:LEU:HD11	2:U:80:LEU:HD22	1.94	0.49
1:S:106:GLU:HG2	2:U:70:PHE:HA	1.95	0.49
3:L:137:ASN:ND2	4:H:174:PHE:CZ	2.73	0.49
4:F:12:VAL:HG23	4:F:111:VAL:HG22	1.93	0.49
1:M:98:TYR:CD1	1:M:230:MET:HG3	2.48	0.49
1:O:83:PRO:CB	3:Q:49:TYR:CE2	2.95	0.49
1:O:221:PRO:HB3	5:f:1:NAG:H81	1.94	0.49
1:O:230:MET:HE1	1:O:252:ILE:HG12	1.95	0.49
1:S:98:TYR:CD1	1:S:230:MET:HG3	2.48	0.49
3:E:124:GLN:NE2	3:E:131:SER:OG	2.38	0.49
4:T:190:SER:O	4:T:190:SER:OG	2.22	0.49
2:N:127:ARG:HH21	2:U:131:LYS:NZ	2.10	0.49
3:X:174:SER:CB	4:T:174:PHE:CE1	2.96	0.49
4:H:12:VAL:HG23	4:H:111:VAL:HG22	1.93	0.49
4:K:137:MET:HE3	4:K:192:THR:HG22	1.95	0.49
1:A:98:TYR:CD1	1:A:230:MET:HG3	2.48	0.49
1:C:307:LYS:HD3	2:D:59:MET:O	2.13	0.49
3:E:27(B):VAL:HG22	3:E:27(B):VAL:O	2.12	0.49
3:Q:124:GLN:NE2	3:Q:131:SER:OG	2.38	0.49
3:V:119:PRO:HG2	4:W:228:ARG:HE	1.78	0.49
4:F:93:VAL:HG11	4:F:100(C):PHE:HB3	1.94	0.49
3:J:135:PHE:CZ	4:K:124:LEU:HD13	2.48	0.49
4:H:93:VAL:HG11	4:H:100(C):PHE:HB3	1.93	0.49
4:T:93:VAL:HG11	4:T:100(C):PHE:HB3	1.94	0.49
1:O:83(A):GLU:OE1	3:Q:53:ASN:ND2	2.46	0.49
1:O:316:LEU:CD2	2:P:100:VAL:HG22	2.41	0.49
3:J:166:GLN:HB2	3:J:173:TYR:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:MET:HE1	1:A:252:ILE:HG12	1.95	0.48
1:A:244:ASN:HD22	1:G:221:PRO:HD3	1.76	0.48
1:O:98:TYR:CD1	1:O:230:MET:HG3	2.48	0.48
3:E:166:GLN:HB2	3:E:173:TYR:CE1	2.47	0.48
3:Q:166:GLN:HB2	3:Q:173:TYR:CE1	2.47	0.48
3:X:27(B):VAL:O	3:X:27(B):VAL:HG22	2.12	0.48
4:T:137:MET:HE3	4:T:192:THR:HG22	1.95	0.48
1:C:98:TYR:CD1	1:C:230:MET:HG3	2.48	0.48
1:G:230:MET:HE1	1:G:252:ILE:HG12	1.95	0.48
1:S:83:PRO:HG2	4:W:100(B):TYR:OH	2.12	0.48
1:M:19:ALA:O	2:N:15:GLN:HA	2.14	0.48
1:S:230:MET:HE1	1:S:252:ILE:HG12	1.95	0.48
3:L:166:GLN:HB2	3:L:173:TYR:CE1	2.47	0.48
1:G:179:LEU:HD23	1:G:234:TRP:HB3	1.95	0.48
4:F:51:ILE:HD13	4:F:71:VAL:HG23	1.96	0.48
1:M:179:LEU:HD23	1:M:234:TRP:HB3	1.95	0.48
4:T:51:ILE:HD13	4:T:71:VAL:HG23	1.96	0.48
1:M:230:MET:HE1	1:M:252:ILE:HG12	1.95	0.48
1:M:323:THR:HG21	2:N:13:GLY:H	1.78	0.48
4:H:19:LYS:HZ3	4:H:81:ASP:HB2	1.77	0.48
4:R:137:MET:HE3	4:R:192:THR:HG22	1.95	0.48
1:A:56:VAL:HG21	3:L:30:LYS:HZ1	1.77	0.48
1:A:179:LEU:HD23	1:A:234:TRP:HB3	1.96	0.48
1:C:56:VAL:CG2	3:E:50:ARG:HH12	2.26	0.48
3:J:53:ASN:OD1	3:J:53:ASN:N	2.47	0.48
3:J:119:PRO:HG2	4:K:228:ARG:HE	1.79	0.48
3:X:118:PHE:HB3	4:T:124:LEU:HD22	1.95	0.48
3:Q:195:GLU:HG3	3:Q:206:VAL:HG22	1.96	0.48
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.96	0.48
2:B:51:LYS:CE	1:G:30:MET:HE2	2.34	0.48
1:C:56:VAL:HG22	3:E:50:ARG:NH1	2.28	0.48
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.96	0.48
1:G:134:GLY:HA3	1:G:153:TRP:HB3	1.96	0.48
3:E:33:MET:HB3	3:E:51:ALA:HB2	1.96	0.48
3:X:124:GLN:NE2	3:X:131:SER:OG	2.38	0.48
4:H:137:MET:HE3	4:H:192:THR:HG22	1.95	0.48
4:F:137:MET:HE3	4:F:192:THR:HG22	1.95	0.48
1:G:83(A):GLU:N	3:J:49:TYR:OH	2.29	0.48
2:N:47:GLY:O	1:S:30:MET:HG2	2.14	0.48
1:O:106:GLU:OE1	2:P:71:ASN:ND2	2.28	0.48
1:O:134:GLY:HA3	1:O:153:TRP:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:MET:HE1	1:C:252:ILE:HG12	1.95	0.47
1:O:179:LEU:HD23	1:O:234:TRP:HB3	1.95	0.47
3:L:33:MET:HB3	3:L:51:ALA:HB2	1.96	0.47
3:Q:33:MET:HB3	3:Q:51:ALA:HB2	1.96	0.47
4:H:51:ILE:HD13	4:H:71:VAL:HG23	1.96	0.47
4:K:51:ILE:HD13	4:K:71:VAL:HG23	1.96	0.47
1:G:106:GLU:OE1	2:I:71:ASN:ND2	2.24	0.47
1:O:83(A):GLU:H	3:Q:49:TYR:HH	1.61	0.47
3:J:195:GLU:HG3	3:J:206:VAL:HG22	1.96	0.47
3:V:33:MET:HB3	3:V:51:ALA:HB2	1.96	0.47
1:S:134:GLY:HA3	1:S:153:TRP:HB3	1.96	0.47
1:S:179:LEU:HD23	1:S:234:TRP:HB3	1.95	0.47
4:F:183:ASP:O	4:F:184:LEU:HD23	2.15	0.47
4:W:51:ILE:HD13	4:W:71:VAL:HG23	1.96	0.47
1:A:276:ASN:ND2	4:H:52:PHE:CE1	2.82	0.47
5:d:1:NAG:H61	5:d:2:NAG:N2	2.29	0.47
1:M:134:GLY:HA3	1:M:153:TRP:HB3	1.96	0.47
3:L:174:SER:HB3	4:H:174:PHE:CE1	2.49	0.47
3:X:53:ASN:OD1	3:X:53:ASN:N	2.47	0.47
4:R:183:ASP:O	4:R:184:LEU:HD23	2.15	0.47
2:D:31:GLY:HA3	4:W:219:VAL:HG22	1.97	0.47
2:N:80:LEU:CD2	2:U:80:LEU:HD11	2.44	0.47
1:O:56:VAL:CG2	3:Q:30:LYS:HZ1	2.27	0.47
1:S:316:LEU:HD21	2:U:100:VAL:HG22	1.95	0.47
3:J:33:MET:HB3	3:J:51:ALA:HB2	1.96	0.47
3:Q:53:ASN:OD1	3:Q:53:ASN:N	2.47	0.47
4:K:29:PHE:CD2	4:K:76:SER:HA	2.50	0.47
4:T:183:ASP:O	4:T:184:LEU:HD23	2.15	0.47
1:C:274:TYR:HD2	4:F:31:GLU:O	1.97	0.47
1:M:17:TYR:CE2	2:N:13:GLY:HA2	2.47	0.47
3:V:53:ASN:OD1	3:V:53:ASN:N	2.47	0.47
4:H:183:ASP:O	4:H:184:LEU:HD23	2.15	0.47
4:F:48:ILE:HG12	4:F:63:PHE:CD2	2.50	0.47
4:K:183:ASP:O	4:K:184:LEU:HD23	2.15	0.47
4:W:137:MET:HE3	4:W:192:THR:HG22	1.95	0.47
1:M:30:MET:HE1	2:P:110:PHE:CD1	2.50	0.47
3:V:135:PHE:CZ	4:W:124:LEU:CD1	2.98	0.47
4:R:29:PHE:CD2	4:R:76:SER:HA	2.50	0.47
2:N:165:GLU:HA	2:N:168:LEU:HD23	1.96	0.47
3:E:53:ASN:OD1	3:E:53:ASN:N	2.47	0.47
4:F:29:PHE:CD2	4:F:76:SER:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:51:ILE:HD13	4:R:71:VAL:HG23	1.96	0.47
1:C:179:LEU:HD23	1:C:234:TRP:HB3	1.95	0.47
1:G:32:LYS:HB3	8:b:1:NAG:C8	2.44	0.47
3:E:195:GLU:HG3	3:E:206:VAL:HG22	1.96	0.47
4:T:29:PHE:CD2	4:T:76:SER:HA	2.50	0.47
4:W:19:LYS:HZ3	4:W:81:ASP:HB2	1.78	0.47
3:V:24:ARG:NH1	3:V:70:ASP:HB3	2.31	0.46
3:V:195:GLU:HG3	3:V:206:VAL:HG22	1.96	0.46
4:K:48:ILE:HG12	4:K:63:PHE:CD2	2.50	0.46
4:T:48:ILE:HG12	4:T:63:PHE:CD2	2.50	0.46
1:M:16:GLY:O	2:N:17:MET:HE1	2.15	0.46
2:N:110:PHE:CG	1:S:30:MET:HE1	2.50	0.46
3:L:195:GLU:HG3	3:L:206:VAL:HG22	1.96	0.46
3:X:195:GLU:HG3	3:X:206:VAL:HG22	1.96	0.46
3:Q:24:ARG:NH1	3:Q:70:ASP:HB3	2.31	0.46
4:W:29:PHE:CD2	4:W:76:SER:HA	2.50	0.46
4:W:183:ASP:O	4:W:184:LEU:HD23	2.15	0.46
2:D:76:ARG:HH22	2:I:74:GLU:CD	2.06	0.46
2:N:74:GLU:CD	2:U:76:ARG:HH12	2.23	0.46
3:E:24:ARG:NH1	3:E:70:ASP:HB3	2.31	0.46
3:X:33:MET:HB3	3:X:51:ALA:HB2	1.96	0.46
4:R:48:ILE:HG12	4:R:63:PHE:CD2	2.49	0.46
2:N:76:ARG:CZ	1:O:110:HIS:HB2	2.46	0.46
3:X:131:SER:OG	4:T:145:LYS:HE2	2.16	0.46
4:H:29:PHE:CD2	4:H:76:SER:HA	2.50	0.46
3:E:135:PHE:CE2	4:F:190:SER:HB2	2.50	0.46
4:H:48:ILE:HG12	4:H:63:PHE:CD2	2.50	0.46
3:X:43:SER:HB3	4:T:91:TYR:CE1	2.51	0.46
4:W:48:ILE:HG12	4:W:63:PHE:CD2	2.50	0.46
1:C:268:MET:HE3	1:C:268:MET:HB2	1.83	0.46
1:S:141:TYR:CZ	1:S:149:ARG:NH2	2.84	0.46
3:J:11:LEU:HD12	3:X:8:PRO:HG3	1.98	0.46
4:H:73:ARG:H	4:H:73:ARG:HG2	1.49	0.46
1:A:12:GLN:N	2:B:27:SER:O	2.45	0.46
1:A:141:TYR:CZ	1:A:149:ARG:NH2	2.84	0.46
1:G:141:TYR:CZ	1:G:149:ARG:NH2	2.84	0.46
1:O:16:GLY:HA3	2:P:14:TRP:CZ3	2.51	0.46
3:L:24:ARG:NH1	3:L:70:ASP:HB3	2.31	0.46
3:V:174:SER:CB	4:W:174:PHE:CZ	2.99	0.46
4:F:60:ASN:OD1	4:F:61:GLN:N	2.49	0.46
3:L:167:ASP:HB3	3:L:170:ASP:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:167:ASP:HB3	3:J:170:ASP:OD1	2.16	0.46
3:X:24:ARG:NH1	3:X:70:ASP:HB3	2.31	0.46
3:Q:167:ASP:HB3	3:Q:170:ASP:OD1	2.16	0.46
3:V:169:LYS:HD2	3:V:169:LYS:HA	1.79	0.46
4:K:37:MET:HE3	4:K:46:GLU:O	2.16	0.46
4:K:60:ASN:OD1	4:K:61:GLN:N	2.49	0.46
4:K:66:ARG:H	4:K:66:ARG:HG3	1.53	0.46
4:T:37:MET:HE3	4:T:46:GLU:O	2.17	0.46
1:A:16:GLY:HA3	2:B:14:TRP:CH2	2.51	0.45
1:C:106:GLU:OE2	2:D:71:ASN:HB3	2.15	0.45
2:D:128:ASP:OD1	2:D:159:TYR:OH	2.22	0.45
1:M:141:TYR:CZ	1:M:149:ARG:NH2	2.84	0.45
3:X:167:ASP:HB3	3:X:170:ASP:OD1	2.16	0.45
1:C:16:GLY:HA3	2:D:14:TRP:CE2	2.51	0.45
1:G:15:ILE:O	2:I:10:ILE:HD13	2.16	0.45
3:L:44:PRO:CG	4:H:45:LEU:HD11	2.38	0.45
3:L:118:PHE:CE2	4:H:124:LEU:HB3	2.52	0.45
3:L:90:GLN:HE21	3:L:97:THR:HG22	1.82	0.45
3:E:50:ARG:HE	3:E:50:ARG:HB2	1.53	0.45
3:J:24:ARG:NH1	3:J:70:ASP:HB3	2.31	0.45
4:H:37:MET:HE3	4:H:46:GLU:O	2.17	0.45
4:F:37:MET:HE3	4:F:46:GLU:O	2.17	0.45
4:R:37:MET:HE3	4:R:46:GLU:O	2.16	0.45
1:A:14:CYS:O	2:B:24:TYR:HA	2.17	0.45
1:A:55(A):GLY:HA3	3:L:32:PHE:CZ	2.51	0.45
1:S:53:ASP:OD1	1:S:56:VAL:C	2.60	0.45
3:L:174:SER:CB	4:H:174:PHE:CE1	2.96	0.45
3:E:167:ASP:HB3	3:E:170:ASP:OD1	2.16	0.45
4:K:73:ARG:H	4:K:73:ARG:HG2	1.49	0.45
2:D:163:SER:O	2:D:167:ARG:HG3	2.17	0.45
2:N:127:ARG:HH21	2:U:131:LYS:HZ2	1.62	0.45
3:Q:90:GLN:HE21	3:Q:97:THR:HG22	1.82	0.45
3:V:167:ASP:HB3	3:V:170:ASP:OD1	2.16	0.45
4:W:60:ASN:OD1	4:W:61:GLN:N	2.49	0.45
1:C:11:ASP:HA	2:D:27:SER:O	2.17	0.45
1:G:53:ASP:OD1	1:G:56:VAL:C	2.60	0.45
1:M:244:ASN:HD22	1:S:221:PRO:HD3	1.82	0.45
1:O:141:TYR:CZ	1:O:149:ARG:NH2	2.84	0.45
4:H:60:ASN:OD1	4:H:61:GLN:N	2.49	0.45
1:A:83:PRO:CB	3:L:49:TYR:CE2	3.00	0.45
1:C:141:TYR:CZ	1:C:149:ARG:NH2	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:34:HIS:O	3:V:88:CYS:HA	2.17	0.45
4:T:60:ASN:OD1	4:T:61:GLN:N	2.49	0.45
4:R:30:THR:HB	4:R:53:ASN:HB2	1.99	0.45
1:C:53:ASP:OD1	1:C:56:VAL:C	2.60	0.45
1:M:53:ASP:OD1	1:M:56:VAL:C	2.60	0.45
2:N:84:MET:HE2	2:N:84:MET:HB3	1.85	0.45
1:O:53:ASP:HA	1:O:58:PRO:HD3	1.99	0.45
3:E:169:LYS:HD2	3:E:169:LYS:HA	1.80	0.45
3:X:111:ALA:O	3:X:200:THR:HG21	2.17	0.45
1:A:53:ASP:OD1	1:A:56:VAL:C	2.60	0.45
1:C:17:TYR:CZ	2:D:12:GLY:C	2.95	0.45
1:M:11:ASP:OD1	2:N:28:ASN:HA	2.16	0.45
1:M:17:TYR:CD2	2:N:13:GLY:HA2	2.52	0.45
1:O:53:ASP:OD1	1:O:56:VAL:C	2.60	0.45
3:Q:111:ALA:O	3:Q:200:THR:HG21	2.17	0.45
4:H:30:THR:HB	4:H:53:ASN:HB2	1.99	0.45
4:R:142:CYS:HB2	4:R:157:TRP:CH2	2.52	0.45
1:C:16:GLY:HA3	2:D:14:TRP:CH2	2.52	0.45
2:P:128:ASP:OD1	2:P:159:TYR:OH	2.22	0.45
3:L:135:PHE:C	3:L:136:LEU:HD12	2.42	0.45
3:L:164:THR:HG22	4:H:175:PRO:HD3	1.98	0.45
2:N:128:ASP:OD1	2:N:159:TYR:OH	2.22	0.44
3:E:111:ALA:O	3:E:200:THR:HG21	2.17	0.44
3:X:90:GLN:HE21	3:X:97:THR:HG22	1.82	0.44
3:V:135:PHE:C	3:V:136:LEU:HD12	2.42	0.44
3:V:160:LEU:HD21	4:W:179:GLN:NE2	2.21	0.44
4:H:142:CYS:HB2	4:H:157:TRP:CH2	2.52	0.44
4:F:30:THR:HB	4:F:53:ASN:HB2	1.99	0.44
4:F:142:CYS:HB2	4:F:157:TRP:CH2	2.52	0.44
4:K:30:THR:HB	4:K:53:ASN:HB2	1.99	0.44
4:R:60:ASN:OD1	4:R:61:GLN:N	2.49	0.44
3:Q:34:HIS:O	3:Q:88:CYS:HA	2.17	0.44
2:B:124:LEU:CD1	2:I:9:PHE:HB2	2.47	0.44
3:J:118:PHE:CE2	4:K:124:LEU:HB3	2.50	0.44
3:X:34:HIS:O	3:X:88:CYS:HA	2.17	0.44
4:T:142:CYS:HB2	4:T:157:TRP:CH2	2.52	0.44
2:D:19:ASP:OD1	2:D:19:ASP:N	2.42	0.44
3:L:34:HIS:O	3:L:88:CYS:HA	2.17	0.44
3:E:135:PHE:C	3:E:136:LEU:HD12	2.42	0.44
3:J:34:HIS:O	3:J:88:CYS:HA	2.17	0.44
3:J:135:PHE:C	3:J:136:LEU:HD12	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:135:PHE:C	3:X:136:LEU:HD12	2.42	0.44
3:Q:135:PHE:C	3:Q:136:LEU:HD12	2.42	0.44
4:K:142:CYS:HB2	4:K:157:TRP:CH2	2.52	0.44
4:W:30:THR:HB	4:W:53:ASN:HB2	1.99	0.44
4:W:37:MET:HE3	4:W:46:GLU:O	2.16	0.44
1:S:62:ARG:CG	1:S:63:ASP:H	2.29	0.44
3:J:39:LYS:NZ	3:J:39:LYS:HB3	2.33	0.44
3:X:124:GLN:HG3	4:T:122:TYR:CE2	2.53	0.44
2:U:128:ASP:OD1	2:U:159:TYR:OH	2.22	0.44
4:T:30:THR:HB	4:T:53:ASN:HB2	1.99	0.44
1:A:53:ASP:HA	1:A:58:PRO:HD3	1.99	0.44
1:A:58:PRO:HG2	1:A:60:ILE:HD11	2.00	0.44
1:C:53:ASP:HA	1:C:58:PRO:HD3	1.99	0.44
1:S:58:PRO:HG2	1:S:60:ILE:HD11	2.00	0.44
3:E:34:HIS:O	3:E:88:CYS:HA	2.17	0.44
3:E:90:GLN:HE21	3:E:97:THR:HG22	1.82	0.44
3:Q:148:TRP:CD2	3:Q:179:LEU:HD13	2.53	0.44
3:V:135:PHE:HZ	4:W:124:LEU:CD1	2.31	0.44
4:W:142:CYS:HB2	4:W:157:TRP:CH2	2.52	0.44
1:O:16:GLY:HA3	2:P:14:TRP:CH2	2.53	0.44
3:L:148:TRP:CD2	3:L:179:LEU:HD13	2.53	0.44
3:X:124:GLN:HG3	4:T:122:TYR:CZ	2.52	0.44
1:C:62:ARG:CG	1:C:63:ASP:N	2.73	0.44
1:G:53:ASP:HA	1:G:58:PRO:HD3	1.99	0.44
3:E:98:PHE:CE1	4:F:37:MET:CE	3.00	0.44
3:J:148:TRP:CD2	3:J:179:LEU:HD13	2.53	0.44
3:Q:39:LYS:NZ	3:Q:39:LYS:HB3	2.33	0.44
3:V:39:LYS:NZ	3:V:39:LYS:HB3	2.33	0.44
5:f:1:NAG:H61	5:f:2:NAG:N2	2.33	0.44
3:E:150:ILE:HG12	3:E:192:TYR:CD1	2.53	0.44
3:V:111:ALA:O	3:V:200:THR:HG21	2.17	0.44
4:F:52:PHE:CE2	4:F:53:ASN:HB3	2.53	0.44
4:T:52:PHE:CE2	4:T:53:ASN:HB3	2.53	0.44
7:c:1:NAG:H61	7:c:2:NAG:N2	2.33	0.44
1:M:53:ASP:HA	1:M:58:PRO:HD3	1.99	0.43
1:O:58:PRO:HG2	1:O:60:ILE:HD11	2.00	0.43
3:L:150:ILE:HG12	3:L:192:TYR:CD1	2.53	0.43
3:J:111:ALA:O	3:J:200:THR:HG21	2.17	0.43
3:J:164:THR:HG22	4:K:174:PHE:HA	2.00	0.43
3:X:169:LYS:HD2	3:X:169:LYS:HA	1.79	0.43
3:Q:150:ILE:HG12	3:Q:192:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:52:PHE:CE2	4:K:53:ASN:HB3	2.53	0.43
1:A:274:TYR:CZ	4:H:97:GLY:HA2	2.53	0.43
3:X:39:LYS:HB3	3:X:39:LYS:NZ	2.33	0.43
2:I:128:ASP:OD1	2:I:159:TYR:OH	2.22	0.43
4:R:52:PHE:CE2	4:R:53:ASN:HB3	2.53	0.43
1:A:55(A):GLY:HA3	3:L:32:PHE:CE1	2.54	0.43
1:A:135:VAL:HG22	1:A:146:SER:HA	2.00	0.43
2:N:76:ARG:HB2	1:O:107:GLU:OE2	2.17	0.43
1:S:53:ASP:HA	1:S:58:PRO:HD3	1.99	0.43
3:J:118:PHE:HA	3:J:119:PRO:HD3	1.87	0.43
3:X:148:TRP:CD2	3:X:179:LEU:HD13	2.53	0.43
3:L:111:ALA:O	3:L:200:THR:HG21	2.17	0.43
3:V:148:TRP:CD2	3:V:179:LEU:HD13	2.53	0.43
4:R:48:ILE:HG12	4:R:63:PHE:CE2	2.54	0.43
4:W:48:ILE:HG12	4:W:63:PHE:CE2	2.54	0.43
1:C:55:ASN:O	3:E:30:LYS:HE3	2.19	0.43
1:C:135:VAL:HG22	1:C:146:SER:HA	2.00	0.43
1:M:276:ASN:ND2	4:T:31:GLU:O	2.50	0.43
3:E:148:TRP:CD2	3:E:179:LEU:HD13	2.53	0.43
3:J:118:PHE:HE2	4:K:124:LEU:O	2.01	0.43
3:J:169:LYS:HD2	3:J:169:LYS:HA	1.80	0.43
3:X:162:SER:HB2	4:T:177:VAL:CG2	2.47	0.43
3:X:174:SER:HB3	4:T:174:PHE:CE1	2.53	0.43
4:R:19:LYS:HZ1	4:R:81:ASP:HB2	1.82	0.43
5:Y:1:NAG:H61	5:Y:2:NAG:N2	2.33	0.43
1:G:32:LYS:CG	8:b:1:NAG:H81	2.47	0.43
1:G:58:PRO:HG2	1:G:60:ILE:HD11	2.00	0.43
1:G:135:VAL:HG22	1:G:146:SER:HA	2.00	0.43
2:N:3:PHE:CE1	2:P:3:PHE:HE1	2.36	0.43
1:O:135:VAL:HG22	1:O:146:SER:HA	2.00	0.43
3:L:39:LYS:NZ	3:L:39:LYS:HB3	2.33	0.43
3:V:150:ILE:HG12	3:V:192:TYR:CD1	2.53	0.43
2:I:58:LYS:HA	2:I:58:LYS:HD2	1.83	0.43
1:A:62:ARG:NH1	1:A:63:ASP:OD2	2.52	0.43
1:A:206:THR:HG23	1:A:241:ASP:OD2	2.19	0.43
1:C:16:GLY:HA3	2:D:14:TRP:CZ2	2.53	0.43
3:L:169:LYS:HD2	3:L:169:LYS:HA	1.80	0.43
2:I:169:ASN:O	2:I:172:GLU:OE1	2.37	0.43
4:R:66:ARG:H	4:R:66:ARG:HG3	1.53	0.43
7:a:1:NAG:H61	7:a:2:NAG:N2	2.33	0.43
1:G:25:GLN:OE1	1:G:33:ASN:CG	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:206:THR:HG23	1:S:241:ASP:OD2	2.19	0.43
3:E:203:SER:HA	3:E:204:PRO:HD3	1.91	0.43
3:J:150:ILE:HG12	3:J:192:TYR:CD1	2.53	0.43
1:A:176:LEU:HD12	1:A:258:TYR:C	2.44	0.43
2:B:58:LYS:HA	2:B:58:LYS:HD2	1.83	0.43
3:E:39:LYS:NZ	3:E:39:LYS:HB3	2.33	0.43
4:H:48:ILE:HG12	4:H:63:PHE:CE2	2.54	0.43
4:H:137:MET:SD	4:H:194:PRO:HA	2.59	0.43
1:C:11:ASP:CA	2:D:27:SER:O	2.67	0.43
3:L:186:TYR:CE1	3:L:192:TYR:CE2	3.07	0.43
3:Q:186:TYR:CE1	3:Q:192:TYR:CE2	3.07	0.43
4:R:137:MET:SD	4:R:194:PRO:HA	2.59	0.43
1:C:316:LEU:HD23	2:D:100:VAL:HG13	2.01	0.42
3:J:8:PRO:CG	3:X:11:LEU:HD12	2.49	0.42
3:J:135:PHE:CZ	4:K:124:LEU:CD1	3.02	0.42
4:K:137:MET:SD	4:K:194:PRO:HA	2.59	0.42
4:W:137:MET:SD	4:W:194:PRO:HA	2.59	0.42
1:C:16:GLY:HA3	2:D:14:TRP:CZ3	2.55	0.42
1:C:16:GLY:CA	2:D:14:TRP:CH2	3.01	0.42
1:M:20:ASN:HA	2:N:15:GLN:OE1	2.19	0.42
2:N:169:ASN:O	2:N:172:GLU:OE1	2.37	0.42
2:P:76:ARG:CZ	2:U:69:GLU:H	2.32	0.42
1:S:176:LEU:HD12	1:S:258:TYR:C	2.44	0.42
3:L:4:LEU:HD23	3:L:4:LEU:HA	1.73	0.42
3:E:59:PRO:HG2	3:E:62:PHE:CE2	2.55	0.42
3:E:186:TYR:CE1	3:E:192:TYR:CE2	3.07	0.42
3:J:160:LEU:HD11	4:K:179:GLN:CD	2.42	0.42
3:J:193:THR:HG22	3:J:194:CYS:N	2.34	0.42
3:X:4:LEU:HD23	3:X:4:LEU:HA	1.73	0.42
3:Q:59:PRO:HG2	3:Q:62:PHE:CE2	2.55	0.42
1:C:176:LEU:HD12	1:C:258:TYR:C	2.44	0.42
1:G:131:ASP:OD2	1:G:133(A):SER:OG	2.37	0.42
1:M:58:PRO:HG2	1:M:60:ILE:HD11	2.00	0.42
1:O:323:THR:HA	1:O:324:PRO:HD3	1.77	0.42
3:L:133:VAL:HG21	4:H:143:LEU:HD13	2.00	0.42
3:J:62:PHE:CD1	3:J:75:ILE:HG12	2.55	0.42
3:X:150:ILE:HG12	3:X:192:TYR:CD1	2.53	0.42
3:Q:118:PHE:HA	3:Q:119:PRO:HD3	1.87	0.42
4:H:52:PHE:CE2	4:H:53:ASN:HB3	2.53	0.42
4:K:48:ILE:HG12	4:K:63:PHE:CE2	2.54	0.42
4:T:37:MET:HE3	4:T:37:MET:HB3	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:48:ILE:HG12	4:T:63:PHE:CE2	2.54	0.42
1:C:14:CYS:O	2:D:24:TYR:HA	2.19	0.42
1:C:17:TYR:CE2	2:D:13:GLY:HA3	2.55	0.42
1:C:58:PRO:HG2	1:C:60:ILE:HD11	2.00	0.42
2:D:169:ASN:O	2:D:172:GLU:OE1	2.37	0.42
1:G:28:THR:HA	2:I:101:LEU:HD22	2.01	0.42
1:M:135:VAL:HG22	1:M:146:SER:HA	2.00	0.42
1:M:176:LEU:HD12	1:M:258:TYR:C	2.44	0.42
1:O:176:LEU:HD12	1:O:258:TYR:C	2.44	0.42
3:J:119:PRO:HB3	3:J:209:PHE:CE2	2.55	0.42
3:X:119:PRO:HB3	3:X:209:PHE:CE2	2.55	0.42
4:T:19:LYS:NZ	4:T:81:ASP:HB3	2.34	0.42
1:M:11:ASP:CG	2:N:28:ASN:CA	2.85	0.42
1:O:206:THR:HG23	1:O:241:ASP:OD2	2.19	0.42
3:X:186:TYR:CE1	3:X:192:TYR:CE2	3.07	0.42
3:Q:119:PRO:HB3	3:Q:209:PHE:CE2	2.55	0.42
3:V:59:PRO:HG2	3:V:62:PHE:CE2	2.55	0.42
4:R:19:LYS:HE2	4:R:81:ASP:OD1	2.20	0.42
4:W:136:SER:C	4:W:195:SER:HG	2.24	0.42
1:A:280:LYS:HE3	1:A:304:GLU:CG	2.50	0.42
1:C:206:THR:HG23	1:C:241:ASP:OD2	2.19	0.42
2:P:169:ASN:O	2:P:172:GLU:OE1	2.37	0.42
1:S:106:GLU:HG2	2:U:70:PHE:C	2.44	0.42
3:E:62:PHE:CD1	3:E:75:ILE:HG12	2.55	0.42
3:J:186:TYR:CE1	3:J:192:TYR:CE2	3.07	0.42
3:Q:62:PHE:CD1	3:Q:75:ILE:HG12	2.55	0.42
3:V:186:TYR:CE1	3:V:192:TYR:CE2	3.07	0.42
4:K:19:LYS:HE2	4:K:81:ASP:OD1	2.20	0.42
1:C:280:LYS:HE3	1:C:304:GLU:CG	2.50	0.42
2:D:3:PHE:CE2	2:D:113:SER:HB2	2.55	0.42
1:M:323:THR:HA	1:M:324:PRO:HD3	1.77	0.42
3:E:44:PRO:HG2	4:F:45:LEU:HD11	2.02	0.42
3:E:119:PRO:HG3	3:E:209:PHE:CD2	2.55	0.42
3:V:119:PRO:HG3	3:V:209:PHE:CD2	2.55	0.42
4:F:19:LYS:HE2	4:F:81:ASP:OD1	2.20	0.42
4:T:93:VAL:CG1	4:T:100(C):PHE:HB3	2.50	0.42
4:T:137:MET:SD	4:T:194:PRO:HA	2.59	0.42
4:R:19:LYS:HZ3	4:R:81:ASP:HB2	1.82	0.42
2:B:169:ASN:O	2:B:172:GLU:OE1	2.37	0.42
1:C:16:GLY:CA	2:D:14:TRP:CZ3	3.03	0.42
1:G:206:THR:HG23	1:G:241:ASP:OD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:76:ARG:NH1	2:U:69:GLU:H	2.17	0.42
3:L:119:PRO:HB3	3:L:209:PHE:CE2	2.55	0.42
3:E:27(B):VAL:HG23	3:E:92:ASN:HB2	2.02	0.42
3:X:18:ARG:O	3:X:18:ARG:HG3	2.20	0.42
3:X:62:PHE:CD1	3:X:75:ILE:HG12	2.55	0.42
3:V:27(B):VAL:HG23	3:V:92:ASN:HB2	2.02	0.42
4:T:125:ALA:HA	4:T:126:PRO:HD3	1.85	0.42
1:A:268:MET:HE3	1:A:268:MET:HB2	1.82	0.42
2:D:83:GLN:CD	2:I:68:ARG:HH22	2.25	0.42
1:M:280:LYS:HE3	1:M:304:GLU:CG	2.50	0.42
2:N:3:PHE:CE2	2:N:113:SER:HB2	2.55	0.42
1:O:280:LYS:HE3	1:O:304:GLU:CG	2.50	0.42
1:S:14:CYS:O	2:U:24:TYR:HA	2.20	0.42
1:S:18:HIS:HB2	2:U:20:GLY:O	2.20	0.42
1:S:135:VAL:HG22	1:S:146:SER:HA	2.00	0.42
3:L:59:PRO:HG2	3:L:62:PHE:CE2	2.55	0.42
3:E:119:PRO:HB3	3:E:209:PHE:CE2	2.55	0.42
3:J:174:SER:CB	4:K:174:PHE:HE1	2.28	0.42
3:V:119:PRO:HB3	3:V:209:PHE:CE2	2.55	0.42
4:F:48:ILE:HG12	4:F:63:PHE:CE2	2.54	0.42
1:G:280:LYS:HE3	1:G:304:GLU:CG	2.50	0.42
1:M:17:TYR:OH	2:N:13:GLY:N	2.52	0.42
1:M:206:THR:HG23	1:M:241:ASP:OD2	2.19	0.42
2:N:168:LEU:HD12	2:N:169:ASN:CA	2.48	0.42
1:O:62:ARG:CG	1:O:63:ASP:H	2.29	0.42
3:L:62:PHE:CD1	3:L:75:ILE:HG12	2.55	0.42
3:L:174:SER:HB2	4:H:174:PHE:CE1	2.54	0.42
3:X:59:PRO:HG2	3:X:62:PHE:CE2	2.55	0.42
3:X:124:GLN:CB	4:T:122:TYR:CZ	3.03	0.42
3:V:62:PHE:CD1	3:V:75:ILE:HG12	2.55	0.42
3:V:98:PHE:CZ	4:W:45:LEU:HB3	2.55	0.42
2:U:73:LEU:HD23	2:U:73:LEU:HA	1.91	0.42
4:H:199:THR:O	4:H:204:GLU:N	2.50	0.42
4:W:19:LYS:HE2	4:W:81:ASP:OD1	2.20	0.42
2:N:62:GLN:HG3	2:N:92:TRP:CD2	2.55	0.41
1:S:323:THR:HG21	2:U:13:GLY:H	1.85	0.41
3:E:193:THR:HG22	3:E:194:CYS:N	2.34	0.41
3:J:4:LEU:HA	3:J:4:LEU:HD23	1.73	0.41
3:J:119:PRO:CG	4:K:228:ARG:HH21	2.33	0.41
4:H:19:LYS:HE2	4:H:81:ASP:OD1	2.20	0.41
4:F:137:MET:SD	4:F:194:PRO:HA	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:95:ASN:HA	4:T:100(C):PHE:HA	2.02	0.41
1:C:164:ILE:O	1:C:246:GLU:HA	2.20	0.41
2:D:73:LEU:HD23	2:D:73:LEU:HA	1.91	0.41
1:M:221:PRO:HB3	5:d:1:NAG:H81	2.02	0.41
1:O:16:GLY:CA	2:P:14:TRP:CZ3	3.03	0.41
2:P:3:PHE:CE2	2:P:113:SER:HB2	2.55	0.41
3:J:119:PRO:HG3	3:J:209:PHE:CD2	2.55	0.41
3:Q:87:PHE:CE1	3:Q:101:GLY:HA3	2.56	0.41
3:V:135:PHE:CE2	4:W:124:LEU:HD13	2.55	0.41
2:U:169:ASN:O	2:U:172:GLU:OE1	2.37	0.41
4:F:95:ASN:HA	4:F:100(C):PHE:HA	2.02	0.41
4:W:66:ARG:H	4:W:66:ARG:HG3	1.53	0.41
1:C:16:GLY:HA3	2:D:14:TRP:CD2	2.55	0.41
1:S:307:LYS:HB3	2:U:62:GLN:NE2	2.36	0.41
3:E:18:ARG:O	3:E:18:ARG:HG3	2.20	0.41
3:J:90:GLN:HE21	3:J:97:THR:HG22	1.82	0.41
3:X:87:PHE:CE1	3:X:101:GLY:HA3	2.56	0.41
2:U:3:PHE:CE2	2:U:113:SER:HB2	2.55	0.41
4:H:66:ARG:H	4:H:66:ARG:HG3	1.53	0.41
2:B:3:PHE:CE2	2:B:113:SER:HB2	2.55	0.41
1:G:176:LEU:HD12	1:G:258:TYR:C	2.44	0.41
1:G:238:LYS:HA	1:G:239:PRO:HD3	1.94	0.41
1:M:268:MET:HE3	1:M:268:MET:HB2	1.82	0.41
3:L:27(B):VAL:HG23	3:L:92:ASN:HB2	2.02	0.41
3:E:124:GLN:HG3	4:F:122:TYR:CE2	2.54	0.41
3:J:59:PRO:HG2	3:J:62:PHE:CE2	2.54	0.41
3:V:4:LEU:HA	3:V:4:LEU:HD23	1.73	0.41
4:H:11:LEU:HA	4:H:110:THR:O	2.21	0.41
4:W:93:VAL:CG1	4:W:100(C):PHE:HB3	2.50	0.41
1:A:265:SER:OG	1:A:266:ALA:N	2.53	0.41
3:L:18:ARG:O	3:L:18:ARG:HG3	2.20	0.41
3:E:24:ARG:HH11	3:E:70:ASP:HB3	1.86	0.41
3:J:18:ARG:O	3:J:18:ARG:HG3	2.20	0.41
3:J:27(B):VAL:HG23	3:J:92:ASN:HB2	2.02	0.41
3:Q:18:ARG:O	3:Q:18:ARG:HG3	2.20	0.41
2:I:62:GLN:HG3	2:I:92:TRP:CD2	2.55	0.41
4:H:148:PHE:HA	4:H:149:PRO:HA	1.85	0.41
4:F:93:VAL:CG1	4:F:100(C):PHE:HB3	2.50	0.41
4:W:19:LYS:HZ1	4:W:81:ASP:HB2	1.86	0.41
1:C:17:TYR:CE2	2:D:13:GLY:CA	3.04	0.41
1:G:13:ILE:O	2:I:137:CYS:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:18:ARG:O	3:V:18:ARG:HG3	2.20	0.41
4:K:95:ASN:HA	4:K:100(C):PHE:HA	2.03	0.41
2:D:58:LYS:HD2	2:D:58:LYS:HA	1.83	0.41
1:G:164:ILE:O	1:G:246:GLU:HA	2.20	0.41
2:N:11:GLU:O	2:N:11:GLU:HG3	2.21	0.41
2:N:55:ILE:HG23	2:N:99:LEU:HD23	2.03	0.41
1:S:18:HIS:HB2	2:U:21:TRP:HA	2.01	0.41
3:X:95:PRO:O	3:X:97:THR:HG22	2.21	0.41
3:V:193:THR:HG22	3:V:194:CYS:N	2.34	0.41
4:F:176:ALA:HA	4:F:187:LEU:HB3	2.03	0.41
4:K:33:THR:HG23	4:K:95:ASN:HD22	1.86	0.41
4:T:11:LEU:HA	4:T:110:THR:O	2.21	0.41
4:W:199:THR:O	4:W:204:GLU:N	2.51	0.41
2:B:62:GLN:HG3	2:B:92:TRP:CD2	2.55	0.41
1:O:164:ILE:O	1:O:246:GLU:HA	2.20	0.41
1:O:265:SER:OG	1:O:266:ALA:N	2.53	0.41
2:P:11:GLU:O	2:P:11:GLU:HG3	2.21	0.41
2:P:62:GLN:HG3	2:P:92:TRP:CD2	2.55	0.41
1:S:131:ASP:OD2	1:S:133(A):SER:OG	2.37	0.41
1:S:164:ILE:O	1:S:246:GLU:HA	2.21	0.41
1:S:280:LYS:HE3	1:S:304:GLU:CG	2.50	0.41
3:L:87:PHE:CE1	3:L:101:GLY:HA3	2.56	0.41
3:E:139:PHE:HD2	3:E:198:HIS:HE2	1.69	0.41
2:I:3:PHE:CE2	2:I:113:SER:HB2	2.55	0.41
4:H:157:TRP:CZ2	4:H:191:VAL:HG12	2.56	0.41
4:F:140:LEU:HD23	4:F:140:LEU:HA	1.90	0.41
4:K:11:LEU:HA	4:K:110:THR:O	2.21	0.41
4:W:11:LEU:HA	4:W:110:THR:O	2.21	0.41
4:W:157:TRP:CZ2	4:W:191:VAL:HG12	2.56	0.41
1:A:218:ALA:CB	1:C:203:SER:HB2	2.46	0.41
1:C:62:ARG:NH1	1:C:63:ASP:OD2	2.53	0.41
2:D:83:GLN:NE2	2:I:63:PHE:CZ	2.89	0.41
1:G:265:SER:OG	1:G:266:ALA:N	2.53	0.41
1:M:52:CYS:HB2	1:M:279:THR:HG22	2.03	0.41
2:N:168:LEU:C	2:N:168:LEU:CD1	2.92	0.41
2:P:55:ILE:HG23	2:P:99:LEU:HD23	2.03	0.41
2:P:150:GLU:CB	10:P:2001:NAG:H62	2.47	0.41
1:S:52:CYS:HB2	1:S:279:THR:HG22	2.03	0.41
3:L:119:PRO:HG3	3:L:209:PHE:CD2	2.55	0.41
3:J:87:PHE:CE1	3:J:101:GLY:HA3	2.56	0.41
3:X:24:ARG:HH11	3:X:70:ASP:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:119:PRO:HG3	3:X:209:PHE:CD2	2.55	0.41
3:X:193:THR:HG22	3:X:194:CYS:N	2.34	0.41
3:Q:193:THR:HG22	3:Q:194:CYS:N	2.35	0.41
3:V:38:GLN:CD	4:W:39:GLN:HE22	2.28	0.41
3:V:87:PHE:CE1	3:V:101:GLY:HA3	2.56	0.41
3:V:95:PRO:O	3:V:97:THR:HG22	2.21	0.41
2:I:11:GLU:HG3	2:I:11:GLU:O	2.21	0.41
2:U:11:GLU:HG3	2:U:11:GLU:O	2.21	0.41
2:U:55:ILE:HG23	2:U:99:LEU:HD23	2.03	0.41
2:U:62:GLN:HG3	2:U:92:TRP:CD2	2.55	0.41
4:H:36:TRP:CZ3	4:H:92:CYS:HB2	2.56	0.41
4:H:176:ALA:HA	4:H:187:LEU:HB3	2.03	0.41
4:F:33:THR:HG23	4:F:95:ASN:HD22	1.86	0.41
4:K:36:TRP:CZ3	4:K:92:CYS:HB2	2.56	0.41
4:T:176:ALA:HA	4:T:187:LEU:HB3	2.03	0.41
2:B:11:GLU:HG3	2:B:11:GLU:O	2.21	0.41
1:C:211:GLN:NE2	1:C:213:LEU:HD11	2.36	0.41
1:G:62:ARG:NH1	1:G:63:ASP:OD2	2.53	0.41
1:M:106:GLU:HG2	2:N:70:PHE:HA	2.03	0.41
1:M:164:ILE:O	1:M:246:GLU:HA	2.20	0.41
2:P:168:LEU:HD23	2:P:168:LEU:HA	1.96	0.41
3:Q:119:PRO:HG3	3:Q:209:PHE:CD2	2.55	0.41
3:Q:124:GLN:HB2	4:R:122:TYR:CG	2.56	0.41
4:H:33:THR:HG23	4:H:95:ASN:HD22	1.86	0.41
4:H:93:VAL:CG1	4:H:100(C):PHE:HB3	2.50	0.41
4:F:36:TRP:CZ3	4:F:92:CYS:HB2	2.56	0.41
4:R:11:LEU:HA	4:R:110:THR:O	2.21	0.41
4:R:33:THR:HG23	4:R:95:ASN:HD22	1.86	0.41
4:R:93:VAL:CG1	4:R:100(C):PHE:HB3	2.50	0.41
4:R:157:TRP:CZ2	4:R:191:VAL:HG12	2.56	0.41
1:A:211:GLN:NE2	1:A:213:LEU:HD11	2.36	0.40
1:C:52:CYS:HB2	1:C:279:THR:HG22	2.03	0.40
1:G:28:THR:CA	2:I:101:LEU:HD22	2.52	0.40
1:G:211:GLN:NE2	1:G:213:LEU:HD11	2.36	0.40
1:M:62:ARG:NH1	1:M:63:ASP:OD2	2.53	0.40
1:O:147:PHE:HZ	1:O:230:MET:HE1	1.86	0.40
3:L:24:ARG:HH11	3:L:70:ASP:HB3	1.86	0.40
2:I:55:ILE:HG23	2:I:99:LEU:HD23	2.03	0.40
2:I:84:MET:HE2	2:I:84:MET:HB3	1.85	0.40
4:K:93:VAL:CG1	4:K:100(C):PHE:HB3	2.50	0.40
4:W:95:ASN:HA	4:W:100(C):PHE:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:15:ILE:HG13	2:I:119:TYR:HA	2.03	0.40
1:G:62:ARG:CG	1:G:63:ASP:H	2.29	0.40
1:G:147:PHE:HZ	1:G:230:MET:HE1	1.86	0.40
1:M:323:THR:HG21	2:N:12:GLY:HA2	2.02	0.40
1:O:211:GLN:NE2	1:O:213:LEU:HD11	2.36	0.40
3:L:95:PRO:O	3:L:97:THR:HG22	2.21	0.40
3:L:193:THR:HG22	3:L:194:CYS:N	2.34	0.40
3:X:27(B):VAL:HG23	3:X:92:ASN:HB2	2.02	0.40
3:X:162:SER:HB2	4:T:177:VAL:HG21	2.04	0.40
3:Q:139:PHE:HD2	3:Q:198:HIS:HE2	1.69	0.40
4:H:24:THR:HG22	4:H:76:SER:OG	2.21	0.40
4:H:37:MET:HE3	4:H:37:MET:HB3	1.72	0.40
4:F:157:TRP:CZ2	4:F:191:VAL:HG12	2.56	0.40
4:T:36:TRP:CH2	4:T:92:CYS:HB2	2.56	0.40
1:C:62:ARG:CG	1:C:63:ASP:H	2.29	0.40
2:D:11:GLU:O	2:D:11:GLU:HG3	2.21	0.40
2:D:55:ILE:HG23	2:D:99:LEU:HD23	2.03	0.40
1:O:62:ARG:NH1	1:O:63:ASP:OD2	2.53	0.40
3:L:118:PHE:HA	3:L:119:PRO:HD3	1.87	0.40
3:Q:24:ARG:HH11	3:Q:70:ASP:HB3	1.86	0.40
3:Q:27(B):VAL:HG23	3:Q:92:ASN:HB2	2.02	0.40
3:Q:95:PRO:O	3:Q:97:THR:HG22	2.21	0.40
3:V:24:ARG:HH11	3:V:70:ASP:HB3	1.86	0.40
4:T:66:ARG:H	4:T:66:ARG:HG3	1.53	0.40
4:W:36:TRP:CH2	4:W:92:CYS:HB2	2.57	0.40
1:A:164:ILE:O	1:A:246:GLU:HA	2.21	0.40
1:C:147:PHE:HZ	1:C:230:MET:HE1	1.86	0.40
2:D:62:GLN:HG3	2:D:92:TRP:CD2	2.55	0.40
3:J:24:ARG:HH11	3:J:70:ASP:HB3	1.86	0.40
3:J:139:PHE:HD2	3:J:198:HIS:HE2	1.69	0.40
4:F:36:TRP:CH2	4:F:92:CYS:HB2	2.56	0.40
4:K:176:ALA:HA	4:K:187:LEU:HB3	2.03	0.40
4:R:36:TRP:CZ3	4:R:92:CYS:HB2	2.56	0.40
4:W:36:TRP:CZ3	4:W:92:CYS:HB2	2.56	0.40
1:A:186:ASN:CG	1:A:227:SER:HG	2.29	0.40
1:M:147:PHE:HZ	1:M:230:MET:HE1	1.87	0.40
1:S:62:ARG:NH1	1:S:63:ASP:OD2	2.53	0.40
4:K:24:THR:HG22	4:K:76:SER:OG	2.21	0.40
4:K:82(A):ARG:NH1	4:K:82(A):ARG:HB3	2.37	0.40
4:K:222:LYS:H	4:K:222:LYS:HG2	1.69	0.40
4:T:24:THR:HG22	4:T:76:SER:OG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:33:THR:HG23	4:W:95:ASN:HD22	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	318/334 (95%)	309 (97%)	9 (3%)	0	100	100
1	C	315/334 (94%)	305 (97%)	10 (3%)	0	100	100
1	G	315/334 (94%)	306 (97%)	9 (3%)	0	100	100
1	M	318/334 (95%)	309 (97%)	9 (3%)	0	100	100
1	O	314/334 (94%)	305 (97%)	9 (3%)	0	100	100
1	S	318/334 (95%)	308 (97%)	10 (3%)	0	100	100
2	B	168/182 (92%)	164 (98%)	4 (2%)	0	100	100
2	D	168/182 (92%)	164 (98%)	4 (2%)	0	100	100
2	I	171/182 (94%)	167 (98%)	4 (2%)	0	100	100
2	N	163/182 (90%)	160 (98%)	3 (2%)	0	100	100
2	P	168/182 (92%)	164 (98%)	4 (2%)	0	100	100
2	U	171/182 (94%)	167 (98%)	4 (2%)	0	100	100
3	E	212/218 (97%)	194 (92%)	18 (8%)	0	100	100
3	J	203/218 (93%)	185 (91%)	18 (9%)	0	100	100
3	L	209/218 (96%)	191 (91%)	18 (9%)	0	100	100
3	Q	209/218 (96%)	191 (91%)	18 (9%)	0	100	100
3	V	206/218 (94%)	189 (92%)	17 (8%)	0	100	100
3	X	212/218 (97%)	194 (92%)	18 (8%)	0	100	100
4	F	217/222 (98%)	187 (86%)	26 (12%)	4 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	217/222 (98%)	189 (87%)	24 (11%)	4 (2%)	6	34
4	K	217/222 (98%)	188 (87%)	25 (12%)	4 (2%)	6	34
4	R	217/222 (98%)	189 (87%)	24 (11%)	4 (2%)	6	34
4	T	216/222 (97%)	188 (87%)	25 (12%)	3 (1%)	9	40
4	W	217/222 (98%)	188 (87%)	25 (12%)	4 (2%)	6	34
All	All	5459/5736 (95%)	5101 (93%)	335 (6%)	23 (0%)	30	67

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	135	ASN
4	F	135	ASN
4	K	135	ASN
4	R	135	ASN
4	W	135	ASN
4	H	229	ASP
4	F	229	ASP
4	K	229	ASP
4	T	229	ASP
4	R	229	ASP
4	W	229	ASP
4	H	96	TYR
4	F	96	TYR
4	K	96	TYR
4	T	96	TYR
4	R	96	TYR
4	W	96	TYR
4	H	41	HIS
4	F	41	HIS
4	K	41	HIS
4	T	41	HIS
4	R	41	HIS
4	W	41	HIS

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	286/297 (96%)	271 (95%)	15 (5%)	21	42
1	C	285/297 (96%)	269 (94%)	16 (6%)	19	40
1	G	285/297 (96%)	270 (95%)	15 (5%)	20	41
1	M	286/297 (96%)	271 (95%)	15 (5%)	21	42
1	O	283/297 (95%)	268 (95%)	15 (5%)	20	41
1	S	286/297 (96%)	271 (95%)	15 (5%)	21	42
2	B	147/155 (95%)	144 (98%)	3 (2%)	48	66
2	D	147/155 (95%)	144 (98%)	3 (2%)	48	66
2	I	148/155 (96%)	145 (98%)	3 (2%)	48	66
2	N	144/155 (93%)	142 (99%)	2 (1%)	59	72
2	P	147/155 (95%)	144 (98%)	3 (2%)	48	66
2	U	148/155 (96%)	144 (97%)	4 (3%)	39	61
3	E	189/191 (99%)	171 (90%)	18 (10%)	8	25
3	J	185/191 (97%)	167 (90%)	18 (10%)	8	24
3	L	188/191 (98%)	170 (90%)	18 (10%)	8	25
3	Q	188/191 (98%)	171 (91%)	17 (9%)	9	27
3	V	187/191 (98%)	169 (90%)	18 (10%)	8	25
3	X	189/191 (99%)	172 (91%)	17 (9%)	9	27
4	F	192/193 (100%)	167 (87%)	25 (13%)	4	15
4	H	192/193 (100%)	167 (87%)	25 (13%)	4	15
4	K	192/193 (100%)	167 (87%)	25 (13%)	4	15
4	R	192/193 (100%)	168 (88%)	24 (12%)	4	16
4	T	191/193 (99%)	165 (86%)	26 (14%)	3	14
4	W	192/193 (100%)	166 (86%)	26 (14%)	4	14
All	All	4869/5016 (97%)	4503 (92%)	366 (8%)	12	33

All (366) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	29	ILE
1	A	36	VAL

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Mol	Chain	Res	Type
1	A	82	VAL
1	A	111	LEU
1	A	123	ILE
1	A	135	VAL
1	A	151	VAL
1	A	195	TYR
1	A	206	THR
1	A	260	ILE
1	A	260(A)	VAL
1	A	283	THR
1	A	307	LYS
1	A	309	VAL
2	B	69	GLU
2	B	83	GLN
2	B	93	THR
1	C	26	VAL
1	C	29	ILE
1	C	36	VAL
1	C	82	VAL
1	C	111	LEU
1	C	123	ILE
1	C	135	VAL
1	C	151	VAL
1	C	195	TYR
1	C	206	THR
1	C	210	ASN
1	C	260	ILE
1	C	260(A)	VAL
1	C	283	THR
1	C	307	LYS
1	C	309	VAL
2	D	69	GLU
2	D	83	GLN
2	D	93	THR
1	G	26	VAL
1	G	29	ILE
1	G	36	VAL
1	G	82	VAL
1	G	111	LEU
1	G	123	ILE
1	G	135	VAL
1	G	151	VAL

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Mol	Chain	Res	Type
1	G	195	TYR
1	G	206	THR
1	G	260	ILE
1	G	260(A)	VAL
1	G	283	THR
1	G	307	LYS
1	G	309	VAL
1	M	26	VAL
1	M	29	ILE
1	M	36	VAL
1	M	82	VAL
1	M	111	LEU
1	M	123	ILE
1	M	135	VAL
1	M	151	VAL
1	M	195	TYR
1	M	206	THR
1	M	260	ILE
1	M	260(A)	VAL
1	M	283	THR
1	M	307	LYS
1	M	309	VAL
2	N	83	GLN
2	N	93	THR
1	O	26	VAL
1	O	29	ILE
1	O	36	VAL
1	O	82	VAL
1	O	111	LEU
1	O	123	ILE
1	O	135	VAL
1	O	151	VAL
1	O	195	TYR
1	O	206	THR
1	O	260	ILE
1	O	260(A)	VAL
1	O	283	THR
1	O	307	LYS
1	O	309	VAL
2	P	69	GLU
2	P	83	GLN
2	P	93	THR

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Mol	Chain	Res	Type
1	S	26	VAL
1	S	29	ILE
1	S	36	VAL
1	S	82	VAL
1	S	111	LEU
1	S	123	ILE
1	S	135	VAL
1	S	151	VAL
1	S	195	TYR
1	S	206	THR
1	S	260	ILE
1	S	260(A)	VAL
1	S	283	THR
1	S	307	LYS
1	S	309	VAL
3	L	14	SER
3	L	24	ARG
3	L	30	LYS
3	L	39	LYS
3	L	42	GLN
3	L	43	SER
3	L	53	ASN
3	L	69	THR
3	L	70	ASP
3	L	83	VAL
3	L	97	THR
3	L	116	SER
3	L	142	LYS
3	L	184	ASP
3	L	197	THR
3	L	202	THR
3	L	207	LYS
3	L	213	GLU
3	E	14	SER
3	E	24	ARG
3	E	30	LYS
3	E	39	LYS
3	E	42	GLN
3	E	43	SER
3	E	53	ASN
3	E	69	THR
3	E	70	ASP

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Mol	Chain	Res	Type
3	E	83	VAL
3	E	97	THR
3	E	116	SER
3	E	142	LYS
3	E	184	ASP
3	E	197	THR
3	E	202	THR
3	E	207	LYS
3	E	213	GLU
3	J	14	SER
3	J	24	ARG
3	J	30	LYS
3	J	39	LYS
3	J	42	GLN
3	J	43	SER
3	J	53	ASN
3	J	69	THR
3	J	70	ASP
3	J	83	VAL
3	J	97	THR
3	J	116	SER
3	J	142	LYS
3	J	184	ASP
3	J	197	THR
3	J	202	THR
3	J	207	LYS
3	J	213	GLU
3	X	14	SER
3	X	24	ARG
3	X	30	LYS
3	X	39	LYS
3	X	42	GLN
3	X	43	SER
3	X	53	ASN
3	X	69	THR
3	X	70	ASP
3	X	83	VAL
3	X	97	THR
3	X	116	SER
3	X	142	LYS
3	X	184	ASP
3	X	197	THR

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Mol	Chain	Res	Type
3	X	202	THR
3	X	213	GLU
3	Q	14	SER
3	Q	24	ARG
3	Q	30	LYS
3	Q	39	LYS
3	Q	42	GLN
3	Q	43	SER
3	Q	53	ASN
3	Q	69	THR
3	Q	70	ASP
3	Q	83	VAL
3	Q	97	THR
3	Q	116	SER
3	Q	142	LYS
3	Q	184	ASP
3	Q	197	THR
3	Q	207	LYS
3	Q	213	GLU
3	V	14	SER
3	V	24	ARG
3	V	30	LYS
3	V	39	LYS
3	V	42	GLN
3	V	43	SER
3	V	53	ASN
3	V	69	THR
3	V	70	ASP
3	V	83	VAL
3	V	97	THR
3	V	116	SER
3	V	142	LYS
3	V	184	ASP
3	V	197	THR
3	V	202	THR
3	V	207	LYS
3	V	213	GLU
2	I	69	GLU
2	I	83	GLN
2	I	93	THR
2	U	69	GLU
2	U	83	GLN

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Mol	Chain	Res	Type
2	U	93	THR
2	U	97	GLU
4	H	1	GLU
4	H	2	VAL
4	H	11	LEU
4	H	12	VAL
4	H	18	VAL
4	H	24	THR
4	H	30	THR
4	H	33	THR
4	H	34	ILE
4	H	58	THR
4	H	71	VAL
4	H	73	ARG
4	H	75	SER
4	H	109	VAL
4	H	113	SER
4	H	134	THR
4	H	144	VAL
4	H	166	LEU
4	H	177	VAL
4	H	190	SER
4	H	204	GLU
4	H	209	ASN
4	H	218	LYS
4	H	222	LYS
4	H	229	ASP
4	F	1	GLU
4	F	2	VAL
4	F	11	LEU
4	F	12	VAL
4	F	18	VAL
4	F	24	THR
4	F	30	THR
4	F	33	THR
4	F	34	ILE
4	F	58	THR
4	F	71	VAL
4	F	73	ARG
4	F	75	SER
4	F	109	VAL
4	F	113	SER

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Mol	Chain	Res	Type
4	F	144	VAL
4	F	166	LEU
4	F	177	VAL
4	F	190	SER
4	F	195	SER
4	F	204	GLU
4	F	209	ASN
4	F	218	LYS
4	F	222	LYS
4	F	229	ASP
4	K	1	GLU
4	K	2	VAL
4	K	11	LEU
4	K	12	VAL
4	K	18	VAL
4	K	24	THR
4	K	30	THR
4	K	33	THR
4	K	34	ILE
4	K	58	THR
4	K	71	VAL
4	K	73	ARG
4	K	75	SER
4	K	109	VAL
4	K	113	SER
4	K	144	VAL
4	K	166	LEU
4	K	177	VAL
4	K	190	SER
4	K	195	SER
4	K	204	GLU
4	K	209	ASN
4	K	218	LYS
4	K	222	LYS
4	K	229	ASP
4	T	1	GLU
4	T	2	VAL
4	T	11	LEU
4	T	12	VAL
4	T	18	VAL
4	T	24	THR
4	T	30	THR

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Mol	Chain	Res	Type
4	T	33	THR
4	T	34	ILE
4	T	58	THR
4	T	71	VAL
4	T	73	ARG
4	T	75	SER
4	T	81	ASP
4	T	109	VAL
4	T	113	SER
4	T	144	VAL
4	T	166	LEU
4	T	177	VAL
4	T	190	SER
4	T	195	SER
4	T	204	GLU
4	T	209	ASN
4	T	218	LYS
4	T	222	LYS
4	T	229	ASP
4	R	1	GLU
4	R	2	VAL
4	R	11	LEU
4	R	12	VAL
4	R	18	VAL
4	R	24	THR
4	R	30	THR
4	R	33	THR
4	R	34	ILE
4	R	58	THR
4	R	71	VAL
4	R	73	ARG
4	R	75	SER
4	R	109	VAL
4	R	113	SER
4	R	144	VAL
4	R	166	LEU
4	R	177	VAL
4	R	190	SER
4	R	204	GLU
4	R	209	ASN
4	R	218	LYS
4	R	222	LYS

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Mol	Chain	Res	Type
4	R	229	ASP
4	W	1	GLU
4	W	2	VAL
4	W	11	LEU
4	W	12	VAL
4	W	18	VAL
4	W	24	THR
4	W	30	THR
4	W	33	THR
4	W	34	ILE
4	W	58	THR
4	W	71	VAL
4	W	73	ARG
4	W	75	SER
4	W	109	VAL
4	W	113	SER
4	W	144	VAL
4	W	166	LEU
4	W	177	VAL
4	W	179	GLN
4	W	190	SER
4	W	195	SER
4	W	204	GLU
4	W	209	ASN
4	W	218	LYS
4	W	222	LYS
4	W	229	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
2	B	161	GLN
1	C	276	ASN
1	M	276	ASN
1	S	278	ASN
3	L	27(D)	ASN
3	L	92	ASN
3	L	161	ASN
3	L	190	ASN
3	L	210	ASN
3	E	27(D)	ASN

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Mol	Chain	Res	Type
3	E	38	GLN
3	E	161	ASN
3	E	190	ASN
3	E	210	ASN
3	J	27(D)	ASN
3	J	161	ASN
3	J	190	ASN
3	J	210	ASN
3	X	17	GLN
3	X	27(D)	ASN
3	X	38	GLN
3	X	92	ASN
3	X	161	ASN
3	X	190	ASN
3	X	210	ASN
3	Q	27(D)	ASN
3	Q	92	ASN
3	Q	161	ASN
3	Q	190	ASN
3	Q	210	ASN
3	V	27(D)	ASN
3	V	38	GLN
3	V	92	ASN
3	V	161	ASN
3	V	190	ASN
3	V	210	ASN
4	H	95	ASN
4	F	39	GLN
4	F	95	ASN
4	K	95	ASN
4	K	172	HIS
4	T	39	GLN
4	T	95	ASN
4	R	95	ASN
4	W	39	GLN
4	W	95	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 ⓘ

28 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
5	NAG	Y	1	5,1	14,14,15	1.32	2 (14%)	17,19,21	2.08	4 (23%)
5	NAG	Y	2	5	14,14,15	1.89	5 (35%)	17,19,21	1.53	2 (11%)
5	MAN	Y	3	5	11,11,12	1.94	3 (27%)	15,15,17	1.83	5 (33%)
6	NAG	Z	1	6,1	14,14,15	0.49	0	17,19,21	2.27	3 (17%)
6	NAG	Z	2	6	14,14,15	0.50	0	17,19,21	1.33	3 (17%)
6	BMA	Z	3	6	11,11,12	0.63	0	15,15,17	1.43	3 (20%)
6	MAN	Z	4	6	11,11,12	0.60	0	15,15,17	2.22	3 (20%)
6	MAN	Z	5	6	11,11,12	0.57	0	15,15,17	1.92	5 (33%)
6	MAN	Z	6	6	11,11,12	0.59	0	15,15,17	1.87	5 (33%)
6	MAN	Z	7	6	11,11,12	0.59	0	15,15,17	2.27	7 (46%)
6	MAN	Z	8	6	11,11,12	0.60	0	15,15,17	2.33	5 (33%)
7	NAG	a	1	7,1	14,14,15	1.41	3 (21%)	17,19,21	2.00	4 (23%)
7	NAG	a	2	7	14,14,15	1.76	4 (28%)	17,19,21	1.78	6 (35%)
8	NAG	b	1	8,1	14,14,15	0.53	0	17,19,21	1.28	3 (17%)
8	NAG	b	2	8	14,14,15	0.44	0	17,19,21	0.64	0
8	BMA	b	3	8	11,11,12	0.61	0	15,15,17	0.57	0
7	NAG	c	1	7,1	14,14,15	1.31	2 (14%)	17,19,21	2.08	4 (23%)
7	NAG	c	2	7	14,14,15	1.87	5 (35%)	17,19,21	1.53	2 (11%)
5	NAG	d	1	5,1	14,14,15	1.31	2 (14%)	17,19,21	1.84	4 (23%)
5	NAG	d	2	5	14,14,15	1.83	4 (28%)	17,19,21	1.77	5 (29%)
5	MAN	d	3	5	11,11,12	1.83	4 (36%)	15,15,17	1.86	4 (26%)
9	NAG	e	1	9,1	14,14,15	0.59	0	17,19,21	1.28	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	e	2	9	14,14,15	0.46	0	17,19,21	1.14	1 (5%)
9	BMA	e	3	9	11,11,12	0.72	0	15,15,17	0.59	0
9	MAN	e	4	9	11,11,12	0.59	0	15,15,17	1.02	1 (6%)
5	NAG	f	1	5,1	14,14,15	1.41	3 (21%)	17,19,21	2.01	4 (23%)
5	NAG	f	2	5	14,14,15	1.77	4 (28%)	17,19,21	1.79	6 (35%)
5	MAN	f	3	5	11,11,12	1.79	3 (27%)	15,15,17	1.96	5 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	Y	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	0/6/23/26	0/1/1/1
5	MAN	Y	3	5	-	2/2/19/22	0/1/1/1
6	NAG	Z	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	0/6/23/26	0/1/1/1
6	BMA	Z	3	6	-	2/2/19/22	0/1/1/1
6	MAN	Z	4	6	-	0/2/19/22	0/1/1/1
6	MAN	Z	5	6	-	0/2/19/22	0/1/1/1
6	MAN	Z	6	6	-	0/2/19/22	0/1/1/1
6	MAN	Z	7	6	-	0/2/19/22	0/1/1/1
6	MAN	Z	8	6	-	0/2/19/22	0/1/1/1
7	NAG	a	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	a	2	7	-	0/6/23/26	0/1/1/1
8	NAG	b	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	b	2	8	-	0/6/23/26	0/1/1/1
8	BMA	b	3	8	-	1/2/19/22	0/1/1/1
7	NAG	c	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	c	2	7	-	0/6/23/26	0/1/1/1
5	NAG	d	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	d	2	5	-	0/6/23/26	0/1/1/1
5	MAN	d	3	5	-	2/2/19/22	0/1/1/1
9	NAG	e	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	e	2	9	-	0/6/23/26	0/1/1/1
9	BMA	e	3	9	-	0/2/19/22	0/1/1/1
9	MAN	e	4	9	-	0/2/19/22	0/1/1/1
5	NAG	f	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	f	2	5	-	0/6/23/26	0/1/1/1
5	MAN	f	3	5	-	2/2/19/22	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	2	NAG	C1-C2	3.87	1.57	1.52
7	c	2	NAG	C1-C2	3.76	1.57	1.52
7	a	2	NAG	C1-C2	3.74	1.57	1.52
5	f	2	NAG	C1-C2	3.70	1.57	1.52
5	d	2	NAG	C1-C2	3.23	1.56	1.52
5	Y	3	MAN	C4-C3	3.00	1.60	1.52
5	f	3	MAN	C2-C3	2.99	1.57	1.52
5	d	2	NAG	O4-C4	2.98	1.50	1.43
5	Y	2	NAG	C4-C3	2.96	1.60	1.52
7	c	2	NAG	C4-C3	2.96	1.60	1.52
5	d	1	NAG	C1-C2	2.86	1.56	1.52
5	Y	3	MAN	C2-C3	2.85	1.56	1.52
5	d	3	MAN	C2-C3	2.84	1.56	1.52
5	d	3	MAN	C1-C2	2.78	1.58	1.52
5	f	2	NAG	C4-C3	2.71	1.59	1.52
5	Y	2	NAG	O4-C4	2.69	1.49	1.43
7	c	2	NAG	O4-C4	2.67	1.49	1.43
7	a	2	NAG	C4-C3	2.66	1.59	1.52
5	f	2	NAG	C3-C2	2.57	1.57	1.52
7	a	2	NAG	C3-C2	2.52	1.57	1.52
5	d	2	NAG	C4-C5	2.45	1.58	1.53
5	f	1	NAG	C1-C2	2.39	1.55	1.52
7	c	1	NAG	O3-C3	2.34	1.48	1.43
7	a	1	NAG	C1-C2	2.33	1.55	1.52
5	d	2	NAG	C4-C3	2.30	1.58	1.52
5	Y	1	NAG	O3-C3	2.29	1.48	1.43
5	f	3	MAN	C1-C2	2.28	1.57	1.52
7	c	2	NAG	C4-C5	2.27	1.57	1.53
5	Y	2	NAG	C4-C5	2.27	1.57	1.53
5	f	3	MAN	C4-C3	2.26	1.58	1.52
5	d	3	MAN	C4-C3	2.25	1.58	1.52
5	f	1	NAG	C3-C2	2.24	1.57	1.52
5	Y	1	NAG	C3-C2	2.24	1.57	1.52
7	a	1	NAG	C3-C2	2.21	1.57	1.52
7	c	1	NAG	C3-C2	2.21	1.57	1.52
5	Y	3	MAN	C1-C2	2.17	1.57	1.52
5	f	2	NAG	O4-C4	2.11	1.48	1.43
7	a	2	NAG	O4-C4	2.10	1.48	1.43
5	d	3	MAN	O5-C5	2.09	1.47	1.43
7	a	1	NAG	C4-C5	2.08	1.57	1.53
5	f	1	NAG	C4-C5	2.08	1.57	1.53
7	c	2	NAG	O5-C5	2.07	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	d	1	NAG	C3-C2	2.04	1.56	1.52
5	Y	2	NAG	O5-C5	2.00	1.47	1.43

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	1	NAG	O5-C1-C2	-7.51	99.67	111.29
6	Z	4	MAN	C1-C2-C3	5.91	118.25	109.64
6	Z	8	MAN	C1-O5-C5	5.84	120.02	112.19
7	c	1	NAG	C1-O5-C5	5.16	119.10	112.19
5	Y	1	NAG	C1-O5-C5	5.14	119.07	112.19
5	f	3	MAN	C1-O5-C5	4.95	118.82	112.19
6	Z	7	MAN	C6-C5-C4	-4.82	101.18	113.02
5	f	1	NAG	C1-O5-C5	4.64	118.41	112.19
7	a	1	NAG	C1-O5-C5	4.63	118.39	112.19
5	d	1	NAG	C1-O5-C5	4.45	118.15	112.19
5	Y	3	MAN	C1-O5-C5	4.20	117.82	112.19
5	f	1	NAG	C8-C7-N2	-4.10	109.32	116.12
7	a	1	NAG	C8-C7-N2	-4.02	109.44	116.12
6	Z	4	MAN	C2-C3-C4	-4.01	103.80	110.86
6	Z	5	MAN	O4-C4-C3	-3.86	101.27	110.38
5	d	3	MAN	O2-C2-C1	3.72	117.73	109.22
5	d	3	MAN	C1-O5-C5	3.66	117.09	112.19
6	Z	7	MAN	O4-C4-C3	-3.52	102.07	110.38
5	d	2	NAG	O3-C3-C4	3.47	118.57	110.38
7	c	1	NAG	C2-N2-C7	3.46	127.54	122.90
5	Y	1	NAG	C2-N2-C7	3.45	127.52	122.90
6	Z	6	MAN	O4-C4-C3	-3.36	102.46	110.38
6	Z	8	MAN	C3-C4-C5	3.35	116.30	110.23
9	e	4	MAN	C1-O5-C5	3.29	116.60	112.19
6	Z	5	MAN	O4-C4-C5	3.24	117.31	109.32
5	f	3	MAN	C2-C3-C4	3.23	116.55	110.86
6	Z	6	MAN	C2-C3-C4	3.21	116.51	110.86
8	b	1	NAG	C2-N2-C7	-3.21	118.60	122.90
9	e	1	NAG	C1-O5-C5	3.14	116.39	112.19
5	f	2	NAG	C1-O5-C5	3.14	116.39	112.19
6	Z	2	NAG	O5-C5-C6	-3.09	101.64	107.66
6	Z	7	MAN	C3-C4-C5	-3.09	104.64	110.23
5	d	3	MAN	C2-C3-C4	3.08	116.28	110.86
7	a	2	NAG	C1-O5-C5	3.07	116.30	112.19
5	Y	3	MAN	O2-C2-C1	3.06	116.24	109.22
5	f	2	NAG	C3-C4-C5	-3.04	104.72	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	2	NAG	C3-C4-C5	-3.04	104.73	110.23
5	Y	1	NAG	C8-C7-N2	-3.03	111.09	116.12
7	c	1	NAG	C8-C7-N2	-3.00	111.15	116.12
5	d	2	NAG	C4-C3-C2	2.97	115.37	111.02
5	d	1	NAG	C8-C7-N2	-2.95	111.23	116.12
7	a	2	NAG	O3-C3-C4	2.95	117.33	110.38
5	f	2	NAG	O3-C3-C4	2.93	117.28	110.38
5	Y	2	NAG	O3-C3-C4	2.93	117.28	110.38
7	c	2	NAG	O3-C3-C4	2.90	117.21	110.38
6	Z	7	MAN	O2-C2-C3	-2.88	104.19	110.15
6	Z	3	BMA	O2-C2-C3	2.86	116.08	110.15
5	d	2	NAG	C2-N2-C7	2.86	126.73	122.90
6	Z	1	NAG	O7-C7-C8	-2.85	116.98	122.05
5	Y	3	MAN	O5-C5-C6	2.83	113.17	107.66
9	e	1	NAG	C1-C2-N2	2.81	114.86	110.43
6	Z	8	MAN	O4-C4-C5	2.80	116.22	109.32
7	c	2	NAG	C3-C4-C5	-2.75	105.24	110.23
5	Y	2	NAG	C3-C4-C5	-2.70	105.33	110.23
6	Z	6	MAN	O5-C5-C6	-2.69	102.43	107.66
6	Z	1	NAG	C4-C3-C2	-2.68	107.09	111.02
6	Z	3	BMA	O4-C4-C5	-2.65	102.79	109.32
5	Y	3	MAN	C2-C3-C4	2.64	115.51	110.86
5	f	3	MAN	O2-C2-C1	2.62	115.23	109.22
5	f	1	NAG	O3-C3-C2	2.62	114.84	109.40
6	Z	8	MAN	O2-C2-C1	2.60	115.19	109.22
7	a	1	NAG	O3-C3-C2	2.58	114.76	109.40
5	d	2	NAG	C8-C7-N2	-2.56	111.87	116.12
5	Y	1	NAG	O3-C3-C2	2.55	114.70	109.40
6	Z	7	MAN	O5-C5-C6	2.54	112.61	107.66
7	a	2	NAG	C1-C2-N2	2.54	114.43	110.43
5	f	2	NAG	C1-C2-N2	2.52	114.41	110.43
7	c	1	NAG	O3-C3-C2	2.49	114.56	109.40
6	Z	5	MAN	O5-C5-C6	-2.47	102.85	107.66
5	d	3	MAN	O5-C5-C6	2.44	112.42	107.66
8	b	1	NAG	O3-C3-C2	-2.43	104.35	109.40
8	b	1	NAG	O5-C1-C2	-2.42	107.55	111.29
6	Z	8	MAN	O5-C5-C6	-2.33	103.12	107.66
6	Z	2	NAG	O5-C1-C2	-2.31	107.71	111.29
6	Z	3	BMA	C6-C5-C4	-2.31	107.34	113.02
6	Z	6	MAN	O3-C3-C2	2.31	114.77	110.05
5	d	1	NAG	C2-N2-C7	2.31	126.00	122.90
6	Z	5	MAN	C1-O5-C5	2.31	115.28	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	f	3	MAN	O5-C5-C6	2.27	112.08	107.66
6	Z	4	MAN	O5-C1-C2	-2.26	105.41	110.79
5	d	1	NAG	O3-C3-C2	2.21	114.00	109.40
5	f	2	NAG	O4-C4-C3	2.21	115.59	110.38
6	Z	6	MAN	C1-O5-C5	2.20	115.14	112.19
5	f	3	MAN	C3-C4-C5	2.20	114.22	110.23
6	Z	2	NAG	C4-C3-C2	-2.20	107.80	111.02
7	a	2	NAG	O4-C4-C3	2.18	115.52	110.38
5	f	1	NAG	O7-C7-N2	2.14	125.77	121.98
5	f	2	NAG	C8-C7-N2	-2.14	112.57	116.12
6	Z	7	MAN	O2-C2-C1	2.13	114.11	109.22
7	a	1	NAG	O7-C7-N2	2.12	125.73	121.98
6	Z	5	MAN	O3-C3-C2	-2.12	105.72	110.05
6	Z	7	MAN	C2-C3-C4	2.08	114.52	110.86
7	a	2	NAG	C8-C7-N2	-2.08	112.67	116.12
9	e	2	NAG	C1-O5-C5	2.07	114.96	112.19
5	d	2	NAG	O4-C4-C3	2.04	115.17	110.38
5	Y	3	MAN	C3-C4-C5	2.01	113.88	110.23

There are no chirality outliers.

All (15) torsion outliers are listed below:

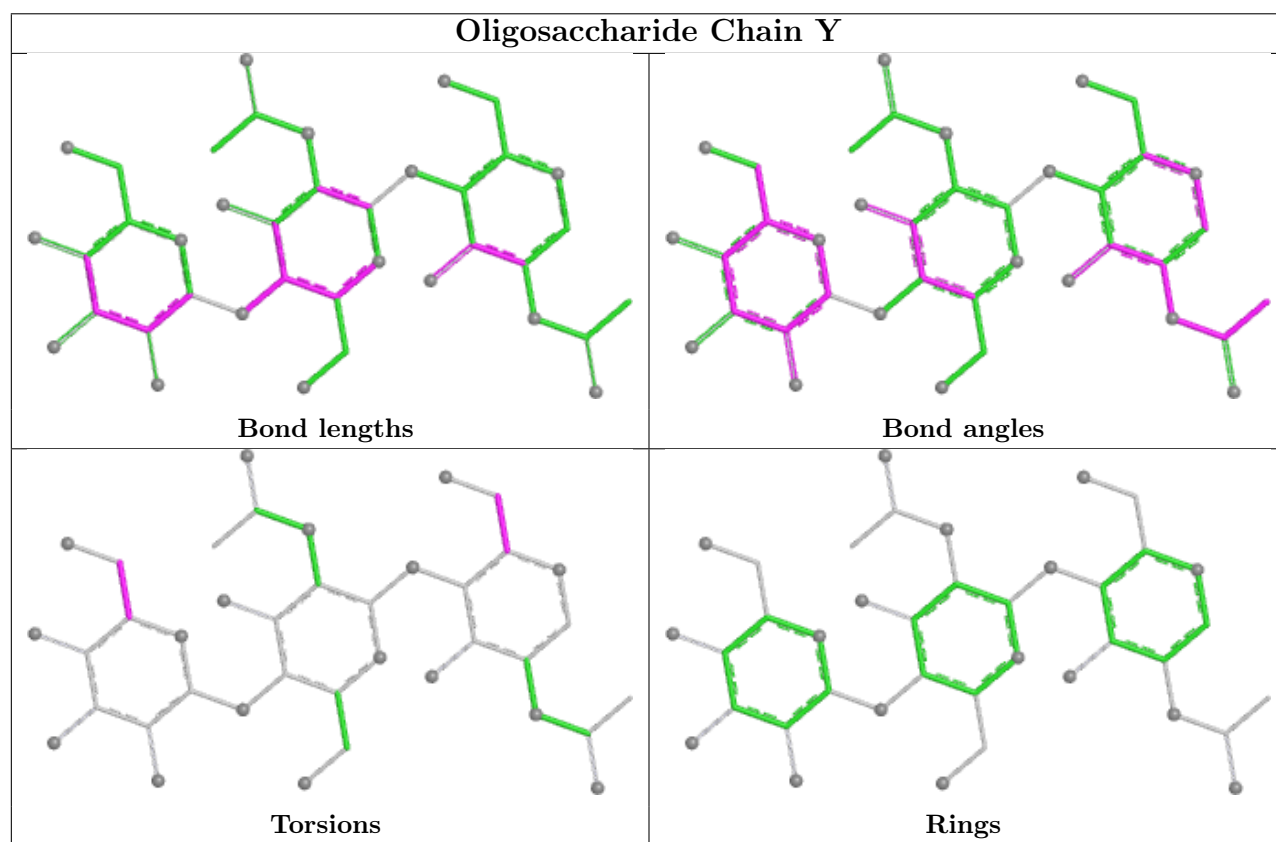
Mol	Chain	Res	Type	Atoms
5	d	3	MAN	C4-C5-C6-O6
5	f	3	MAN	C4-C5-C6-O6
5	Y	3	MAN	C4-C5-C6-O6
5	d	3	MAN	O5-C5-C6-O6
5	f	3	MAN	O5-C5-C6-O6
7	a	1	NAG	C4-C5-C6-O6
5	f	1	NAG	C4-C5-C6-O6
5	Y	3	MAN	O5-C5-C6-O6
5	Y	1	NAG	C4-C5-C6-O6
7	c	1	NAG	C4-C5-C6-O6
5	d	1	NAG	C4-C5-C6-O6
8	b	3	BMA	O5-C5-C6-O6
6	Z	3	BMA	C4-C5-C6-O6
6	Z	3	BMA	O5-C5-C6-O6
6	Z	1	NAG	O7-C7-N2-C2

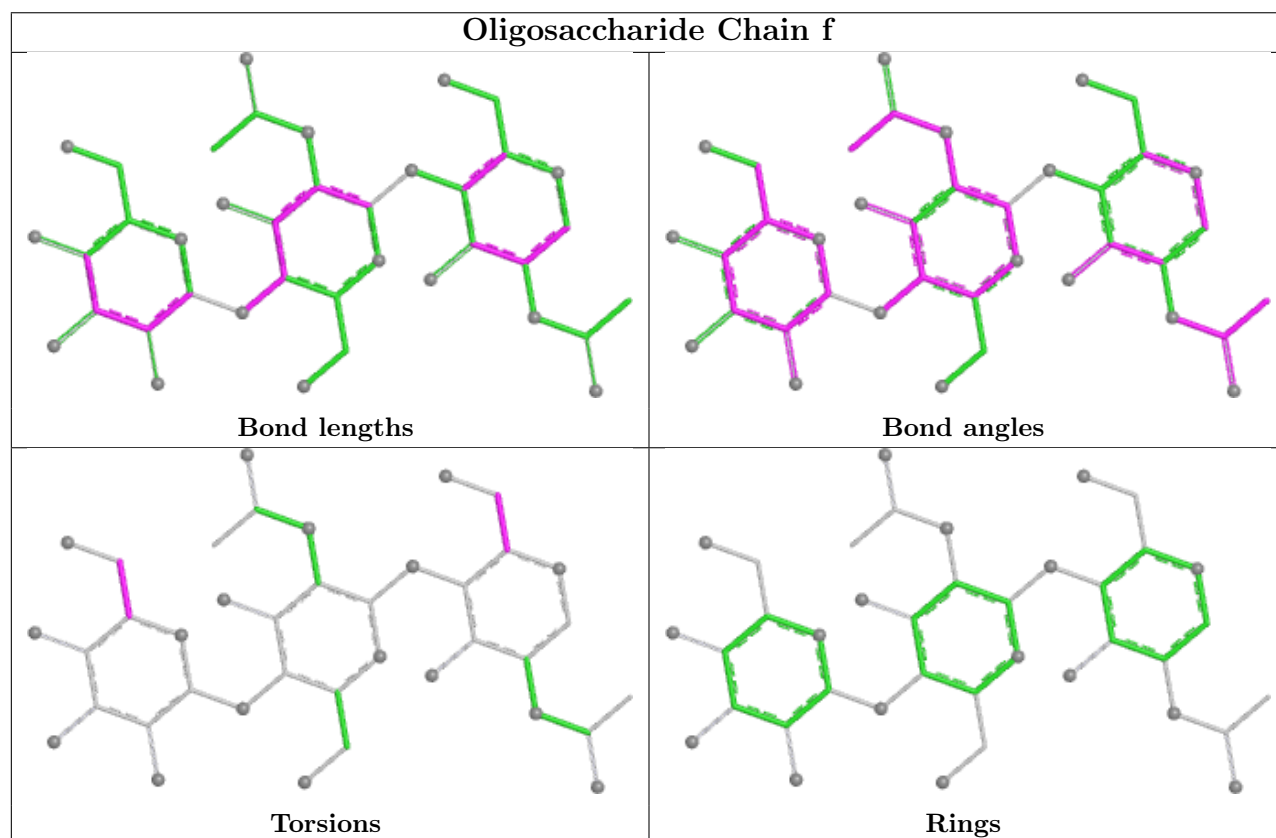
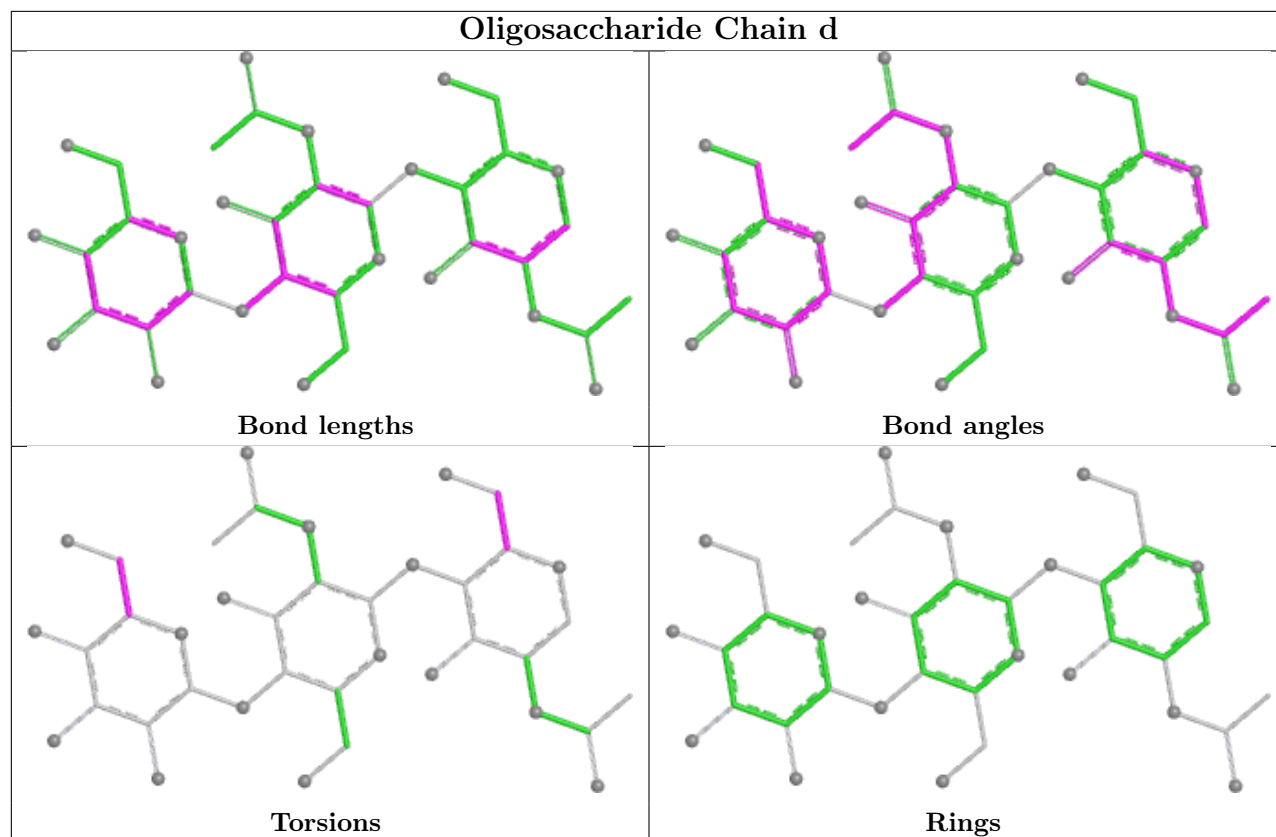
There are no ring outliers.

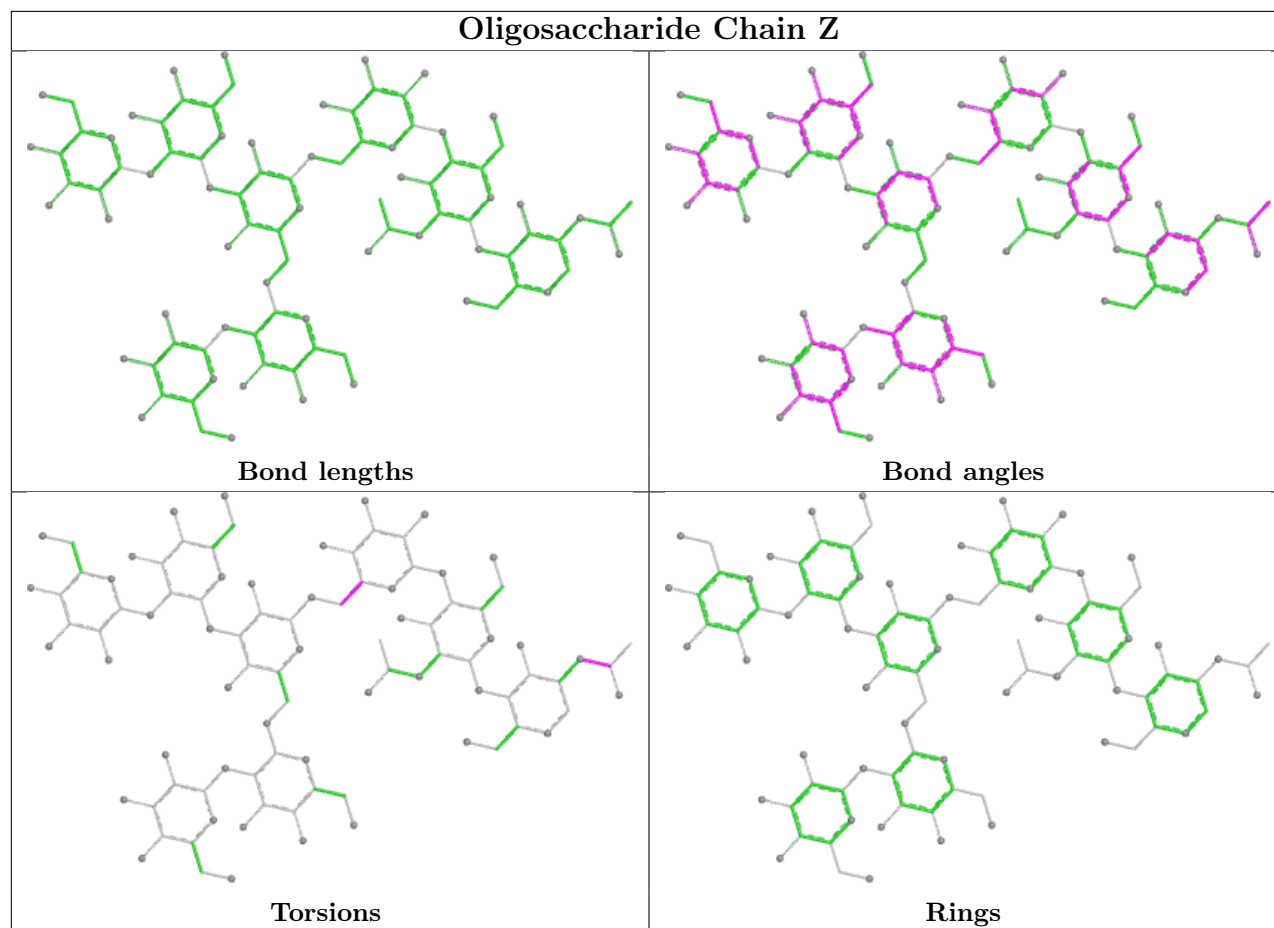
11 monomers are involved in 10 short contacts:

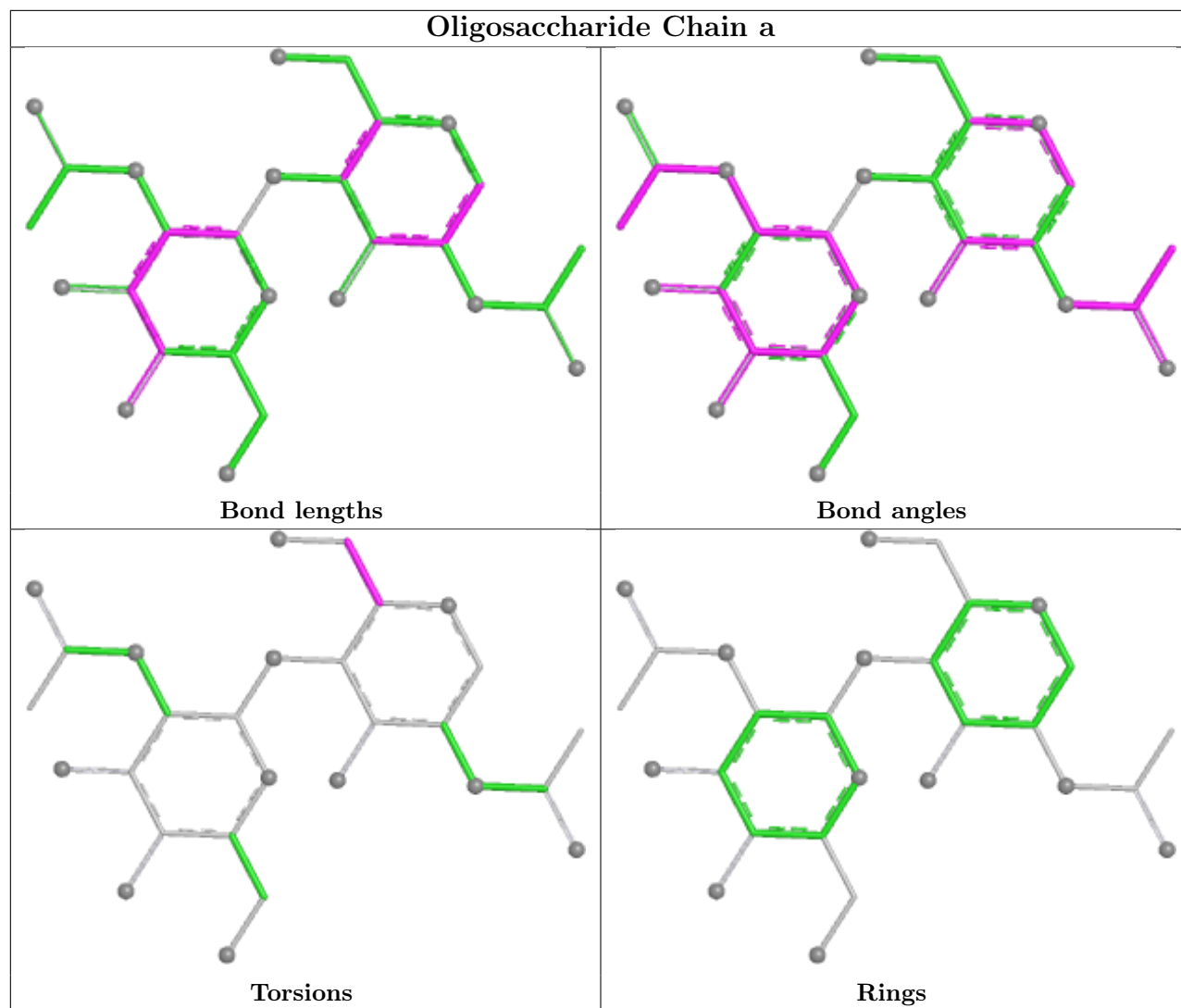
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	c	1	NAG	1	0
5	d	1	NAG	2	0
7	a	2	NAG	1	0
5	Y	1	NAG	1	0
5	f	2	NAG	1	0
5	f	1	NAG	2	0
7	a	1	NAG	1	0
8	b	1	NAG	3	0
5	Y	2	NAG	1	0
7	c	2	NAG	1	0
5	d	2	NAG	1	0

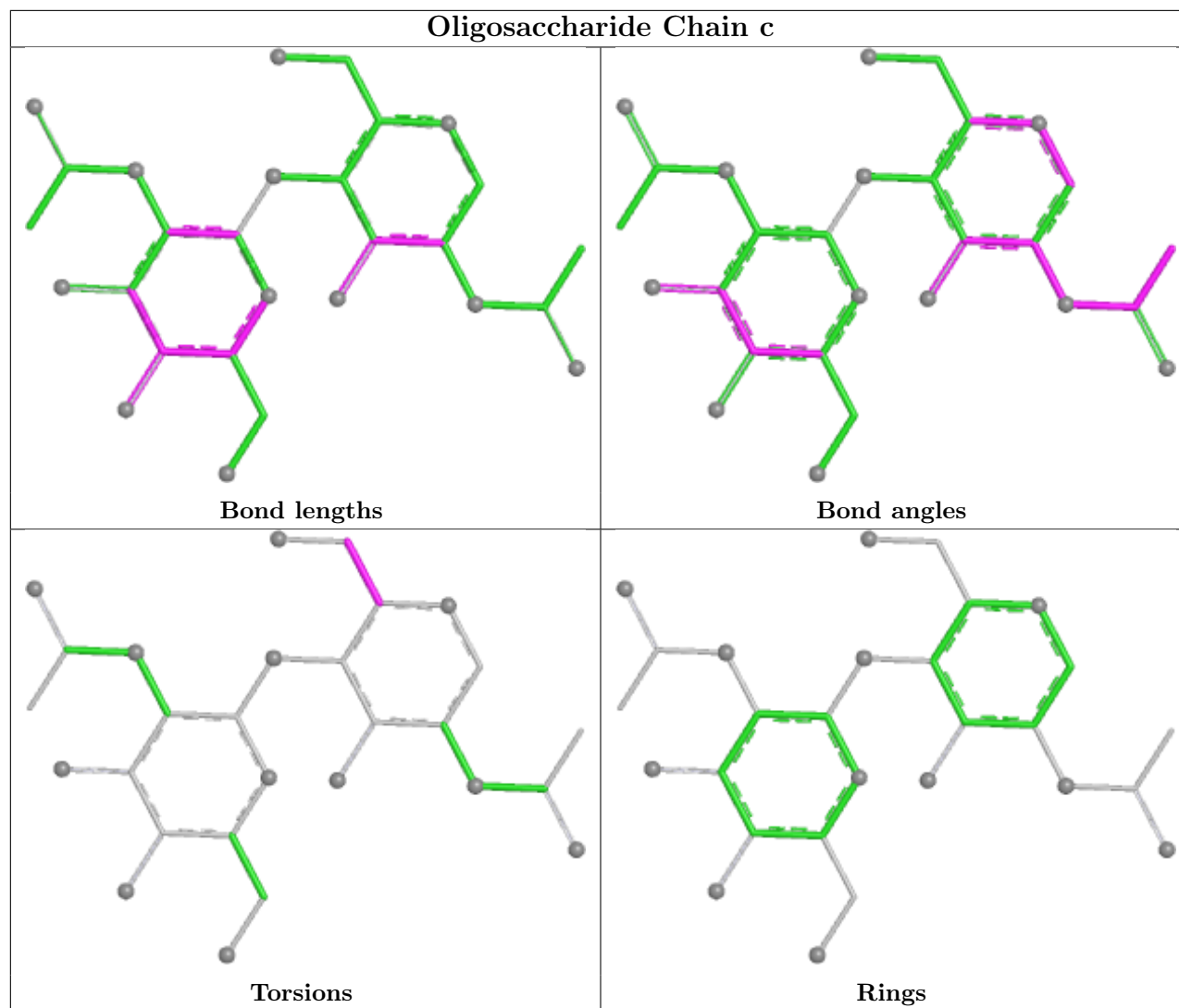
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

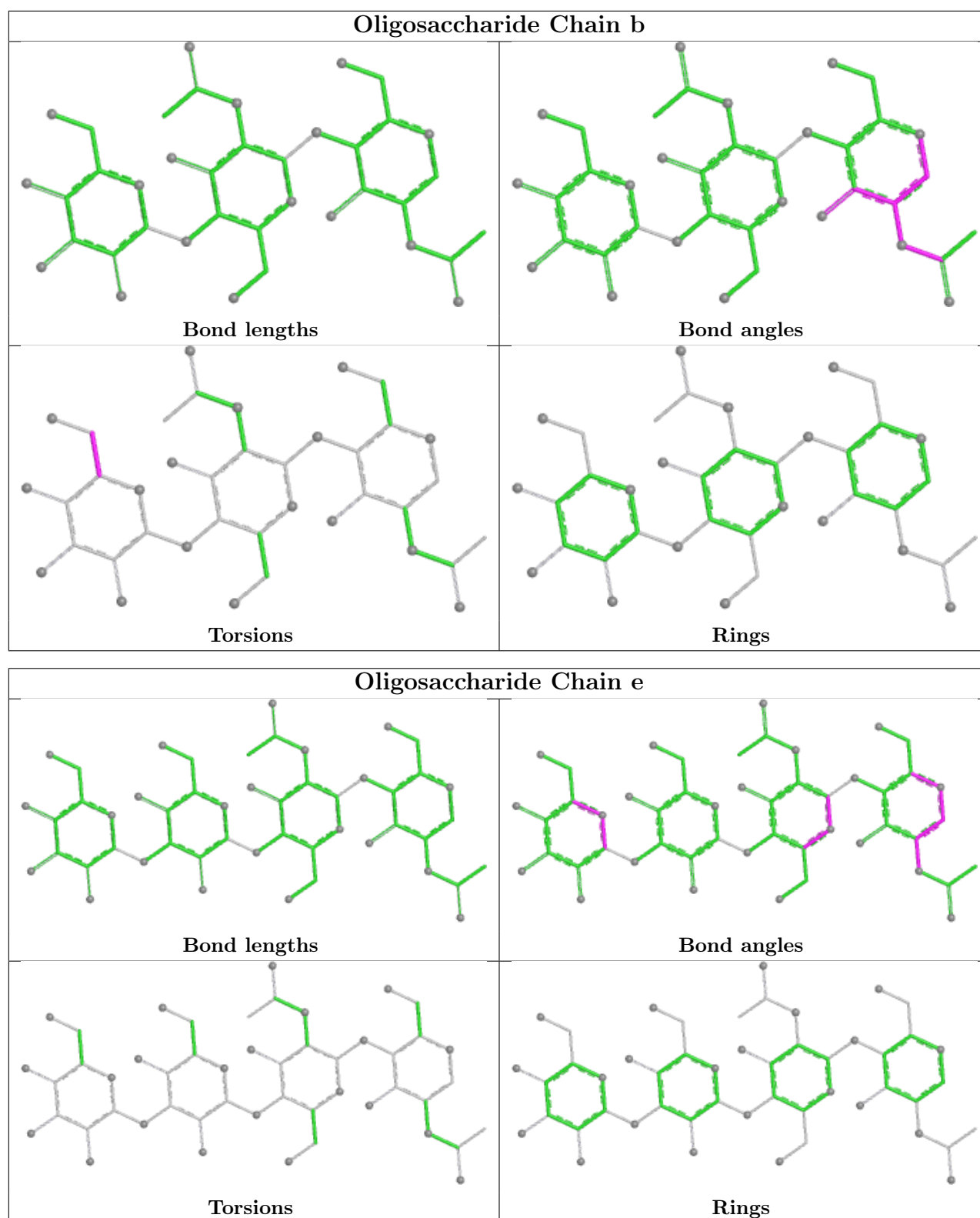












5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
10	NAG	O	2004	1	14,14,15	1.91	4 (28%)	17,19,21	2.60	8 (47%)
10	NAG	M	2003	1	14,14,15	1.94	4 (28%)	17,19,21	2.55	8 (47%)
10	NAG	A	2004	1	14,14,15	1.96	4 (28%)	17,19,21	2.56	8 (47%)
10	NAG	C	2001	1	14,14,15	1.32	2 (14%)	17,19,21	1.84	4 (23%)
10	NAG	P	2001	2	14,14,15	2.26	6 (42%)	17,19,21	2.79	8 (47%)
10	NAG	S	2004	1	14,14,15	1.86	4 (28%)	17,19,21	2.53	8 (47%)

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
10	NAG	O	2004	1	-	2/6/23/26	0/1/1/1
10	NAG	M	2003	1	-	1/6/23/26	0/1/1/1
10	NAG	A	2004	1	-	1/6/23/26	0/1/1/1
10	NAG	C	2001	1	-	1/6/23/26	0/1/1/1
10	NAG	P	2001	2	-	2/6/23/26	0/1/1/1
10	NAG	S	2004	1	-	1/6/23/26	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	P	2001	NAG	C1-C2	4.73	1.58	1.52
10	A	2004	NAG	C1-C2	3.90	1.57	1.52
10	O	2004	NAG	C1-C2	3.88	1.57	1.52
10	M	2003	NAG	C1-C2	3.86	1.57	1.52
10	P	2001	NAG	C2-N2	3.43	1.51	1.46
10	S	2004	NAG	O4-C4	3.15	1.50	1.43
10	P	2001	NAG	C4-C5	3.11	1.59	1.53
10	S	2004	NAG	C1-C2	3.06	1.56	1.52
10	A	2004	NAG	C4-C3	3.02	1.60	1.52
10	M	2003	NAG	C4-C3	2.99	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	2001	NAG	C1-C2	2.95	1.56	1.52
10	S	2004	NAG	C4-C3	2.90	1.59	1.52
10	M	2003	NAG	O3-C3	2.89	1.50	1.43
10	O	2004	NAG	C4-C3	2.86	1.59	1.52
10	A	2004	NAG	O3-C3	2.86	1.50	1.43
10	M	2003	NAG	O4-C4	2.82	1.49	1.43
10	A	2004	NAG	O4-C4	2.81	1.49	1.43
10	O	2004	NAG	O4-C4	2.61	1.49	1.43
10	P	2001	NAG	C3-C2	2.44	1.57	1.52
10	O	2004	NAG	O3-C3	2.44	1.49	1.43
10	S	2004	NAG	C2-N2	2.42	1.50	1.46
10	P	2001	NAG	C4-C3	2.06	1.57	1.52
10	C	2001	NAG	C3-C2	2.05	1.56	1.52
10	P	2001	NAG	C7-N2	2.00	1.40	1.34

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	2001	NAG	C2-N2-C7	8.56	134.38	122.90
10	O	2004	NAG	C1-C2-N2	6.21	120.21	110.43
10	S	2004	NAG	C4-C3-C2	5.62	119.26	111.02
10	A	2004	NAG	C1-C2-N2	5.54	119.16	110.43
10	M	2003	NAG	C1-C2-N2	5.50	119.11	110.43
10	A	2004	NAG	C4-C3-C2	4.94	118.26	111.02
10	M	2003	NAG	C4-C3-C2	4.91	118.22	111.02
10	C	2001	NAG	C1-O5-C5	4.47	118.18	112.19
10	S	2004	NAG	C1-C2-N2	4.17	117.01	110.43
10	O	2004	NAG	C4-C3-C2	3.84	116.65	111.02
10	S	2004	NAG	O5-C5-C6	3.77	115.00	107.66
10	O	2004	NAG	C1-O5-C5	3.26	116.55	112.19
10	P	2001	NAG	O5-C1-C2	3.21	116.26	111.29
10	S	2004	NAG	O3-C3-C4	3.20	117.92	110.38
10	A	2004	NAG	O3-C3-C4	3.09	117.67	110.38
10	M	2003	NAG	O3-C3-C4	3.06	117.60	110.38
10	C	2001	NAG	C8-C7-N2	-2.94	111.23	116.12
10	P	2001	NAG	O7-C7-N2	2.94	127.18	121.98
10	A	2004	NAG	C3-C4-C5	2.89	115.47	110.23
10	O	2004	NAG	O5-C5-C6	2.87	113.26	107.66
10	M	2003	NAG	C3-C4-C5	2.87	115.43	110.23
10	P	2001	NAG	C1-O5-C5	2.86	116.02	112.19
10	M	2003	NAG	O5-C5-C6	2.84	113.20	107.66
10	S	2004	NAG	C2-N2-C7	2.84	126.71	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2004	NAG	O5-C5-C6	2.82	113.14	107.66
10	O	2004	NAG	O4-C4-C5	-2.78	102.47	109.32
10	O	2004	NAG	C3-C4-C5	2.67	115.08	110.23
10	O	2004	NAG	O5-C5-C4	2.60	117.16	110.83
10	P	2001	NAG	O3-C3-C2	2.54	114.68	109.40
10	S	2004	NAG	C3-C4-C5	2.35	114.50	110.23
10	S	2004	NAG	O5-C5-C4	2.35	116.54	110.83
10	C	2001	NAG	C2-N2-C7	2.30	125.98	122.90
10	M	2003	NAG	O5-C5-C4	2.30	116.42	110.83
10	A	2004	NAG	O5-C5-C4	2.25	116.31	110.83
10	C	2001	NAG	O3-C3-C2	2.21	113.99	109.40
10	P	2001	NAG	O4-C4-C5	2.18	114.70	109.32
10	A	2004	NAG	C8-C7-N2	-2.12	112.60	116.12
10	P	2001	NAG	C8-C7-N2	-2.10	112.63	116.12
10	M	2003	NAG	C8-C7-N2	-2.10	112.64	116.12
10	S	2004	NAG	O4-C4-C5	-2.08	104.19	109.32
10	P	2001	NAG	C4-C3-C2	2.08	114.06	111.02
10	O	2004	NAG	O3-C3-C4	2.06	115.23	110.38
10	A	2004	NAG	O4-C4-C5	-2.04	104.30	109.32
10	M	2003	NAG	O4-C4-C5	-2.03	104.32	109.32

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	S	2004	NAG	O5-C5-C6-O6
10	O	2004	NAG	O5-C5-C6-O6
10	A	2004	NAG	O5-C5-C6-O6
10	M	2003	NAG	O5-C5-C6-O6
10	C	2001	NAG	C4-C5-C6-O6
10	P	2001	NAG	O5-C5-C6-O6
10	O	2004	NAG	C1-C2-N2-C7
10	P	2001	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	P	2001	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	322/334 (96%)	-0.24	8 (2%) 58 50	60, 90, 90, 90	0
1	C	321/334 (96%)	-0.19	8 (2%) 58 50	60, 90, 90, 90	0
1	G	321/334 (96%)	-0.15	11 (3%) 48 44	60, 90, 90, 90	0
1	M	322/334 (96%)	-0.29	4 (1%) 76 65	60, 90, 90, 90	0
1	O	318/334 (95%)	-0.20	7 (2%) 62 53	90, 90, 90, 90	0
1	S	322/334 (96%)	-0.22	8 (2%) 58 50	60, 90, 90, 90	0
2	B	172/182 (94%)	-0.32	1 (0%) 85 76	90, 90, 90, 90	0
2	D	172/182 (94%)	-0.36	1 (0%) 85 76	90, 90, 90, 90	0
2	I	173/182 (95%)	-0.19	4 (2%) 61 53	90, 90, 90, 90	0
2	N	169/182 (92%)	-0.35	1 (0%) 85 76	90, 90, 90, 90	0
2	P	172/182 (94%)	-0.37	2 (1%) 76 65	90, 90, 90, 90	0
2	U	173/182 (95%)	-0.27	3 (1%) 69 59	90, 90, 90, 90	0
3	E	216/218 (99%)	-0.29	4 (1%) 66 56	90, 90, 90, 90	0
3	J	211/218 (96%)	-0.26	1 (0%) 87 77	90, 90, 90, 90	0
3	L	215/218 (98%)	-0.33	3 (1%) 73 62	90, 90, 90, 90	0
3	Q	215/218 (98%)	-0.31	3 (1%) 73 62	90, 90, 90, 90	0
3	V	214/218 (98%)	-0.26	2 (0%) 81 70	90, 90, 90, 90	0
3	X	216/218 (99%)	-0.28	4 (1%) 66 56	90, 90, 90, 90	0
4	F	221/222 (99%)	-0.42	1 (0%) 87 77	80, 90, 90, 90	1 (0%)
4	H	221/222 (99%)	-0.41	3 (1%) 73 62	80, 90, 90, 90	1 (0%)
4	K	221/222 (99%)	-0.16	2 (0%) 81 70	80, 90, 90, 90	1 (0%)
4	R	221/222 (99%)	-0.32	2 (0%) 81 70	80, 90, 90, 90	1 (0%)
4	T	220/222 (99%)	-0.23	4 (1%) 67 58	80, 90, 90, 90	1 (0%)
4	W	221/222 (99%)	-0.29	2 (0%) 81 70	80, 90, 90, 90	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	5569/5736 (97%)	-0.27	89 (1%) 70 59	60, 90, 90, 90	6 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	T	45	LEU	5.0
2	P	52	VAL	5.0
1	G	245	PHE	4.4
1	A	112	LEU	4.0
3	L	21	ILE	4.0
1	O	98	TYR	3.9
1	C	66	VAL	3.9
1	O	179	LEU	3.9
1	G	267	ILE	3.9
1	C	70	LEU	3.8
2	I	55	ILE	3.7
1	G	243	ILE	3.5
4	K	100(A)	GLY	3.5
1	C	245	PHE	3.5
1	C	179	LEU	3.5
1	G	294	PHE	3.4
3	X	73	LEU	3.3
2	I	96	ALA	3.2
2	U	77	ILE	3.2
3	Q	104	LEU	3.2
1	S	245	PHE	3.1
1	A	179	LEU	3.1
4	H	45	LEU	2.9
1	M	66	VAL	2.9
3	L	73	LEU	2.9
3	Q	21	ILE	2.9
1	C	71	LEU	2.9
1	O	70	LEU	2.9
2	U	126	LEU	2.8
4	T	69	LEU	2.8
2	D	122	VAL	2.8
1	S	102	PHE	2.8
4	W	191	VAL	2.8
1	O	66	VAL	2.8
1	S	98	TYR	2.7
1	G	66	VAL	2.7
2	N	55	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
3	J	91	SER	2.7
1	A	96(A)	LEU	2.6
3	E	196	ALA	2.6
3	Q	19	ALA	2.6
1	A	316	LEU	2.6
1	C	112	LEU	2.5
1	G	42	ILE	2.5
2	I	1	GLY	2.5
1	G	179	LEU	2.5
2	B	52	VAL	2.5
3	V	181	LEU	2.5
2	U	55	ILE	2.5
1	S	71	LEU	2.5
2	P	48	VAL	2.4
4	R	78	ALA	2.4
1	O	112	LEU	2.4
1	A	232	PHE	2.4
4	T	67	ALA	2.3
4	R	108	THR	2.3
1	S	243	ILE	2.3
1	A	71	LEU	2.3
1	M	87	ILE	2.3
1	A	69	TRP	2.3
3	X	62	PHE	2.3
1	C	164	ILE	2.3
4	H	97	GLY	2.3
1	O	58	PRO	2.2
4	W	140	LEU	2.2
4	K	82	LEU	2.2
3	V	93	GLU	2.2
3	E	115	VAL	2.2
4	H	202	PRO	2.2
1	G	191	GLN	2.2
3	L	35	TRP	2.2
1	G	112	LEU	2.1
3	X	47	LEU	2.1
1	S	153	TRP	2.1
3	X	21	ILE	2.1
1	C	251	PHE	2.1
1	G	124	ILE	2.1
1	M	70	LEU	2.1
2	I	59	MET	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	63	ASN	2.1
1	M	71	LEU	2.1
3	E	186	TYR	2.1
1	O	87	ILE	2.1
4	F	30	THR	2.1
1	G	314	LEU	2.0
4	T	133	GLN	2.0
1	A	13	ILE	2.0
1	S	69	TRP	2.0
1	S	96	ASP	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.

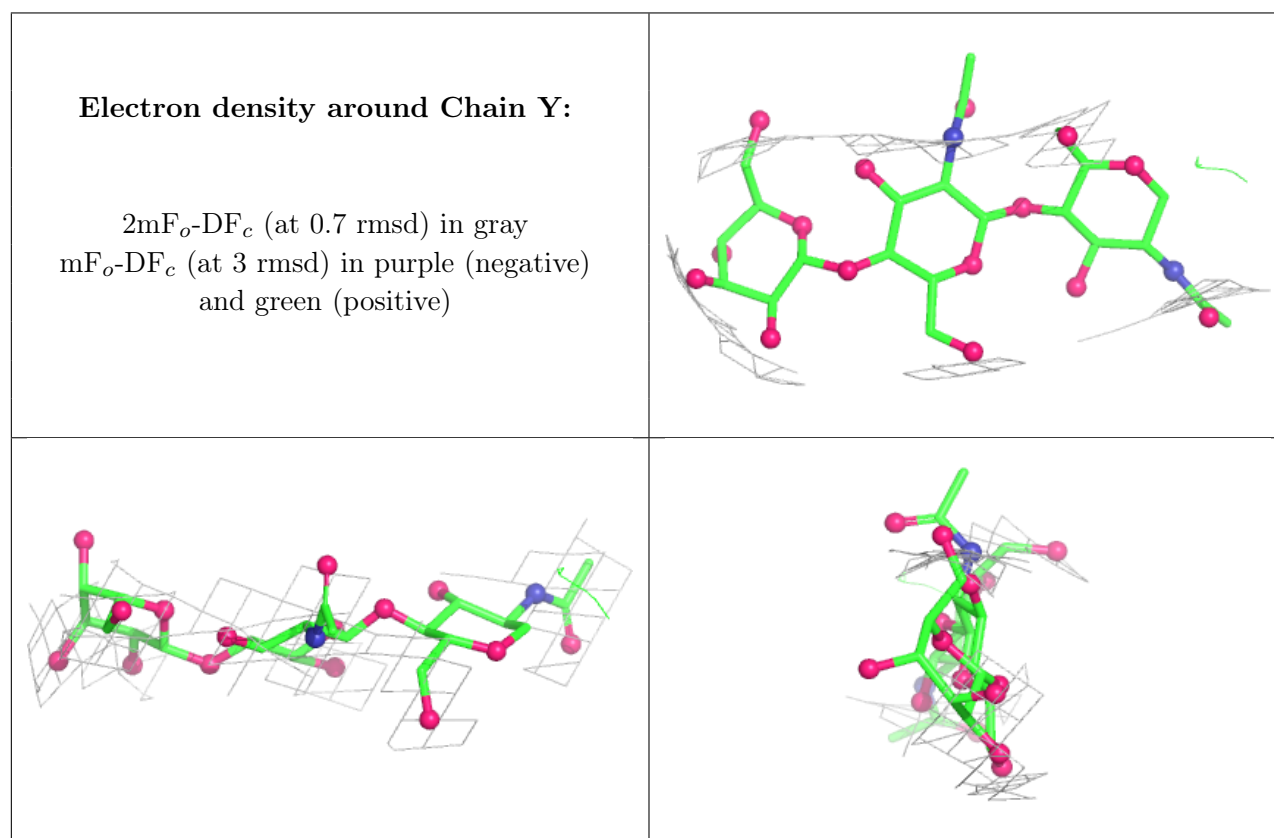
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MAN	Z	8	11/12	0.11	0.09	90,90,90,90	0
6	MAN	Z	6	11/12	0.47	0.08	90,90,90,90	0
6	NAG	Z	2	14/15	0.52	0.08	90,90,90,90	0
5	NAG	d	1	14/15	-	-	90,90,90,90	0
5	NAG	d	2	14/15	-	-	90,90,90,90	0
5	MAN	d	3	11/12	-	-	90,90,90,90	0
5	NAG	f	1	14/15	-	-	90,90,90,90	0
5	NAG	f	2	14/15	-	-	90,90,90,90	0
5	MAN	f	3	11/12	-	-	90,90,90,90	0
6	NAG	Z	1	14/15	0.53	0.11	90,90,90,90	0
5	MAN	Y	3	11/12	0.65	0.06	90,90,90,90	0
6	MAN	Z	5	11/12	0.67	0.07	90,90,90,90	0
6	MAN	Z	7	11/12	0.70	0.06	90,90,90,90	0
6	MAN	Z	4	11/12	0.70	0.07	90,90,90,90	0
6	BMA	Z	3	11/12	0.79	0.05	90,90,90,90	0
5	NAG	Y	2	14/15	0.85	0.13	90,90,90,90	0
5	NAG	Y	1	14/15	0.93	0.09	90,90,90,90	0
7	NAG	a	1	14/15	-	-	90,90,90,90	0

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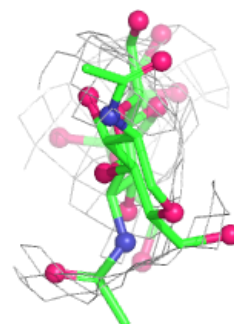
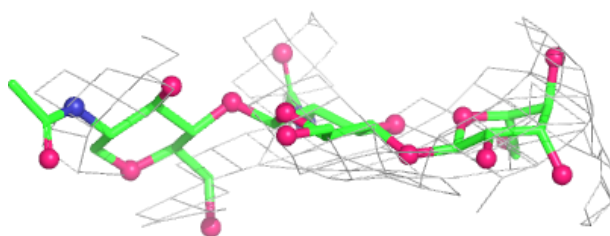
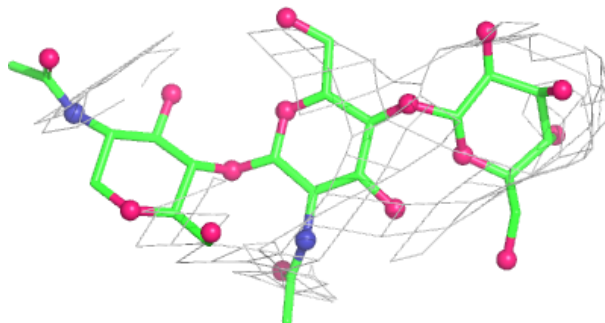
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	a	2	14/15	-	-	90,90,90,90	0
7	NAG	c	1	14/15	-	-	90,90,90,90	0
7	NAG	c	2	14/15	-	-	90,90,90,90	0
8	NAG	b	1	14/15	-	-	38,47,53,63	0
8	NAG	b	2	14/15	-	-	48,62,76,87	0
8	BMA	b	3	11/12	-	-	102,115,122,126	0
9	NAG	e	1	14/15	-	-	32,37,44,45	0
9	NAG	e	2	14/15	-	-	37,38,39,42	0
9	BMA	e	3	11/12	-	-	43,47,56,63	0
9	MAN	e	4	11/12	-	-	47,49,50,52	0

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

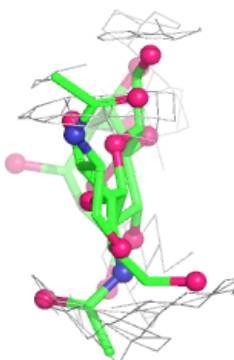
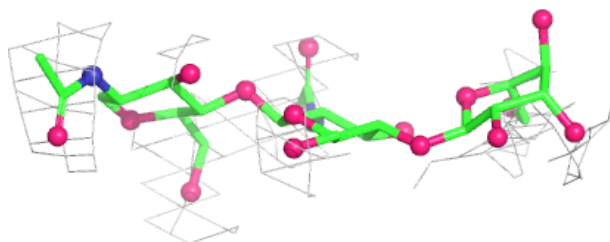
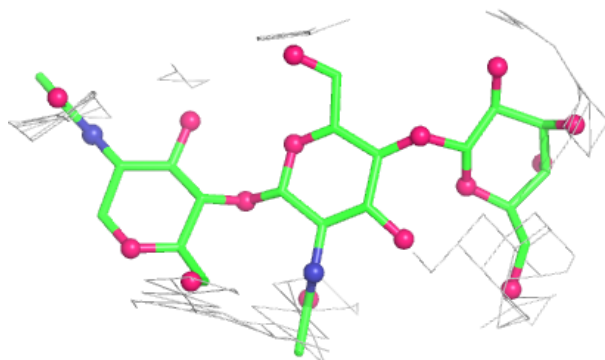


Electron density around Chain d:

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

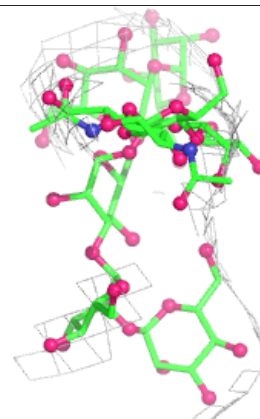
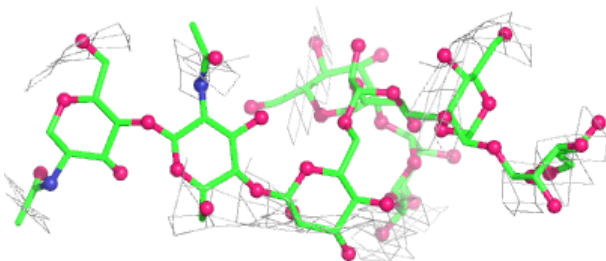
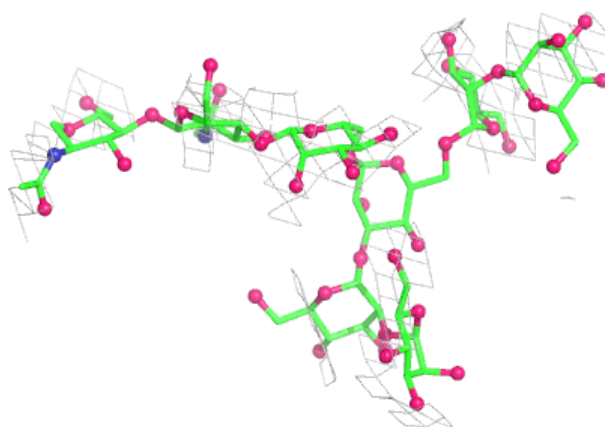
**Electron density around Chain f:**

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



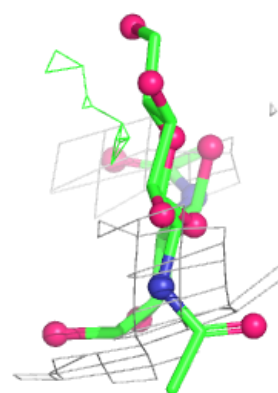
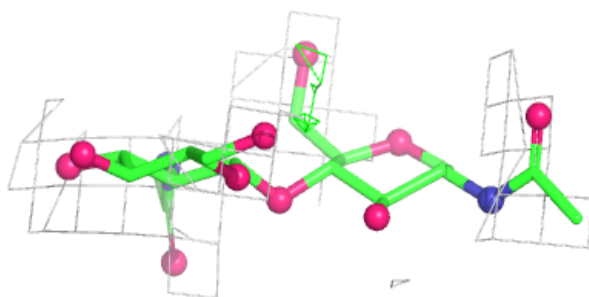
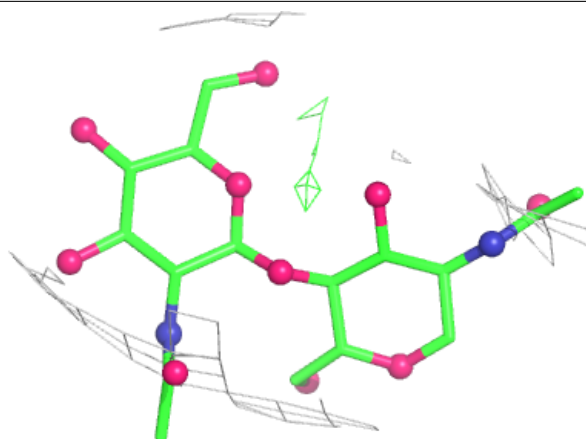
Electron density around Chain Z:

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



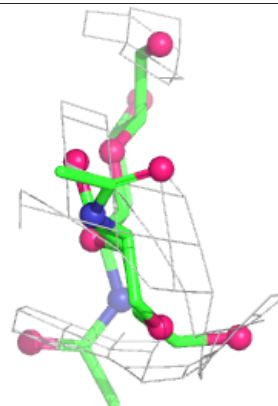
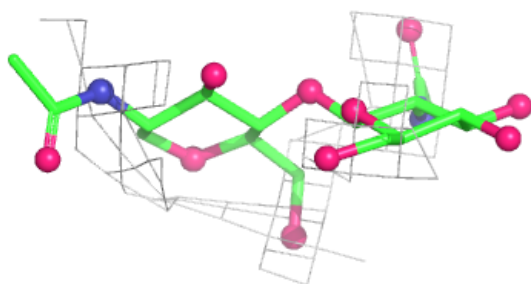
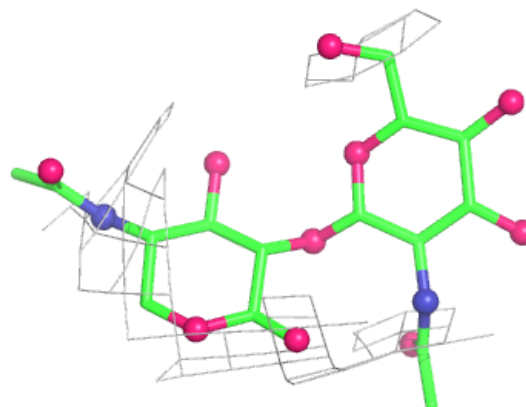
Electron density around Chain a:

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

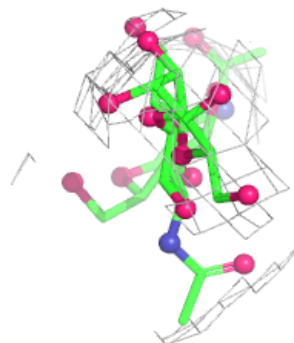
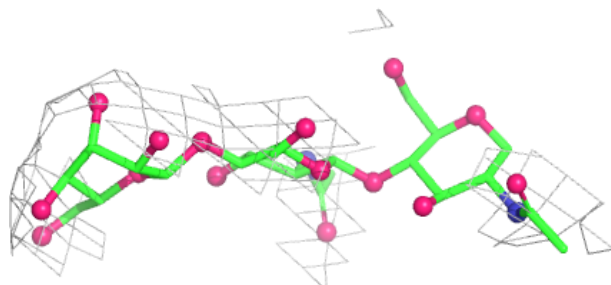
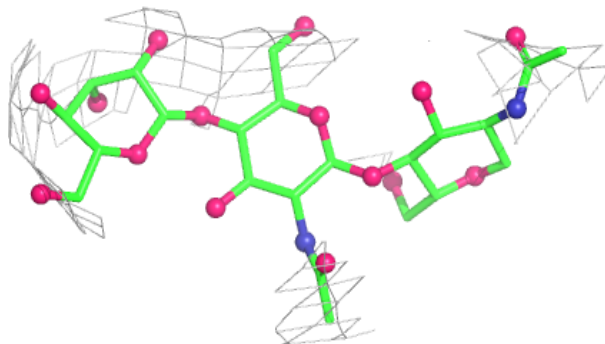


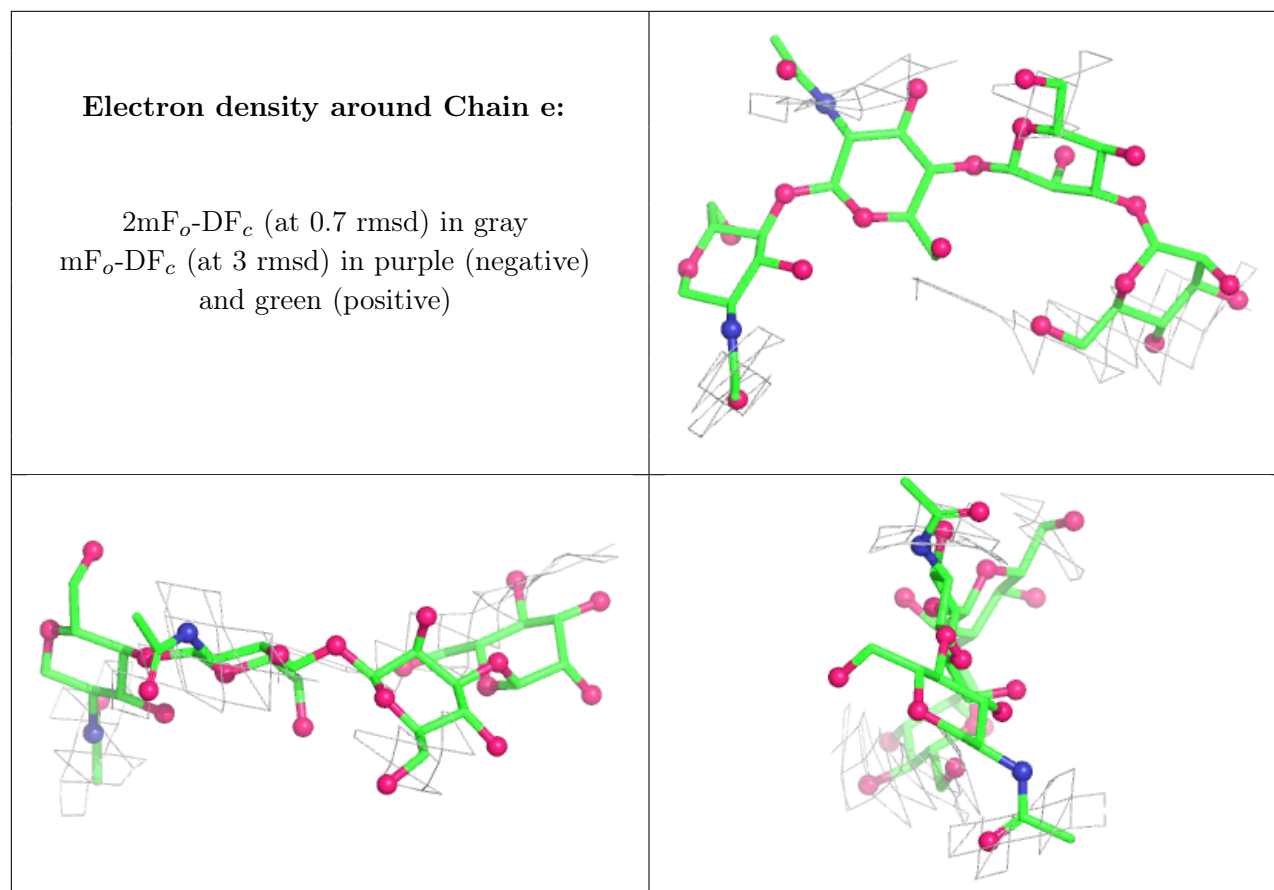
Electron density around Chain c:

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

**Electron density around Chain b:**

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
10	NAG	S	2004	14/15	0.40	0.12	90,90,90,90	0
10	NAG	O	2004	14/15	0.45	0.17	90,90,90,90	0
10	NAG	P	2001	14/15	0.58	0.08	90,90,90,90	0
10	NAG	A	2004	14/15	0.58	0.14	90,90,90,90	0
10	NAG	M	2003	14/15	0.62	0.12	90,90,90,90	0
10	NAG	C	2001	14/15	0.85	0.12	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.