



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:41 AM UTC

PDB ID : 6OUS / pdb_00006ous
Title : Structure of fusion glycoprotein from human respiratory syncytial virus
Authors : Su, H.P.
Deposited on : 2019-05-05
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

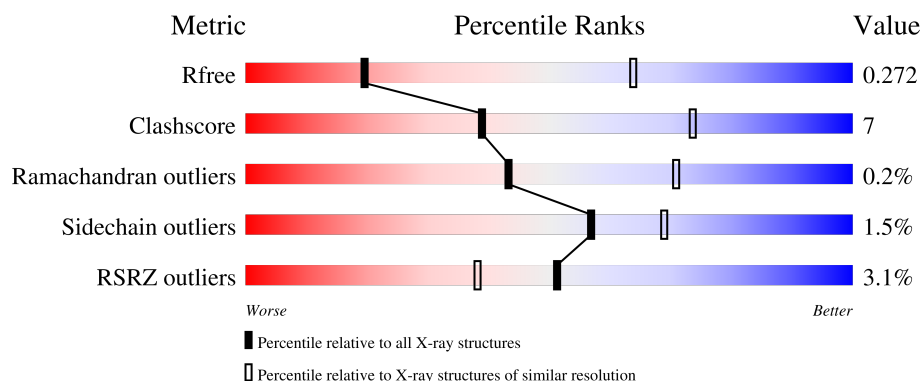
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	84	
1	C	84	
1	E	84	
1	G	84	
1	I	84	

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Mol	Chain	Length	Quality of chain
1	K	84	
2	B	414	
2	D	414	
2	F	414	
2	H	414	
2	J	414	
2	L	414	
3	M	231	
3	O	231	
3	Q	231	
3	S	231	
3	U	231	
3	W	231	
4	N	214	
4	P	214	
4	R	214	
4	T	214	
4	V	214	
4	X	214	
5	Y	4	
5	Z	4	
5	a	4	
5	b	4	
5	c	4	
5	d	4	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 41597 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 Fusion glycoprotein F2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	73	Total	C	N	O	S	0	0	0
			567	360	90	115	2			
1	C	76	Total	C	N	O	S	0	0	0
			583	369	94	117	3			
1	E	73	Total	C	N	O	S	0	0	0
			569	361	91	114	3			
1	G	76	Total	C	N	O	S	0	0	0
			581	367	93	118	3			
1	I	78	Total	C	N	O	S	0	0	0
			601	380	96	122	3			
1	K	70	Total	C	N	O	S	0	0	0
			546	347	87	109	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	PRO	conflict	UNP P03420
C	102	ALA	PRO	conflict	UNP P03420
E	102	ALA	PRO	conflict	UNP P03420
G	102	ALA	PRO	conflict	UNP P03420
I	102	ALA	PRO	conflict	UNP P03420
K	102	ALA	PRO	conflict	UNP P03420

- Molecule 2 is a protein called Fusion glycoprotein F1 fused with Fibrin trimerization domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	0	0
			3057	1939	501	597	20			
2	D	404	Total	C	N	O	S	0	0	0
			3038	1920	501	597	20			
2	F	401	Total	C	N	O	S	0	0	0
			3056	1939	502	596	19			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	395	Total	C	N	O	S	0	0	0
			2977	1885	492	581	19			
2	J	389	Total	C	N	O	S	0	0	0
			2952	1866	489	577	20			
2	L	396	Total	C	N	O	S	0	0	0
			2982	1888	491	583	20			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	155	CYS	SER	conflict	UNP P03420
B	190	PHE	SER	conflict	UNP P03420
B	207	LEU	VAL	conflict	UNP P03420
B	290	CYS	SER	conflict	UNP P03420
B	379	VAL	ILE	conflict	UNP P03420
B	447	VAL	MET	conflict	UNP P03420
B	514	SER	-	linker	UNP P03420
B	515	ALA	-	linker	UNP P03420
B	516	ILE	-	linker	UNP P03420
B	517	GLY	-	linker	UNP P03420
B	546	GLY	-	expression tag	UNP M1E1E4
B	547	LEU	-	expression tag	UNP M1E1E4
B	548	VAL	-	expression tag	UNP M1E1E4
B	549	PRO	-	expression tag	UNP M1E1E4
B	550	ARG	-	expression tag	UNP M1E1E4
D	155	CYS	SER	conflict	UNP P03420
D	190	PHE	SER	conflict	UNP P03420
D	207	LEU	VAL	conflict	UNP P03420
D	290	CYS	SER	conflict	UNP P03420
D	379	VAL	ILE	conflict	UNP P03420
D	447	VAL	MET	conflict	UNP P03420
D	514	SER	-	linker	UNP P03420
D	515	ALA	-	linker	UNP P03420
D	516	ILE	-	linker	UNP P03420
D	517	GLY	-	linker	UNP P03420
D	546	GLY	-	expression tag	UNP M1E1E4
D	547	LEU	-	expression tag	UNP M1E1E4
D	548	VAL	-	expression tag	UNP M1E1E4
D	549	PRO	-	expression tag	UNP M1E1E4
D	550	ARG	-	expression tag	UNP M1E1E4
F	155	CYS	SER	conflict	UNP P03420
F	190	PHE	SER	conflict	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
F	207	LEU	VAL	conflict	UNP P03420
F	290	CYS	SER	conflict	UNP P03420
F	379	VAL	ILE	conflict	UNP P03420
F	447	VAL	MET	conflict	UNP P03420
F	514	SER	-	linker	UNP P03420
F	515	ALA	-	linker	UNP P03420
F	516	ILE	-	linker	UNP P03420
F	517	GLY	-	linker	UNP P03420
F	546	GLY	-	expression tag	UNP M1E1E4
F	547	LEU	-	expression tag	UNP M1E1E4
F	548	VAL	-	expression tag	UNP M1E1E4
F	549	PRO	-	expression tag	UNP M1E1E4
F	550	ARG	-	expression tag	UNP M1E1E4
H	155	CYS	SER	conflict	UNP P03420
H	190	PHE	SER	conflict	UNP P03420
H	207	LEU	VAL	conflict	UNP P03420
H	290	CYS	SER	conflict	UNP P03420
H	379	VAL	ILE	conflict	UNP P03420
H	447	VAL	MET	conflict	UNP P03420
H	514	SER	-	linker	UNP P03420
H	515	ALA	-	linker	UNP P03420
H	516	ILE	-	linker	UNP P03420
H	517	GLY	-	linker	UNP P03420
H	546	GLY	-	expression tag	UNP M1E1E4
H	547	LEU	-	expression tag	UNP M1E1E4
H	548	VAL	-	expression tag	UNP M1E1E4
H	549	PRO	-	expression tag	UNP M1E1E4
H	550	ARG	-	expression tag	UNP M1E1E4
J	155	CYS	SER	conflict	UNP P03420
J	190	PHE	SER	conflict	UNP P03420
J	207	LEU	VAL	conflict	UNP P03420
J	290	CYS	SER	conflict	UNP P03420
J	379	VAL	ILE	conflict	UNP P03420
J	447	VAL	MET	conflict	UNP P03420
J	514	SER	-	linker	UNP P03420
J	515	ALA	-	linker	UNP P03420
J	516	ILE	-	linker	UNP P03420
J	517	GLY	-	linker	UNP P03420
J	546	GLY	-	expression tag	UNP M1E1E4
J	547	LEU	-	expression tag	UNP M1E1E4
J	548	VAL	-	expression tag	UNP M1E1E4
J	549	PRO	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
J	550	ARG	-	expression tag	UNP M1E1E4
L	155	CYS	SER	conflict	UNP P03420
L	190	PHE	SER	conflict	UNP P03420
L	207	LEU	VAL	conflict	UNP P03420
L	290	CYS	SER	conflict	UNP P03420
L	379	VAL	ILE	conflict	UNP P03420
L	447	VAL	MET	conflict	UNP P03420
L	514	SER	-	linker	UNP P03420
L	515	ALA	-	linker	UNP P03420
L	516	ILE	-	linker	UNP P03420
L	517	GLY	-	linker	UNP P03420
L	546	GLY	-	expression tag	UNP M1E1E4
L	547	LEU	-	expression tag	UNP M1E1E4
L	548	VAL	-	expression tag	UNP M1E1E4
L	549	PRO	-	expression tag	UNP M1E1E4
L	550	ARG	-	expression tag	UNP M1E1E4

- Molecule 3 is a protein called RB1 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	225	Total	C	N	O	S	0	0	0
			1680	1061	281	332	6			
3	O	224	Total	C	N	O	S	0	0	0
			1669	1055	277	330	7			
3	Q	229	Total	C	N	O	S	0	0	0
			1701	1073	283	339	6			
3	S	224	Total	C	N	O	S	0	0	0
			1671	1055	279	331	6			
3	U	215	Total	C	N	O	S	0	0	0
			1583	1002	261	314	6			
3	W	225	Total	C	N	O	S	0	0	0
			1674	1057	279	331	7			

- Molecule 4 is a protein called RB1 Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	213	Total	C	N	O	S	0	0	0
			1636	1028	275	328	5			
4	P	213	Total	C	N	O	S	0	0	0
			1630	1025	272	328	5			
4	R	213	Total	C	N	O	S	0	0	0
			1636	1028	275	328	5			

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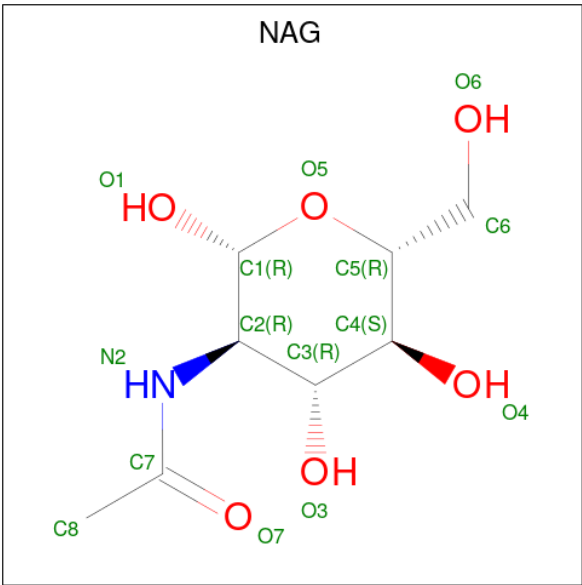
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	T	213	Total	C	N	O	S	0	0	0
			1636	1028	275	328	5			
4	V	209	Total	C	N	O	S	0	0	0
			1580	995	265	315	5			
4	X	213	Total	C	N	O	S	0	0	0
			1636	1028	275	328	5			

- Molecule 5 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
5	Y	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	Z	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	a	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	b	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	c	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	d	4	Total	C	N	O	0	0	0
			50	28	2	20			

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

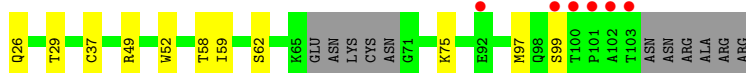


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	L	1	Total	C	N	O	0	0
			14	8	1	5		

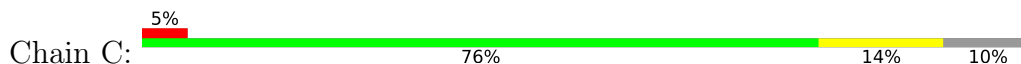
3 Residue-property plots [i](#)

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

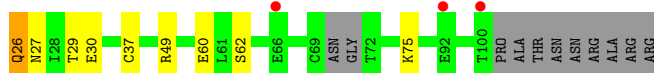
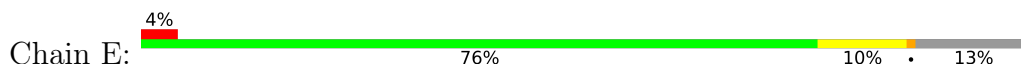
- Molecule 1: Fusion glycoprotein F2



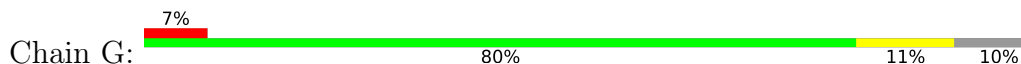
- Molecule 1: Fusion glycoprotein F2



- Molecule 1: Fusion glycoprotein F2



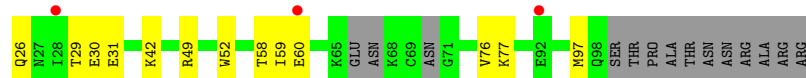
- Molecule 1: Fusion glycoprotein F2



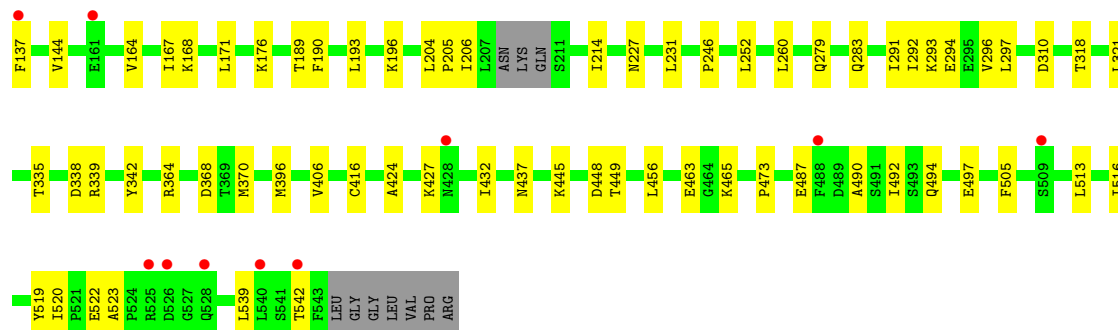
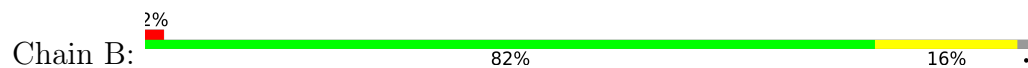
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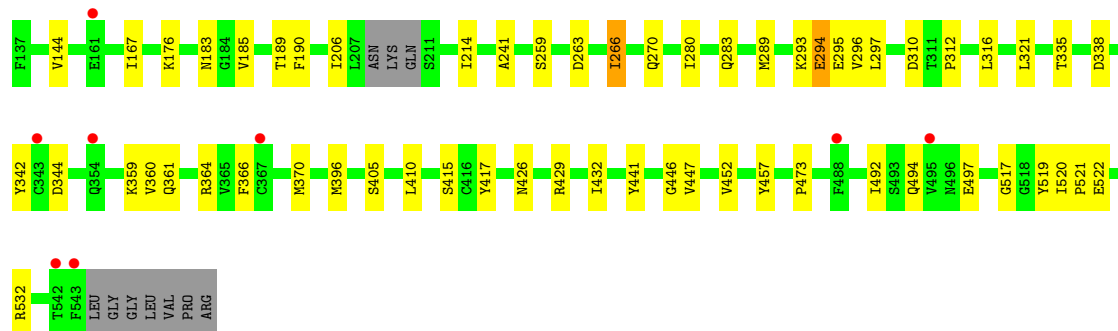
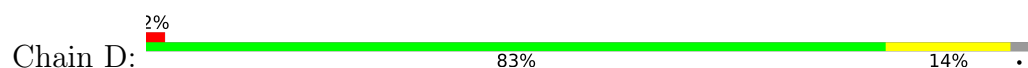
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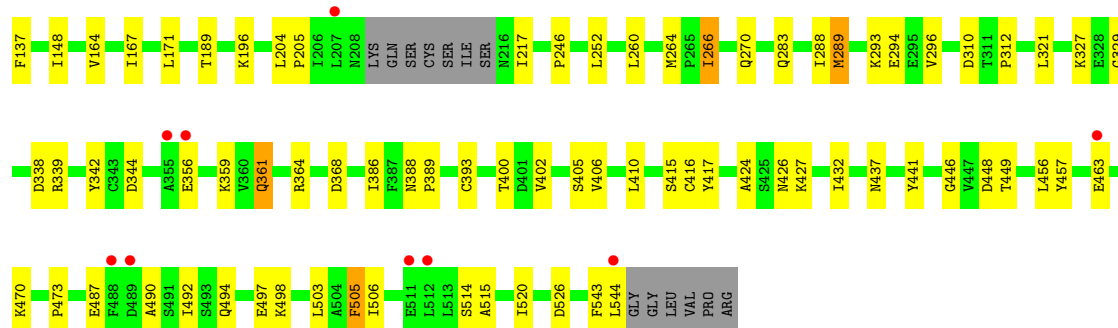
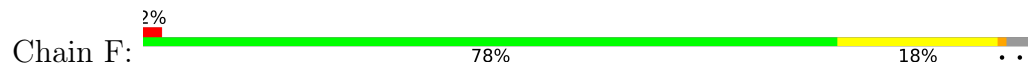
- Molecule 2: Fusion glycoprotein F1 fused with Fibrin trimerization domain



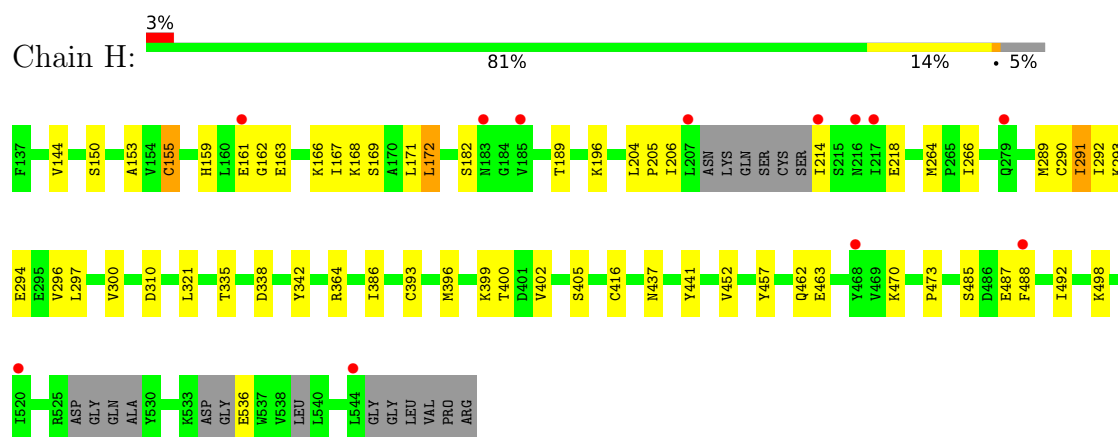
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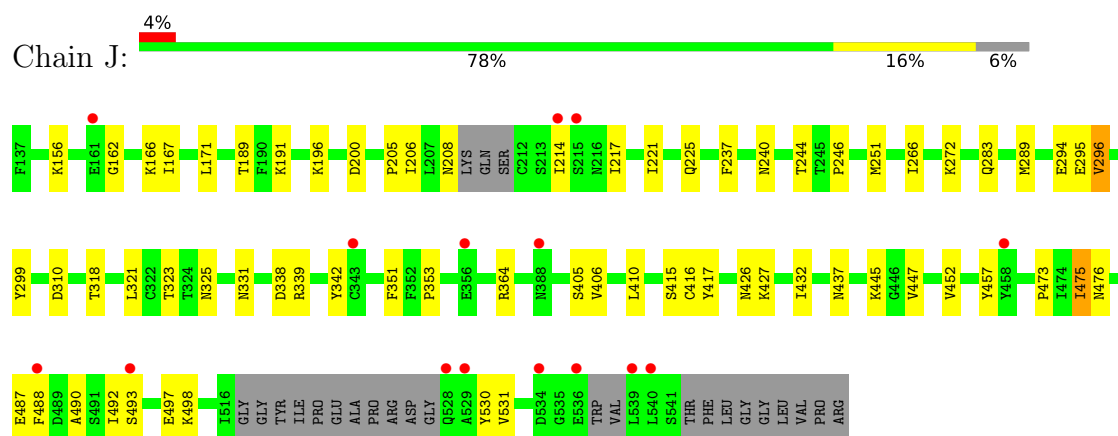
- Molecule 2: Fusion glycoprotein F1 fused with Fibrin trimerization domain



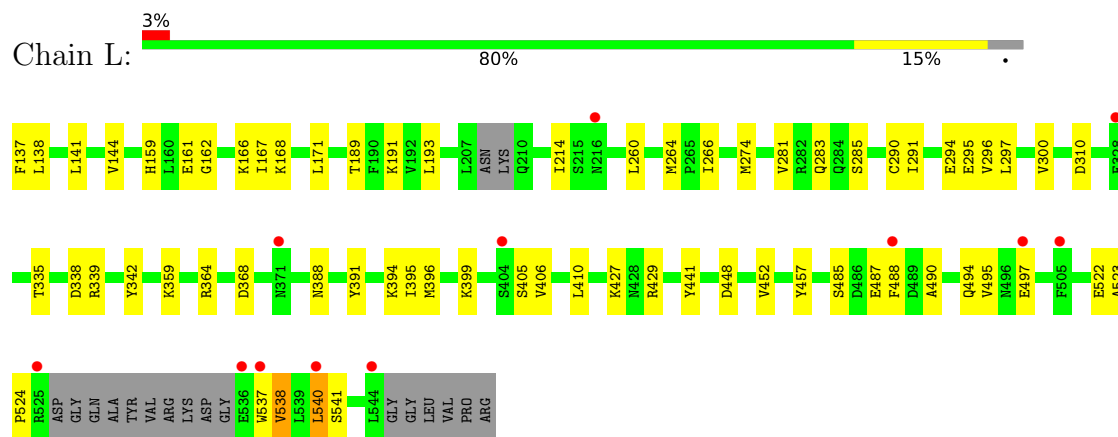
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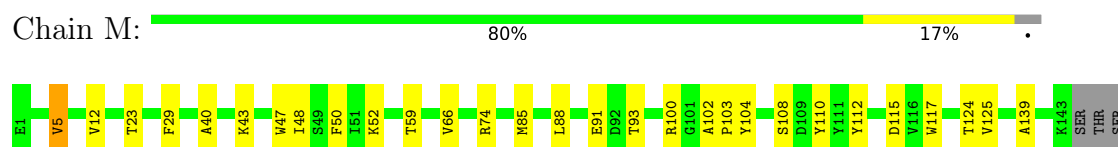
- Molecule 2: Fusion glycoprotein F1 fused with Fibrin trimerization domain



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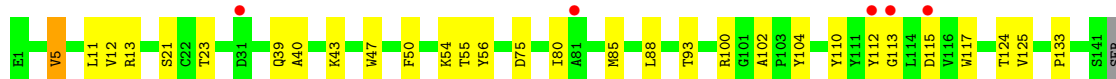
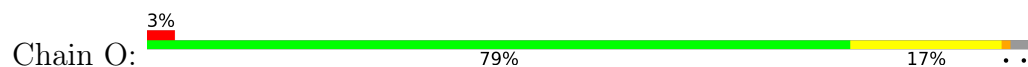


- Molecule 3: RB1 Fab Heavy Chain

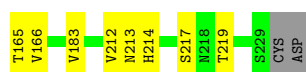
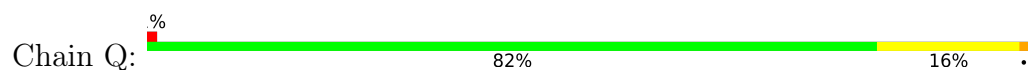




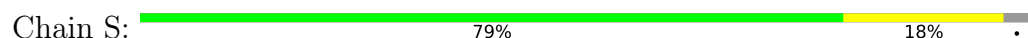
• Molecule 3: RB1 Fab Heavy Chain



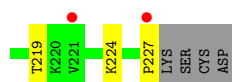
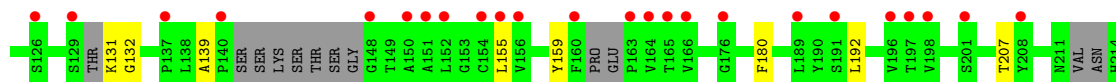
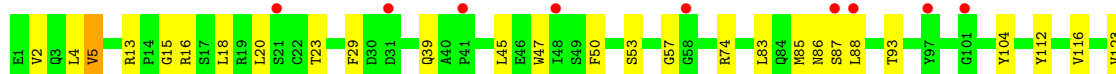
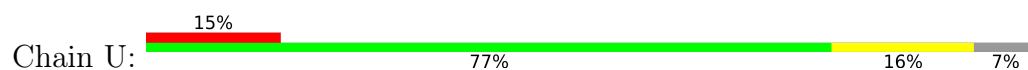
• Molecule 3: RB1 Fab Heavy Chain



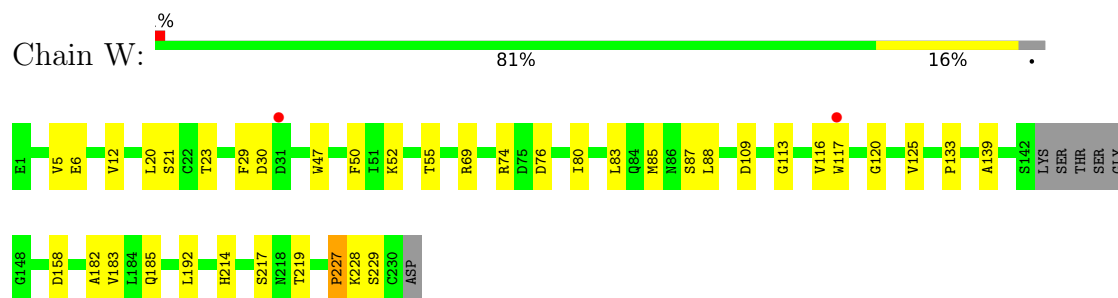
• Molecule 3: RB1 Fab Heavy Chain



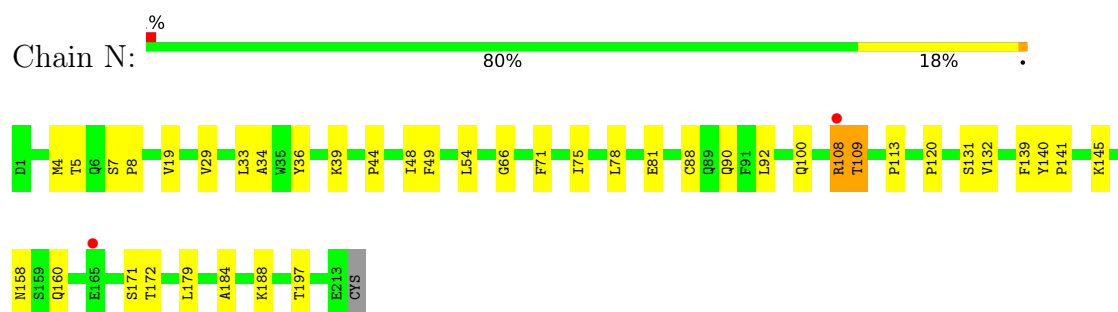
• Molecule 3: RB1 Fab Heavy Chain



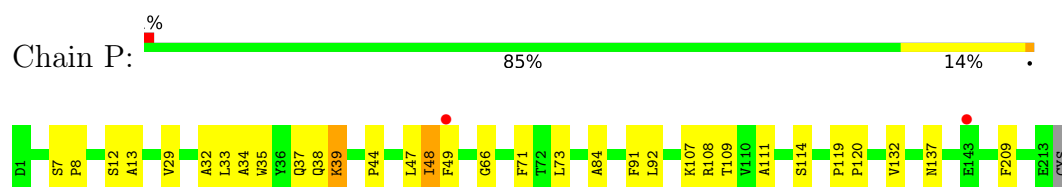
- Molecule 3: RB1 Fab Heavy Chain



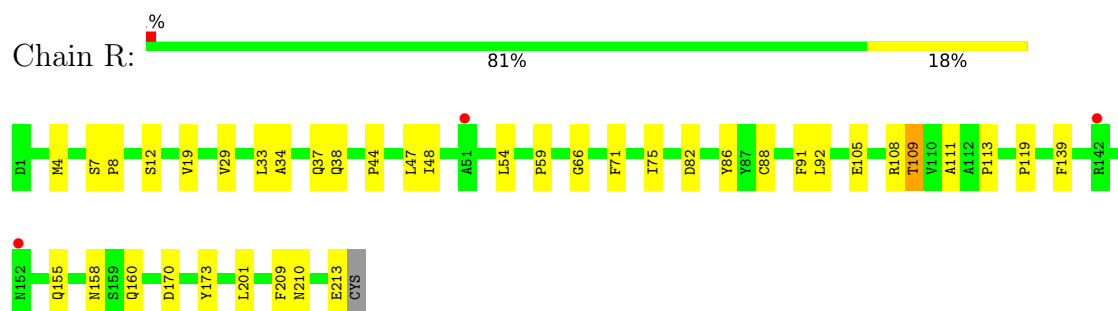
- Molecule 4: RB1 Fab Light chain



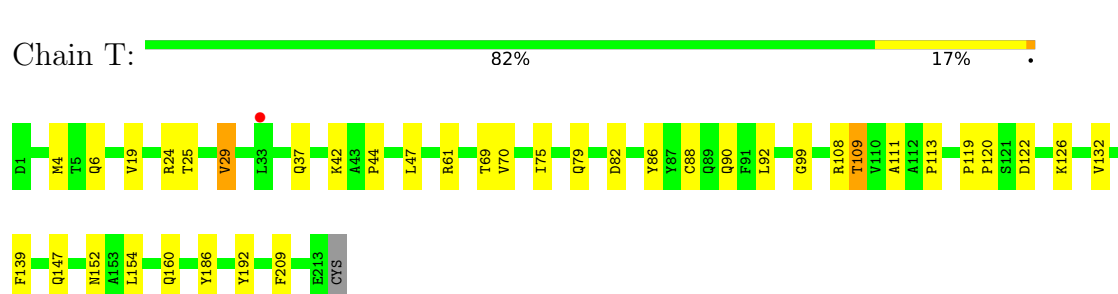
- Molecule 4: RB1 Fab Light chain



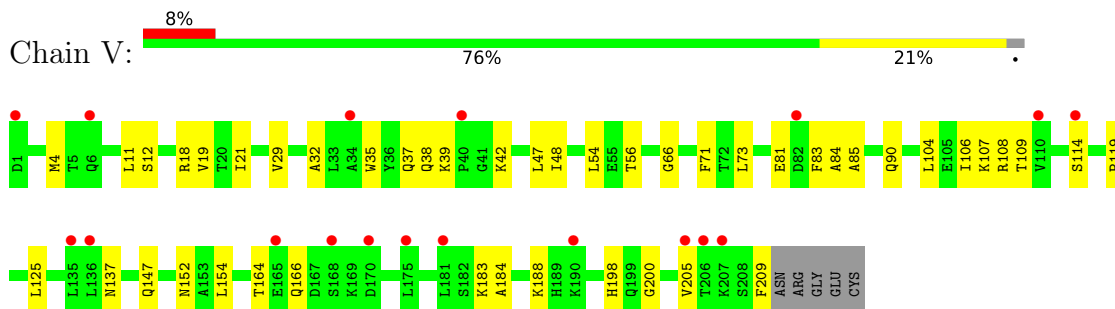
- Molecule 4: RB1 Fab Light chain



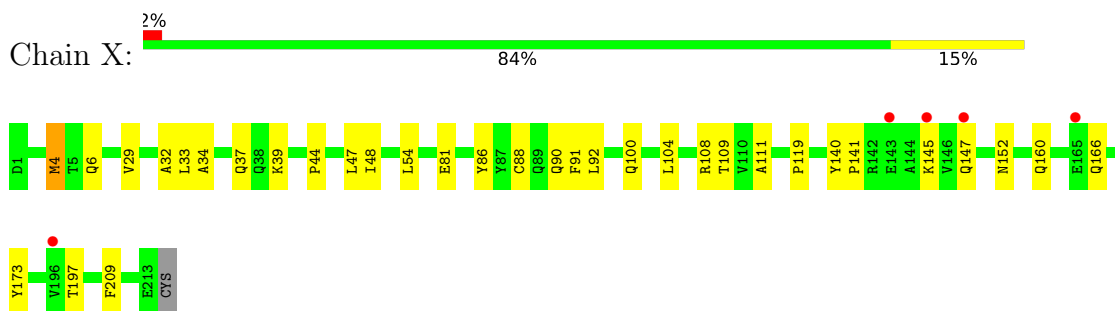
- Molecule 4: RB1 Fab Light chain



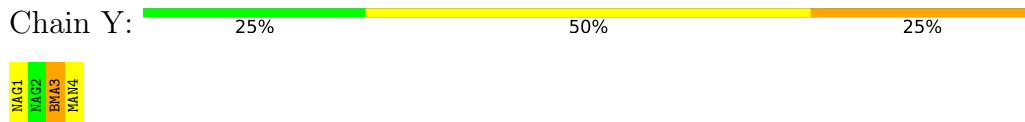
- Molecule 4: RB1 Fab Light chain



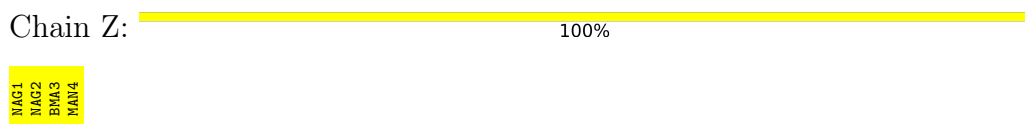
- Molecule 4: RB1 Fab Light chain



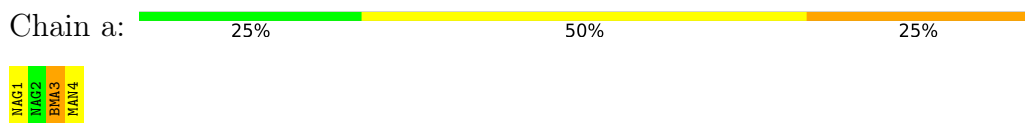
- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 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



- Molecule 5: 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

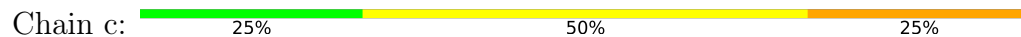


- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

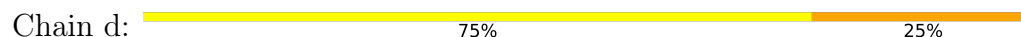




- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	118.15Å 126.59Å 148.16Å 87.24° 79.15° 86.29°	Depositor
Resolution (Å)	49.86 – 3.40 49.86 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.86-3.40) 98.9 (49.86-3.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.245 , 0.275 0.244 , 0.272	Depositor DCC
R_{free} test set	5767 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	77.2	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 26.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	41597	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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, MAN, BMA, PCA

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	0.21	0/566	0.46	0/767
1	C	0.17	0/582	0.38	0/788
1	E	0.16	0/567	0.40	0/766
1	G	0.16	0/580	0.37	0/788
1	I	0.18	0/601	0.41	0/815
1	K	0.17	0/543	0.41	0/732
2	B	0.18	0/3106	0.42	0/4223
2	D	0.17	0/3086	0.40	0/4198
2	F	0.18	0/3106	0.39	0/4221
2	H	0.20	0/3020	0.43	1/4100 (0.0%)
2	J	0.19	0/2994	0.41	0/4061
2	L	0.20	0/3028	0.42	0/4116
3	M	0.16	0/1719	0.41	0/2337
3	O	0.20	0/1708	0.44	0/2323
3	Q	0.15	0/1741	0.42	0/2368
3	S	0.18	0/1710	0.43	0/2326
3	U	0.17	0/1617	0.45	0/2197
3	W	0.15	0/1713	0.41	0/2330
4	N	0.21	0/1671	0.47	3/2267 (0.1%)
4	P	0.22	0/1665	0.45	1/2260 (0.0%)
4	R	0.15	0/1671	0.41	0/2267
4	T	0.16	0/1671	0.41	0/2267
4	V	0.15	0/1614	0.43	0/2195
4	X	0.15	0/1671	0.39	0/2267
All	All	0.18	0/41950	0.42	5/56979 (0.0%)

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
4	P	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	155	CYS	CA-CB-SG	-7.53	97.08	114.40
4	N	108	ARG	NE-CZ-NH1	-6.23	115.27	121.50
4	N	108	ARG	NE-CZ-NH2	5.51	124.16	119.20
4	N	108	ARG	CD-NE-CZ	-5.27	117.02	124.40
4	P	49	PHE	N-CA-CB	-5.11	101.55	110.44

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	P	48	ILE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	567	0	570	9	0
1	C	583	0	575	9	0
1	E	569	0	570	8	0
1	G	581	0	566	8	0
1	I	601	0	598	14	0
1	K	546	0	544	12	0
2	B	3057	0	3035	46	0
2	D	3038	0	2983	43	0
2	F	3056	0	3036	56	0
2	H	2977	0	2950	43	0
2	J	2952	0	2935	50	0
2	L	2982	0	2943	50	0
3	M	1680	0	1644	25	0
3	O	1669	0	1631	31	0
3	Q	1701	0	1665	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	S	1671	0	1631	25	0
3	U	1583	0	1526	26	0
3	W	1674	0	1632	21	0
4	N	1636	0	1594	32	0
4	P	1630	0	1583	25	0
4	R	1636	0	1594	25	0
4	T	1636	0	1594	22	0
4	V	1580	0	1529	28	0
4	X	1636	0	1594	20	0
5	Y	50	0	43	1	0
5	Z	50	0	43	1	0
5	a	50	0	43	1	0
5	b	50	0	43	2	0
5	c	50	0	43	1	0
5	d	50	0	43	1	0
6	B	14	0	13	0	0
6	F	14	0	13	0	0
6	J	14	0	13	0	0
6	L	14	0	13	0	0
All	All	41597	0	40832	560	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 7.

All (560) 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)
2:F:487:GLU:OE2	2:F:498:LYS:NZ	1.84	1.09
1:I:93:LEU:HD22	2:J:289:MET:HE1	1.36	1.04
4:N:108:ARG:NH1	4:N:171:SER:O	1.95	0.99
4:N:108:ARG:HH12	4:N:172:THR:HA	1.28	0.96
2:B:310:ASP:OD1	2:B:364:ARG:NH1	1.99	0.94
2:L:310:ASP:OD1	2:L:364:ARG:NH1	2.03	0.91
3:O:215:LYS:HG3	3:O:216:PRO:HD3	1.60	0.83
2:H:289:MET:HE1	2:H:297:LEU:HD11	1.60	0.82
4:P:108:ARG:HH12	4:P:111:ALA:HB2	1.47	0.80
2:J:310:ASP:OD1	2:J:364:ARG:NH1	2.15	0.80
4:N:108:ARG:NH2	4:N:140:TYR:HB2	1.97	0.80
2:D:176:LYS:NZ	2:D:263:ASP:OD2	2.12	0.78
4:P:29:VAL:HG13	4:P:92:LEU:HB2	1.68	0.76
4:T:108:ARG:HH12	4:T:111:ALA:HB2	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:386:ILE:HG13	2:H:492:ILE:HD11	1.67	0.74
2:J:487:GLU:OE2	2:J:498:LYS:NZ	2.17	0.73
2:H:293:LYS:HG2	2:H:294:GLU:OE2	1.89	0.73
4:X:108:ARG:HH12	4:X:111:ALA:HB2	1.54	0.70
2:J:530:TYR:O	2:L:538:VAL:HG21	1.90	0.70
2:B:522:GLU:HA	2:D:520:ILE:HD11	1.72	0.70
4:N:108:ARG:CZ	4:N:140:TYR:HB2	2.22	0.70
1:G:56:VAL:HG22	2:H:300:VAL:HG22	1.74	0.70
1:K:76:VAL:HG22	2:L:214:ILE:HD13	1.73	0.70
2:F:310:ASP:OD1	2:F:364:ARG:NH2	2.25	0.69
4:V:38:GLN:HB3	4:V:85:ALA:HB3	1.76	0.67
2:L:159:HIS:CG	2:L:291:ILE:HD11	2.29	0.67
2:J:205:PRO:O	2:J:208:ASN:ND2	2.23	0.66
2:F:386:ILE:HG13	2:F:492:ILE:HD11	1.78	0.66
4:P:29:VAL:HG12	4:P:32:ALA:HB3	1.76	0.66
1:K:29:THR:HG23	1:K:42:LYS:HG3	1.78	0.65
1:G:75:LYS:HD2	2:H:214:ILE:HG21	1.77	0.65
1:K:60:GLU:HG3	2:L:296:VAL:HG12	1.78	0.65
1:C:59:ILE:HB	2:D:297:LEU:HB3	1.78	0.65
2:D:310:ASP:OD1	2:D:364:ARG:NH1	2.30	0.65
3:W:228:LYS:HG2	3:W:229:SER:H	1.62	0.65
2:B:505:PHE:HD1	2:F:505:PHE:CE2	2.14	0.64
4:P:29:VAL:HA	4:P:92:LEU:HD22	1.80	0.64
2:H:488:PHE:CZ	2:J:488:PHE:HB3	2.32	0.64
4:V:114:SER:HB2	4:V:137:ASN:HB3	1.78	0.64
2:B:168:LYS:NZ	2:B:294:GLU:O	2.31	0.64
2:H:310:ASP:OD1	2:H:364:ARG:NH1	2.28	0.64
2:J:530:TYR:HB3	2:L:538:VAL:HG23	1.80	0.63
1:G:97:MET:HG3	2:H:291:ILE:HA	1.80	0.62
4:N:108:ARG:HH12	4:N:172:THR:CA	2.08	0.62
1:K:31:GLU:OE2	1:K:42:LYS:NZ	2.28	0.62
3:O:100:ARG:NH2	3:O:115:ASP:OD2	2.27	0.62
3:M:5:VAL:HG23	3:M:23:THR:HB	1.83	0.61
3:W:29:PHE:O	3:W:74:ARG:NH2	2.34	0.61
4:N:108:ARG:CZ	4:N:172:THR:HG22	2.30	0.61
3:O:21:SER:HB3	3:O:80:ILE:HD11	1.82	0.61
3:O:102:ALA:HB2	3:O:115:ASP:HB2	1.83	0.61
2:D:432:ILE:HD11	2:D:447:VAL:HG22	1.81	0.61
2:F:505:PHE:CD1	2:F:505:PHE:C	2.77	0.61
2:H:470:LYS:NZ	3:S:30:ASP:HB2	2.16	0.60
2:J:487:GLU:HB3	2:J:490:ALA:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:406:VAL:HG13	2:L:144:VAL:HB	1.83	0.60
2:L:395:ILE:HD11	2:L:495:VAL:HG21	1.83	0.60
3:U:13:ARG:O	3:U:15:GLY:N	2.31	0.60
4:R:29:VAL:HA	4:R:92:LEU:HD22	1.82	0.60
2:D:293:LYS:HG2	2:D:294:GLU:HG3	1.83	0.60
3:O:85:MET:HB3	3:O:88:LEU:HD21	1.84	0.60
2:J:167:ILE:HG23	2:J:189:THR:HG21	1.82	0.60
4:T:147:GLN:HB3	4:T:154:LEU:HD21	1.83	0.59
2:F:505:PHE:HD1	2:F:505:PHE:O	1.85	0.59
2:L:429:ARG:NH2	4:X:92:LEU:O	2.35	0.59
2:F:321:LEU:HD11	2:F:473:PRO:HB3	1.84	0.59
4:N:33:LEU:HD11	4:N:88:CYS:HB2	1.85	0.59
2:B:206:ILE:HG21	2:B:214:ILE:HD13	1.84	0.58
2:J:325:ASN:H	2:J:331:ASN:ND2	2.01	0.58
2:L:399:LYS:NZ	2:L:485:SER:OG	2.36	0.58
3:M:40:ALA:HB3	3:M:43:LYS:HB2	1.84	0.58
3:O:5:VAL:HG23	3:O:23:THR:HB	1.85	0.58
3:Q:5:VAL:HG23	3:Q:23:THR:HB	1.86	0.58
2:F:505:PHE:C	2:F:505:PHE:HD1	2.12	0.58
1:I:30:GLU:HB2	2:J:410:LEU:HD12	1.86	0.58
2:D:494:GLN:O	2:D:497:GLU:HG2	2.04	0.57
3:S:185:GLN:HG2	3:S:189:LEU:O	2.03	0.57
3:Q:93:THR:HG23	3:Q:124:THR:HA	1.86	0.57
4:T:6:GLN:NE2	4:T:86:TYR:O	2.36	0.57
3:U:53:SER:O	3:U:57:GLY:HA3	2.02	0.57
2:D:176:LYS:HZ1	2:D:259:SER:HB3	1.69	0.57
2:F:470:LYS:NZ	3:Q:30:ASP:HB2	2.19	0.57
4:N:120:PRO:HD3	4:N:132:VAL:HG22	1.87	0.57
3:W:47:TRP:HZ2	3:W:50:PHE:HB2	1.70	0.57
3:Q:47:TRP:HZ2	3:Q:50:PHE:HB2	1.70	0.56
2:B:293:LYS:O	2:B:296:VAL:HG12	2.05	0.56
4:N:145:LYS:HB3	4:N:197:THR:HB	1.86	0.56
2:D:429:ARG:NE	3:O:110:TYR:HD1	2.03	0.56
2:J:493:SER:O	2:J:497:GLU:HG2	2.06	0.56
3:O:47:TRP:HZ2	3:O:50:PHE:HB2	1.70	0.56
2:J:432:ILE:HD11	2:J:447:VAL:HG22	1.88	0.56
2:D:289:MET:HE1	2:D:297:LEU:HD11	1.86	0.56
3:Q:183:VAL:HG11	4:R:160:GLN:HG2	1.88	0.56
2:H:393:CYS:HB2	2:H:492:ILE:HD12	1.88	0.56
3:U:20:LEU:HD12	3:U:83:LEU:HD23	1.88	0.56
3:M:52:LYS:HE2	3:M:59:THR:HB	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:108:ARG:HG2	4:V:109:THR:H	1.69	0.55
3:O:11:LEU:HD21	3:O:13:ARG:HH21	1.70	0.55
3:O:75:ASP:HB3	3:O:80:ILE:HG22	1.87	0.55
4:X:145:LYS:HE2	4:X:147:GLN:OE1	2.07	0.55
3:M:93:THR:HG23	3:M:124:THR:HA	1.87	0.55
3:U:5:VAL:HG23	3:U:23:THR:HB	1.88	0.55
2:F:167:ILE:HG23	2:F:189:THR:HG21	1.88	0.55
2:D:335:THR:HB	2:D:396:MET:HE2	1.89	0.55
2:L:523:ALA:HB1	2:L:524:PRO:HD2	1.88	0.55
2:H:386:ILE:HG13	2:H:492:ILE:CD1	2.36	0.55
2:B:252:LEU:HD21	2:B:260:LEU:HD12	1.89	0.55
2:H:163:GLU:OE2	2:H:182:SER:N	2.40	0.54
1:I:37:CYS:HB2	2:J:321:LEU:HD13	1.88	0.54
4:X:145:LYS:HB3	4:X:197:THR:HB	1.88	0.54
2:H:168:LYS:NZ	2:H:294:GLU:HB3	2.23	0.54
1:I:73:ASP:HB3	1:I:76:VAL:HB	1.89	0.54
3:W:139:ALA:HB1	3:W:227:PRO:HA	1.89	0.54
1:E:49:ARG:NH2	2:F:368:ASP:OD1	2.40	0.54
4:T:119:PRO:HB3	4:T:209:PHE:CE1	2.42	0.54
3:W:52:LYS:NZ	3:W:109:ASP:OD2	2.29	0.54
3:U:39:GLN:HB2	3:U:45:LEU:HD23	1.88	0.54
2:B:167:ILE:HG23	2:B:189:THR:HG21	1.90	0.54
1:E:37:CYS:HB2	2:F:321:LEU:HD13	1.89	0.54
4:X:29:VAL:HG12	4:X:32:ALA:HB3	1.89	0.54
1:A:75:LYS:HB2	2:B:214:ILE:HB	1.89	0.54
4:P:66:GLY:HA3	4:P:71:PHE:HA	1.88	0.54
4:V:108:ARG:HG2	4:V:109:THR:N	2.23	0.54
2:F:487:GLU:HB3	2:F:490:ALA:HB2	1.89	0.54
3:O:93:THR:HG23	3:O:124:THR:HA	1.89	0.54
4:T:120:PRO:HD3	4:T:132:VAL:HG22	1.90	0.54
3:S:183:VAL:HG11	4:T:160:GLN:HG2	1.90	0.53
3:M:47:TRP:HZ2	3:M:50:PHE:HB2	1.73	0.53
2:D:266:ILE:HD13	2:D:270:GLN:HB2	1.91	0.53
2:L:167:ILE:HG23	2:L:189:THR:HG21	1.90	0.53
3:M:29:PHE:O	3:M:74:ARG:NH2	2.41	0.53
4:N:5:THR:HA	4:N:100:GLN:HE22	1.74	0.53
3:Q:39:GLN:OE1	4:R:38:GLN:NE2	2.41	0.53
1:K:30:GLU:OE1	2:L:441:TYR:OH	2.22	0.53
4:V:39:LYS:NZ	4:V:81:GLU:O	2.42	0.53
1:C:30:GLU:OE1	2:D:441:TYR:OH	2.19	0.53
2:L:168:LYS:HZ3	2:L:295:GLU:H	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:5:VAL:HG23	3:W:23:THR:HB	1.91	0.53
2:B:513:LEU:HG	2:B:516:ILE:HD12	1.91	0.53
2:D:360:VAL:O	2:D:361:GLN:NE2	2.41	0.53
3:M:139:ALA:HB1	3:M:227:PRO:HA	1.89	0.53
3:W:30:ASP:OD2	3:W:76:ASP:HB3	2.09	0.53
2:H:487:GLU:OE2	2:H:498:LYS:NZ	2.37	0.52
2:L:388:ASN:OD1	2:L:391:TYR:N	2.42	0.52
3:M:214:HIS:CD2	3:M:216:PRO:HD2	2.43	0.52
2:F:171:LEU:HD11	2:F:189:THR:HG22	1.91	0.52
2:J:221:ILE:O	2:J:225:GLN:HG2	2.09	0.52
4:R:105:GLU:OE1	4:R:173:TYR:OH	2.18	0.52
4:T:186:TYR:O	4:T:192:TYR:OH	2.27	0.52
4:N:108:ARG:NH1	4:N:171:SER:C	2.68	0.52
3:S:104:TYR:N	3:S:110:TYR:O	2.39	0.52
5:d:1:NAG:H62	5:d:2:NAG:HN2	1.74	0.52
1:A:97:MET:SD	2:B:292:ILE:HG22	2.50	0.52
2:L:335:THR:HB	2:L:396:MET:HE2	1.92	0.52
4:R:59:PRO:HD3	5:a:3:BMA:H61	1.91	0.52
4:V:66:GLY:HA3	4:V:71:PHE:HA	1.92	0.52
2:J:432:ILE:HD13	3:U:104:TYR:HB3	1.92	0.52
2:J:473:PRO:HG2	2:J:476:ASN:ND2	2.25	0.52
3:Q:102:ALA:HB2	3:Q:115:ASP:CG	2.35	0.52
5:b:2:NAG:H61	5:b:3:BMA:O5	2.10	0.52
2:H:206:ILE:HG21	2:H:214:ILE:HD12	1.91	0.51
3:U:159:TYR:OH	3:U:192:LEU:HD23	2.10	0.51
3:O:39:GLN:OE1	4:P:38:GLN:NE2	2.40	0.51
4:P:107:LYS:HZ3	4:V:205:VAL:HG22	1.76	0.51
3:U:47:TRP:HZ2	3:U:50:PHE:HB2	1.74	0.51
3:O:47:TRP:CZ2	3:O:50:PHE:HB2	2.45	0.51
4:V:37:GLN:HB2	4:V:47:LEU:HD11	1.93	0.51
1:E:30:GLU:OE1	2:F:441:TYR:OH	2.18	0.51
3:U:207:THR:HG22	3:U:224:LYS:HE3	1.92	0.51
2:B:445:LYS:HZ3	2:B:465:LYS:HD3	1.76	0.51
2:B:171:LEU:HD11	2:B:189:THR:HG22	1.93	0.51
3:S:47:TRP:HZ2	3:S:50:PHE:HB2	1.75	0.51
4:V:147:GLN:HB3	4:V:154:LEU:HD21	1.93	0.51
3:W:85:MET:HB3	3:W:88:LEU:HD21	1.93	0.51
2:F:426:ASN:ND2	2:F:446:GLY:O	2.43	0.51
2:H:536:GLU:N	2:L:522:GLU:OE2	2.44	0.51
4:V:83:PHE:HD1	4:V:104:LEU:HB3	1.76	0.51
2:B:445:LYS:NZ	2:B:465:LYS:HD3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:VAL:HB	2:F:406:VAL:HG13	1.93	0.50
4:P:107:LYS:NZ	4:V:205:VAL:HG22	2.25	0.50
3:Q:117:TRP:CE3	4:R:44:PRO:HD2	2.47	0.50
1:G:30:GLU:OE1	2:H:441:TYR:OH	2.24	0.50
2:H:321:LEU:HD11	2:H:473:PRO:HB3	1.92	0.50
2:L:538:VAL:O	2:L:540:LEU:N	2.40	0.50
4:P:114:SER:HB2	4:P:137:ASN:HB3	1.93	0.50
4:P:119:PRO:HB3	4:P:209:PHE:CE1	2.46	0.50
4:V:12:SER:HB2	4:V:107:LYS:HG3	1.94	0.50
1:A:59:ILE:HG23	2:B:193:LEU:HB3	1.93	0.50
2:F:386:ILE:O	2:F:492:ILE:HD13	2.12	0.50
3:O:173:LEU:HD21	3:O:196:VAL:HG21	1.93	0.50
4:R:155:GLN:HB3	4:R:158:ASN:HD21	1.76	0.50
3:S:21:SER:HB3	3:S:80:ILE:HD11	1.94	0.50
2:J:530:TYR:HB3	2:L:538:VAL:CG2	2.41	0.50
3:M:85:MET:HB3	3:M:88:LEU:HD21	1.92	0.50
2:F:526:ASP:OD1	2:F:526:ASP:N	2.44	0.50
4:N:39:LYS:NZ	4:N:81:GLU:O	2.27	0.50
3:O:112:TYR:CD1	3:O:112:TYR:C	2.90	0.50
4:T:25:THR:HG22	4:T:69:THR:O	2.10	0.50
4:P:12:SER:HB3	4:P:107:LYS:HG3	1.93	0.50
3:Q:85:MET:HB3	3:Q:88:LEU:HD21	1.94	0.50
3:U:53:SER:HA	3:U:74:ARG:HH12	1.76	0.50
4:V:108:ARG:HE	4:V:109:THR:HG22	1.77	0.50
4:X:48:ILE:HG12	4:X:54:LEU:HD12	1.92	0.50
2:B:427:LYS:HG2	2:B:448:ASP:OD2	2.11	0.50
2:D:206:ILE:HG21	2:D:214:ILE:HD13	1.94	0.50
1:I:62:SER:OG	2:J:200:ASP:OD1	2.30	0.50
4:T:122:ASP:O	4:T:126:LYS:HG3	2.12	0.50
2:H:161:GLU:OE1	2:H:161:GLU:N	2.41	0.50
2:H:335:THR:HB	2:H:396:MET:HE2	1.93	0.50
4:V:119:PRO:HB3	4:V:209:PHE:CE1	2.47	0.50
2:F:470:LYS:HE3	3:Q:31:ASP:HB2	1.92	0.49
2:H:162:GLY:O	2:H:166:LYS:HG3	2.12	0.49
2:H:169:SER:HA	2:H:172:LEU:HD13	1.94	0.49
2:H:218:GLU:OE2	1:I:75:LYS:NZ	2.34	0.49
1:C:59:ILE:HD12	2:D:297:LEU:HD23	1.94	0.49
2:D:176:LYS:HG3	2:D:189:THR:O	2.12	0.49
3:M:112:TYR:CG	4:N:49:PHE:HD2	2.29	0.49
3:S:158:ASP:OD2	3:S:185:GLN:NE2	2.45	0.49
4:V:35:TRP:HB2	4:V:48:ILE:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:60:GLU:OE2	2:J:296:VAL:HB	2.12	0.49
2:L:138:LEU:HB3	2:L:141:LEU:HD12	1.95	0.49
2:D:426:ASN:ND2	2:D:446:GLY:O	2.40	0.49
3:S:133:PRO:HB3	3:S:159:TYR:HB3	1.94	0.49
2:H:400:THR:HG22	2:H:402:VAL:HG13	1.93	0.49
4:R:108:ARG:NH2	4:R:111:ALA:HB2	2.28	0.49
2:H:405:SER:HB3	2:H:457:TYR:CE1	2.48	0.49
1:K:97:MET:SD	2:L:291:ILE:HG23	2.53	0.49
2:L:137:PHE:HE1	2:L:339:ARG:HH21	1.59	0.49
4:X:119:PRO:HB3	4:X:209:PHE:CE1	2.48	0.49
2:J:323:THR:HG23	2:J:475:ILE:HG12	1.94	0.49
3:O:133:PRO:HB3	3:O:159:TYR:HB3	1.93	0.48
4:P:37:GLN:HB2	4:P:47:LEU:HD11	1.95	0.48
3:S:17:SER:OG	3:S:86:ASN:OD1	2.24	0.48
4:V:48:ILE:HG12	4:V:54:LEU:HD12	1.95	0.48
2:F:393:CYS:HB2	2:F:492:ILE:CD1	2.43	0.48
4:X:6:GLN:NE2	4:X:86:TYR:O	2.41	0.48
3:S:75:ASP:HB3	3:S:80:ILE:HG22	1.95	0.48
1:A:59:ILE:HB	2:B:297:LEU:HB3	1.96	0.48
2:B:406:VAL:HG13	2:D:144:VAL:HB	1.93	0.48
2:D:405:SER:HB3	2:D:457:TYR:CE1	2.48	0.48
3:S:102:ALA:HB2	3:S:115:ASP:CG	2.38	0.48
3:U:180:PHE:CD2	4:V:164:THR:HG23	2.49	0.48
3:W:12:VAL:HG13	3:W:125:VAL:HG22	1.95	0.48
3:W:133:PRO:HD2	3:W:219:THR:HG21	1.96	0.48
3:O:12:VAL:HG13	3:O:125:VAL:HG22	1.94	0.48
4:V:29:VAL:HG12	4:V:32:ALA:HB3	1.94	0.48
2:B:279:GLN:HB2	2:D:241:ALA:HA	1.95	0.48
3:O:158:ASP:OD1	3:O:185:GLN:NE2	2.42	0.48
1:I:75:LYS:HE3	2:J:217:ILE:HB	1.95	0.48
4:N:48:ILE:HG13	4:N:54:LEU:HD12	1.96	0.48
4:R:108:ARG:HG2	4:R:109:THR:N	2.29	0.48
2:B:523:ALA:HB3	2:D:532:ARG:HG2	1.96	0.48
2:H:171:LEU:HD11	2:H:189:THR:HG22	1.95	0.47
4:T:29:VAL:HA	4:T:92:LEU:HD22	1.96	0.47
2:B:338:ASP:OD1	2:B:338:ASP:N	2.47	0.47
4:N:29:VAL:HA	4:N:92:LEU:HD22	1.96	0.47
4:N:66:GLY:HA3	4:N:71:PHE:HA	1.96	0.47
3:Q:21:SER:HB3	3:Q:80:ILE:HD11	1.96	0.47
2:B:338:ASP:O	2:B:342:TYR:OH	2.28	0.47
2:F:514:SER:HA	2:F:515:ALA:HA	1.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:30:GLU:HB2	2:L:410:LEU:HD12	1.97	0.47
3:W:69:ARG:NH2	3:W:87:SER:O	2.46	0.47
3:O:112:TYR:CD1	3:O:113:GLY:N	2.82	0.47
3:U:16:ARG:CB	3:U:87:SER:H	2.27	0.47
1:C:29:THR:HG22	1:C:30:GLU:N	2.29	0.47
2:H:167:ILE:HG23	2:H:189:THR:HG21	1.97	0.47
2:H:393:CYS:HB2	2:H:492:ILE:CD1	2.45	0.47
2:L:338:ASP:HB2	2:L:342:TYR:OH	2.14	0.47
3:M:158:ASP:OD1	3:M:185:GLN:NE2	2.45	0.47
2:F:312:PRO:HG2	2:F:344:ASP:OD2	2.15	0.47
2:L:162:GLY:O	2:L:166:LYS:HG3	2.14	0.47
2:L:523:ALA:HB2	2:L:537:TRP:NE1	2.30	0.47
3:M:47:TRP:CZ2	3:M:50:PHE:HB2	2.50	0.47
3:M:112:TYR:CG	4:N:49:PHE:CD2	3.03	0.47
4:P:35:TRP:HB2	4:P:48:ILE:HB	1.97	0.47
2:B:321:LEU:HD11	2:B:473:PRO:HB3	1.96	0.47
2:D:520:ILE:HG22	2:D:521:PRO:O	2.15	0.47
2:F:427:LYS:HG2	2:F:448:ASP:OD2	2.15	0.47
3:M:183:VAL:HG11	4:N:160:GLN:HG2	1.96	0.47
3:W:20:LEU:HD12	3:W:83:LEU:HD23	1.97	0.47
2:D:321:LEU:HD11	2:D:473:PRO:HB3	1.97	0.46
2:J:338:ASP:OD1	2:J:338:ASP:N	2.48	0.46
2:J:405:SER:HB3	2:J:457:TYR:CE1	2.50	0.46
3:O:104:TYR:HA	3:O:112:TYR:HD2	1.80	0.46
3:Q:75:ASP:HB3	3:Q:80:ILE:HG22	1.97	0.46
4:R:108:ARG:HH21	4:R:111:ALA:HB2	1.80	0.46
3:U:104:TYR:HA	3:U:112:TYR:HD2	1.79	0.46
2:J:171:LEU:HD13	2:J:191:LYS:HB2	1.96	0.46
4:P:33:LEU:HD13	4:P:34:ALA:N	2.29	0.46
2:F:148:ILE:HB	2:F:288:ILE:HD11	1.98	0.46
2:L:487:GLU:HB3	2:L:490:ALA:HB2	1.97	0.46
3:U:2:VAL:HG11	3:U:116:VAL:HG11	1.98	0.46
2:D:293:LYS:O	2:D:296:VAL:HG12	2.15	0.46
3:O:102:ALA:HB3	3:O:112:TYR:CZ	2.50	0.46
4:T:24:ARG:HG3	4:T:70:VAL:HG22	1.98	0.46
2:D:405:SER:HB2	2:D:452:VAL:HG21	1.97	0.46
2:L:405:SER:HB3	2:L:457:TYR:CE1	2.50	0.46
2:L:427:LYS:HG2	2:L:448:ASP:OD2	2.16	0.46
2:L:494:GLN:O	2:L:497:GLU:HG2	2.16	0.46
3:Q:47:TRP:CZ2	3:Q:50:PHE:HB2	2.50	0.46
3:W:47:TRP:CZ2	3:W:50:PHE:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:283:GLN:HB3	2:F:359:LYS:HE2	1.96	0.46
2:F:338:ASP:HB2	2:F:342:TYR:OH	2.16	0.46
2:F:405:SER:HB3	2:F:457:TYR:CE1	2.51	0.46
2:F:449:THR:HB	2:F:456:LEU:HD11	1.97	0.46
2:F:361:GLN:HE21	2:F:361:GLN:HA	1.80	0.46
3:M:100:ARG:NH1	3:M:115:ASP:OD2	2.49	0.46
2:F:266:ILE:HD13	2:F:270:GLN:HB2	1.98	0.46
3:M:48:ILE:HG23	3:M:66:VAL:HG21	1.97	0.46
4:T:113:PRO:HB3	4:T:139:PHE:HB3	1.98	0.46
3:U:93:THR:HA	3:U:123:VAL:O	2.16	0.46
3:U:139:ALA:HB1	3:U:227:PRO:HA	1.98	0.46
3:O:54:LYS:HB3	3:O:54:LYS:HE2	1.70	0.45
2:F:137:PHE:HD1	2:F:339:ARG:HE	1.63	0.45
4:P:38:GLN:O	4:P:84:ALA:HB1	2.16	0.45
3:S:93:THR:HG23	3:S:124:THR:HA	1.98	0.45
2:J:530:TYR:CD2	2:L:538:VAL:HB	2.51	0.45
2:L:290:CYS:SG	2:L:300:VAL:HG23	2.56	0.45
3:M:104:TYR:N	3:M:110:TYR:O	2.40	0.45
4:N:33:LEU:HG	4:N:34:ALA:N	2.32	0.45
4:P:12:SER:CB	4:P:107:LYS:HG3	2.47	0.45
4:R:37:GLN:HB2	4:R:47:LEU:HD11	1.98	0.45
3:S:5:VAL:HG23	3:S:23:THR:HB	1.98	0.45
4:T:25:THR:HG21	4:T:29:VAL:CG2	2.46	0.45
3:U:131:LYS:HD3	3:U:132:GLY:O	2.17	0.45
4:X:4:MET:O	4:X:100:GLN:NE2	2.47	0.45
2:B:494:GLN:O	2:B:497:GLU:HG2	2.16	0.45
2:F:252:LEU:HD21	2:F:260:LEU:HD12	1.98	0.45
2:F:327:LYS:NZ	2:F:329:GLY:H	2.14	0.45
2:J:272:LYS:HB2	2:J:272:LYS:HE3	1.66	0.45
2:L:523:ALA:HB2	2:L:537:TRP:CD1	2.52	0.45
4:N:140:TYR:CG	4:N:141:PRO:HA	2.52	0.45
3:Q:133:PRO:HB3	3:Q:159:TYR:HB3	1.97	0.45
4:X:108:ARG:HG2	4:X:109:THR:N	2.32	0.45
5:Y:3:BMA:O4	5:Y:3:BMA:O6	2.35	0.45
2:B:519:TYR:HB2	2:D:519:TYR:CZ	2.51	0.45
1:G:97:MET:C	1:G:99:SER:H	2.24	0.45
1:I:64:ILE:HD11	2:J:200:ASP:OD1	2.16	0.45
2:H:144:VAL:HB	2:L:406:VAL:HG13	1.98	0.45
1:I:47:ALA:HB2	2:J:364:ARG:HD2	1.98	0.45
1:K:49:ARG:NH1	1:K:52:TRP:CE2	2.85	0.45
2:L:161:GLU:OE1	2:L:161:GLU:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:39:LYS:HD2	4:P:84:ALA:HB2	1.97	0.45
3:W:158:ASP:OD1	3:W:185:GLN:NE2	2.48	0.45
2:D:176:LYS:NZ	2:D:259:SER:HB3	2.32	0.45
4:P:13:ALA:HA	4:P:107:LYS:HD2	1.97	0.45
3:Q:20:LEU:HD12	3:Q:83:LEU:HD23	1.98	0.45
4:T:42:LYS:HA	4:T:42:LYS:HD3	1.82	0.45
3:W:21:SER:HB3	3:W:80:ILE:HD11	1.98	0.45
2:F:246:PRO:HB3	2:F:283:GLN:HA	1.99	0.45
2:H:470:LYS:HE3	3:S:31:ASP:HB2	1.99	0.45
2:J:338:ASP:HB2	2:J:342:TYR:OH	2.17	0.45
4:V:184:ALA:O	4:V:188:LYS:HG3	2.17	0.45
4:X:37:GLN:HB2	4:X:47:LEU:HD11	1.98	0.45
1:A:49:ARG:NH1	1:A:52:TRP:CE2	2.84	0.45
1:E:26:PCA:HB2	1:E:27:ASN:H	1.46	0.45
3:O:12:VAL:O	3:O:125:VAL:HA	2.17	0.45
4:X:166:GLN:HG3	4:X:173:TYR:CZ	2.52	0.45
5:b:4:MAN:O6	5:b:4:MAN:O4	2.35	0.45
2:B:246:PRO:HB3	2:B:283:GLN:HA	1.99	0.44
3:O:214:HIS:HB3	3:O:219:THR:OG1	2.16	0.44
2:H:204:LEU:N	2:H:205:PRO:HD2	2.32	0.44
2:J:323:THR:C	2:J:331:ASN:HD21	2.25	0.44
3:S:52:LYS:O	3:S:74:ARG:NH1	2.50	0.44
2:B:176:LYS:HE3	2:B:190:PHE:CE2	2.52	0.44
2:D:415:SER:HB3	2:D:417:TYR:CE2	2.52	0.44
3:U:16:ARG:O	3:U:86:ASN:HA	2.16	0.44
2:B:292:ILE:HG21	2:B:292:ILE:HD13	1.70	0.44
2:H:338:ASP:HB3	2:H:342:TYR:OH	2.17	0.44
4:R:119:PRO:HB3	4:R:209:PHE:CE1	2.53	0.44
3:S:214:HIS:CD2	3:S:216:PRO:HD2	2.53	0.44
3:U:4:LEU:HD11	3:U:116:VAL:HG23	1.98	0.44
2:J:237:PHE:CE2	2:J:251:MET:SD	3.11	0.44
2:J:415:SER:HB3	2:J:417:TYR:CE2	2.52	0.44
3:M:12:VAL:HG13	3:M:125:VAL:HG22	1.98	0.44
2:L:264:MET:HE1	2:L:274:MET:HE1	1.99	0.44
3:M:103:PRO:HB3	3:M:108:SER:O	2.18	0.44
3:M:157:LYS:NZ	4:N:131:SER:OG	2.40	0.44
3:S:4:LEU:HD22	3:S:24:VAL:HG22	1.99	0.44
3:U:18:LEU:HD23	3:U:85:MET:CE	2.48	0.44
1:K:58:THR:HA	2:L:297:LEU:O	2.18	0.44
3:M:215:LYS:HB3	3:M:215:LYS:HE2	1.75	0.44
2:F:289:MET:HE2	2:F:289:MET:HB2	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:184:ALA:O	4:N:188:LYS:HG3	2.18	0.43
3:S:12:VAL:HG13	3:S:125:VAL:HG22	2.00	0.43
2:B:424:ALA:O	2:B:432:ILE:HG13	2.19	0.43
2:J:426:ASN:OD1	2:J:427:LYS:N	2.51	0.43
2:L:338:ASP:O	2:L:342:TYR:OH	2.34	0.43
3:U:47:TRP:CZ2	3:U:50:PHE:HB2	2.53	0.43
3:U:155:LEU:HD12	3:U:192:LEU:O	2.17	0.43
2:F:400:THR:HG22	2:F:402:VAL:HG13	2.00	0.43
2:H:405:SER:HB2	2:H:452:VAL:HG21	2.01	0.43
4:N:108:ARG:NH2	4:N:172:THR:HG22	2.33	0.43
4:R:210:ASN:HB2	4:R:213:GLU:OE1	2.18	0.43
4:X:34:ALA:O	4:X:88:CYS:HA	2.19	0.43
4:X:39:LYS:NZ	4:X:81:GLU:O	2.27	0.43
2:B:449:THR:HB	2:B:456:LEU:HD11	1.99	0.43
2:D:176:LYS:HD3	2:D:190:PHE:CD2	2.53	0.43
2:F:415:SER:HB3	2:F:417:TYR:CE2	2.53	0.43
2:J:294:GLU:HA	2:J:295:GLU:HA	1.58	0.43
4:R:34:ALA:O	4:R:88:CYS:HA	2.18	0.43
4:V:38:GLN:O	4:V:84:ALA:HB1	2.18	0.43
1:G:75:LYS:HD2	2:H:214:ILE:CG2	2.46	0.43
1:I:49:ARG:NH1	1:I:52:TRP:CE2	2.87	0.43
2:J:351:PHE:CE2	2:J:353:PRO:HG3	2.53	0.43
2:D:338:ASP:HB3	2:D:342:TYR:OH	2.18	0.43
2:L:283:GLN:HB3	2:L:359:LYS:HE2	2.00	0.43
3:U:85:MET:HB3	3:U:88:LEU:HD21	2.00	0.43
1:C:49:ARG:NH1	1:C:52:TRP:CE2	2.87	0.43
2:F:356:GLU:CD	2:F:356:GLU:H	2.27	0.43
2:L:291:ILE:HD13	2:L:291:ILE:HG21	1.75	0.43
4:P:108:ARG:HG2	4:P:109:THR:N	2.33	0.43
3:S:141:SER:OG	3:S:142:SER:N	2.50	0.43
2:D:183:ASN:OD1	2:D:185:VAL:HG12	2.18	0.43
2:H:416:CYS:O	2:H:437:ASN:HA	2.18	0.43
4:N:19:VAL:HG22	4:N:75:ILE:HB	2.01	0.43
4:X:33:LEU:HD13	4:X:34:ALA:N	2.34	0.43
2:B:318:THR:HG23	2:B:339:ARG:HB3	2.00	0.43
1:C:76:VAL:HA	1:C:79:ILE:HG22	2.01	0.43
2:D:312:PRO:HG2	2:D:344:ASP:OD2	2.19	0.43
2:L:294:GLU:HA	2:L:295:GLU:HA	1.55	0.43
4:N:33:LEU:HG	4:N:34:ALA:H	1.83	0.43
4:T:108:ARG:HG2	4:T:109:THR:N	2.34	0.43
2:D:316:LEU:HD23	2:D:338:ASP:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:GLU:HA	2:F:296:VAL:HG23	2.00	0.43
4:T:37:GLN:HB2	4:T:47:LEU:HD11	2.01	0.43
2:B:463:GLU:CD	2:B:463:GLU:H	2.27	0.42
2:J:318:THR:HG23	2:J:339:ARG:HB3	2.01	0.42
4:N:113:PRO:HB3	4:N:139:PHE:HB3	2.01	0.42
3:U:29:PHE:O	3:U:74:ARG:NH2	2.51	0.42
2:D:522:GLU:HB3	2:F:520:ILE:HG22	2.02	0.42
2:F:327:LYS:HZ3	2:F:329:GLY:H	1.66	0.42
2:F:388:ASN:OD1	2:F:389:PRO:HD2	2.19	0.42
1:K:77:LYS:HD2	1:K:77:LYS:HA	1.91	0.42
3:Q:2:VAL:HG12	3:Q:116:VAL:HG11	2.02	0.42
4:T:25:THR:HG21	4:T:29:VAL:HG23	2.01	0.42
4:T:61:ARG:NE	4:T:82:ASP:OD2	2.46	0.42
4:V:11:LEU:HD21	4:V:19:VAL:HB	2.00	0.42
2:H:150:SER:O	2:H:153:ALA:HB3	2.19	0.42
3:O:55:THR:C	3:O:56:TYR:HD1	2.28	0.42
5:Z:1:NAG:H5	5:Z:2:NAG:C7	2.49	0.42
1:A:58:THR:HA	2:B:297:LEU:O	2.19	0.42
2:B:164:VAL:CG2	2:B:291:ILE:HD11	2.50	0.42
2:L:396:MET:HG3	2:L:488:PHE:HA	2.01	0.42
4:R:33:LEU:HD13	4:R:34:ALA:N	2.34	0.42
3:W:113:GLY:HA2	4:X:91:PHE:CE1	2.54	0.42
4:X:140:TYR:CG	4:X:141:PRO:HA	2.54	0.42
2:B:137:PHE:CD2	2:B:137:PHE:C	2.97	0.42
4:N:158:ASN:HB3	4:N:179:LEU:HD12	2.02	0.42
4:R:66:GLY:HA3	4:R:71:PHE:HA	2.01	0.42
1:A:62:SER:HB3	2:B:196:LYS:HA	2.00	0.42
2:B:335:THR:HB	2:B:396:MET:HE2	2.01	0.42
3:W:183:VAL:HG11	4:X:160:GLN:HG2	2.01	0.42
1:I:62:SER:HB2	2:J:196:LYS:HA	2.01	0.42
4:T:88:CYS:O	4:T:99:GLY:N	2.52	0.42
5:c:3:BMA:O4	5:c:3:BMA:O6	2.32	0.42
2:B:204:LEU:N	2:B:205:PRO:HD2	2.35	0.42
1:E:30:GLU:HB2	2:F:410:LEU:HD12	2.02	0.42
2:F:393:CYS:HB2	2:F:492:ILE:HD11	2.01	0.42
4:N:108:ARG:HG2	4:N:109:THR:N	2.34	0.42
4:T:19:VAL:HG22	4:T:75:ILE:HB	2.01	0.42
2:H:292:ILE:HD12	2:H:297:LEU:HD13	2.02	0.41
2:J:246:PRO:HB3	2:J:283:GLN:HA	2.01	0.41
2:L:260:LEU:O	2:L:264:MET:HG3	2.20	0.41
2:L:394:LYS:HE3	2:L:394:LYS:HB3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:182:ALA:HA	3:W:192:LEU:HB3	2.01	0.41
1:E:62:SER:HB3	2:F:196:LYS:HA	2.02	0.41
2:F:204:LEU:N	2:F:205:PRO:HD2	2.36	0.41
2:F:338:ASP:N	2:F:338:ASP:OD1	2.51	0.41
2:J:405:SER:HB2	2:J:452:VAL:HG21	2.02	0.41
3:O:40:ALA:HB3	3:O:43:LYS:HB2	2.02	0.41
4:P:7:SER:HA	4:P:8:PRO:HA	1.83	0.41
3:Q:160:PHE:HA	3:Q:161:PRO:HA	1.86	0.41
4:R:7:SER:HA	4:R:8:PRO:HA	1.83	0.41
1:A:49:ARG:HE	2:B:368:ASP:CG	2.28	0.41
2:D:293:LYS:HG2	2:D:294:GLU:N	2.35	0.41
1:G:62:SER:HB3	2:H:196:LYS:HA	2.02	0.41
1:I:75:LYS:HB2	2:J:214:ILE:HB	2.01	0.41
2:J:240:ASN:HB2	2:J:244:THR:HG22	2.01	0.41
2:J:416:CYS:O	2:J:437:ASN:HA	2.20	0.41
3:O:117:TRP:CE3	4:P:44:PRO:HD2	2.55	0.41
4:V:21:ILE:HD12	4:V:73:LEU:HD23	2.02	0.41
2:F:503:LEU:HD23	2:F:503:LEU:HA	1.88	0.41
2:J:251:MET:HG3	2:J:299:TYR:CE2	2.55	0.41
1:K:49:ARG:HE	2:L:368:ASP:CG	2.28	0.41
3:M:151:ALA:HB2	3:M:197:THR:HG22	2.02	0.41
3:S:215:LYS:HE2	3:S:215:LYS:HB3	1.72	0.41
4:V:106:ILE:H	4:V:166:GLN:HE22	1.67	0.41
2:B:338:ASP:HB2	2:B:342:TYR:OH	2.20	0.41
2:B:370:MET:HE2	2:B:370:MET:HB2	1.89	0.41
2:F:463:GLU:CD	2:F:463:GLU:H	2.29	0.41
3:M:117:TRP:CE3	4:N:44:PRO:HD2	2.56	0.41
4:N:75:ILE:HG21	4:N:78:LEU:HD23	2.01	0.41
3:W:117:TRP:CE3	4:X:44:PRO:HD2	2.56	0.41
2:D:167:ILE:HG23	2:D:189:THR:HG21	2.02	0.41
2:F:494:GLN:HA	2:F:497:GLU:HG2	2.03	0.41
2:J:445:LYS:HE3	4:V:56:THR:HG23	2.03	0.41
4:N:7:SER:HA	4:N:8:PRO:HA	1.85	0.41
3:S:117:TRP:CE3	4:T:44:PRO:HD2	2.56	0.41
4:T:61:ARG:CZ	4:T:79:GLN:HG3	2.51	0.41
1:A:37:CYS:HB2	2:B:321:LEU:HD13	2.03	0.41
2:B:416:CYS:O	2:B:437:ASN:HA	2.21	0.41
2:H:159:HIS:HA	2:H:291:ILE:HD13	2.03	0.41
2:L:405:SER:HB2	2:L:452:VAL:HG21	2.03	0.41
4:V:38:GLN:NE2	4:V:42:LYS:O	2.54	0.41
3:W:214:HIS:ND1	3:W:217:SER:OG	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ALA:HB2	2:D:364:ARG:HD2	2.03	0.41
2:F:424:ALA:O	2:F:432:ILE:HG13	2.21	0.41
2:J:432:ILE:CD1	3:U:104:TYR:HB3	2.50	0.41
1:K:59:ILE:HG23	2:L:193:LEU:HB3	2.02	0.41
4:P:120:PRO:HD3	4:P:132:VAL:HG22	2.02	0.41
3:Q:113:GLY:HA2	4:R:91:PHE:CE1	2.56	0.41
4:R:82:ASP:O	4:R:86:TYR:OH	2.30	0.41
2:D:289:MET:HE1	2:D:297:LEU:CD1	2.51	0.41
2:L:161:GLU:HG3	4:V:18:ARG:HH12	1.84	0.41
2:L:171:LEU:HD13	2:L:191:LYS:HB2	2.02	0.41
3:O:113:GLY:HA2	4:P:91:PHE:CE1	2.56	0.41
4:R:48:ILE:HG12	4:R:54:LEU:HD12	2.03	0.41
4:R:108:ARG:HG2	4:R:109:THR:H	1.85	0.41
4:R:108:ARG:HD2	4:R:170:ASP:O	2.21	0.41
3:U:53:SER:HA	3:U:74:ARG:NH1	2.36	0.41
4:V:125:LEU:O	4:V:183:LYS:HD2	2.21	0.41
3:W:6:GLU:CD	3:W:120:GLY:H	2.29	0.41
1:C:28:ILE:HG22	2:D:410:LEU:HD11	2.03	0.41
1:G:32:PHE:CD1	2:H:441:TYR:HB2	2.56	0.41
2:J:162:GLY:O	2:J:166:LYS:HG3	2.21	0.41
3:O:113:GLY:HA2	4:P:91:PHE:CZ	2.56	0.41
3:Q:166:VAL:HG22	3:Q:212:VAL:HG22	2.03	0.41
3:Q:214:HIS:ND1	3:Q:217:SER:OG	2.38	0.41
4:R:12:SER:OG	4:R:105:GLU:OE2	2.26	0.41
4:R:113:PRO:HB3	4:R:139:PHE:HB3	2.02	0.41
3:S:20:LEU:HD12	3:S:83:LEU:HD23	2.02	0.41
2:B:227:ASN:O	2:B:231:LEU:HG	2.21	0.40
1:C:58:THR:HA	2:D:297:LEU:O	2.21	0.40
1:E:75:LYS:NZ	2:F:217:ILE:HB	2.36	0.40
3:S:173:LEU:HD21	3:S:196:VAL:HG21	2.03	0.40
2:D:283:GLN:HB3	2:D:359:LYS:HE2	2.03	0.40
4:R:19:VAL:HG22	4:R:75:ILE:HB	2.03	0.40
3:S:12:VAL:O	3:S:125:VAL:HA	2.21	0.40
3:S:47:TRP:CZ2	3:S:50:PHE:HB2	2.53	0.40
2:F:164:VAL:HG21	2:F:293:LYS:HD3	2.03	0.40
2:F:416:CYS:O	2:F:437:ASN:HA	2.21	0.40
2:H:462:GLN:HG2	2:J:156:LYS:NZ	2.35	0.40
3:M:112:TYR:CD1	4:N:49:PHE:CD2	3.10	0.40
3:O:100:ARG:HH21	3:O:115:ASP:CG	2.22	0.40
3:O:200:SER:O	3:O:203:LEU:HD12	2.21	0.40
4:V:198:HIS:CE1	4:V:200:GLY:H	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:86:TYR:HE2	4:X:104:LEU:HD12	1.87	0.40
2:B:487:GLU:HB3	2:B:490:ALA:HB2	2.03	0.40
2:J:171:LEU:HD11	2:J:189:THR:HG22	2.03	0.40
3:M:102:ALA:HB2	3:M:115:ASP:CG	2.46	0.40
4:P:35:TRP:CD2	4:P:73:LEU:HB2	2.57	0.40
3:Q:165:THR:OG1	3:Q:213:ASN:HB3	2.21	0.40
2:D:280:ILE:HG21	2:D:366:PHE:CG	2.56	0.40
2:F:543:PHE:HA	2:F:544:LEU:HA	1.76	0.40
2:H:399:LYS:NZ	2:H:485:SER:HB3	2.36	0.40
2:H:463:GLU:H	2:H:463:GLU:CD	2.29	0.40
1:I:26:PCA:HA	1:I:27:ASN:HA	1.82	0.40
2:L:281:VAL:O	2:L:285:SER:OG	2.33	0.40
3:Q:104:TYR:N	3:Q:110:TYR:O	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	69/84 (82%)	66 (96%)	3 (4%)	0	100	100
1	C	72/84 (86%)	69 (96%)	2 (3%)	1 (1%)	9	31
1	E	69/84 (82%)	65 (94%)	4 (6%)	0	100	100
1	G	72/84 (86%)	68 (94%)	3 (4%)	1 (1%)	9	31
1	I	76/84 (90%)	72 (95%)	4 (5%)	0	100	100
1	K	64/84 (76%)	62 (97%)	2 (3%)	0	100	100
2	B	400/414 (97%)	376 (94%)	23 (6%)	1 (0%)	36	65
2	D	400/414 (97%)	378 (94%)	19 (5%)	3 (1%)	16	44
2	F	397/414 (96%)	372 (94%)	24 (6%)	1 (0%)	36	65
2	H	385/414 (93%)	366 (95%)	19 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	381/414 (92%)	362 (95%)	18 (5%)	1 (0%)	36	65
2	L	390/414 (94%)	365 (94%)	25 (6%)	0	100	100
3	M	221/231 (96%)	212 (96%)	8 (4%)	1 (0%)	24	54
3	O	220/231 (95%)	210 (96%)	10 (4%)	0	100	100
3	Q	227/231 (98%)	214 (94%)	12 (5%)	1 (0%)	30	59
3	S	220/231 (95%)	208 (94%)	12 (6%)	0	100	100
3	U	205/231 (89%)	197 (96%)	8 (4%)	0	100	100
3	W	221/231 (96%)	209 (95%)	11 (5%)	1 (0%)	24	54
4	N	211/214 (99%)	202 (96%)	9 (4%)	0	100	100
4	P	211/214 (99%)	200 (95%)	11 (5%)	0	100	100
4	R	211/214 (99%)	200 (95%)	11 (5%)	0	100	100
4	T	211/214 (99%)	201 (95%)	10 (5%)	0	100	100
4	V	207/214 (97%)	200 (97%)	7 (3%)	0	100	100
4	X	211/214 (99%)	202 (96%)	9 (4%)	0	100	100
All	All	5351/5658 (95%)	5076 (95%)	264 (5%)	11 (0%)	43	71

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	531	VAL
1	C	67	ASN
2	D	295	GLU
2	F	294	GLU
2	B	542	THR
1	G	98	GLN
2	D	294	GLU
2	D	517	GLY
3	Q	140	PRO
3	W	227	PRO
3	M	163	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	63/74 (85%)	61 (97%)	2 (3%)	34	58
1	C	63/74 (85%)	63 (100%)	0	100	100
1	E	63/74 (85%)	62 (98%)	1 (2%)	55	68
1	G	63/74 (85%)	63 (100%)	0	100	100
1	I	66/74 (89%)	65 (98%)	1 (2%)	57	69
1	K	60/74 (81%)	60 (100%)	0	100	100
2	B	350/373 (94%)	347 (99%)	3 (1%)	70	76
2	D	344/373 (92%)	341 (99%)	3 (1%)	70	76
2	F	350/373 (94%)	344 (98%)	6 (2%)	53	67
2	H	339/373 (91%)	332 (98%)	7 (2%)	47	64
2	J	340/373 (91%)	335 (98%)	5 (2%)	57	69
2	L	340/373 (91%)	336 (99%)	4 (1%)	63	72
3	M	187/194 (96%)	184 (98%)	3 (2%)	55	68
3	O	186/194 (96%)	184 (99%)	2 (1%)	65	74
3	Q	190/194 (98%)	185 (97%)	5 (3%)	40	61
3	S	186/194 (96%)	183 (98%)	3 (2%)	55	68
3	U	173/194 (89%)	171 (99%)	2 (1%)	63	72
3	W	186/194 (96%)	184 (99%)	2 (1%)	65	74
4	N	185/187 (99%)	181 (98%)	4 (2%)	45	63
4	P	184/187 (98%)	183 (100%)	1 (0%)	81	81
4	R	185/187 (99%)	182 (98%)	3 (2%)	55	68
4	T	185/187 (99%)	180 (97%)	5 (3%)	39	60
4	V	176/187 (94%)	173 (98%)	3 (2%)	53	67
4	X	185/187 (99%)	182 (98%)	3 (2%)	55	68
All	All	4649/4968 (94%)	4581 (98%)	68 (2%)	57	69

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	99	SER
2	B	492	ILE

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Mol	Chain	Res	Type
2	B	520	ILE
2	B	539	LEU
2	D	266	ILE
2	D	370	MET
2	D	492	ILE
1	E	29	THR
2	F	264	MET
2	F	266	ILE
2	F	289	MET
2	F	361	GLN
2	F	505	PHE
2	F	506	ILE
2	H	155	CYS
2	H	172	LEU
2	H	264	MET
2	H	266	ILE
2	H	290	CYS
2	H	291	ILE
2	H	296	VAL
1	I	66	GLU
2	J	206	ILE
2	J	266	ILE
2	J	296	VAL
2	J	475	ILE
2	J	492	ILE
2	L	266	ILE
2	L	538	VAL
2	L	540	LEU
2	L	541	SER
3	M	5	VAL
3	M	91	GLU
3	M	219	THR
4	N	4	MET
4	N	36	TYR
4	N	90	GLN
4	N	109	THR
3	O	5	VAL
3	O	203	LEU
4	P	39	LYS
3	Q	5	VAL
3	Q	107	ASN
3	Q	116	VAL

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Mol	Chain	Res	Type
3	Q	164	VAL
3	Q	219	THR
4	R	4	MET
4	R	109	THR
4	R	201	LEU
3	S	55	THR
3	S	116	VAL
3	S	193	SER
4	T	4	MET
4	T	29	VAL
4	T	90	GLN
4	T	109	THR
4	T	152	ASN
3	U	5	VAL
3	U	219	THR
4	V	4	MET
4	V	90	GLN
4	V	152	ASN
3	W	55	THR
3	W	116	VAL
4	X	4	MET
4	X	90	GLN
4	X	152	ASN

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

Mol	Chain	Res	Type
2	B	165	ASN
2	B	197	ASN
2	B	225	GLN
2	B	283	GLN
2	B	383	ASN
2	B	428	ASN
2	B	454	ASN
1	C	94	GLN
2	D	165	ASN
2	D	225	GLN
2	D	276	ASN
2	D	354	GLN
2	D	380	ASN
2	D	460	ASN
2	F	225	GLN

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Mol	Chain	Res	Type
2	F	254	ASN
2	F	276	ASN
2	F	371	ASN
2	F	496	ASN
2	F	500	ASN
1	G	94	GLN
2	H	225	GLN
2	H	276	ASN
2	H	462	GLN
1	I	94	GLN
2	J	216	ASN
2	J	276	ASN
2	J	383	ASN
1	K	81	GLN
2	L	276	ASN
2	L	283	GLN
2	L	496	ASN
3	M	178	HIS
4	N	137	ASN
4	N	160	GLN
3	O	178	HIS
3	O	185	GLN
3	O	213	ASN
3	O	218	ASN
3	Q	84	GLN
3	Q	86	ASN
3	Q	213	ASN
3	S	84	GLN
4	T	147	GLN
4	V	27	GLN
3	W	84	GLN
4	X	210	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PCA	E	26	1	7,8,9	1.92	1 (14%)	9,10,12	2.15	5 (55%)
1	PCA	C	26	1,2	7,8,9	1.94	1 (14%)	9,10,12	2.09	5 (55%)
1	PCA	A	26	1	7,8,9	1.91	1 (14%)	9,10,12	2.34	5 (55%)
1	PCA	I	26	1	7,8,9	1.95	1 (14%)	9,10,12	2.22	6 (66%)
1	PCA	G	26	1	7,8,9	1.97	1 (14%)	9,10,12	2.20	5 (55%)
1	PCA	K	26	1	7,8,9	1.95	1 (14%)	9,10,12	2.30	5 (55%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	E	26	1	-	0/0/11/13	0/1/1/1
1	PCA	C	26	1,2	-	0/0/11/13	0/1/1/1
1	PCA	A	26	1	-	0/0/11/13	0/1/1/1
1	PCA	I	26	1	-	0/0/11/13	0/1/1/1
1	PCA	G	26	1	-	0/0/11/13	0/1/1/1
1	PCA	K	26	1	-	0/0/11/13	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	26	PCA	CD-N	5.08	1.47	1.34
1	I	26	PCA	CD-N	5.05	1.47	1.34
1	K	26	PCA	CD-N	5.03	1.47	1.34
1	C	26	PCA	CD-N	4.98	1.46	1.34
1	E	26	PCA	CD-N	4.95	1.46	1.34
1	A	26	PCA	CD-N	4.89	1.46	1.34

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	PCA	CB-CA-C	-3.45	107.93	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	26	PCA	OE-CD-CG	-3.14	121.11	126.72
1	K	26	PCA	CA-N-CD	-3.13	102.87	113.58
1	A	26	PCA	OE-CD-CG	-3.12	121.15	126.72
1	I	26	PCA	OE-CD-CG	-3.06	121.27	126.72
1	K	26	PCA	CB-CA-N	3.06	111.65	103.24
1	G	26	PCA	OE-CD-CG	-3.00	121.36	126.72
1	G	26	PCA	CB-CA-C	-2.97	108.59	112.66
1	C	26	PCA	CA-N-CD	-2.95	103.46	113.58
1	I	26	PCA	CA-N-CD	-2.95	103.46	113.58
1	A	26	PCA	CA-N-CD	-2.94	103.51	113.58
1	E	26	PCA	CA-N-CD	-2.90	103.64	113.58
1	C	26	PCA	CB-CA-N	2.89	111.19	103.24
1	G	26	PCA	CA-N-CD	-2.86	103.77	113.58
1	I	26	PCA	CB-CA-N	2.85	111.07	103.24
1	E	26	PCA	OE-CD-CG	-2.83	121.66	126.72
1	E	26	PCA	CB-CA-N	2.81	110.98	103.24
1	A	26	PCA	CG-CD-N	2.78	115.19	108.39
1	E	26	PCA	CB-CA-C	-2.72	108.92	112.66
1	C	26	PCA	OE-CD-CG	-2.71	121.89	126.72
1	K	26	PCA	CG-CD-N	2.69	114.96	108.39
1	G	26	PCA	CB-CA-N	2.65	110.54	103.24
1	A	26	PCA	CB-CA-N	2.65	110.53	103.24
1	K	26	PCA	O-C-CA	-2.62	118.04	124.77
1	G	26	PCA	CG-CD-N	2.54	114.61	108.39
1	I	26	PCA	CG-CD-N	2.52	114.56	108.39
1	C	26	PCA	CG-CD-N	2.51	114.53	108.39
1	I	26	PCA	O-C-CA	-2.47	118.41	124.77
1	E	26	PCA	CG-CD-N	2.45	114.38	108.39
1	C	26	PCA	CB-CA-C	-2.17	109.67	112.66
1	I	26	PCA	CB-CA-C	-2.03	109.87	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	26	PCA	1	0
1	I	26	PCA	1	0

5.5 Carbohydrates ⓘ

24 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	Y	1	1,5	14,14,15	0.75	1 (7%)	17,19,21	0.52	0
5	NAG	Y	2	5	14,14,15	0.28	0	17,19,21	0.50	0
5	BMA	Y	3	5	11,11,12	1.26	1 (9%)	15,15,17	0.84	0
5	MAN	Y	4	5	11,11,12	1.29	2 (18%)	15,15,17	1.32	1 (6%)
5	NAG	Z	1	1,5	14,14,15	0.79	0	17,19,21	0.53	0
5	NAG	Z	2	5	14,14,15	0.26	0	17,19,21	0.56	0
5	BMA	Z	3	5	11,11,12	1.08	1 (9%)	15,15,17	0.82	0
5	MAN	Z	4	5	11,11,12	1.02	0	15,15,17	1.19	1 (6%)
5	NAG	a	1	1,5	14,14,15	0.79	1 (7%)	17,19,21	0.47	0
5	NAG	a	2	5	14,14,15	0.32	0	17,19,21	0.61	0
5	BMA	a	3	5	11,11,12	1.00	1 (9%)	15,15,17	0.85	0
5	MAN	a	4	5	11,11,12	1.16	2 (18%)	15,15,17	1.44	1 (6%)
5	NAG	b	1	1,5	14,14,15	0.58	0	17,19,21	0.44	0
5	NAG	b	2	5	14,14,15	0.47	0	17,19,21	1.09	1 (5%)
5	BMA	b	3	5	11,11,12	1.45	2 (18%)	15,15,17	1.22	2 (13%)
5	MAN	b	4	5	11,11,12	1.17	1 (9%)	15,15,17	1.35	2 (13%)
5	NAG	c	1	1,5	14,14,15	0.85	1 (7%)	17,19,21	0.63	0
5	NAG	c	2	5	14,14,15	0.44	0	17,19,21	0.48	0
5	BMA	c	3	5	11,11,12	1.02	1 (9%)	15,15,17	0.78	0
5	MAN	c	4	5	11,11,12	1.09	1 (9%)	15,15,17	1.33	2 (13%)
5	NAG	d	1	1,5	14,14,15	0.98	2 (14%)	17,19,21	0.64	0
5	NAG	d	2	5	14,14,15	0.40	0	17,19,21	0.53	0
5	BMA	d	3	5	11,11,12	1.23	2 (18%)	15,15,17	0.86	0
5	MAN	d	4	5	11,11,12	1.37	2 (18%)	15,15,17	1.34	1 (6%)

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	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	1/6/23/26	0/1/1/1
5	BMA	Y	3	5	-	1/2/19/22	0/1/1/1
5	MAN	Y	4	5	-	1/2/19/22	0/1/1/1
5	NAG	Z	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	1/6/23/26	0/1/1/1
5	BMA	Z	3	5	-	1/2/19/22	0/1/1/1
5	MAN	Z	4	5	-	1/2/19/22	0/1/1/1
5	NAG	a	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	a	2	5	-	1/6/23/26	0/1/1/1
5	BMA	a	3	5	-	2/2/19/22	0/1/1/1
5	MAN	a	4	5	-	1/2/19/22	0/1/1/1
5	NAG	b	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	0/6/23/26	0/1/1/1
5	BMA	b	3	5	-	2/2/19/22	0/1/1/1
5	MAN	b	4	5	-	1/2/19/22	0/1/1/1
5	NAG	c	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	1/6/23/26	0/1/1/1
5	BMA	c	3	5	-	1/2/19/22	0/1/1/1
5	MAN	c	4	5	-	1/2/19/22	0/1/1/1
5	NAG	d	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	d	2	5	-	1/6/23/26	0/1/1/1
5	BMA	d	3	5	-	1/2/19/22	0/1/1/1
5	MAN	d	4	5	-	1/2/19/22	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	b	3	BMA	C1-C2	3.76	1.61	1.52
5	d	3	BMA	C1-C2	3.04	1.59	1.52
5	d	4	MAN	C1-C2	2.97	1.59	1.52
5	Y	3	BMA	C1-C2	2.95	1.59	1.52
5	d	4	MAN	C2-C3	2.65	1.56	1.52
5	c	3	BMA	C1-C2	2.65	1.58	1.52
5	b	4	MAN	C1-C2	2.63	1.58	1.52
5	a	4	MAN	C2-C3	2.61	1.56	1.52
5	c	4	MAN	C1-C2	2.59	1.58	1.52
5	Y	4	MAN	C1-C2	2.57	1.58	1.52
5	Y	4	MAN	C2-C3	2.55	1.56	1.52
5	Z	3	BMA	C1-C2	2.44	1.58	1.52
5	d	1	NAG	O5-C1	-2.43	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	d	1	NAG	C1-C2	2.38	1.55	1.52
5	b	3	BMA	C2-C3	2.31	1.56	1.52
5	c	1	NAG	C1-C2	2.25	1.55	1.52
5	a	3	BMA	C1-C2	2.20	1.57	1.52
5	d	3	BMA	C2-C3	2.19	1.55	1.52
5	Y	1	NAG	C1-C2	2.18	1.55	1.52
5	a	4	MAN	C1-C2	2.06	1.57	1.52
5	a	1	NAG	C1-C2	2.03	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a	4	MAN	C1-O5-C5	3.91	117.43	112.19
5	c	4	MAN	C1-O5-C5	3.55	116.95	112.19
5	Y	4	MAN	C1-O5-C5	3.47	116.84	112.19
5	d	4	MAN	C1-O5-C5	3.47	116.84	112.19
5	b	4	MAN	C1-O5-C5	3.46	116.83	112.19
5	Z	4	MAN	C1-O5-C5	3.42	116.77	112.19
5	b	3	BMA	C1-O5-C5	3.30	116.60	112.19
5	b	2	NAG	O4-C4-C3	-2.84	103.67	110.38
5	c	4	MAN	O2-C2-C3	-2.30	105.39	110.15
5	b	4	MAN	O2-C2-C3	-2.05	105.90	110.15
5	b	3	BMA	O3-C3-C2	2.03	114.20	110.05

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	c	1	NAG	C4-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
5	b	3	BMA	C4-C5-C6-O6
5	a	3	BMA	O5-C5-C6-O6
5	b	3	BMA	O5-C5-C6-O6
5	c	3	BMA	O5-C5-C6-O6
5	Y	2	NAG	O5-C5-C6-O6
5	a	4	MAN	O5-C5-C6-O6
5	d	2	NAG	O5-C5-C6-O6
5	Y	3	BMA	O5-C5-C6-O6
5	Y	4	MAN	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
5	d	3	BMA	O5-C5-C6-O6
5	d	4	MAN	O5-C5-C6-O6

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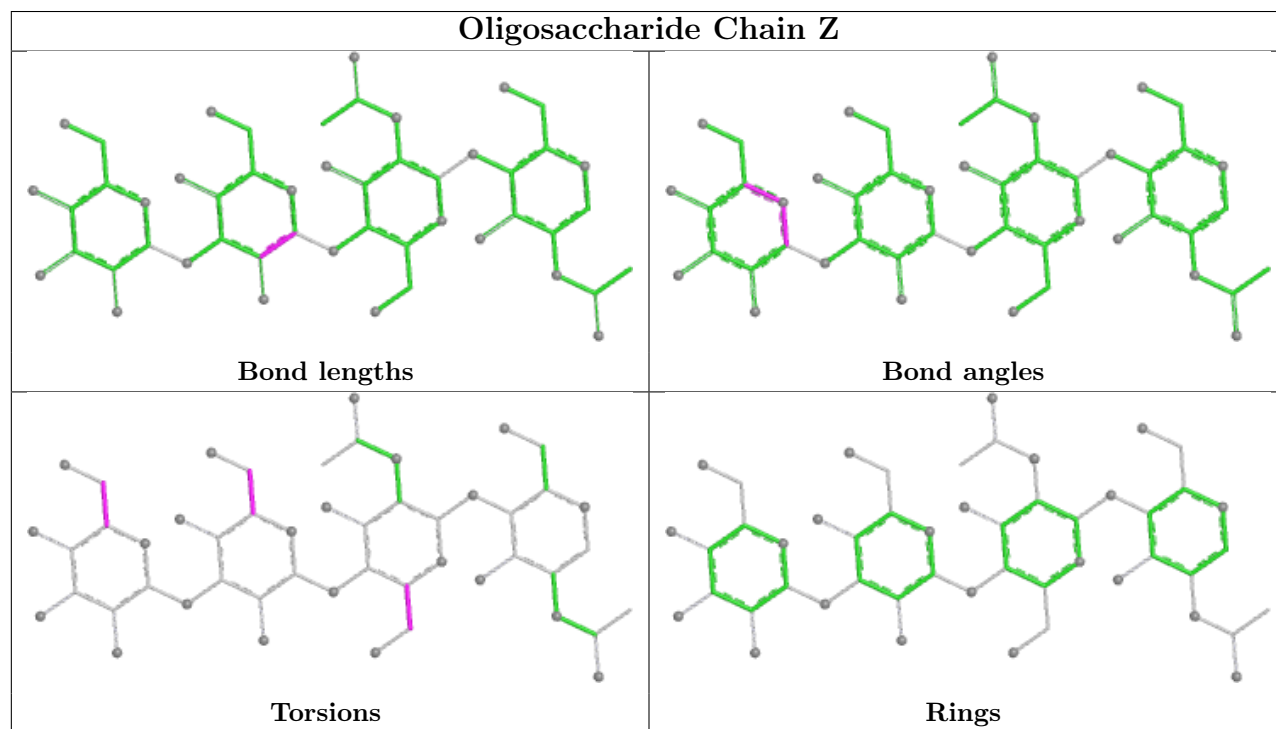
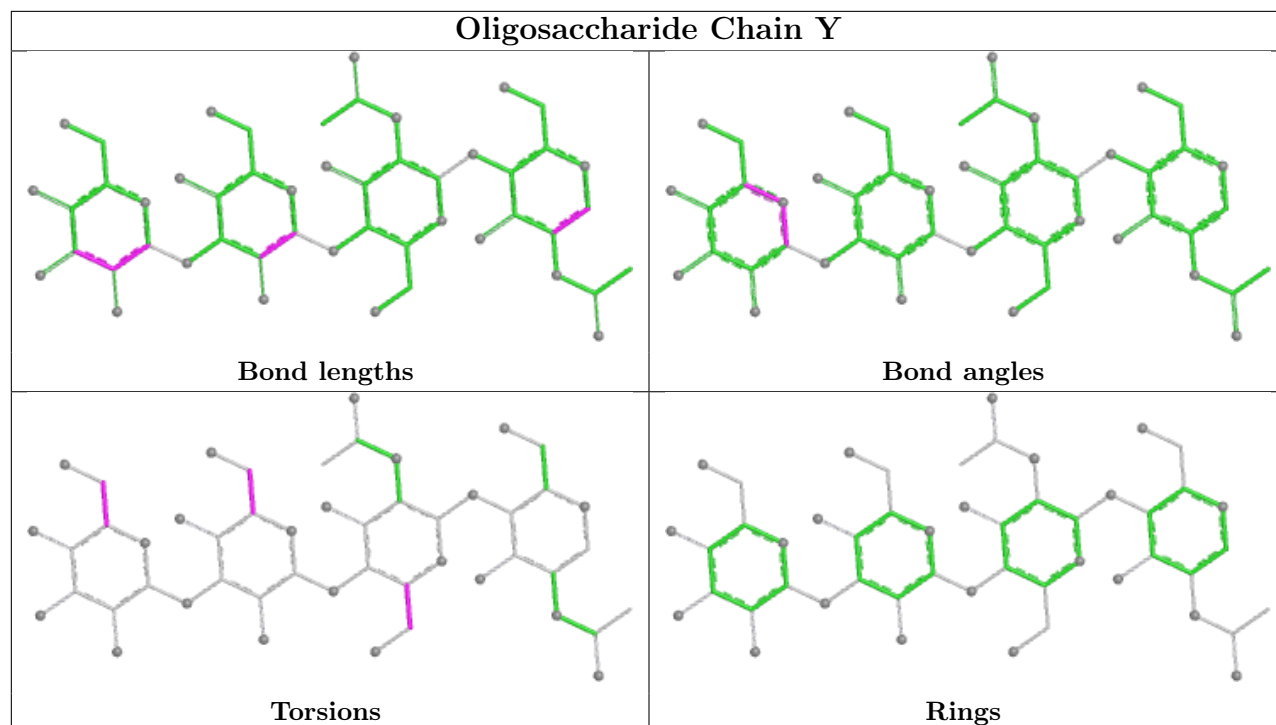
Mol	Chain	Res	Type	Atoms
5	Z	2	NAG	O5-C5-C6-O6
5	Z	3	BMA	O5-C5-C6-O6
5	Z	4	MAN	O5-C5-C6-O6
5	a	2	NAG	O5-C5-C6-O6
5	b	4	MAN	O5-C5-C6-O6
5	c	4	MAN	O5-C5-C6-O6
5	a	3	BMA	C4-C5-C6-O6

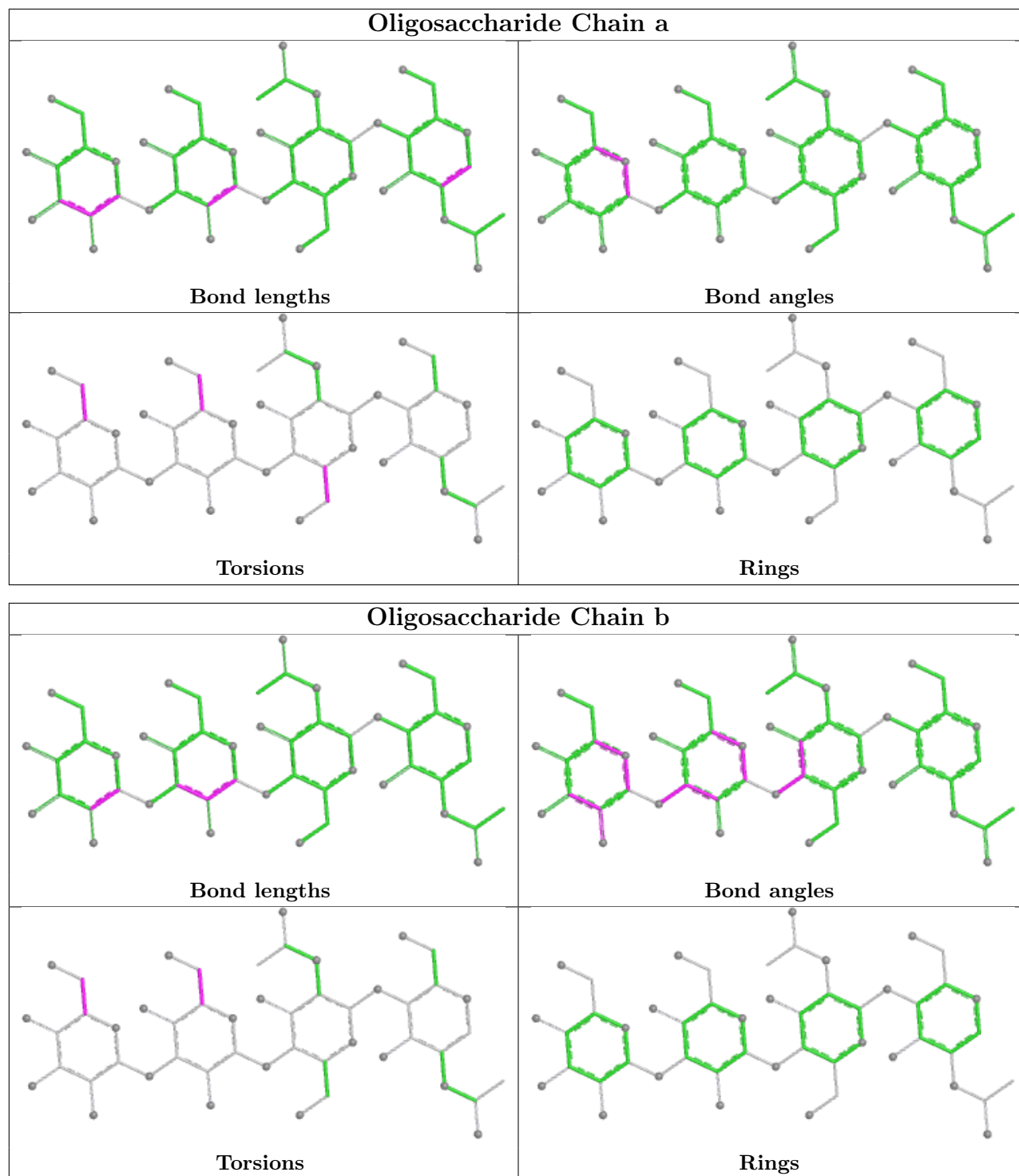
There are no ring outliers.

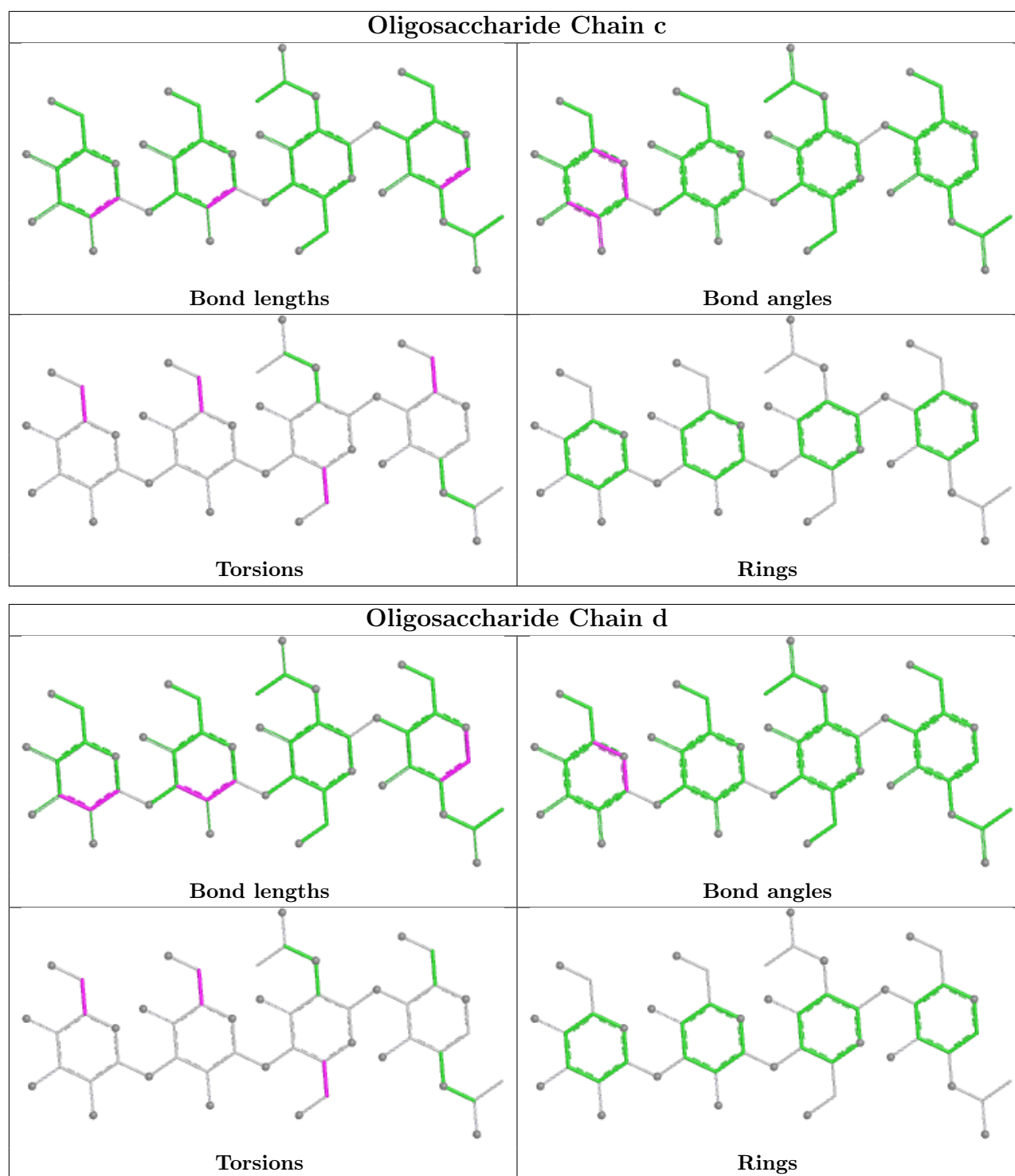
10 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	b	2	NAG	1	0
5	a	3	BMA	1	0
5	c	3	BMA	1	0
5	Z	1	NAG	1	0
5	b	4	MAN	1	0
5	d	1	NAG	1	0
5	Y	3	BMA	1	0
5	b	3	BMA	1	0
5	Z	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](#)

4 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	$\# Z > 2$
6	NAG	F	1001	-	14,14,15	0.28	0	17,19,21	0.50	0
6	NAG	B	1001	2	14,14,15	0.40	0	17,19,21	0.54	0
6	NAG	J	1001	2	14,14,15	0.56	0	17,19,21	0.44	0
6	NAG	L	1001	2	14,14,15	0.55	0	17,19,21	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	F	1001	-	-	1/6/23/26	0/1/1/1
6	NAG	B	1001	2	-	4/6/23/26	0/1/1/1
6	NAG	J	1001	2	-	1/6/23/26	0/1/1/1
6	NAG	L	1001	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1001	NAG	O5-C5-C6-O6
6	B	1001	NAG	C4-C5-C6-O6
6	F	1001	NAG	O5-C5-C6-O6
6	J	1001	NAG	O5-C5-C6-O6
6	B	1001	NAG	C3-C2-N2-C7
6	L	1001	NAG	C3-C2-N2-C7
6	B	1001	NAG	C1-C2-N2-C7
6	L	1001	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	72/84 (85%)	0.71	6 (8%)	17 15	57, 89, 118, 123	0
1	C	75/84 (89%)	0.65	4 (5%)	32 24	61, 88, 124, 127	0
1	E	72/84 (85%)	0.43	3 (4%)	40 29	54, 96, 122, 124	0
1	G	75/84 (89%)	0.78	6 (8%)	18 16	59, 96, 126, 137	0
1	I	77/84 (91%)	0.69	5 (6%)	25 20	60, 95, 125, 129	0
1	K	69/84 (82%)	0.55	3 (4%)	40 29	67, 93, 122, 134	0
2	B	404/414 (97%)	0.49	10 (2%)	58 43	55, 70, 109, 130	0
2	D	404/414 (97%)	0.40	8 (1%)	65 49	61, 75, 110, 131	0
2	F	401/414 (96%)	0.45	9 (2%)	62 47	52, 75, 109, 122	0
2	H	395/414 (95%)	0.47	12 (3%)	52 39	55, 80, 120, 131	0
2	J	389/414 (93%)	0.56	15 (3%)	43 31	60, 77, 118, 130	0
2	L	396/414 (95%)	0.60	12 (3%)	52 39	64, 80, 123, 133	0
3	M	225/231 (97%)	0.23	0	100 100	56, 70, 79, 100	0
3	O	224/231 (96%)	0.38	6 (2%)	56 42	65, 71, 79, 94	1 (0%)
3	Q	229/231 (99%)	0.32	2 (0%)	81 68	55, 78, 93, 96	0
3	S	224/231 (96%)	0.18	1 (0%)	88 81	53, 58, 69, 83	0
3	U	215/231 (93%)	1.16	35 (16%)	4 6	74, 115, 150, 152	0
3	W	225/231 (97%)	0.31	2 (0%)	81 68	64, 71, 81, 103	1 (0%)
4	N	213/214 (99%)	0.31	2 (0%)	81 68	55, 69, 85, 96	0
4	P	213/214 (99%)	0.48	2 (0%)	81 68	71, 81, 90, 93	0
4	R	213/214 (99%)	0.29	3 (1%)	73 59	61, 79, 92, 95	0
4	T	213/214 (99%)	0.22	1 (0%)	87 78	56, 65, 72, 79	0
4	V	209/214 (97%)	0.98	18 (8%)	16 15	91, 124, 152, 156	0
4	X	213/214 (99%)	0.30	5 (2%)	61 46	64, 72, 88, 103	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	5445/5658 (96%)	0.47	170 (3%)	51	38	52, 75, 123, 156	2 (0%)

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	102	ALA	5.1
1	G	103	THR	4.6
1	I	101	PRO	4.4
1	A	103	THR	4.3
1	C	103	THR	4.2
1	C	101	PRO	4.1
4	V	175	LEU	3.9
3	U	58	GLY	3.9
1	G	100	THR	3.8
4	X	145	LYS	3.8
3	U	101	GLY	3.6
3	U	129	SER	3.6
2	B	509	SER	3.6
1	I	102	ALA	3.5
2	B	137	PHE	3.4
1	E	100	THR	3.4
3	U	140	PRO	3.4
4	V	1	ASP	3.4
3	O	112	TYR	3.4
3	Q	145	THR	3.4
4	P	49	PHE	3.4
4	V	110	VAL	3.3
3	U	163	PRO	3.3
1	A	102	ALA	3.2
1	I	103	THR	3.2
2	L	540	LEU	3.2
1	C	102	ALA	3.1
1	G	92	GLU	3.1
3	U	227	PRO	3.1
1	A	101	PRO	3.0
3	U	197	THR	3.0
3	U	152	LEU	3.0
3	O	115	ASP	3.0
4	V	205	VAL	2.9
2	F	489	ASP	2.9
3	U	156	VAL	2.9
4	V	190	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
4	V	82	ASP	2.9
3	U	196	VAL	2.8
2	H	520	ILE	2.8
1	A	99	SER	2.8
2	D	354	GLN	2.8
2	F	512	LEU	2.8
2	H	216	ASN	2.8
2	J	536	GLU	2.8
2	J	534	ASP	2.7
2	F	511	GLU	2.7
3	U	176	GLY	2.7
4	V	170	ASP	2.7
2	L	371	ASN	2.7
1	E	66	GLU	2.6
2	H	161	GLU	2.6
3	U	150	ALA	2.6
2	B	542	THR	2.6
2	H	544	LEU	2.6
2	L	537	TRP	2.6
3	U	88	LEU	2.6
2	L	216	ASN	2.6
4	X	147	GLN	2.6
1	A	100	THR	2.6
2	F	356	GLU	2.6
2	D	367	CYS	2.5
3	O	113	GLY	2.5
4	V	40	PRO	2.5
3	U	221	VAL	2.5
1	I	97	MET	2.5
2	L	505	PHE	2.5
3	U	154	CYS	2.5
1	K	92	GLU	2.5
2	L	536	GLU	2.5
1	K	28	ILE	2.5
3	W	31	ASP	2.5
2	F	488	PHE	2.5
2	J	488	PHE	2.5
1	G	101	PRO	2.5
1	I	92	GLU	2.5
3	U	151	ALA	2.4
2	D	543	PHE	2.4
2	L	488	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	542	THR	2.4
4	V	206	THR	2.4
4	V	168	SER	2.4
4	V	207	LYS	2.4
2	J	458	TYR	2.4
3	U	41	PRO	2.4
2	H	468	TYR	2.4
2	D	488	PHE	2.4
2	J	539	LEU	2.4
3	U	87	SER	2.4
3	U	198	VAL	2.4
2	H	279	GLN	2.4
2	J	528	GLN	2.4
4	V	135	LEU	2.4
3	U	97	TYR	2.3
4	V	34	ALA	2.3
3	U	160	PHE	2.3
3	U	189	LEU	2.3
4	V	114	SER	2.3
3	U	31	ASP	2.3
4	V	165	GLU	2.3
4	R	142	ARG	2.3
3	U	21	SER	2.3
4	V	136	LEU	2.3
2	J	161	GLU	2.3
4	P	143	GLU	2.3
2	J	529	ALA	2.3
4	R	51	ALA	2.3
2	L	544	LEU	2.3
2	H	185	VAL	2.3
2	B	161	GLU	2.2
3	U	155	LEU	2.2
2	J	215	SER	2.2
3	U	164	VAL	2.2
4	X	196	VAL	2.2
1	A	92	GLU	2.2
3	O	31	ASP	2.2
2	B	488	PHE	2.2
3	U	126	SER	2.2
2	J	214	ILE	2.2
2	H	207	LEU	2.2
3	U	48	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	J	540	LEU	2.2
4	X	165	GLU	2.2
2	H	488	PHE	2.2
2	B	528	GLN	2.2
3	U	191	SER	2.2
2	F	463	GLU	2.2
2	J	356	GLU	2.2
4	R	152	ASN	2.2
3	U	148	GLY	2.2
3	O	230	CYS	2.2
2	H	217	ILE	2.1
2	B	540	LEU	2.1
2	F	207	LEU	2.1
4	V	181	LEU	2.1
2	J	493	SER	2.1
1	K	60	GLU	2.1
2	L	497	GLU	2.1
2	J	343	CYS	2.1
2	D	161	GLU	2.1
3	Q	126	SER	2.1
2	D	343	CYS	2.1
4	N	108	ARG	2.1
1	G	74	ALA	2.1
3	U	137	PRO	2.1
4	N	165	GLU	2.1
3	U	201	SER	2.1
2	B	526	ASP	2.1
4	T	33	LEU	2.1
2	L	525	ARG	2.1
4	V	6	GLN	2.1
2	L	404	SER	2.1
2	B	428	ASN	2.1
2	H	183	ASN	2.1
2	F	544	LEU	2.1
3	S	31	ASP	2.1
3	U	208	TYR	2.1
2	F	355	ALA	2.1
2	L	328	GLU	2.1
4	X	143	GLU	2.1
3	U	166	VAL	2.0
2	B	525	ARG	2.0
2	H	214	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
3	W	117	TRP	2.0
3	O	81	ALA	2.0
3	U	165	THR	2.0
1	C	92	GLU	2.0
2	J	388	ASN	2.0
1	E	92	GLU	2.0
2	D	495	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PCA	I	26	8/9	0.69	0.24	97,98,99,99	0
1	PCA	E	26	8/9	0.74	0.18	81,81,82,82	0
1	PCA	C	26	8/9	0.77	0.17	76,76,77,77	0
1	PCA	K	26	8/9	0.78	0.15	79,79,80,81	0
1	PCA	A	26	8/9	0.80	0.15	68,70,71,72	0
1	PCA	G	26	8/9	0.86	0.13	76,77,78,78	0

6.3 Carbohydrates [i](#)

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

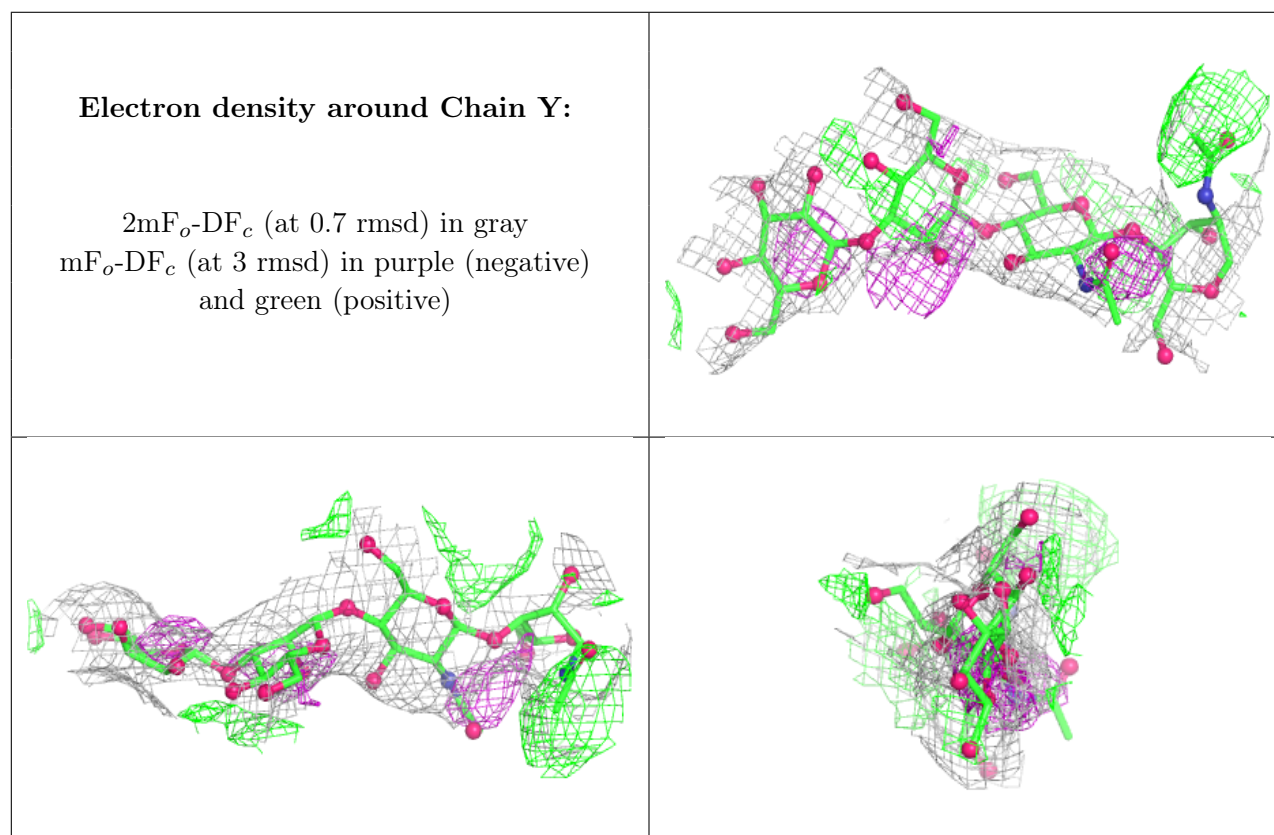
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	Y	1	14/15	0.25	0.20	81,85,86,86	0
5	NAG	Z	1	14/15	0.27	0.19	85,88,90,90	0
5	NAG	Z	2	14/15	0.41	0.22	92,93,94,94	0
5	BMA	Z	3	11/12	0.48	0.23	90,92,93,94	0
5	BMA	Y	3	11/12	0.53	0.20	84,85,86,86	0
5	NAG	Y	2	14/15	0.54	0.16	86,87,88,88	0
5	MAN	Z	4	11/12	0.54	0.17	88,90,90,91	0
5	MAN	Y	4	11/12	0.57	0.15	83,84,85,85	0
5	NAG	a	1	14/15	-	-	83,86,88,88	0
5	NAG	a	2	14/15	-	-	85,88,88,89	0

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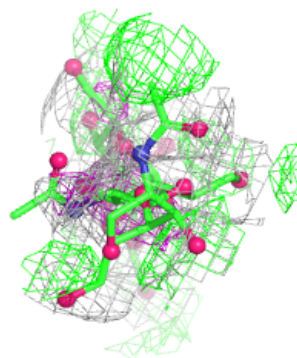
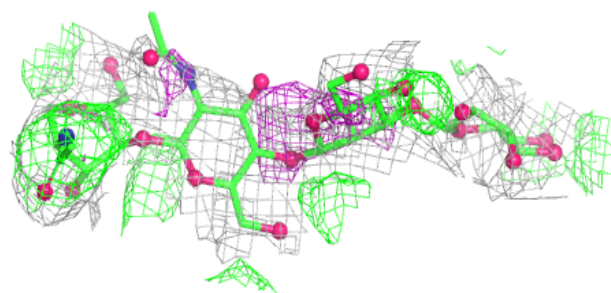
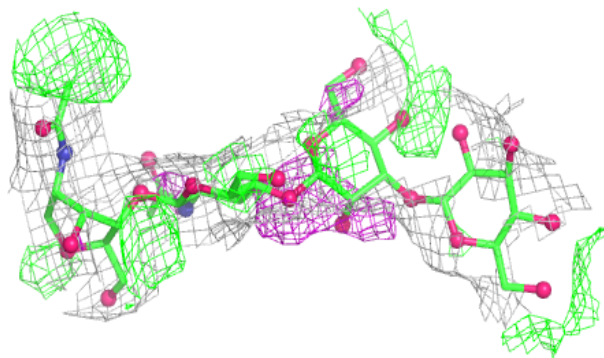
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BMA	a	3	11/12	-	-	84,85,87,88	0
5	MAN	a	4	11/12	-	-	82,84,85,85	0
5	NAG	b	1	14/15	-	-	76,79,80,80	0
5	NAG	b	2	14/15	-	-	79,81,81,82	0
5	BMA	b	3	11/12	-	-	77,80,82,82	0
5	MAN	b	4	11/12	-	-	75,77,77,78	0
5	NAG	c	1	14/15	-	-	104,108,109,109	0
5	NAG	c	2	14/15	-	-	114,115,115,116	0
5	BMA	c	3	11/12	-	-	116,118,118,118	0
5	MAN	c	4	11/12	-	-	117,118,119,119	0
5	NAG	d	1	14/15	-	-	87,91,93,93	0
5	NAG	d	2	14/15	-	-	89,92,94,94	0
5	BMA	d	3	11/12	-	-	89,90,91,91	0
5	MAN	d	4	11/12	-	-	86,87,88,88	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.

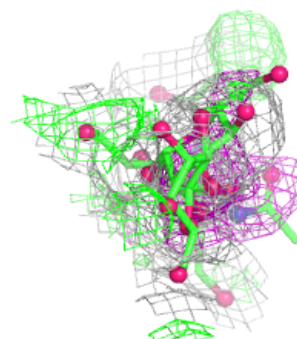
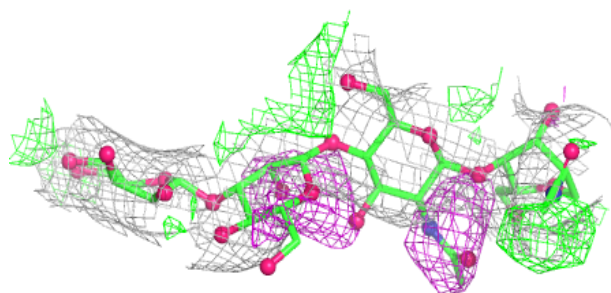
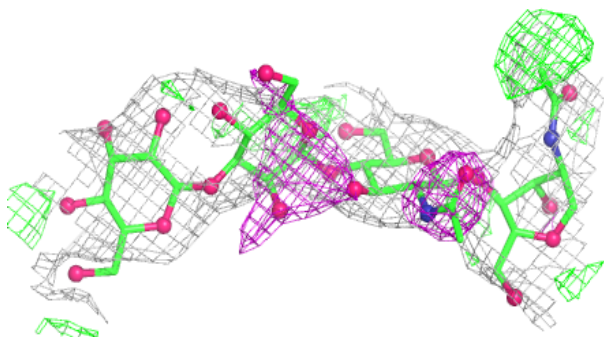


Electron density around Chain Z:

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

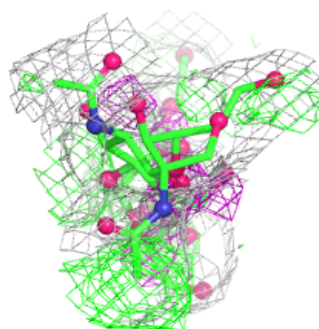
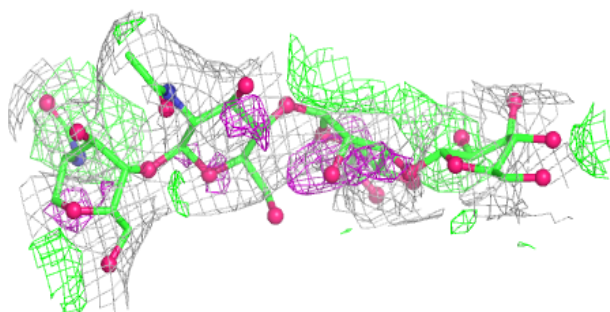
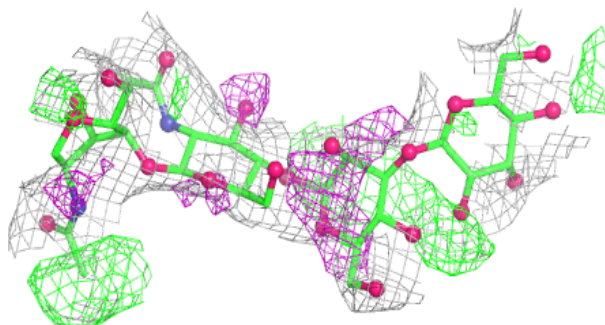
**Electron density around Chain a:**

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

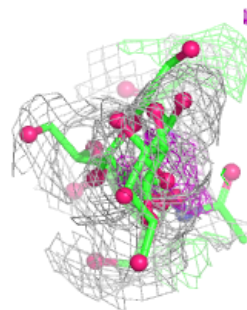
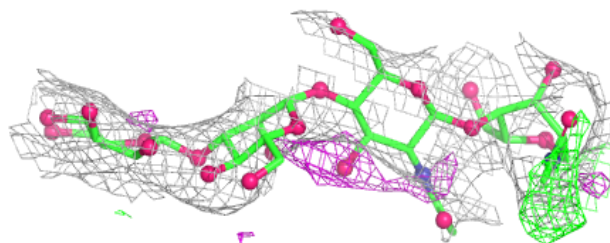
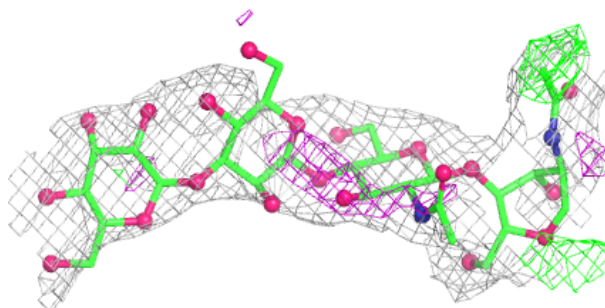


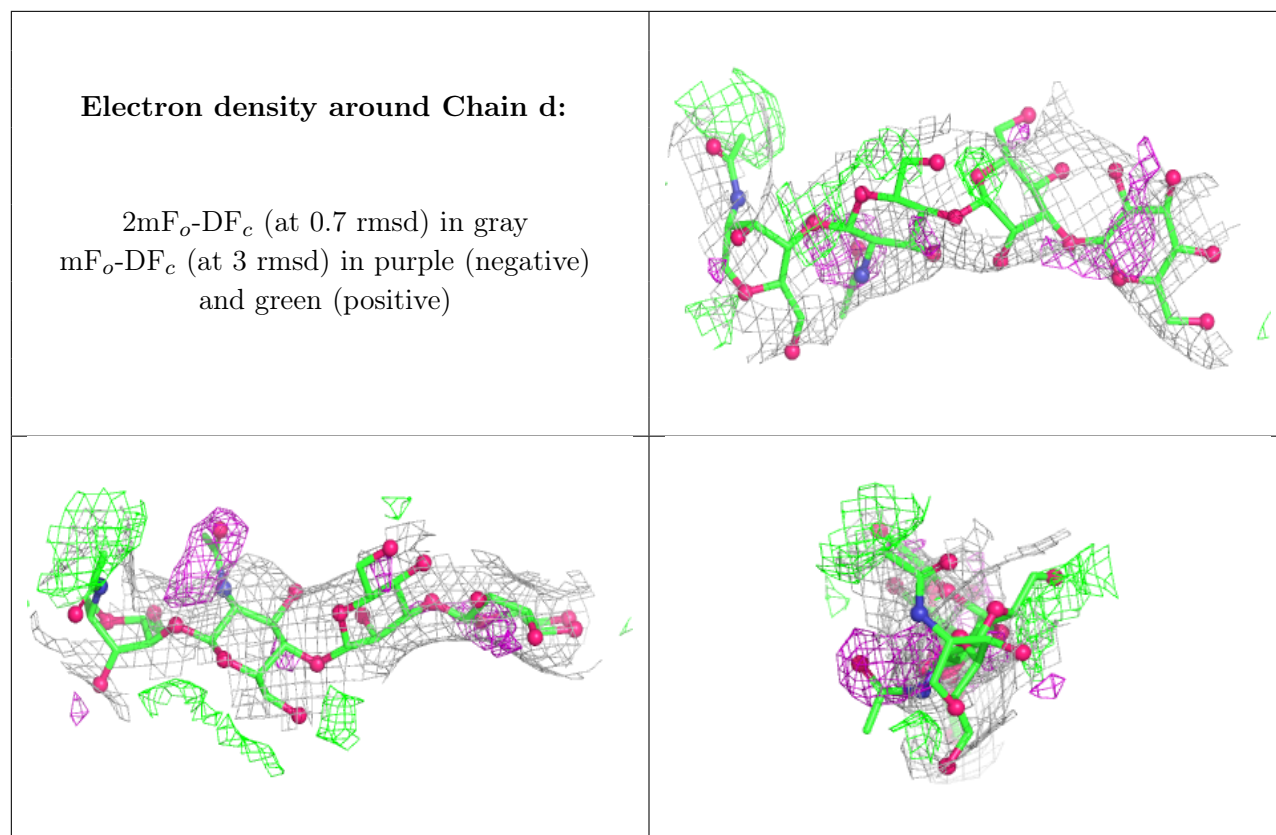
Electron density around Chain b:

$2mF_o-DF_c$ (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)





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
6	NAG	F	1001	14/15	0.35	0.19	100,102,103,103	0
6	NAG	B	1001	14/15	0.48	0.15	100,101,101,102	0
6	NAG	J	1001	14/15	0.49	0.14	92,94,95,95	0
6	NAG	L	1001	14/15	0.51	0.13	105,107,107,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.