



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:01 PM UTC

PDB ID : 8E0P / pdb_00008e0p
Title : Crystal structure of mouse APCDD1 in fusion with engineered MBP
Authors : Hsieh, F.L.; Chang, T.H.; Gabelli, S.B.; Nathans, J.
Deposited on : 2022-08-09
Resolution : 2.33 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

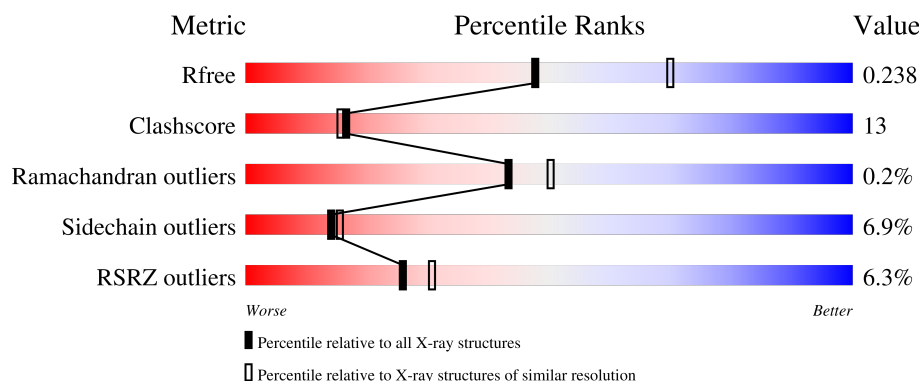
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	818	
1	B	818	
1	C	818	
1	D	818	
2	F	2	

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Mol	Chain	Length	Quality of chain
2	G	2	 50%50%
2	H	2	 100%
2	I	2	 50%50%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 25921 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 Maltodextrin-binding protein, Protein APCDD1 complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	778	Total	C	N	O	S	0	3	0
			6184	3943	1076	1139	26			
1	B	789	Total	C	N	O	S	0	2	0
			6242	3975	1086	1153	28			
1	C	782	Total	C	N	O	S	0	4	0
			6221	3967	1078	1150	26			
1	D	784	Total	C	N	O	S	0	6	0
			6251	3978	1088	1159	26			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	-	expression tag	UNP C3SHQ8
A	2	THR	-	expression tag	UNP C3SHQ8
A	3	GLY	-	expression tag	UNP C3SHQ8
A	4	LYS	-	expression tag	UNP C3SHQ8
A	5	THR	-	expression tag	UNP C3SHQ8
A	85	ALA	ASP	engineered mutation	UNP C3SHQ8
A	86	ALA	LYS	engineered mutation	UNP C3SHQ8
A	175	ALA	GLU	engineered mutation	UNP C3SHQ8
A	176	ALA	ASN	engineered mutation	UNP C3SHQ8
A	218	HIS	ALA	engineered mutation	UNP C3SHQ8
A	222	HIS	LYS	engineered mutation	UNP C3SHQ8
A	242	ALA	LYS	engineered mutation	UNP C3SHQ8
A	315	VAL	ALA	engineered mutation	UNP C3SHQ8
A	320	VAL	ILE	engineered mutation	UNP C3SHQ8
A	362	ALA	GLU	engineered mutation	UNP C3SHQ8
A	365	ALA	LYS	engineered mutation	UNP C3SHQ8
A	366	ALA	ASP	engineered mutation	UNP C3SHQ8
A	370	ASN	-	linker	UNP C3SHQ8
A	371	ALA	-	linker	UNP C3SHQ8
A	372	ALA	-	linker	UNP C3SHQ8
A	810	THR	-	expression tag	UNP Q3U128

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Chain	Residue	Modelled	Actual	Comment	Reference
A	811	HIS	-	expression tag	UNP Q3U128
A	812	HIS	-	expression tag	UNP Q3U128
A	813	HIS	-	expression tag	UNP Q3U128
A	814	HIS	-	expression tag	UNP Q3U128
A	815	HIS	-	expression tag	UNP Q3U128
A	816	HIS	-	expression tag	UNP Q3U128
A	817	HIS	-	expression tag	UNP Q3U128
A	818	HIS	-	expression tag	UNP Q3U128
B	1	GLU	-	expression tag	UNP C3SHQ8
B	2	THR	-	expression tag	UNP C3SHQ8
B	3	GLY	-	expression tag	UNP C3SHQ8
B	4	LYS	-	expression tag	UNP C3SHQ8
B	5	THR	-	expression tag	UNP C3SHQ8
B	85	ALA	ASP	engineered mutation	UNP C3SHQ8
B	86	ALA	LYS	engineered mutation	UNP C3SHQ8
B	175	ALA	GLU	engineered mutation	UNP C3SHQ8
B	176	ALA	ASN	engineered mutation	UNP C3SHQ8
B	218	HIS	ALA	engineered mutation	UNP C3SHQ8
B	222	HIS	LYS	engineered mutation	UNP C3SHQ8
B	242	ALA	LYS	engineered mutation	UNP C3SHQ8
B	315	VAL	ALA	engineered mutation	UNP C3SHQ8
B	320	VAL	ILE	engineered mutation	UNP C3SHQ8
B	362	ALA	GLU	engineered mutation	UNP C3SHQ8
B	365	ALA	LYS	engineered mutation	UNP C3SHQ8
B	366	ALA	ASP	engineered mutation	UNP C3SHQ8
B	370	ASN	-	linker	UNP C3SHQ8
B	371	ALA	-	linker	UNP C3SHQ8
B	372	ALA	-	linker	UNP C3SHQ8
B	810	THR	-	expression tag	UNP Q3U128
B	811	HIS	-	expression tag	UNP Q3U128
B	812	HIS	-	expression tag	UNP Q3U128
B	813	HIS	-	expression tag	UNP Q3U128
B	814	HIS	-	expression tag	UNP Q3U128
B	815	HIS	-	expression tag	UNP Q3U128
B	816	HIS	-	expression tag	UNP Q3U128
B	817	HIS	-	expression tag	UNP Q3U128
B	818	HIS	-	expression tag	UNP Q3U128
C	1	GLU	-	expression tag	UNP C3SHQ8
C	2	THR	-	expression tag	UNP C3SHQ8
C	3	GLY	-	expression tag	UNP C3SHQ8
C	4	LYS	-	expression tag	UNP C3SHQ8
C	5	THR	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	85	ALA	ASP	engineered mutation	UNP C3SHQ8
C	86	ALA	LYS	engineered mutation	UNP C3SHQ8
C	175	ALA	GLU	engineered mutation	UNP C3SHQ8
C	176	ALA	ASN	engineered mutation	UNP C3SHQ8
C	218	HIS	ALA	engineered mutation	UNP C3SHQ8
C	222	HIS	LYS	engineered mutation	UNP C3SHQ8
C	242	ALA	LYS	engineered mutation	UNP C3SHQ8
C	315	VAL	ALA	engineered mutation	UNP C3SHQ8
C	320	VAL	ILE	engineered mutation	UNP C3SHQ8
C	362	ALA	GLU	engineered mutation	UNP C3SHQ8
C	365	ALA	LYS	engineered mutation	UNP C3SHQ8
C	366	ALA	ASP	engineered mutation	UNP C3SHQ8
C	370	ASN	-	linker	UNP C3SHQ8
C	371	ALA	-	linker	UNP C3SHQ8
C	372	ALA	-	linker	UNP C3SHQ8
C	810	THR	-	expression tag	UNP Q3U128
C	811	HIS	-	expression tag	UNP Q3U128
C	812	HIS	-	expression tag	UNP Q3U128
C	813	HIS	-	expression tag	UNP Q3U128
C	814	HIS	-	expression tag	UNP Q3U128
C	815	HIS	-	expression tag	UNP Q3U128
C	816	HIS	-	expression tag	UNP Q3U128
C	817	HIS	-	expression tag	UNP Q3U128
C	818	HIS	-	expression tag	UNP Q3U128
D	1	GLU	-	expression tag	UNP C3SHQ8
D	2	THR	-	expression tag	UNP C3SHQ8
D	3	GLY	-	expression tag	UNP C3SHQ8
D	4	LYS	-	expression tag	UNP C3SHQ8
D	5	THR	-	expression tag	UNP C3SHQ8
D	85	ALA	ASP	engineered mutation	UNP C3SHQ8
D	86	ALA	LYS	engineered mutation	UNP C3SHQ8
D	175	ALA	GLU	engineered mutation	UNP C3SHQ8
D	176	ALA	ASN	engineered mutation	UNP C3SHQ8
D	218	HIS	ALA	engineered mutation	UNP C3SHQ8
D	222	HIS	LYS	engineered mutation	UNP C3SHQ8
D	242	ALA	LYS	engineered mutation	UNP C3SHQ8
D	315	VAL	ALA	engineered mutation	UNP C3SHQ8
D	320	VAL	ILE	engineered mutation	UNP C3SHQ8
D	362	ALA	GLU	engineered mutation	UNP C3SHQ8
D	365	ALA	LYS	engineered mutation	UNP C3SHQ8
D	366	ALA	ASP	engineered mutation	UNP C3SHQ8
D	370	ASN	-	linker	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	371	ALA	-	linker	UNP C3SHQ8
D	372	ALA	-	linker	UNP C3SHQ8
D	810	THR	-	expression tag	UNP Q3U128
D	811	HIS	-	expression tag	UNP Q3U128
D	812	HIS	-	expression tag	UNP Q3U128
D	813	HIS	-	expression tag	UNP Q3U128
D	814	HIS	-	expression tag	UNP Q3U128
D	815	HIS	-	expression tag	UNP Q3U128
D	816	HIS	-	expression tag	UNP Q3U128
D	817	HIS	-	expression tag	UNP Q3U128
D	818	HIS	-	expression tag	UNP Q3U128

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



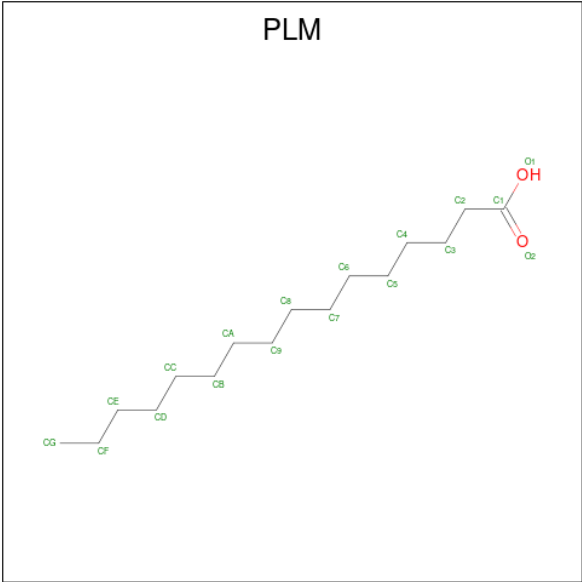
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	F	2	Total	C	O	0	0	0
			23	12	11			
2	G	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			
2	I	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



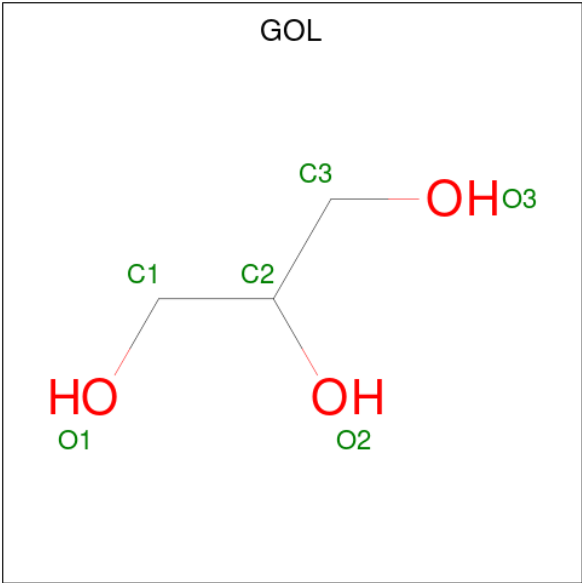
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1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

- Molecule 4 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			18	16	2		
4	C	1	Total	C	O	0	0
			18	16	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

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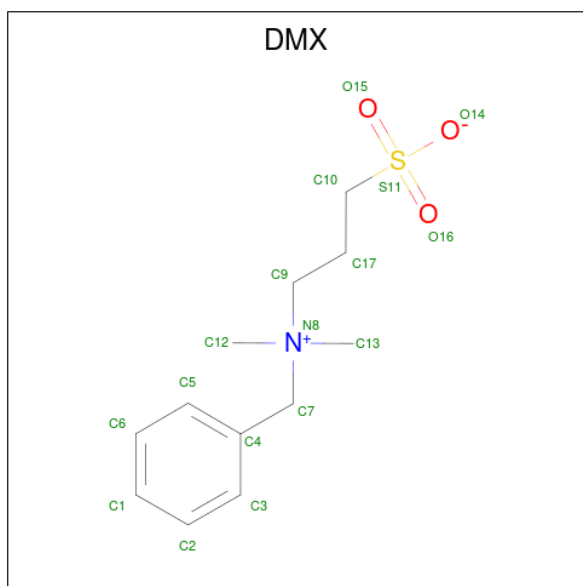
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	B	1	Total	Cl	0	0
			1	1		
6	D	1	Total	Cl	0	0
			1	1		

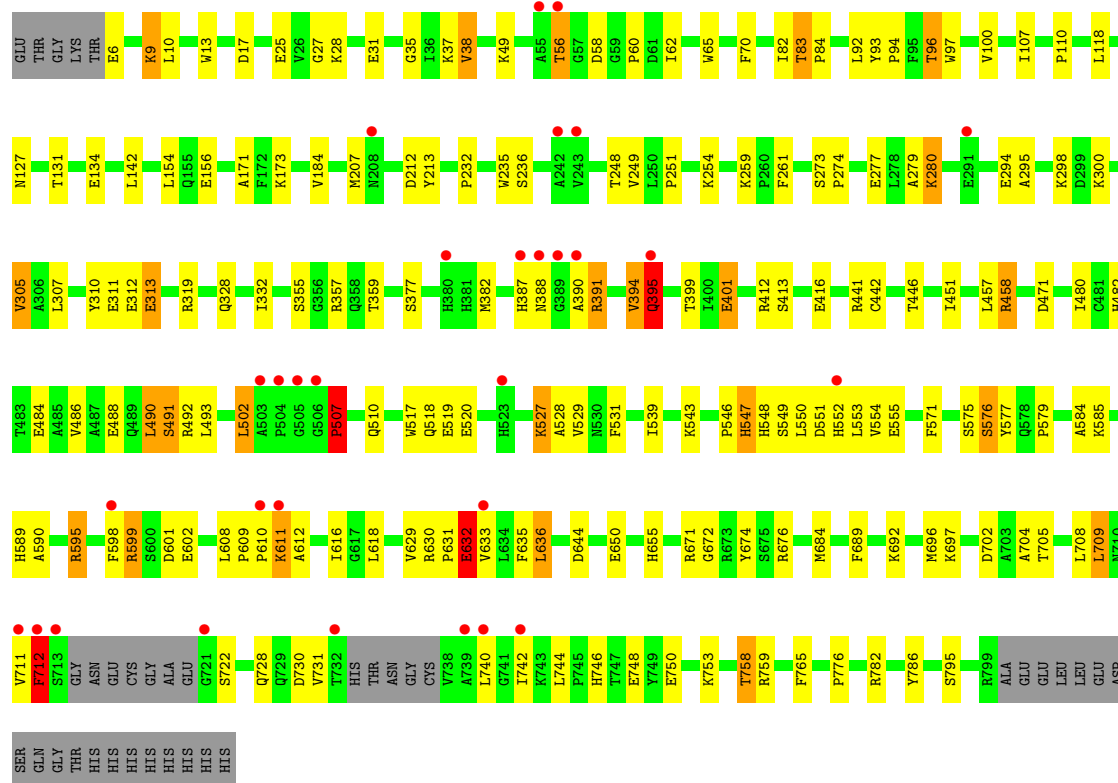
- Molecule 7 is 3-[BENZYL(DIMETHYL)AMMONIO]PROPANE-1-SULFONATE (CCD ID: DMX) (formula: C₁₂H₁₉NO₃S).



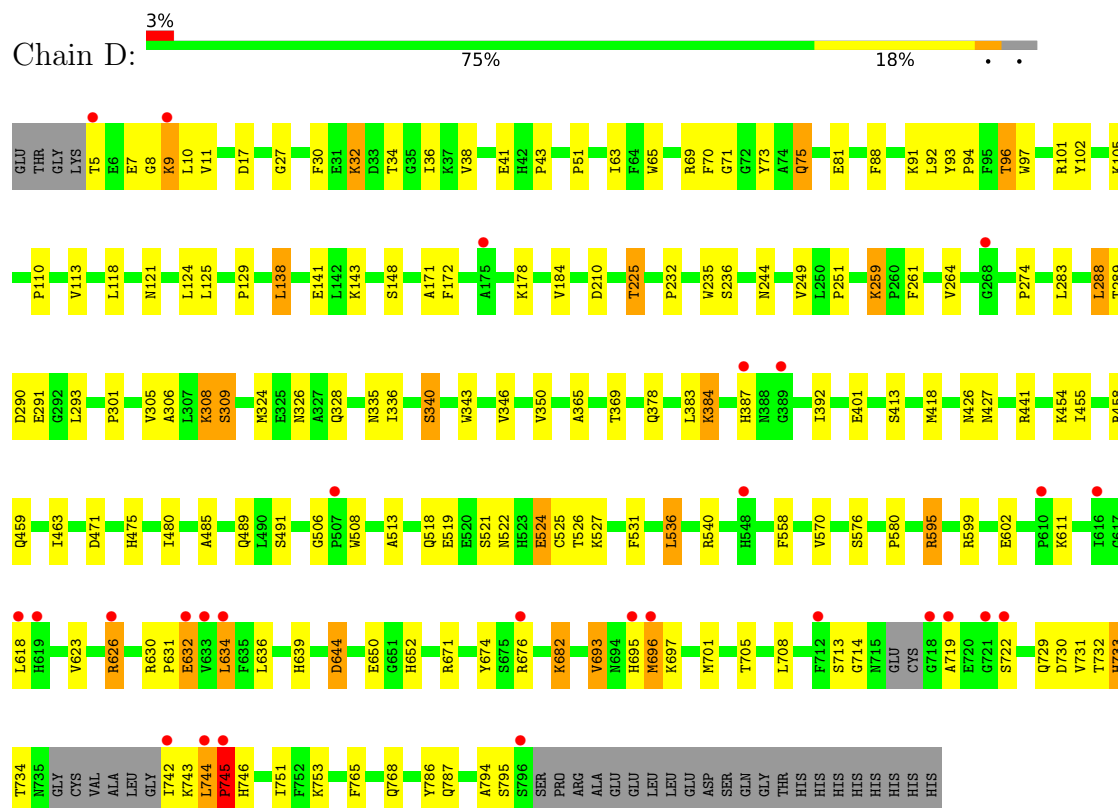
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
7	C	1	Total	C	N	O	S	0	0
			17	12	1	3	1		
7	D	1	Total	C	N	O	S	0	0
			17	12	1	3	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	160	Total 160	O 160	0	0
8	B	79	Total 79	O 79	0	0
8	C	184	Total 184	O 184	0	0
8	D	220	Total 220	O 220	0	0



- Molecule 1: Maltodextrin-binding protein, Protein APCDD1 complex



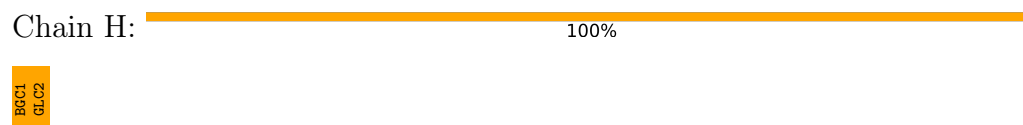
- Molecule 2: alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	123.91Å 98.36Å 156.51Å 90.00° 109.73° 90.00°	Depositor
Resolution (Å)	39.67 – 2.33 39.67 – 2.33	Depositor EDS
% Data completeness (in resolution range)	87.7 (39.67-2.33) 88.5 (39.67-2.33)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.192 , 0.239 0.206 , 0.238	Depositor DCC
R_{free} test set	1990 reflections (1.48%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25921	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.79% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, DMX, BGC, GLC, CL, PLM, NAG

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	0.50	6/6356 (0.1%)	0.85	25/8638 (0.3%)
1	B	0.45	0/6417	0.76	10/8724 (0.1%)
1	C	0.59	6/6394 (0.1%)	1.04	43/8690 (0.5%)
1	D	0.45	3/6427 (0.0%)	0.71	12/8734 (0.1%)
All	All	0.50	15/25594 (0.1%)	0.85	90/34786 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	4
1	D	0	6
All	All	0	19

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	579	PRO	CA-C	-14.54	1.43	1.51
1	C	611	LYS	CE-NZ	13.42	1.89	1.49
1	C	458	ARG	CA-C	11.74	1.60	1.53
1	A	579	PRO	CA-C	11.47	1.58	1.51
1	C	609	PRO	CA-C	-11.02	1.45	1.51
1	A	128	PRO	CA-C	-7.79	1.47	1.51
1	A	605	PRO	CA-C	-6.87	1.47	1.52
1	A	573	ARG	CD-NE	-6.62	1.36	1.46
1	D	32	LYS	CD-CE	6.29	1.71	1.52
1	C	599	ARG	CD-NE	-6.27	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	759	ARG	CG-CD	5.70	1.69	1.52
1	D	32	LYS	CA-CB	5.44	1.62	1.53
1	A	573	ARG	N-CA	-5.24	1.41	1.46
1	A	572	TYR	C-N	-5.12	1.27	1.33
1	D	9	LYS	CA-CB	5.05	1.60	1.53

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	488	GLU	CG-CD-OE1	19.01	162.12	118.40
1	A	391	ARG	CB-CG-CD	-18.68	68.33	111.30
1	A	391	ARG	CA-CB-CG	17.96	150.02	114.10
1	C	759	ARG	CB-CG-CD	-17.70	70.58	111.30
1	C	488	GLU	CG-CD-OE2	-17.18	78.89	118.40
1	C	313	GLU	CA-CB-CG	15.90	145.90	114.10
1	C	611	LYS	N-CA-CB	15.34	134.05	111.05
1	C	611	LYS	CB-CA-C	-15.12	81.81	110.24
1	C	488	GLU	OE1-CD-OE2	-15.06	86.76	122.90
1	C	394	VAL	CA-C-N	-13.54	102.69	123.13
1	C	394	VAL	C-N-CA	-13.54	102.69	123.13
1	C	312	GLU	CA-C-N	12.73	141.98	120.71
1	C	312	GLU	C-N-CA	12.73	141.98	120.71
1	C	611	LYS	N-CA-C	-12.57	90.58	109.81
1	A	141	GLU	CA-CB-CG	12.51	139.13	114.10
1	B	397	PRO	N-CA-C	-12.23	95.78	110.70
1	C	313	GLU	CB-CA-C	11.95	130.86	110.79
1	C	599	ARG	CD-NE-CZ	-11.41	108.42	124.40
1	C	611	LYS	CG-CD-CE	11.22	137.10	111.30
1	A	391	ARG	CG-CD-NE	11.18	136.59	112.00
1	C	488	GLU	CA-CB-CG	10.95	135.99	114.10
1	C	759	ARG	CA-CB-CG	10.93	135.97	114.10
1	C	313	GLU	N-CA-CB	-10.90	94.00	110.13
1	C	395	GLN	CA-CB-CG	-10.80	92.49	114.10
1	C	579	PRO	O-C-N	-10.64	116.42	121.31
1	D	682	LYS	CB-CG-CD	10.61	135.71	111.30
1	C	488	GLU	CB-CG-CD	-10.56	94.65	112.60
1	C	611	LYS	CD-CE-NZ	-10.13	79.47	111.90
1	A	759	ARG	CB-CG-CD	9.37	132.85	111.30
1	B	599	ARG	CD-NE-CZ	9.33	137.46	124.40
1	C	313	GLU	CG-CD-OE1	-8.79	98.17	118.40
1	B	328	GLN	CA-C-N	8.76	133.62	120.31
1	B	328	GLN	C-N-CA	8.76	133.62	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	579	PRO	O-C-N	8.67	125.30	121.31
1	C	313	GLU	CG-CD-OE2	8.65	138.31	118.40
1	D	32	LYS	CB-CG-CD	8.29	130.37	111.30
1	C	609	PRO	O-C-N	-8.06	117.60	121.31
1	C	300	LYS	CA-CB-CG	8.00	130.09	114.10
1	A	391	ARG	N-CA-CB	7.82	121.87	110.06
1	A	391	ARG	CD-NE-CZ	-7.66	113.67	124.40
1	A	141	GLU	CB-CA-C	7.28	122.47	110.17
1	C	395	GLN	N-CA-C	-7.23	93.16	107.69
1	C	401	GLU	N-CA-CB	7.13	121.03	109.69
1	A	605	PRO	O-C-N	-7.12	117.80	121.15
1	C	401	GLU	CA-CB-CG	7.04	128.19	114.10
1	A	573	ARG	CG-CD-NE	-7.04	96.52	112.00
1	C	599	ARG	CG-CD-NE	7.04	127.48	112.00
1	C	610	PRO	CA-C-N	-7.02	110.47	123.03
1	C	610	PRO	C-N-CA	-7.02	110.47	123.03
1	A	484	GLU	CA-CB-CG	7.01	128.11	114.10
1	A	128	PRO	O-C-N	-6.99	118.09	121.31
1	A	759	ARG	CA-CB-CG	-6.98	100.14	114.10
1	D	32	LYS	CG-CD-CE	-6.95	95.31	111.30
1	C	758	THR	CA-C-N	-6.70	111.52	122.65
1	C	758	THR	C-N-CA	-6.70	111.52	122.65
1	C	611	LYS	CA-CB-CG	6.60	127.29	114.10
1	C	401	GLU	CB-CA-C	-6.59	99.09	109.70
1	D	32	LYS	CB-CA-C	6.56	122.71	110.70
1	A	83	THR	OG1-CB-CG2	6.56	122.42	109.30
1	A	143	LYS	CA-CB-CG	6.52	127.13	114.10
1	B	75	GLN	CG-CD-NE2	-6.50	106.64	116.40
1	D	9	LYS	N-CA-CB	6.50	121.56	110.65
1	C	759	ARG	CG-CD-NE	6.49	126.29	112.00
1	A	48	GLU	CA-CB-CG	-6.41	101.28	114.10
1	C	313	GLU	CB-CG-CD	-6.36	101.78	112.60
1	C	507	PRO	N-CA-CB	-6.33	96.61	103.25
1	D	9	LYS	CB-CG-CD	-6.27	96.88	111.30
1	C	300	LYS	CB-CG-CD	-6.23	96.97	111.30
1	D	32	LYS	CA-CB-CG	6.08	126.27	114.10
1	C	759	ARG	CD-NE-CZ	6.03	132.85	124.40
1	D	682	LYS	CA-CB-CG	-5.91	102.29	114.10
1	D	745	PRO	N-CA-C	-5.90	100.31	112.47
1	A	391	ARG	CB-CA-C	-5.84	99.67	109.53
1	B	329	LYS	CA-CB-CG	5.82	125.73	114.10
1	A	759	ARG	CG-CD-NE	5.78	124.71	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	682	LYS	N-CA-CB	-5.67	101.75	110.20
1	B	454	LYS	CA-CB-CG	5.64	125.39	114.10
1	A	758	THR	CA-C-N	-5.62	114.17	122.83
1	A	758	THR	C-N-CA	-5.62	114.17	122.83
1	C	712	PHE	CB-CA-C	5.61	118.74	111.50
1	D	522	ASN	N-CA-C	-5.60	106.40	113.23
1	D	32	LYS	CD-CE-NZ	-5.53	94.22	111.90
1	A	522	ASN	N-CA-C	-5.50	106.24	113.17
1	B	264	VAL	CG1-CB-CG2	5.48	122.87	110.80
1	B	29	LYS	CD-CE-NZ	-5.43	94.53	111.90
1	A	573	ARG	CB-CG-CD	5.34	123.57	111.30
1	A	475	HIS	N-CA-C	-5.25	107.53	114.04
1	B	465	ARG	CG-CD-NE	5.20	123.43	112.00
1	A	186	VAL	N-CA-C	-5.12	105.87	113.39
1	C	712	PHE	CA-CB-CG	5.11	118.91	113.80

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	ARG	Sidechain
1	A	141	GLU	Peptide
1	A	391	ARG	Sidechain
1	A	573	ARG	Sidechain
1	A	759	ARG	Sidechain
1	B	465	ARG	Sidechain
1	B	599	ARG	Sidechain
1	B	69	ARG	Sidechain
1	B	75	GLN	Sidechain
1	C	394	VAL	Peptide
1	C	395	GLN	Sidechain
1	C	595	ARG	Sidechain
1	C	599	ARG	Sidechain
1	D	536	LEU	Mainchain
1	D	595	ARG	Sidechain
1	D	626	ARG	Sidechain
1	D	745	PRO	Mainchain
1	D	8	GLY	Peptide

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	6184	0	5991	142	1
1	B	6242	0	6036	231	1
1	C	6221	0	6019	147	1
1	D	6251	0	6034	126	1
2	F	23	0	21	2	0
2	G	23	0	21	1	0
2	H	23	0	21	3	0
2	I	23	0	21	2	0
3	A	42	0	39	1	0
3	B	42	0	39	1	0
3	C	42	0	39	0	0
3	D	42	0	39	0	0
4	A	18	0	31	6	0
4	C	18	0	31	4	0
5	A	6	0	8	0	0
5	B	12	0	16	1	0
5	C	6	0	8	1	0
5	D	6	0	8	0	0
6	A	1	0	0	0	0
6	B	1	0	0	1	0
6	D	1	0	0	1	0
7	C	34	0	38	8	0
7	D	17	0	19	5	0
8	A	160	0	0	6	1
8	B	79	0	0	3	1
8	C	184	0	0	3	0
8	D	220	0	0	3	2
All	All	25921	0	24479	640	4

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 13.

All (640) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:611:LYS:CE	1:C:611:LYS:NZ	1.89	1.36
1:C:611:LYS:NZ	1:C:611:LYS:CD	2.22	1.01
1:C:6:GLU:HB2	1:C:9:LYS:HD3	1.44	0.98
1:D:387:HIS:CD2	1:D:626:ARG:HE	1.83	0.97
1:D:731:VAL:HG23	1:D:744:LEU:HD11	1.51	0.92
1:A:391:ARG:NH1	1:A:393:THR:OG1	2.04	0.91
1:D:94:PRO:HD2	7:D:905:DMX:H1	1.53	0.89
1:C:401:GLU:OE2	8:C:1001:HOH:O	1.89	0.88
1:C:611:LYS:HG3	1:C:612:ALA:C	1.98	0.87
1:C:27:GLY:HA3	1:C:38:VAL:HG21	1.53	0.86
1:B:617:GLY:H	1:B:754:MET:HE1	1.37	0.86
1:B:621:GLU:HG2	1:B:641:ILE:HG12	1.57	0.86
1:B:47:GLU:HG3	1:B:69:ARG:HE	1.38	0.86
1:A:724:GLN:HG3	1:A:727:ILE:HG13	1.59	0.84
1:C:94:PRO:HD2	7:C:905:DMX:H1	1.60	0.83
1:C:611:LYS:HG3	1:C:612:ALA:N	1.95	0.82
1:A:46:LEU:HD13	1:A:63:ILE:HD11	1.62	0.81
1:B:293:LEU:HD13	1:B:305:VAL:HG21	1.62	0.81
1:C:62:ILE:HD11	1:C:279:ALA:HB1	1.62	0.80
1:C:212:ASP:OD1	1:C:213:TYR:N	2.14	0.80
1:D:732:THR:HA	1:D:744:LEU:HD13	1.64	0.80
1:C:611:LYS:NZ	1:C:611:LYS:HD2	1.94	0.80
1:B:714:GLY:O	1:B:715:ASN:ND2	2.17	0.78
1:B:283:LEU:HA	1:B:287:LEU:HB3	1.66	0.77
1:A:17:ASP:OD2	2:F:1:BGC:O1	2.01	0.77
1:B:326:ASN:O	1:B:329:LYS:HB2	1.85	0.77
1:C:118:LEU:HD22	1:C:251:PRO:HD3	1.66	0.77
1:B:96:THR:OG1	1:B:110:PRO:HB3	1.85	0.77
1:B:116:LEU:HD22	1:B:229:ILE:HG22	1.67	0.77
1:D:524:GLU:HG2	1:D:526:THR:H	1.50	0.76
1:C:611:LYS:HG3	1:C:612:ALA:O	1.85	0.76
1:B:649:TRP:HZ2	1:B:693:VAL:HG22	1.49	0.76
1:B:109:TYR:HE1	1:B:284:GLU:HG3	1.50	0.76
1:B:88:PHE:CE2	1:B:284:GLU:HG2	2.23	0.74
1:A:359:THR:HG22	1:A:362:ALA:H	1.51	0.73
1:B:94:PRO:HA	1:B:97:TRP:CD1	2.22	0.73
1:D:480:ILE:HD12	1:D:602:GLU:HB2	1.70	0.73
1:D:125:LEU:HD21	1:D:129:PRO:HD3	1.70	0.73
1:A:391:ARG:HH12	1:A:393:THR:HG1	1.37	0.72
1:B:441:ARG:NH1	1:B:611:LYS:O	2.22	0.72
1:C:631:PRO:O	1:C:632:GLU:HB2	1.89	0.72
1:C:590:ALA:HB1	1:C:758:THR:HG21	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:PHE:HA	1:D:91:LYS:HD2	1.72	0.72
1:C:294:GLU:O	1:C:298:LYS:HG3	1.90	0.71
1:B:109:TYR:CE1	1:B:284:GLU:HG3	2.25	0.71
1:D:27:GLY:HA3	1:D:38:VAL:HG21	1.73	0.71
1:B:619:HIS:HB3	1:B:644:ASP:HB3	1.72	0.71
1:C:611:LYS:CG	1:C:612:ALA:N	2.44	0.71
1:A:358:GLN:HB2	1:A:363:ALA:HB2	1.72	0.71
1:A:544:GLN:O	1:A:546:PRO:HD3	1.91	0.71
1:D:9:LYS:NZ	1:D:11:VAL:HG22	2.05	0.71
1:A:336:ILE:HG22	1:A:338:GLN:OE1	1.91	0.70
1:A:187:ASP:HB2	1:A:368:GLN:HG3	1.73	0.70
1:D:17:ASP:OD2	2:I:1:BGC:O1	2.10	0.70
1:B:238:ILE:HA	1:B:241:SER:HB3	1.74	0.69
1:C:395:GLN:OE1	1:C:543:LYS:HG3	1.91	0.69
1:D:693:VAL:HG13	1:D:746[A]:HIS:HB3	1.73	0.69
1:B:15:ASN:HD22	1:B:16:GLY:N	1.89	0.69
1:A:769:ARG:HD3	4:A:904:PLM:H22	1.75	0.69
1:C:546:PRO:HB3	1:C:551:ASP:HB2	1.73	0.69
1:A:76:SER:HA	1:A:759:ARG:HA	1.75	0.69
1:B:257:PRO:HB2	1:B:329:LYS:HD2	1.75	0.69
1:D:485:ALA:HB1	1:D:489:GLN:HE22	1.58	0.68
1:A:48:GLU:HA	1:A:51:PRO:HD2	1.76	0.68
1:B:88:PHE:CZ	1:B:284:GLU:HG2	2.28	0.68
1:C:65:TRP:HB3	1:C:70:PHE:HE1	1.59	0.67
1:D:733:HIS:CE1	1:D:734:THR:HG23	2.28	0.67
1:C:595:ARG:HA	1:C:598[A]:PHE:CD2	2.30	0.67
1:A:65:TRP:HB3	1:A:70:PHE:HE1	1.60	0.67
1:B:125:LEU:HD21	1:B:128:PRO:HA	1.77	0.67
1:D:387:HIS:CD2	1:D:626:ARG:NE	2.60	0.67
1:A:778:ARG:HG3	1:A:781:LYS:HE3	1.74	0.66
1:C:27:GLY:HA3	1:C:38:VAL:CG2	2.25	0.66
1:C:390:ALA:HA	1:C:547:HIS:CE1	2.30	0.66
1:B:92:LEU:HB2	1:B:97:TRP:CZ2	2.30	0.66
1:B:631:PRO:O	1:B:632:GLU:HB2	1.95	0.66
1:B:638:ARG:HH12	1:B:766:ASN:HD21	1.44	0.66
1:B:170:TYR:OH	1:B:183:ASP:OD1	2.03	0.66
1:B:15:ASN:HD22	1:B:16:GLY:H	1.42	0.65
1:B:92:LEU:HB2	1:B:97:TRP:CH2	2.31	0.65
1:C:518:GLN:HG3	1:C:520:GLU:HB2	1.79	0.65
1:A:739:ALA:O	1:A:742:ILE:HD12	1.97	0.65
1:A:254:LYS:O	1:A:254:LYS:HG2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:TRP:CD2	1:B:60:PRO:HG3	2.31	0.65
1:D:30:PHE:O	1:D:34:THR:HG22	1.97	0.65
1:A:172:PHE:CE1	1:A:184:VAL:HG13	2.32	0.64
1:C:93:TYR:O	1:C:96:THR:HG22	1.96	0.64
1:B:23:LEU:O	1:B:26:VAL:HG12	1.96	0.64
1:C:25:GLU:HA	1:C:28:LYS:HE2	1.78	0.64
1:C:377:SER:HA	1:C:382:MET:HE2	1.79	0.64
1:B:509:VAL:HG13	1:B:512:VAL:HG21	1.79	0.64
1:C:82:ILE:HD12	1:C:84:PRO:HG3	1.79	0.64
1:B:454:LYS:HA	1:B:454:LYS:HE2	1.79	0.63
1:C:611:LYS:CD	1:C:611:LYS:HZ2	2.06	0.63
1:B:67:HIS:HE1	1:B:263:GLY:HA2	1.63	0.63
1:A:724:GLN:CG	1:A:727:ILE:HG13	2.28	0.63
1:B:160:THR:HG23	1:B:198:LEU:HD13	1.81	0.63
1:A:180:ASP:OD2	1:A:182:LYS:HE3	1.97	0.63
1:B:137:ALA:HA	1:B:140:LYS:HD3	1.80	0.63
1:B:102:TYR:HB3	1:B:107:ILE:HG21	1.80	0.62
1:B:269:ILE:HG21	1:B:276:LYS:HD3	1.81	0.62
1:B:82:ILE:HD11	1:B:109:TYR:CZ	2.34	0.62
1:B:284:GLU:HA	1:B:288:LEU:HD12	1.82	0.62
1:B:283:LEU:HD23	1:B:287:LEU:HD23	1.81	0.62
1:B:396:MET:O	1:B:398:PRO:HD3	1.99	0.62
1:D:27:GLY:CA	1:D:38:VAL:HG21	2.30	0.62
1:B:616:ILE:HA	1:B:754:MET:HE3	1.81	0.62
1:B:167:ASP:HA	1:B:256:GLN:NE2	2.15	0.62
1:D:101:ARG:O	8:D:1001:HOH:O	2.16	0.61
1:B:17:ASP:OD2	1:B:18:LYS:NZ	2.34	0.61
1:B:51:PRO:HG3	1:B:73:TYR:CE1	2.36	0.61
1:A:262:VAL:HB	1:A:332:ILE:HA	1.82	0.61
1:B:27:GLY:HA3	1:B:38:VAL:HG21	1.81	0.61
1:B:142:LEU:HB3	1:B:147:LYS:HB2	1.82	0.61
1:D:454:LYS:HG2	1:D:475:HIS:HE2	1.65	0.61
1:A:676:ARG:HA	1:A:689:PHE:CE2	2.36	0.60
1:C:611:LYS:HG3	1:C:612:ALA:CA	2.30	0.60
1:A:172:PHE:CE1	1:A:181:ILE:HA	2.37	0.60
1:B:488:GLU:HG2	1:B:492:ARG:HH11	1.65	0.60
1:C:49:LYS:HD3	1:C:550:LEU:HD21	1.84	0.60
1:D:293:LEU:HD13	1:D:305:VAL:HG21	1.84	0.60
1:D:9:LYS:HZ3	1:D:11:VAL:HG22	1.65	0.59
1:D:631:PRO:O	1:D:632:GLU:HB2	2.02	0.59
1:A:139:ASP:O	1:A:143:LYS:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:708:LEU:HD22	1:D:705:THR:HG23	1.84	0.59
1:C:17:ASP:OD2	2:H:1:BGC:O1	2.19	0.59
1:A:67:HIS:CE1	1:A:263:GLY:HA2	2.38	0.59
1:D:454:LYS:HG2	1:D:475:HIS:NE2	2.18	0.59
1:B:109:TYR:HB2	1:B:267:ALA:HB3	1.83	0.59
1:C:310:TYR:HD1	1:C:313:GLU:OE1	1.86	0.59
1:D:118:LEU:HD22	1:D:251:PRO:HD3	1.85	0.59
1:A:293:LEU:HD13	1:A:305:VAL:HG11	1.85	0.58
1:A:506:GLY:N	1:A:507:PRO:HD3	2.18	0.58
1:D:695[A]:HIS:HE1	1:D:697:LYS:HG3	1.69	0.58
1:D:92:LEU:HB2	1:D:97:TRP:NE1	2.19	0.58
1:A:135:ILE:HD13	1:A:227:MET:HE1	1.85	0.57
1:B:213:TYR:OH	1:B:233:TRP:NE1	2.36	0.57
1:A:650:GLU:HG2	1:A:671:ARG:HG3	1.86	0.57
1:B:276:LYS:HD2	1:B:280:LYS:HG3	1.85	0.57
1:C:156:GLU:HG3	2:H:2:GLC:O6	2.04	0.57
1:B:638:ARG:HH12	1:B:766:ASN:ND2	2.02	0.57
1:B:125:LEU:HD21	1:B:129:PRO:HD3	1.86	0.57
1:B:617:GLY:H	1:B:754:MET:CE	2.14	0.57
1:C:750:GLU:O	1:C:782:ARG:NH1	2.38	0.57
1:D:531:PHE:N	8:D:1006:HOH:O	2.36	0.57
1:A:67:HIS:HE1	1:A:263:GLY:HA2	1.70	0.56
1:A:616:ILE:HD11	1:A:753:LYS:HA	1.86	0.56
1:C:446:THR:HB	7:C:906:DMX:H171	1.85	0.56
1:D:94:PRO:HB2	7:D:905:DMX:H6	1.85	0.56
1:B:68:ASP:OD2	1:B:69:ARG:N	2.38	0.56
1:D:693:VAL:CG1	1:D:746[A]:HIS:HB3	2.36	0.56
1:B:198:LEU:O	1:B:202:ILE:HD12	2.06	0.56
1:B:649:TRP:CZ2	1:B:693:VAL:HG22	2.37	0.56
1:C:6:GLU:HB2	1:C:9:LYS:CD	2.28	0.56
1:B:171:ALA:O	1:B:184:VAL:HA	2.05	0.56
1:C:705:THR:HG22	1:C:709:LEU:HD12	1.88	0.56
1:C:709:LEU:HA	1:C:712:PHE:CD2	2.40	0.56
1:B:480:ILE:HD12	1:B:602:GLU:HB2	1.86	0.56
1:D:730:ASP:OD1	1:D:732:THR:HG22	2.06	0.56
1:A:548:HIS:O	8:A:1001:HOH:O	2.17	0.56
1:B:94:PRO:HA	1:B:97:TRP:HD1	1.68	0.56
1:B:82:ILE:HD11	1:B:109:TYR:CE1	2.42	0.55
1:B:235:TRP:HA	1:B:238:ILE:HD12	1.88	0.55
1:C:650:GLU:HG2	1:C:671:ARG:HG3	1.89	0.55
1:D:92:LEU:HB2	1:D:97:TRP:HE1	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:SER:O	1:B:242:ALA:HB3	2.04	0.55
1:A:81:GLU:OE1	1:A:105:LYS:HG2	2.06	0.55
1:B:179:TYR:HD2	1:B:336:ILE:HD11	1.71	0.55
1:B:294:GLU:HA	1:B:310:TYR:OH	2.07	0.55
1:A:457:LEU:HD11	1:A:539:ILE:HD12	1.89	0.55
1:B:590:ALA:HB1	1:B:758:THR:HG21	1.89	0.54
1:D:458:ARG:HD2	1:D:471:ASP:OD2	2.06	0.54
1:D:713:SER:OG	1:D:714:GLY:N	2.40	0.54
1:B:490:LEU:HD22	1:B:508:TRP:HZ3	1.71	0.54
1:D:27:GLY:C	1:D:38:VAL:HG21	2.32	0.54
1:A:140:LYS:O	1:A:143:LYS:HB3	2.07	0.54
1:B:717:CYS:O	8:B:1001:HOH:O	2.18	0.54
1:A:167:ASP:OD2	1:A:190:GLY:HA2	2.06	0.54
1:B:142:LEU:O	1:B:147:LYS:N	2.38	0.54
1:A:139:ASP:OD2	1:A:143:LYS:NZ	2.40	0.54
1:A:479:VAL:HG12	1:A:516:LEU:HD13	1.90	0.54
1:A:724:GLN:HG3	1:A:727:ILE:CG1	2.35	0.54
1:B:53:VAL:HG12	1:B:59:GLY:HA2	1.88	0.54
1:C:630:ARG:HG3	1:C:636:LEU:CD2	2.38	0.54
1:A:573:ARG:CZ	8:A:1008:HOH:O	2.55	0.54
1:B:491:SER:HB2	3:B:902:NAG:H82	1.90	0.54
1:D:650:GLU:HG2	1:D:671:ARG:HG3	1.89	0.54
1:A:129:PRO:HG3	1:A:138:LEU:CD1	2.38	0.54
1:A:197:PHE:CE1	1:A:201:LEU:HD11	2.43	0.54
1:B:96:THR:OG1	1:B:110:PRO:CB	2.56	0.54
1:C:6:GLU:O	1:C:274:PRO:HG2	2.08	0.53
1:B:20:TYR:HA	1:B:23:LEU:HD23	1.90	0.53
1:A:67:HIS:NE2	1:A:333:MET:O	2.37	0.53
1:A:338:GLN:OE1	1:A:338:GLN:N	2.37	0.53
1:B:14:ILE:HD11	1:B:18:LYS:HB2	1.91	0.53
1:B:311:GLU:O	1:B:315:VAL:HG23	2.07	0.53
1:B:485:ALA:O	1:B:489:GLN:HG3	2.08	0.53
1:C:92:LEU:HD12	1:C:97:TRP:CZ2	2.44	0.53
1:D:401:GLU:OE1	1:D:426:ASN:ND2	2.42	0.53
1:C:576:SER:OG	1:C:577:TYR:N	2.40	0.53
1:B:95:PHE:HA	1:B:98:ASP:OD2	2.09	0.53
1:C:746:HIS:CE1	1:C:748:GLU:HG3	2.44	0.53
1:D:88:PHE:HZ	1:D:288:LEU:HD13	1.74	0.53
1:A:544:GLN:HG3	1:A:554:VAL:HB	1.91	0.52
1:B:79:LEU:HD12	1:B:107:ILE:HD12	1.91	0.52
1:B:235:TRP:HB2	1:B:301:PRO:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:GLU:O	1:B:492:ARG:HD3	2.07	0.52
1:A:36:ILE:HG13	1:A:278:LEU:HD13	1.92	0.52
1:D:289:THR:OG1	1:D:291:GLU:HG2	2.09	0.52
1:A:631:PRO:O	1:A:632:GLU:HB2	2.09	0.52
1:D:232:PRO:HA	1:D:235:TRP:CE2	2.44	0.52
1:B:283:LEU:HA	1:B:287:LEU:CB	2.39	0.52
1:C:391:ARG:HA	1:C:391:ARG:HH11	1.73	0.52
1:B:67:HIS:HE2	1:B:332:ILE:HG22	1.74	0.52
1:B:179:TYR:CD2	1:B:336:ILE:HD11	2.44	0.52
1:D:324:MET:O	1:D:328:GLN:HG2	2.10	0.52
1:D:69:ARG:NH1	1:D:340:SER:OG	2.43	0.52
1:D:51:PRO:HG3	1:D:73:TYR:CE1	2.45	0.52
1:A:197:PHE:CE1	1:A:201:LEU:HD21	2.46	0.51
1:B:232:PRO:HD2	1:B:233:TRP:CE3	2.44	0.51
1:B:82:ILE:HA	1:B:280:LYS:NZ	2.25	0.51
1:C:584:ALA:HA	1:C:598[A]:PHE:CZ	2.45	0.51
1:B:619:HIS:HB3	1:B:644:ASP:CB	2.40	0.51
1:D:540[B]:ARG:HB3	1:D:558:PHE:HB2	1.92	0.51
1:B:20:TYR:CD2	1:B:42:HIS:HD2	2.28	0.51
1:B:179:TYR:CE2	1:B:334:PRO:HB3	2.46	0.51
1:C:451:ILE:HG12	1:C:531:PHE:CZ	2.46	0.51
1:C:553:LEU:HD12	1:C:554:VAL:N	2.26	0.51
1:D:387:HIS:HD2	1:D:626:ARG:HE	1.51	0.51
1:A:305:VAL:HG12	1:A:307:LEU:H	1.74	0.51
1:B:232:PRO:O	1:B:301:PRO:HG2	2.11	0.51
1:D:631:PRO:O	1:D:632:GLU:CB	2.58	0.51
1:A:138:LEU:O	1:A:142:LEU:HD12	2.10	0.51
1:B:68:ASP:HB3	1:B:333:MET:HE3	1.93	0.51
1:A:67:HIS:ND1	1:A:264:VAL:HG22	2.26	0.51
1:C:543:LYS:HG2	1:C:555:GLU:HG2	1.92	0.51
1:A:505:GLY:O	1:D:384:LYS:HD2	2.11	0.51
1:B:50:PHE:CE1	1:B:54:ALA:HB2	2.46	0.51
1:B:451:ILE:HG12	1:B:531:PHE:CZ	2.46	0.50
1:B:456:ARG:HD3	1:C:571:PHE:CZ	2.46	0.50
1:A:119:ILE:HG23	1:A:245:TYR:HD2	1.77	0.50
1:D:731:VAL:HG23	1:D:744:LEU:CD1	2.35	0.50
1:A:172:PHE:CD1	1:A:184:VAL:HG13	2.46	0.50
1:B:257:PRO:HB3	1:B:329:LYS:HE3	1.93	0.50
1:A:753:LYS:HG2	1:A:765:PHE:HB2	1.92	0.50
1:D:121:ASN:HD22	1:D:124:LEU:HD22	1.75	0.50
1:B:691:PHE:CE1	1:B:752:PHE:HE1	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:THR:HG23	1:D:36:ILE:H	1.77	0.50
1:B:456:ARG:O	1:B:456:ARG:HG2	2.11	0.50
1:A:197:PHE:HE1	1:A:201:LEU:HD11	1.77	0.50
1:A:241:SER:HB2	1:A:243:VAL:HG22	1.94	0.50
1:A:534:HIS:CD2	8:A:1008:HOH:O	2.64	0.50
1:B:67:HIS:CE1	1:B:263:GLY:HA2	2.45	0.50
1:B:143:LYS:HD2	1:B:147:LYS:O	2.12	0.50
1:D:9:LYS:HZ3	1:D:11:VAL:CG2	2.24	0.50
1:A:490:LEU:O	1:A:494:VAL:HG23	2.11	0.49
1:D:518:GLN:HB2	1:D:521:SER:OG	2.12	0.49
1:B:132:TRP:CD1	1:B:251:PRO:HB2	2.47	0.49
1:B:735:ASN:OD1	1:B:735:ASN:N	2.45	0.49
1:C:70:PHE:HB3	1:C:107:ILE:CD1	2.42	0.49
1:C:518:GLN:CG	1:C:520:GLU:HB2	2.42	0.49
1:A:195:LEU:HD11	1:A:350:VAL:HG22	1.93	0.49
1:B:282:PHE:HA	1:B:286:TYR:HD2	1.76	0.49
1:B:630:ARG:NH2	6:B:906:CL:CL	2.81	0.49
1:C:517:TRP:CH2	1:C:519:GLU:HB3	2.47	0.49
1:B:11:VAL:HA	1:B:39:THR:OG1	2.13	0.49
1:B:765:PHE:CZ	1:B:789:PRO:HB3	2.48	0.49
1:C:156:GLU:HG3	2:H:2:GLC:HO6	1.77	0.49
1:C:712:PHE:CG	1:C:712:PHE:O	2.65	0.49
1:D:171:ALA:O	1:D:184:VAL:HA	2.13	0.49
1:D:753:LYS:HE2	1:D:786:TYR:CD2	2.48	0.49
1:B:95:PHE:CD1	1:B:96:THR:HG22	2.47	0.49
1:B:692:LYS:HD3	1:B:694:ASN:OD1	2.12	0.49
1:D:88:PHE:CZ	1:D:288:LEU:HD13	2.48	0.49
1:A:534:HIS:CG	8:A:1008:HOH:O	2.65	0.49
1:B:276:LYS:O	1:B:280:LYS:N	2.40	0.49
1:C:441:ARG:NH1	1:C:612:ALA:HA	2.28	0.49
1:C:630:ARG:HG3	1:C:636:LEU:HD21	1.94	0.49
1:C:655:HIS:CE1	4:C:907:PLM:HF1	2.48	0.49
1:B:236:SER:OG	1:B:301:PRO:HD3	2.13	0.49
1:A:47:GLU:O	1:A:48:GLU:HG2	2.13	0.49
1:A:82:ILE:O	1:A:84:PRO:HD3	2.13	0.49
1:A:357:ARG:HD3	1:A:358:GLN:HG3	1.95	0.49
1:B:157:PRO:HD3	1:B:347:ARG:HG3	1.95	0.49
1:C:442:CYS:HB2	1:C:608:LEU:HD22	1.95	0.49
1:D:639:HIS:HB3	1:D:652:HIS:HB2	1.95	0.49
1:B:441:ARG:HH12	1:B:612:ALA:HA	1.76	0.48
1:A:573:ARG:NH1	8:A:1008:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:TYR:HE1	1:B:319:ARG:HD2	1.77	0.48
1:C:655:HIS:NE2	4:C:907:PLM:HF1	2.27	0.48
1:A:693:VAL:HG21	4:A:904:PLM:HC2	1.95	0.48
1:D:96:THR:HG23	1:D:110:PRO:CB	2.43	0.48
1:B:459:GLN:CD	1:B:459:GLN:H	2.21	0.48
1:B:519:GLU:O	1:B:520:GLU:C	2.56	0.48
1:C:709:LEU:HA	1:C:712:PHE:HD2	1.78	0.48
1:A:125:LEU:HD11	1:A:138:LEU:HD11	1.96	0.48
1:A:310:TYR:CE1	1:A:314:LEU:HD21	2.48	0.48
1:D:71:GLY:HA3	1:D:335:ASN:O	2.12	0.48
1:A:504:PRO:HB3	1:D:701:MET:CE	2.44	0.48
1:B:71:GLY:HA3	1:B:335:ASN:O	2.14	0.48
1:B:766:ASN:OD1	1:B:787:GLN:NE2	2.46	0.48
1:A:170:TYR:CD1	1:A:185:GLY:HA3	2.49	0.48
1:A:172:PHE:CZ	1:A:181:ILE:HG22	2.48	0.48
1:A:395:GLN:HE22	1:A:399:THR:HB	1.79	0.48
1:B:131:THR:O	1:B:134:GLU:HG2	2.12	0.48
1:C:94:PRO:HD2	7:C:905:DMX:C1	2.36	0.48
1:C:235:TRP:CH2	1:C:319:ARG:HB3	2.49	0.48
1:C:328:GLN:HE22	7:C:905:DMX:H131	1.79	0.48
1:A:343:TRP:CD1	2:F:2:GLC:H4	2.49	0.48
1:B:30:PHE:CD2	1:B:36:ILE:HB	2.49	0.48
1:B:458:ARG:HG3	1:B:470:ALA:HA	1.95	0.48
1:D:290:ASP:OD1	1:D:309:SER:HB2	2.14	0.48
1:B:724:GLN:HB2	1:B:727:ILE:HG13	1.95	0.48
1:C:131:THR:OG1	1:C:134:GLU:HG2	2.14	0.48
1:C:548:HIS:HB2	1:C:551:ASP:CG	2.39	0.48
1:C:553:LEU:HD12	1:C:554:VAL:H	1.79	0.48
1:C:697:LYS:HG2	1:C:730:ASP:HA	1.96	0.48
1:D:9:LYS:HZ2	1:D:11:VAL:HG22	1.77	0.48
1:A:132:TRP:CD1	1:A:251:PRO:HB2	2.48	0.47
1:C:9:LYS:HE2	1:C:9:LYS:HB2	1.56	0.47
1:B:488:GLU:HG2	1:B:492:ARG:HD2	1.96	0.47
1:D:383:LEU:HG	1:D:623:VAL:HG21	1.95	0.47
1:B:41:GLU:HB3	1:B:43:PRO:HD3	1.95	0.47
1:A:188:ASN:OD1	1:A:189:ALA:N	2.47	0.47
1:B:167:ASP:HA	1:B:256:GLN:HE22	1.78	0.47
1:D:387:HIS:HD2	1:D:626:ARG:NE	2.10	0.47
1:B:336:ILE:HG22	1:B:337:PRO:HD2	1.97	0.47
1:B:374:PHE:HD1	1:B:374:PHE:H	1.62	0.47
1:C:277:GLU:H	1:C:277:GLU:CD	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:HIS:CD2	1:D:392:ILE:HD11	2.49	0.47
1:C:728:GLN:OE1	5:C:904:GOL:H11	2.14	0.47
1:B:110:PRO:O	1:B:111:ILE:HD13	2.15	0.47
1:B:257:PRO:HB2	1:B:329:LYS:CD	2.42	0.47
1:C:696:MET:O	1:C:731:VAL:HG22	2.14	0.47
1:D:540[A]:ARG:HB3	1:D:558:PHE:HB2	1.96	0.47
1:D:768:GLN:HA	1:D:787:GLN:HG3	1.97	0.47
1:C:740:LEU:HB2	1:C:742:ILE:HD12	1.96	0.47
1:C:618:LEU:HD23	1:C:618:LEU:HA	1.77	0.47
1:D:236:SER:OG	1:D:301:PRO:HD3	2.15	0.47
1:D:753:LYS:HG2	1:D:765:PHE:HB2	1.97	0.47
1:B:616:ILE:HB	1:B:676:ARG:NH2	2.30	0.47
1:C:644[B]:ASP:OD1	1:C:674:TYR:OH	2.32	0.47
1:C:748:GLU:OE1	4:C:907:PLM:H82	2.14	0.47
1:A:504:PRO:HB3	1:D:701:MET:HE3	1.95	0.46
1:B:27:GLY:CA	1:B:38:VAL:HG21	2.45	0.46
1:B:204:ASN:HB2	1:B:206:HIS:CD2	2.50	0.46
1:D:365:ALA:O	1:D:369:THR:HG23	2.15	0.46
1:D:644[B]:ASP:HA	1:D:674:TYR:OH	2.15	0.46
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.62	0.46
1:B:19:GLY:N	1:B:300:LYS:HB2	2.30	0.46
1:A:138:LEU:HD22	1:A:142:LEU:HD11	1.97	0.46
1:B:282:PHE:HA	1:B:286:TYR:CD2	2.50	0.46
1:D:536:LEU:HA	1:D:536:LEU:HD23	1.70	0.46
1:D:695[A]:HIS:CE1	1:D:697:LYS:HG3	2.50	0.46
1:C:83:THR:O	1:C:280:LYS:NZ	2.48	0.46
1:D:644[A]:ASP:HA	1:D:674:TYR:OH	2.16	0.46
1:A:47:GLU:HB2	1:A:69:ARG:HD2	1.97	0.46
3:A:903:NAG:O7	1:B:357:ARG:NH2	2.48	0.46
1:B:91:LYS:HB3	1:B:307:LEU:HD12	1.98	0.46
1:C:305:VAL:HG13	1:C:307:LEU:H	1.81	0.46
1:A:139:ASP:CG	1:A:143:LYS:NZ	2.74	0.46
1:B:88:PHE:HZ	1:B:284:GLU:O	1.99	0.46
1:B:135:ILE:N	1:B:136:PRO:CD	2.79	0.46
1:B:240:THR:O	1:B:240:THR:OG1	2.31	0.46
1:A:36:ILE:HG13	1:A:278:LEU:CD1	2.46	0.46
1:B:17:ASP:OD2	2:G:1:BGC:O1	2.33	0.46
1:B:109:TYR:O	1:B:266:SER:HA	2.16	0.46
1:B:132:TRP:O	1:B:135:ILE:HG12	2.16	0.46
1:B:140:LYS:HE3	1:B:140:LYS:HB2	1.56	0.46
1:C:311:GLU:OE1	1:C:311:GLU:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:529:VAL:HG12	7:C:906:DMX:H2	1.96	0.46
1:A:192:LYS:O	1:A:196:THR:HB	2.16	0.46
1:B:550:LEU:HA	1:B:550:LEU:HD12	1.73	0.46
1:A:232:PRO:HA	1:A:235:TRP:CE2	2.51	0.46
1:B:155:GLN:HG3	1:B:212:ASP:HB3	1.98	0.46
1:D:732:THR:CB	1:D:744:LEU:HD22	2.46	0.46
1:A:282:PHE:O	1:A:286:TYR:HB2	2.16	0.46
1:A:550:LEU:O	1:A:553:LEU:HB3	2.16	0.46
1:A:658:ASP:OD2	1:A:660:VAL:HG23	2.16	0.46
1:B:22:GLY:HA3	1:B:299:ASP:HB2	1.97	0.46
1:B:162:PRO:HG3	1:B:260:PRO:HA	1.96	0.46
1:B:689:PHE:CD1	1:B:752:PHE:HD1	2.34	0.46
1:B:752:PHE:CE2	1:B:766:ASN:HB3	2.51	0.46
1:C:56:THR:HG22	1:C:589:HIS:HB2	1.97	0.46
1:C:552:HIS:CD2	1:C:589:HIS:NE2	2.83	0.46
1:D:259:LYS:HB3	1:D:259:LYS:HE2	1.43	0.46
1:A:138:LEU:CD2	1:A:142:LEU:HD11	2.45	0.45
1:B:50:PHE:HA	1:B:53:VAL:HB	1.98	0.45
1:C:552:HIS:CD2	1:C:589:HIS:CD2	3.04	0.45
1:D:491:SER:HB3	1:D:508:TRP:HB2	1.99	0.45
1:A:50:PHE:HB3	1:A:51:PRO:HD3	1.97	0.45
1:A:100:VAL:O	1:A:107:ILE:HG12	2.17	0.45
1:B:13:TRP:CE3	1:B:60:PRO:HG3	2.51	0.45
1:B:375:LYS:HA	1:B:378:GLN:CD	2.41	0.45
1:C:100:VAL:O	1:C:107:ILE:HG13	2.16	0.45
1:A:118:LEU:HD12	1:A:251:PRO:HD3	1.98	0.45
1:A:293:LEU:HD13	1:A:305:VAL:CG1	2.46	0.45
1:C:590:ALA:HB1	1:C:758:THR:CG2	2.45	0.45
1:C:753:LYS:HE2	1:C:786:TYR:CD2	2.51	0.45
1:B:296:VAL:O	1:B:297:ASN:C	2.60	0.45
1:B:692:LYS:HE3	8:B:1068:HOH:O	2.17	0.45
1:D:599:ARG:HE	1:D:599:ARG:HB3	1.49	0.45
1:B:82:ILE:HA	1:B:280:LYS:HZ2	1.81	0.45
1:B:490:LEU:HD22	1:B:508:TRP:CZ3	2.49	0.45
1:C:13:TRP:CD2	1:C:60:PRO:HG3	2.51	0.45
1:C:56:THR:CG2	1:C:589:HIS:HB2	2.46	0.45
1:C:355:SER:OG	1:C:357:ARG:HG3	2.17	0.45
1:C:480:ILE:HD12	1:C:602:GLU:HB2	1.99	0.45
1:A:167:ASP:OD1	1:A:254:LYS:HD2	2.17	0.45
1:A:479:VAL:CG1	1:A:516:LEU:HD13	2.46	0.45
1:B:396:MET:HA	1:B:396:MET:CE	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:ALA:O	1:C:184:VAL:HA	2.17	0.45
4:C:907:PLM:HB1	4:C:907:PLM:HC1	1.62	0.45
1:D:283:LEU:O	1:D:288:LEU:HB2	2.17	0.45
1:A:360:VAL:O	1:A:364:LEU:HB2	2.16	0.45
1:B:74:ALA:HB3	1:B:102:TYR:CD2	2.52	0.45
1:C:391:ARG:HA	1:C:391:ARG:NH1	2.31	0.45
1:C:484:GLU:HG3	1:C:510:GLN:NE2	2.32	0.45
1:A:310:TYR:CD1	1:A:314:LEU:HD21	2.52	0.45
1:B:699:THR:HG23	1:B:727:ILE:C	2.41	0.45
1:C:412:ARG:HB2	1:C:416:GLU:HB2	1.98	0.45
1:C:702:ASP:OD1	1:C:705:THR:N	2.38	0.45
1:D:696:MET:O	1:D:731:VAL:HG22	2.17	0.45
1:A:10:LEU:HA	1:A:61:ASP:OD1	2.17	0.45
1:A:619:HIS:ND1	1:A:644:ASP:HB2	2.31	0.45
1:C:486:VAL:HG13	7:C:906:DMX:H131	1.99	0.45
1:C:753:LYS:HG2	1:C:765:PHE:HB2	1.98	0.45
1:D:41:GLU:C	1:D:43:PRO:HD3	2.41	0.45
1:D:346:VAL:O	1:D:350:VAL:HG12	2.16	0.45
1:A:46:LEU:CD1	1:A:63:ILE:HD11	2.40	0.44
1:A:47:GLU:C	1:A:48:GLU:HG2	2.41	0.44
1:B:65:TRP:CD1	1:B:66:ALA:N	2.86	0.44
1:B:280:LYS:O	1:B:284:GLU:HB2	2.17	0.44
1:C:391:ARG:HA	1:C:391:ARG:HD2	1.39	0.44
1:A:165:ALA:O	1:A:259:LYS:HD3	2.18	0.44
1:D:81:GLU:OE2	1:D:105:LYS:HG2	2.17	0.44
1:D:249:VAL:HA	1:D:326:ASN:HD21	1.82	0.44
1:A:130:LYS:O	1:A:252:THR:HG22	2.17	0.44
1:D:343:TRP:CE3	2:I:2:GLC:H61	2.52	0.44
1:D:719:ALA:HA	1:D:733:HIS:CE1	2.52	0.44
1:D:744:LEU:N	1:D:745:PRO:HD2	2.32	0.44
1:A:71:GLY:HA3	1:A:335:ASN:O	2.18	0.44
1:B:675:SER:HB3	1:B:690:VAL:CG1	2.47	0.44
1:D:94:PRO:CD	7:D:905:DMX:H1	2.38	0.44
1:D:485:ALA:O	1:D:489:GLN:NE2	2.51	0.44
1:A:358:GLN:CB	1:A:363:ALA:HB2	2.44	0.44
1:D:93:TYR:O	1:D:96:THR:HG22	2.17	0.44
1:C:395:GLN:NE2	1:C:543:LYS:HD2	2.33	0.44
1:D:383:LEU:HG	1:D:623:VAL:CG2	2.48	0.44
1:D:634:LEU:HD13	1:D:634:LEU:HA	1.75	0.44
1:B:281:GLU:O	1:B:282:PHE:C	2.60	0.44
1:B:387[B]:HIS:NE2	1:B:626:ARG:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:611:LYS:HD2	1:C:611:LYS:HZ2	1.70	0.44
1:B:179:TYR:CZ	1:B:334:PRO:HG3	2.53	0.43
1:B:387[A]:HIS:CD2	1:B:544:GLN:OE1	2.70	0.43
1:D:125:LEU:HD13	1:D:138:LEU:HD21	1.99	0.43
1:D:753:LYS:HE2	1:D:786:TYR:CE2	2.53	0.43
1:A:28:LYS:HB3	1:A:28:LYS:HE2	1.67	0.43
1:A:112:ALA:HA	1:A:305:VAL:HA	2.00	0.43
1:A:676:ARG:HG2	1:A:689:PHE:CE2	2.53	0.43
1:B:30:PHE:HE1	1:B:286:TYR:HE2	1.65	0.43
1:B:64:PHE:HE1	1:B:111:ILE:HG13	1.83	0.43
1:B:441:ARG:NH2	1:B:613:ASP:H	2.16	0.43
1:B:503:ALA:HB1	1:B:504:PRO:HD2	1.99	0.43
1:B:728:GLN:HE22	5:B:905:GOL:H31	1.82	0.43
1:B:765:PHE:CE2	1:B:789:PRO:HB3	2.53	0.43
1:C:248:THR:OG1	1:C:249:VAL:N	2.51	0.43
1:A:280:LYS:HE3	1:A:284:GLU:CD	2.43	0.43
1:B:336:ILE:H	1:B:336:ILE:HG12	1.30	0.43
1:B:387[A]:HIS:NE2	1:B:544:GLN:OE1	2.51	0.43
1:B:618:LEU:HD23	1:B:618:LEU:HA	1.78	0.43
1:C:319:ARG:HE	1:C:319:ARG:HB2	1.65	0.43
1:C:585:LYS:HA	1:C:585:LYS:HD3	1.73	0.43
1:C:748:GLU:HG2	1:C:776:PRO:HG2	2.00	0.43
1:A:380:HIS:O	1:A:384:LYS:HG3	2.19	0.43
1:B:161:TRP:CE2	1:B:261:PHE:CE1	3.07	0.43
1:C:294:GLU:OE2	1:C:310:TYR:OH	2.36	0.43
1:C:442:CYS:CB	1:C:608:LEU:HD22	2.48	0.43
1:C:629:VAL:HG22	1:C:635:PHE:CD1	2.53	0.43
1:D:235:TRP:HB2	1:D:301:PRO:HG2	2.01	0.43
1:B:144:ALA:C	1:B:146:GLY:H	2.25	0.43
1:B:616:ILE:HA	1:B:754:MET:CE	2.48	0.43
1:B:645:ASN:O	1:B:646:ASN:OD1	2.36	0.43
1:C:295:ALA:HA	1:C:298:LYS:HD3	1.99	0.43
1:C:676:ARG:HG3	1:C:689:PHE:CZ	2.54	0.43
1:D:81:GLU:OE1	1:D:105:LYS:NZ	2.40	0.43
1:D:696:MET:HE3	1:D:696:MET:HB3	1.79	0.43
1:A:451:ILE:HG12	1:A:531:PHE:CZ	2.54	0.43
1:B:9:LYS:HD3	1:B:37:LYS:HB3	2.00	0.43
1:B:140:LYS:O	1:B:143:LYS:HB2	2.18	0.43
1:A:31:GLU:OE2	1:A:37:LYS:HD2	2.19	0.43
1:A:506:GLY:N	1:A:507:PRO:CD	2.82	0.43
4:A:904:PLM:H91	4:A:904:PLM:HC1	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:TRP:CD1	1:B:261:PHE:CD1	3.07	0.43
1:B:278:LEU:HD23	1:B:278:LEU:HA	1.73	0.43
1:C:96:THR:HG23	1:C:110:PRO:HG2	2.01	0.43
1:C:493:LEU:HD21	1:C:528:ALA:O	2.19	0.43
1:D:418:MET:HE2	1:D:418:MET:HB2	1.86	0.43
1:D:671:ARG:HH21	1:D:695[A]:HIS:CD2	2.36	0.43
1:A:120:TYR:CE1	1:A:122:LYS:HG2	2.53	0.43
1:A:759:ARG:H	1:A:759:ARG:HG3	1.57	0.43
1:B:396:MET:HA	1:B:396:MET:HE2	2.01	0.43
1:C:305:VAL:HG11	1:C:310:TYR:HB3	2.01	0.43
1:D:732:THR:HA	1:D:744:LEU:CD1	2.42	0.43
1:B:192:LYS:HE2	1:B:361:ASP:OD1	2.19	0.43
1:B:522:ASN:OD1	1:B:522:ASN:N	2.51	0.43
1:D:65:TRP:HB3	1:D:70:PHE:HE1	1.84	0.43
1:D:595:ARG:HG3	1:D:595:ARG:HH11	1.84	0.43
1:D:682:LYS:H	1:D:682:LYS:HG3	1.38	0.43
1:B:30:PHE:HE1	1:B:286:TYR:CE2	2.36	0.42
1:C:310:TYR:CD1	1:C:313:GLU:OE1	2.68	0.42
1:D:527:LYS:HA	8:D:1006:HOH:O	2.18	0.42
1:D:558:PHE:CE2	1:D:580:PRO:HB3	2.54	0.42
1:B:709:LEU:O	1:B:713:SER:HB2	2.20	0.42
1:C:684:MET:HG3	8:C:1013:HOH:O	2.18	0.42
1:D:10:LEU:HD23	1:D:10:LEU:HA	1.82	0.42
1:A:336:ILE:HD12	1:A:336:ILE:HG23	1.73	0.42
1:B:24:ALA:O	1:B:28:LYS:HG3	2.18	0.42
1:B:395:GLN:HE22	1:B:399:THR:HB	1.83	0.42
1:C:457:LEU:HD11	1:C:539:ILE:HD12	2.02	0.42
1:C:702:ASP:OD1	1:C:704:ALA:N	2.52	0.42
1:D:441:ARG:NE	1:D:611:LYS:O	2.50	0.42
1:D:524:GLU:HG2	1:D:525:CYS:N	2.33	0.42
1:A:240:THR:O	1:A:240:THR:OG1	2.33	0.42
1:A:545:TYR:CD2	1:A:553:LEU:HD13	2.54	0.42
1:B:138:LEU:O	1:B:141:GLU:HG3	2.19	0.42
1:C:10:LEU:HD23	1:C:10:LEU:HA	1.87	0.42
1:C:259:LYS:HB3	1:C:259:LYS:HE2	1.80	0.42
1:C:672:GLY:HA3	1:C:692:LYS:O	2.19	0.42
1:A:46:LEU:HD12	1:A:46:LEU:C	2.44	0.42
1:A:174:TYR:HA	1:A:178:LYS:O	2.20	0.42
1:A:769:ARG:HD3	4:A:904:PLM:C2	2.48	0.42
1:B:122:LYS:H	1:B:122:LYS:HG2	1.43	0.42
1:B:298:LYS:H	1:B:298:LYS:HG2	1.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:LEU:HD11	1:C:207:MET:HE2	2.02	0.42
1:D:5:THR:HG21	1:D:274:PRO:HD3	2.01	0.42
1:D:328:GLN:HE22	7:D:905:DMX:H121	1.83	0.42
1:A:361:ASP:O	1:A:365:ALA:N	2.51	0.42
1:B:143:LYS:HD2	1:B:143:LYS:HA	1.75	0.42
1:C:388:ASN:C	1:C:390:ALA:N	2.76	0.42
1:B:778:ARG:HA	1:B:778:ARG:HD3	1.70	0.42
1:C:207:MET:HE2	1:C:207:MET:HB3	1.97	0.42
1:D:113:VAL:HG22	1:D:264:VAL:HG22	2.02	0.42
1:B:714:GLY:C	1:B:716:GLU:H	2.27	0.42
1:C:492:ARG:HD3	8:C:1021:HOH:O	2.20	0.42
1:C:601:ASP:HB2	1:C:602:GLU:OE1	2.20	0.42
1:A:10:LEU:HA	1:A:10:LEU:HD12	1.75	0.42
1:A:317:ASP:OD2	1:A:320:VAL:HG23	2.20	0.42
1:B:32:LYS:HD3	1:B:32:LYS:HA	1.77	0.42
1:B:72:GLY:HA2	1:B:337:PRO:HG3	2.02	0.42
1:B:364:LEU:HD23	1:B:364:LEU:HA	1.90	0.42
1:C:232:PRO:HA	1:C:235:TRP:CE2	2.55	0.42
1:D:91:LYS:O	1:D:308:LYS:HG3	2.20	0.42
1:B:95:PHE:CE1	1:B:96:THR:HG22	2.55	0.41
1:C:458:ARG:NE	1:C:471:ASP:OD2	2.52	0.41
1:A:121:ASN:C	1:A:121:ASN:HD22	2.27	0.41
1:A:357:ARG:NH2	1:A:358:GLN:HG3	2.35	0.41
1:A:624:SER:HA	1:A:790:LEU:HD23	2.02	0.41
1:B:69:ARG:HG3	1:B:69:ARG:HH11	1.84	0.41
1:C:702:ASP:OD1	1:C:702:ASP:C	2.63	0.41
1:C:740:LEU:HB2	1:C:742:ILE:CD1	2.49	0.41
1:A:681:SER:N	8:A:1004:HOH:O	2.40	0.41
1:B:181:ILE:HD13	1:B:338:GLN:HG2	2.01	0.41
1:B:403:HIS:HD1	1:B:598:PHE:HE2	1.68	0.41
1:B:717:CYS:HB3	1:B:737:CYS:HB3	1.89	0.41
1:B:110:PRO:C	1:B:111:ILE:HD13	2.45	0.41
1:B:122:LYS:HE2	1:B:122:LYS:HB3	1.75	0.41
1:B:235:TRP:HB2	1:B:301:PRO:CG	2.50	0.41
1:B:509:VAL:HG13	1:B:512:VAL:CG2	2.48	0.41
1:B:510:GLN:O	1:B:512:VAL:HG23	2.20	0.41
1:B:709:LEU:O	1:B:713:SER:N	2.53	0.41
1:C:92:LEU:HB2	1:C:97:TRP:NE1	2.35	0.41
1:D:480:ILE:HG12	1:D:513:ALA:HA	2.02	0.41
1:B:374:PHE:CD1	1:B:374:PHE:N	2.89	0.41
1:B:257:PRO:CB	1:B:329:LYS:HE3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:LYS:HB2	1:D:10:LEU:H	1.62	0.41
7:D:905:DMX:H131	7:D:905:DMX:H171	1.69	0.41
1:A:48:GLU:HA	1:A:51:PRO:CD	2.47	0.41
1:B:334:PRO:HB2	1:B:339:MET:CE	2.50	0.41
1:B:714:GLY:C	1:B:715:ASN:HD22	2.29	0.41
1:C:305:VAL:HG13	1:C:307:LEU:N	2.36	0.41
1:D:92:LEU:HD12	1:D:97:TRP:CZ2	2.55	0.41
1:D:618:LEU:HD23	1:D:618:LEU:HA	1.85	0.41
1:A:47:GLU:O	1:A:73:TYR:OH	2.31	0.41
1:A:277:GLU:HG2	1:D:141:GLU:HA	2.03	0.41
1:A:550:LEU:HD23	1:A:550:LEU:HA	1.77	0.41
1:A:678:VAL:HG13	1:B:548:HIS:HA	2.01	0.41
1:B:121:ASN:HD22	1:B:121:ASN:HA	1.75	0.41
1:B:124:LEU:HD12	1:B:124:LEU:HA	1.93	0.41
1:B:672:GLY:HA3	1:B:692:LYS:O	2.20	0.41
1:C:527:LYS:O	1:C:528:ALA:C	2.64	0.41
1:A:33:ASP:HB2	1:A:286:TYR:OH	2.21	0.41
1:A:453:GLY:HA2	1:A:475:HIS:CD2	2.55	0.41
1:A:505:GLY:C	1:A:507:PRO:HD3	2.46	0.41
1:A:630:ARG:NH2	4:A:904:PLM:O1	2.49	0.41
1:B:61:ASP:OD1	1:B:274:PRO:HD2	2.21	0.41
1:B:418:MET:HE1	1:B:434:GLN:HG2	2.02	0.41
1:C:31:GLU:O	1:C:35:GLY:N	2.43	0.41
1:C:280:LYS:HE2	1:C:280:LYS:HB2	1.78	0.41
1:C:490:LEU:HD13	1:C:490:LEU:HA	1.76	0.41
1:C:744:LEU:HD23	1:C:744:LEU:HA	1.85	0.41
1:D:305:VAL:HG22	1:D:306:ALA:H	1.85	0.41
1:B:119:ILE:HA	1:B:246:GLY:O	2.21	0.41
1:B:212:ASP:OD1	1:B:213:TYR:N	2.53	0.41
1:C:273:SER:HA	1:C:274:PRO:HD3	1.88	0.40
1:C:328:GLN:NE2	7:C:905:DMX:H131	2.36	0.40
1:C:575:SER:OG	1:C:631:PRO:HA	2.21	0.40
1:C:705:THR:HG23	1:D:708:LEU:HD13	2.03	0.40
1:A:82:ILE:C	1:A:84:PRO:HD3	2.46	0.40
1:A:172:PHE:CD1	1:A:181:ILE:HA	2.57	0.40
1:A:308:LYS:H	1:A:308:LYS:HG3	1.75	0.40
1:A:352:ASN:O	1:A:357:ARG:N	2.51	0.40
1:A:609:PRO:HA	1:A:610:PRO:HD3	1.92	0.40
1:A:653:TYR:OH	4:A:904:PLM:HB2	2.22	0.40
1:B:65:TRP:CD1	1:B:66:ALA:H	2.39	0.40
1:B:92:LEU:HA	1:B:307:LEU:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:ARG:HD3	1:C:571:PHE:CE2	2.56	0.40
1:B:502:LEU:HB2	8:B:1003:HOH:O	2.20	0.40
1:C:56:THR:HG22	1:C:589:HIS:CB	2.51	0.40
1:C:127:ASN:OD1	1:C:127:ASN:N	2.53	0.40
1:D:172:PHE:CD2	1:D:336:ILE:HD11	2.56	0.40
1:D:441:ARG:HH11	1:D:441:ARG:HG3	1.86	0.40
1:B:92:LEU:HB3	1:B:306:ALA:HB1	2.03	0.40
1:B:205:LYS:HE2	1:B:205:LYS:HB3	1.95	0.40
1:B:474:LEU:HD23	1:B:474:LEU:HA	1.90	0.40
1:C:486:VAL:HG13	7:C:906:DMX:C13	2.51	0.40
1:D:148:SER:OG	1:D:225:THR:HG23	2.21	0.40
1:D:696:MET:HB2	1:D:744:LEU:HD21	2.02	0.40
1:B:270:ASN:O	1:B:273:SER:HB2	2.22	0.40
1:B:311:GLU:O	1:B:314:LEU:N	2.55	0.40
1:B:434:GLN:HB3	1:B:436:TYR:CE1	2.56	0.40
1:D:75:GLN:HG3	1:D:102:TYR:OH	2.21	0.40
1:D:378:GLN:HA	1:D:794:ALA:O	2.21	0.40
1:D:630:ARG:NH2	6:D:906:CL:CL	2.91	0.40
1:A:82:ILE:HG22	1:A:269:ILE:HD12	2.04	0.40
1:B:21:ASN:O	1:B:24:ALA:HB3	2.21	0.40
1:B:295:ALA:HA	1:B:298:LYS:HZ2	1.87	0.40
1:B:338:GLN:HG3	1:B:372:ALA:O	2.22	0.40
1:C:62:ILE:HD11	1:C:279:ALA:CB	2.43	0.40
1:C:491:SER:OG	1:C:502:LEU:HD21	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:NH1	1:C:482:HIS:O[2_546]	1.42	0.78
1:B:313:GLU:OE1	1:D:244:ASN:ND2[2_555]	1.98	0.22
8:A:1002:HOH:O	8:D:1006:HOH:O[2_646]	1.99	0.21
8:B:1071:HOH:O	8:D:1159:HOH:O[2_656]	2.17	0.03

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	775/818 (95%)	746 (96%)	27 (4%)	2 (0%)	36	41
1	B	789/818 (96%)	754 (96%)	34 (4%)	1 (0%)	48	57
1	C	780/818 (95%)	758 (97%)	20 (3%)	2 (0%)	36	41
1	D	784/818 (96%)	755 (96%)	27 (3%)	2 (0%)	36	41
All	All	3128/3272 (96%)	3013 (96%)	108 (4%)	7 (0%)	43	50

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	632	GLU
1	C	507	PRO
1	D	632	GLU
1	A	632	GLU
1	B	632	GLU
1	D	506	GLY
1	A	633	VAL

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	651/681 (96%)	605 (93%)	46 (7%)	13	14
1	B	657/681 (96%)	597 (91%)	60 (9%)	9	9
1	C	656/681 (96%)	618 (94%)	38 (6%)	18	22
1	D	659/681 (97%)	618 (94%)	41 (6%)	16	19
All	All	2623/2724 (96%)	2438 (93%)	185 (7%)	14	14

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	114	GLU
1	A	118	LEU
1	A	141	GLU
1	A	148	SER
1	A	183	ASP
1	A	184	VAL
1	A	186	VAL
1	A	192	LYS
1	A	196	THR
1	A	198	LEU
1	A	199	VAL
1	A	202	ILE
1	A	203	LYS
1	A	205	LYS
1	A	240	THR
1	A	259	LYS
1	A	261	PHE
1	A	275	ASN
1	A	298	LYS
1	A	314	LEU
1	A	315	VAL
1	A	351	ILE
1	A	359	THR
1	A	387[A]	HIS
1	A	387[B]	HIS
1	A	413	SER
1	A	469[A]	GLU
1	A	469[B]	GLU
1	A	490	LEU
1	A	502	LEU
1	A	518	GLN
1	A	520	GLU
1	A	553	LEU
1	A	570	VAL
1	A	576	SER
1	A	588	ASN
1	A	615	THR
1	A	633	VAL
1	A	636	LEU
1	A	660	VAL
1	A	671	ARG
1	A	678	VAL

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Mol	Chain	Res	Type
1	A	732	THR
1	A	759	ARG
1	A	766	ASN
1	B	23	LEU
1	B	26	VAL
1	B	32	LYS
1	B	48	GLU
1	B	69	ARG
1	B	75	GLN
1	B	76	SER
1	B	96	THR
1	B	106	LEU
1	B	122	LYS
1	B	130	LYS
1	B	138	LEU
1	B	140	LYS
1	B	143	LYS
1	B	147	LYS
1	B	182	LYS
1	B	203	LYS
1	B	240	THR
1	B	243	VAL
1	B	244	ASN
1	B	276	LYS
1	B	278	LEU
1	B	285	ASN
1	B	298	LYS
1	B	311	GLU
1	B	331	GLU
1	B	336	ILE
1	B	387[A]	HIS
1	B	387[B]	HIS
1	B	391	ARG
1	B	396	MET
1	B	400	ILE
1	B	459	GLN
1	B	473	GLN
1	B	490	LEU
1	B	502	LEU
1	B	511	ASP
1	B	518	GLN
1	B	519	GLU

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Mol	Chain	Res	Type
1	B	522	ASN
1	B	543	LYS
1	B	548	HIS
1	B	549	SER
1	B	551	ASP
1	B	570	VAL
1	B	573	ARG
1	B	576	SER
1	B	599	ARG
1	B	616	ILE
1	B	619	HIS
1	B	626	ARG
1	B	633	VAL
1	B	673	ARG
1	B	722	SER
1	B	727	ILE
1	B	735	ASN
1	B	743	LYS
1	B	761	ARG
1	B	774	SER
1	B	796	SER
1	C	9	LYS
1	C	37	LYS
1	C	38	VAL
1	C	56	THR
1	C	58[A]	ASP
1	C	58[B]	ASP
1	C	83	THR
1	C	96	THR
1	C	142	LEU
1	C	173	LYS
1	C	236	SER
1	C	254	LYS
1	C	261	PHE
1	C	280	LYS
1	C	305	VAL
1	C	332	ILE
1	C	359	THR
1	C	387	HIS
1	C	391	ARG
1	C	399	THR
1	C	413	SER

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Mol	Chain	Res	Type
1	C	490	LEU
1	C	491	SER
1	C	502	LEU
1	C	507	PRO
1	C	527	LYS
1	C	547	HIS
1	C	549	SER
1	C	576	SER
1	C	616	ILE
1	C	632	GLU
1	C	633	VAL
1	C	636	LEU
1	C	709	LEU
1	C	711	VAL
1	C	712	PHE
1	C	722	SER
1	C	795	SER
1	D	7	GLU
1	D	32	LYS
1	D	63	ILE
1	D	75	GLN
1	D	96	THR
1	D	138	LEU
1	D	143	LYS
1	D	178	LYS
1	D	210	ASP
1	D	225	THR
1	D	259	LYS
1	D	261	PHE
1	D	288	LEU
1	D	308	LYS
1	D	309	SER
1	D	340	SER
1	D	384	LYS
1	D	413	SER
1	D	427	ASN
1	D	455	ILE
1	D	459	GLN
1	D	463	ILE
1	D	519	GLU
1	D	524	GLU
1	D	570	VAL

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Mol	Chain	Res	Type
1	D	576	SER
1	D	634	LEU
1	D	636	LEU
1	D	644[A]	ASP
1	D	644[B]	ASP
1	D	676	ARG
1	D	693	VAL
1	D	696	MET
1	D	722	SER
1	D	729	GLN
1	D	733	HIS
1	D	742	ILE
1	D	743	LYS
1	D	744	LEU
1	D	751	ILE
1	D	795	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	89	GLN
1	A	121	ASN
1	A	218	HIS
1	A	222	HIS
1	A	328	GLN
1	A	368	GLN
1	A	428	ASN
1	A	475	HIS
1	A	489	GLN
1	A	537	GLN
1	A	547	HIS
1	A	587	HIS
1	A	589	HIS
1	A	729	GLN
1	B	15	ASN
1	B	42	HIS
1	B	121	ASN
1	B	155	GLN
1	B	208	ASN
1	B	222	HIS
1	B	244	ASN

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Mol	Chain	Res	Type
1	B	256	GLN
1	B	395	GLN
1	B	426	ASN
1	B	459	GLN
1	B	473	GLN
1	B	587	HIS
1	B	645	ASN
1	B	715	ASN
1	B	766	ASN
1	B	787	GLN
1	B	792	GLN
1	C	89	GLN
1	C	103	ASN
1	C	244	ASN
1	C	370	ASN
1	C	385	HIS
1	C	473	GLN
1	C	475	HIS
1	C	523	HIS
1	C	552	HIS
1	C	652	HIS
1	C	729	GLN
1	C	746	HIS
1	D	21	ASN
1	D	75	GLN
1	D	121	ASN
1	D	378	GLN
1	D	387	HIS
1	D	388	ASN
1	D	395	GLN
1	D	426	ASN
1	D	459	GLN
1	D	489	GLN
1	D	518	GLN
1	D	537	GLN
1	D	587	HIS
1	D	733	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	F	1	2	12,12,12	0.63	0	17,17,17	1.95	3 (17%)
2	GLC	F	2	2	11,11,12	0.59	0	15,15,17	0.74	0
2	BGC	G	1	2	12,12,12	0.67	0	17,17,17	2.14	6 (35%)
2	GLC	G	2	2	11,11,12	0.71	0	15,15,17	0.82	0
2	BGC	H	1	2	12,12,12	0.59	0	17,17,17	1.83	3 (17%)
2	GLC	H	2	2	11,11,12	1.31	1 (9%)	15,15,17	1.23	1 (6%)
2	BGC	I	1	2	12,12,12	0.60	0	17,17,17	2.07	4 (23%)
2	GLC	I	2	2	11,11,12	0.61	0	15,15,17	0.93	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
2	BGC	F	1	2	-	0/2/22/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1
2	BGC	G	1	2	-	0/2/22/22	0/1/1/1
2	GLC	G	2	2	-	0/2/19/22	0/1/1/1
2	BGC	H	1	2	-	0/2/22/22	0/1/1/1
2	GLC	H	2	2	-	0/2/19/22	0/1/1/1
2	BGC	I	1	2	-	0/2/22/22	0/1/1/1
2	GLC	I	2	2	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	GLC	O5-C1	-3.89	1.37	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	BGC	C1-O5-C5	-5.47	103.06	113.65
2	F	1	BGC	C1-O5-C5	-5.32	103.35	113.65
2	I	1	BGC	C1-O5-C5	-5.31	103.39	113.65
2	H	1	BGC	C1-O5-C5	-4.77	104.42	113.65
2	G	1	BGC	C1-C2-C3	-3.90	102.40	110.36
2	I	1	BGC	C1-C2-C3	-3.73	102.74	110.36
2	H	1	BGC	C1-C2-C3	-3.68	102.85	110.36
2	F	1	BGC	C1-C2-C3	-3.63	102.95	110.36
2	H	2	GLC	C1-O5-C5	3.12	116.36	112.19
2	I	1	BGC	O5-C1-C2	-2.92	105.17	110.30
2	H	1	BGC	O5-C1-C2	-2.81	105.35	110.30
2	I	1	BGC	O4-C4-C5	-2.77	102.50	109.32
2	G	1	BGC	O5-C1-C2	-2.72	105.52	110.30
2	F	1	BGC	O5-C1-C2	-2.66	105.62	110.30
2	G	1	BGC	O4-C4-C5	-2.36	103.52	109.32
2	G	1	BGC	O1-C1-C2	2.18	115.31	108.98
2	G	1	BGC	O4-C4-C3	-2.07	105.50	110.38

There are no chirality outliers.

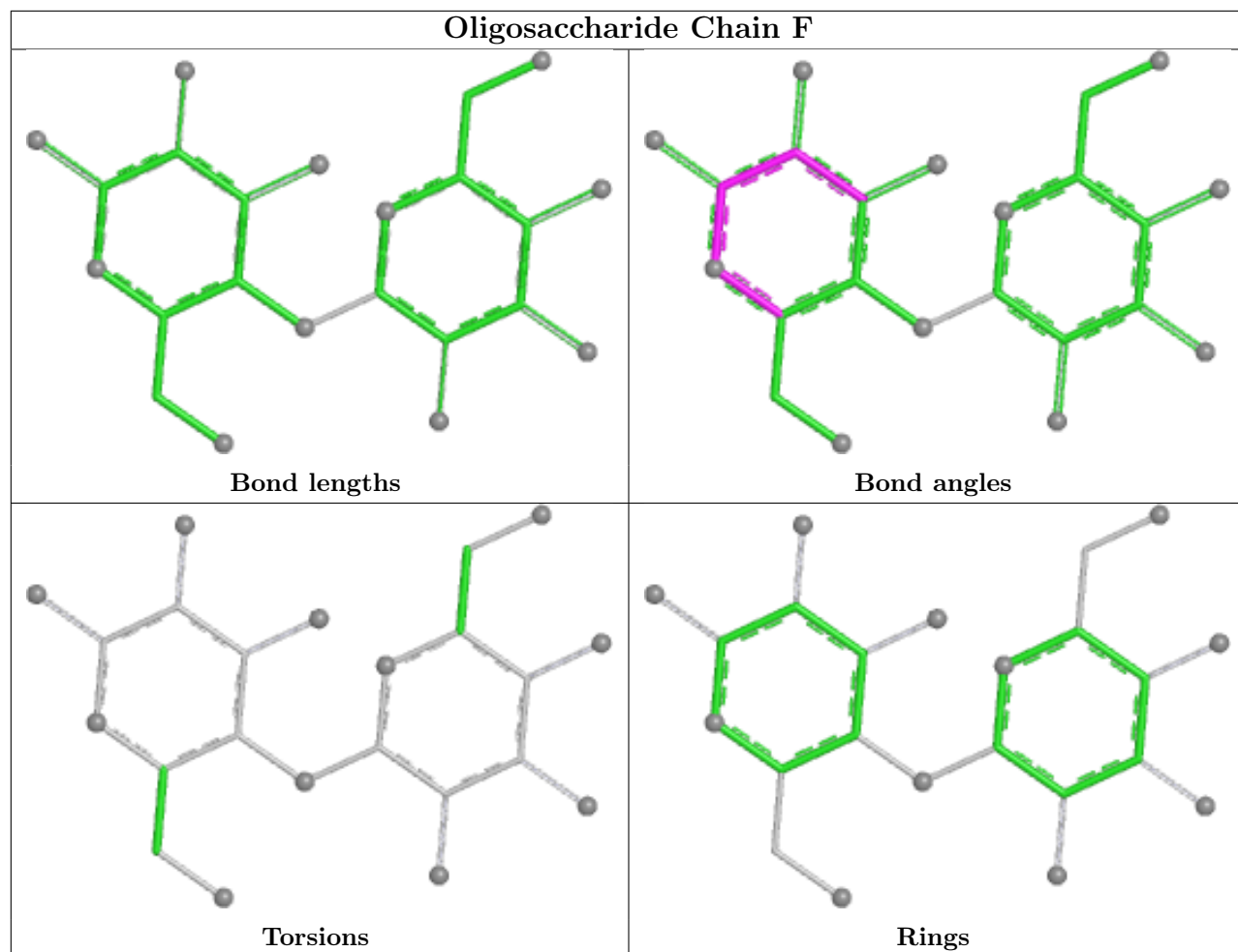
There are no torsion outliers.

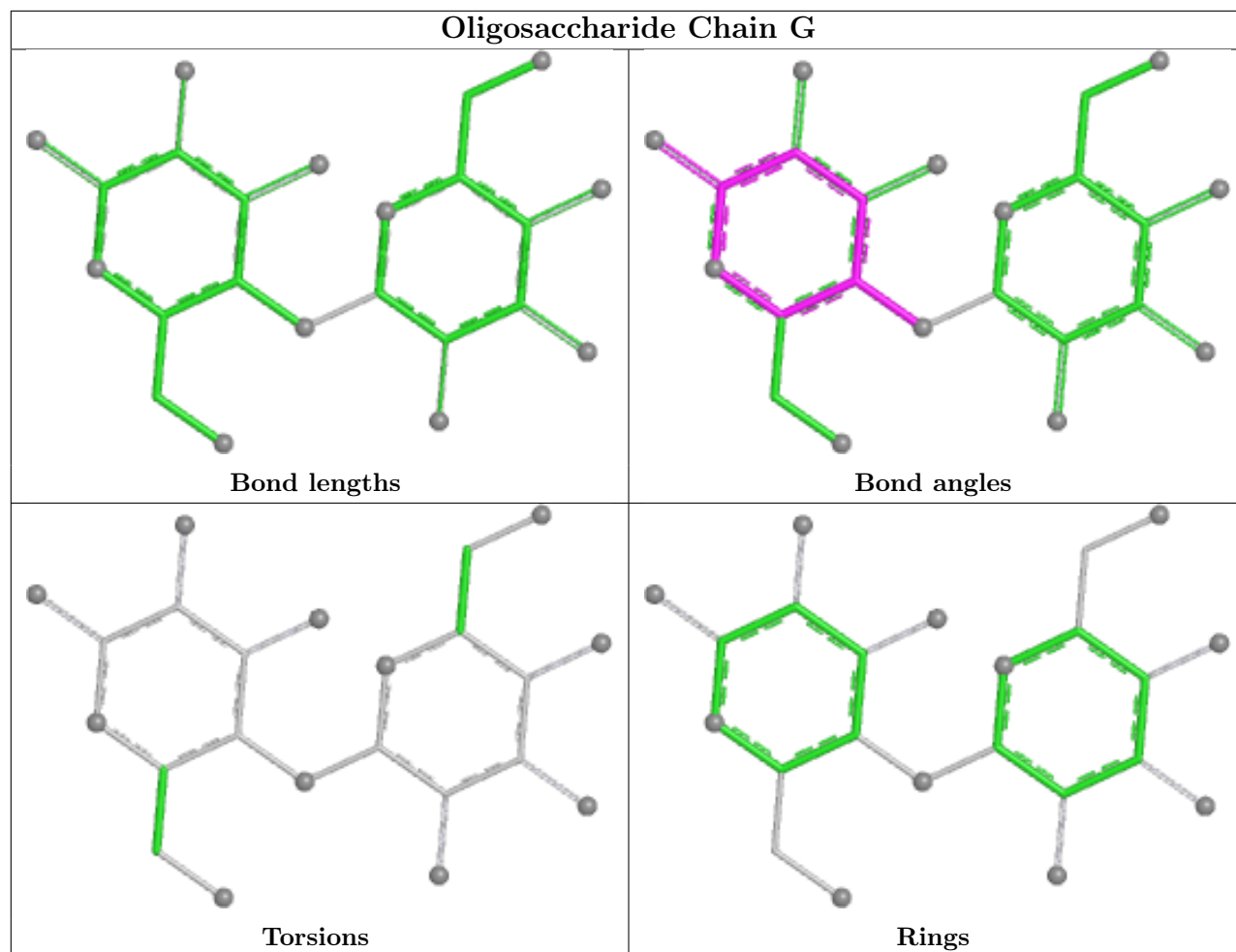
There are no ring outliers.

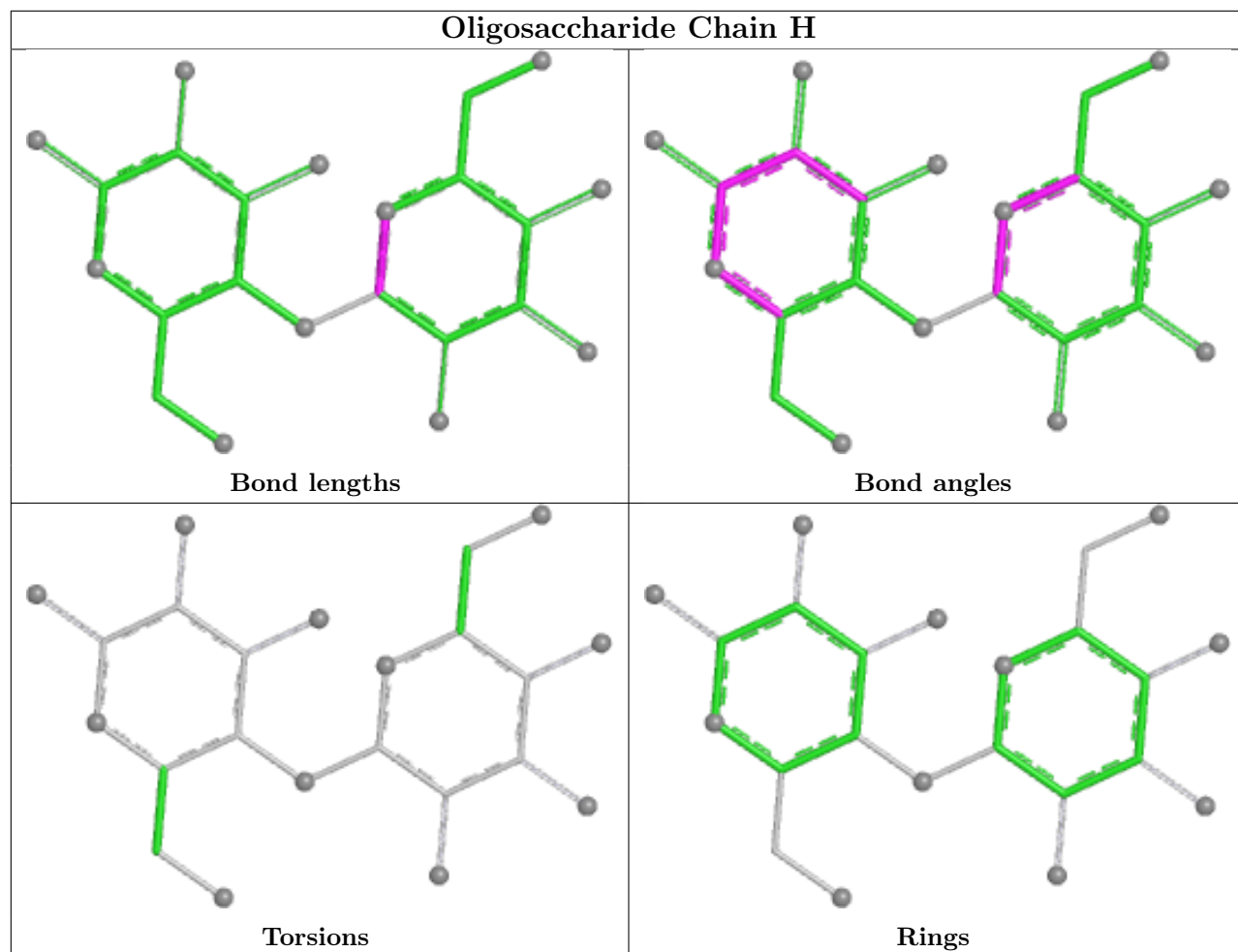
7 monomers are involved in 8 short contacts:

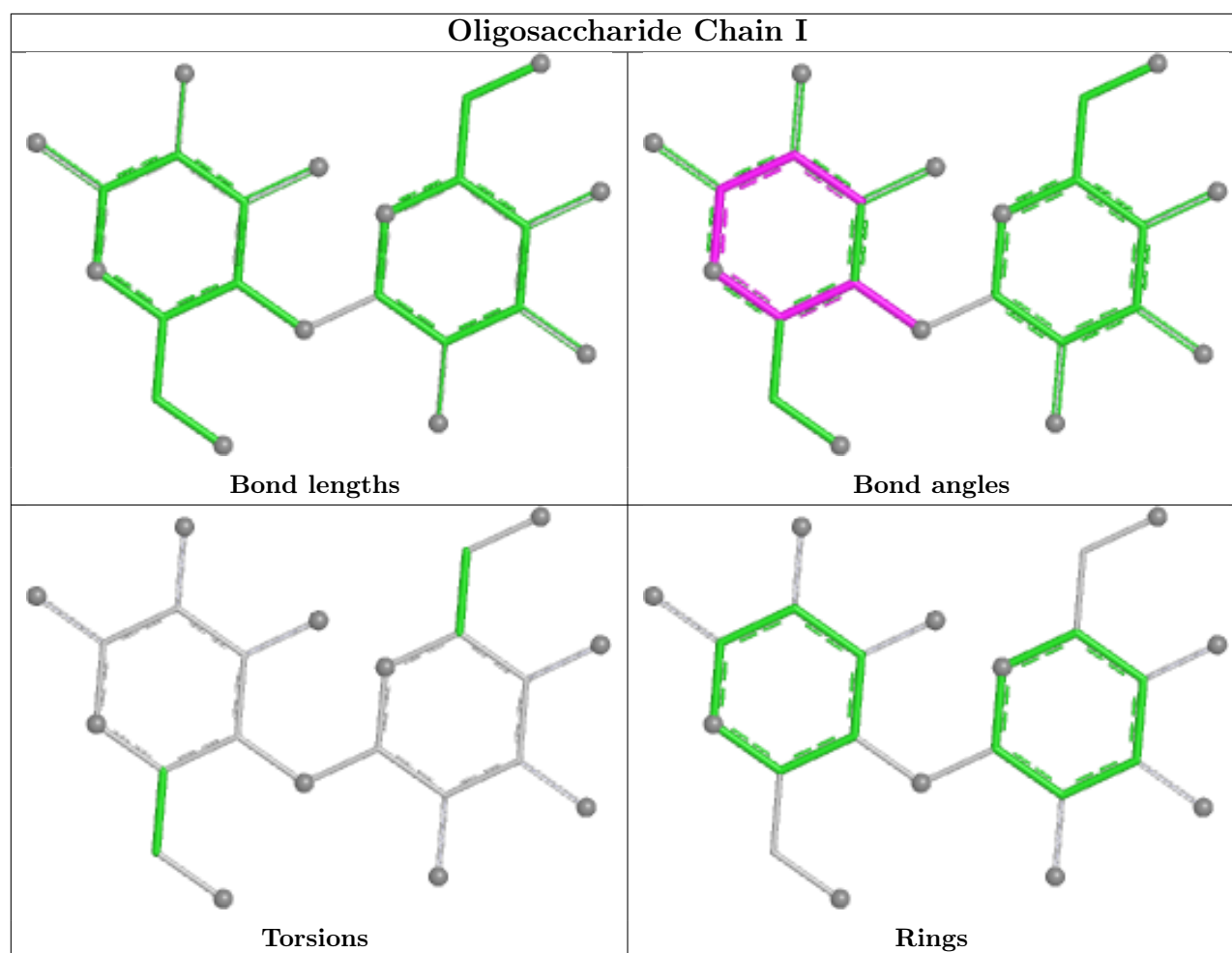
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1	BGC	1	0
2	H	2	GLC	2	0
2	I	2	GLC	1	0
2	G	1	BGC	1	0
2	F	1	BGC	1	0
2	H	1	BGC	1	0
2	F	2	GLC	1	0

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](#)

Of 25 ligands modelled in this entry, 3 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	B	901	1	14,14,15	0.32	0	17,19,21	0.42	0
7	DMX	C	905	-	17,17,17	1.49	2 (11%)	24,24,24	1.43	1 (4%)
3	NAG	C	901	1	14,14,15	0.18	0	17,19,21	0.42	0
3	NAG	A	903	1	14,14,15	0.29	0	17,19,21	0.45	0
3	NAG	B	903	1	14,14,15	0.42	0	17,19,21	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	DMX	C	906	-	17,17,17	1.47	1 (5%)	24,24,24	1.25	2 (8%)
7	DMX	D	905	-	17,17,17	1.28	1 (5%)	24,24,24	1.44	6 (25%)
5	GOL	B	904	-	5,5,5	0.92	0	5,5,5	1.01	0
4	PLM	A	904	-	17,17,17	0.40	0	17,17,17	0.89	0
3	NAG	A	902	1	14,14,15	0.33	0	17,19,21	0.65	0
3	NAG	A	901	1	14,14,15	0.29	0	17,19,21	0.49	0
3	NAG	C	903	1	14,14,15	0.38	0	17,19,21	0.58	0
5	GOL	D	904	-	5,5,5	0.95	0	5,5,5	1.09	0
3	NAG	B	902	1	14,14,15	0.42	0	17,19,21	0.58	0
3	NAG	D	903	1	14,14,15	0.38	0	17,19,21	0.37	0
3	NAG	C	902	1	14,14,15	0.44	0	17,19,21	0.62	0
4	PLM	C	907	-	17,17,17	0.31	0	17,17,17	0.81	0
5	GOL	B	905	-	5,5,5	0.94	0	5,5,5	1.06	0
3	NAG	D	901	1	14,14,15	0.26	0	17,19,21	0.40	0
5	GOL	C	904	-	5,5,5	0.95	0	5,5,5	0.98	0
5	GOL	A	905	-	5,5,5	1.09	0	5,5,5	1.04	0
3	NAG	D	902	1	14,14,15	0.30	0	17,19,21	0.82	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
3	NAG	B	901	1	-	2/6/23/26	0/1/1/1
7	DMX	C	905	-	-	6/13/13/13	0/1/1/1
3	NAG	C	901	1	-	2/6/23/26	0/1/1/1
3	NAG	A	903	1	-	2/6/23/26	0/1/1/1
3	NAG	B	903	1	-	2/6/23/26	0/1/1/1
7	DMX	C	906	-	-	10/13/13/13	0/1/1/1
7	DMX	D	905	-	-	13/13/13/13	0/1/1/1
5	GOL	B	904	-	-	2/4/4/4	-
4	PLM	A	904	-	-	14/15/15/15	-
3	NAG	A	902	1	-	2/6/23/26	0/1/1/1
3	NAG	A	901	1	-	0/6/23/26	0/1/1/1
3	NAG	C	903	1	-	1/6/23/26	0/1/1/1
5	GOL	D	904	-	-	3/4/4/4	-
3	NAG	B	902	1	-	2/6/23/26	0/1/1/1
3	NAG	D	903	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	902	1	-	2/6/23/26	0/1/1/1
4	PLM	C	907	-	-	11/15/15/15	-
5	GOL	B	905	-	-	4/4/4/4	-
3	NAG	D	901	1	-	0/6/23/26	0/1/1/1
5	GOL	C	904	-	-	0/4/4/4	-
5	GOL	A	905	-	-	2/4/4/4	-
3	NAG	D	902	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	906	DMX	C10-S11	5.30	1.85	1.77
7	C	905	DMX	C10-S11	4.97	1.84	1.77
7	D	905	DMX	C10-S11	4.12	1.83	1.77
7	C	905	DMX	C9-N8	2.34	1.57	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	905	DMX	O15-S11-C10	-4.11	100.52	106.73
7	C	906	DMX	O15-S11-C10	-3.35	101.67	106.73
7	D	905	DMX	O16-S11-C10	-2.85	102.42	106.73
7	D	905	DMX	O15-S11-C10	-2.72	102.61	106.73
7	D	905	DMX	O14-S11-C10	-2.33	101.45	106.00
7	D	905	DMX	C17-C10-S11	-2.30	109.73	113.25
7	D	905	DMX	C4-C7-N8	2.24	120.87	114.66
7	C	906	DMX	O16-S11-C10	-2.20	103.40	106.73
7	D	905	DMX	O14-S11-O15	2.05	116.52	111.40

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	904	GOL	C1-C2-C3-O3
5	B	905	GOL	C1-C2-C3-O3
7	C	905	DMX	C10-C17-C9-N8
7	C	905	DMX	C17-C10-S11-O14
7	C	905	DMX	C17-C10-S11-O15
7	C	906	DMX	C4-C7-N8-C9
7	C	906	DMX	C10-C17-C9-N8

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Mol	Chain	Res	Type	Atoms
7	D	905	DMX	C4-C7-N8-C9
7	D	905	DMX	C4-C7-N8-C12
7	D	905	DMX	C4-C7-N8-C13
7	D	905	DMX	C17-C9-N8-C7
7	D	905	DMX	C10-C17-C9-N8
7	D	905	DMX	S11-C10-C17-C9
7	C	906	DMX	C3-C4-C7-N8
7	C	906	DMX	C5-C4-C7-N8
7	D	905	DMX	C3-C4-C7-N8
7	D	905	DMX	C5-C4-C7-N8
7	D	905	DMX	C17-C9-N8-C12
3	B	903	NAG	O5-C5-C6-O6
3	B	901	NAG	O5-C5-C6-O6
7	C	906	DMX	C4-C7-N8-C13
3	B	903	NAG	C4-C5-C6-O6
3	A	903	NAG	O5-C5-C6-O6
3	C	902	NAG	O5-C5-C6-O6
4	C	907	PLM	C9-CA-CB-CC
4	C	907	PLM	C4-C5-C6-C7
7	D	905	DMX	C17-C9-N8-C13
7	D	905	DMX	C17-C10-S11-O14
3	C	902	NAG	C4-C5-C6-O6
7	C	906	DMX	C17-C9-N8-C7
3	A	903	NAG	C4-C5-C6-O6
3	B	901	NAG	C4-C5-C6-O6
7	C	906	DMX	C17-C9-N8-C12
3	B	902	NAG	O5-C5-C6-O6
7	C	906	DMX	S11-C10-C17-C9
7	C	906	DMX	C4-C7-N8-C12
7	C	906	DMX	C17-C9-N8-C13
5	A	905	GOL	O1-C1-C2-C3
5	B	905	GOL	O1-C1-C2-C3
5	D	904	GOL	O1-C1-C2-C3
4	A	904	PLM	C1-C2-C3-C4
4	A	904	PLM	C8-C9-CA-CB
4	A	904	PLM	CB-CC-CD-CE
5	A	905	GOL	O1-C1-C2-O2
5	B	905	GOL	O1-C1-C2-O2
5	B	905	GOL	O2-C2-C3-O3
5	D	904	GOL	O1-C1-C2-O2
4	A	904	PLM	C5-C6-C7-C8
4	C	907	PLM	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
4	C	907	PLM	C5-C6-C7-C8
4	C	907	PLM	CB-CC-CD-CE
7	C	905	DMX	C3-C4-C7-N8
3	C	901	NAG	C4-C5-C6-O6
5	B	904	GOL	O2-C2-C3-O3
7	C	905	DMX	C17-C10-S11-O16
7	D	905	DMX	C17-C10-S11-O15
7	D	905	DMX	C17-C10-S11-O16
4	A	904	PLM	C7-C8-C9-CA
3	C	901	NAG	O5-C5-C6-O6
4	A	904	PLM	CD-CE-CF-CG
4	A	904	PLM	C3-C4-C5-C6
7	C	905	DMX	C5-C4-C7-N8
4	A	904	PLM	C2-C3-C4-C5
4	A	904	PLM	C6-C7-C8-C9
3	D	902	NAG	C1-C2-N2-C7
3	B	902	NAG	C4-C5-C6-O6
4	A	904	PLM	C9-CA-CB-CC
4	C	907	PLM	CA-CB-CC-CD
4	C	907	PLM	C7-C8-C9-CA
3	A	902	NAG	C4-C5-C6-O6
5	D	904	GOL	O2-C2-C3-O3
3	A	902	NAG	O5-C5-C6-O6
4	A	904	PLM	CA-CB-CC-CD
4	C	907	PLM	CD-CE-CF-CG
4	A	904	PLM	O1-C1-C2-C3
4	A	904	PLM	O2-C1-C2-C3
3	C	903	NAG	C1-C2-N2-C7
3	D	902	NAG	C3-C2-N2-C7
3	D	903	NAG	C4-C5-C6-O6
4	A	904	PLM	C4-C5-C6-C7
4	C	907	PLM	O2-C1-C2-C3
4	C	907	PLM	O1-C1-C2-C3
4	C	907	PLM	CC-CD-CE-CF

There are no ring outliers.

9 monomers are involved in 27 short contacts:

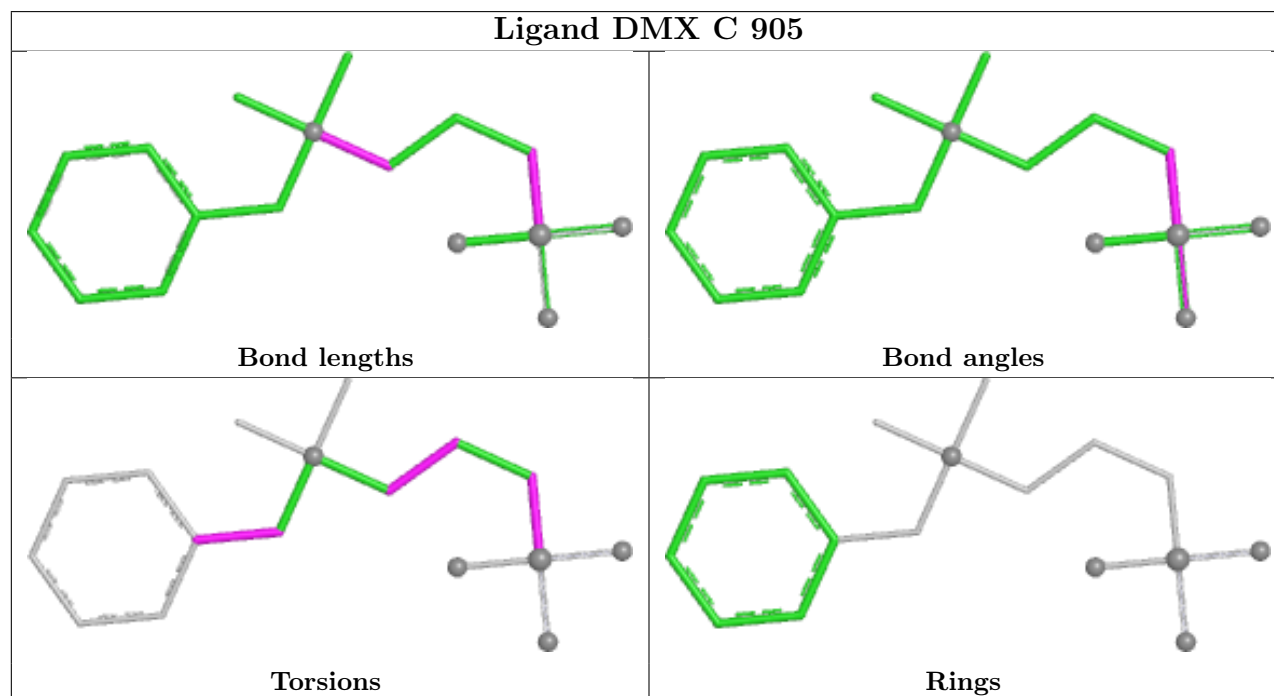
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	905	DMX	4	0
3	A	903	NAG	1	0
7	C	906	DMX	4	0

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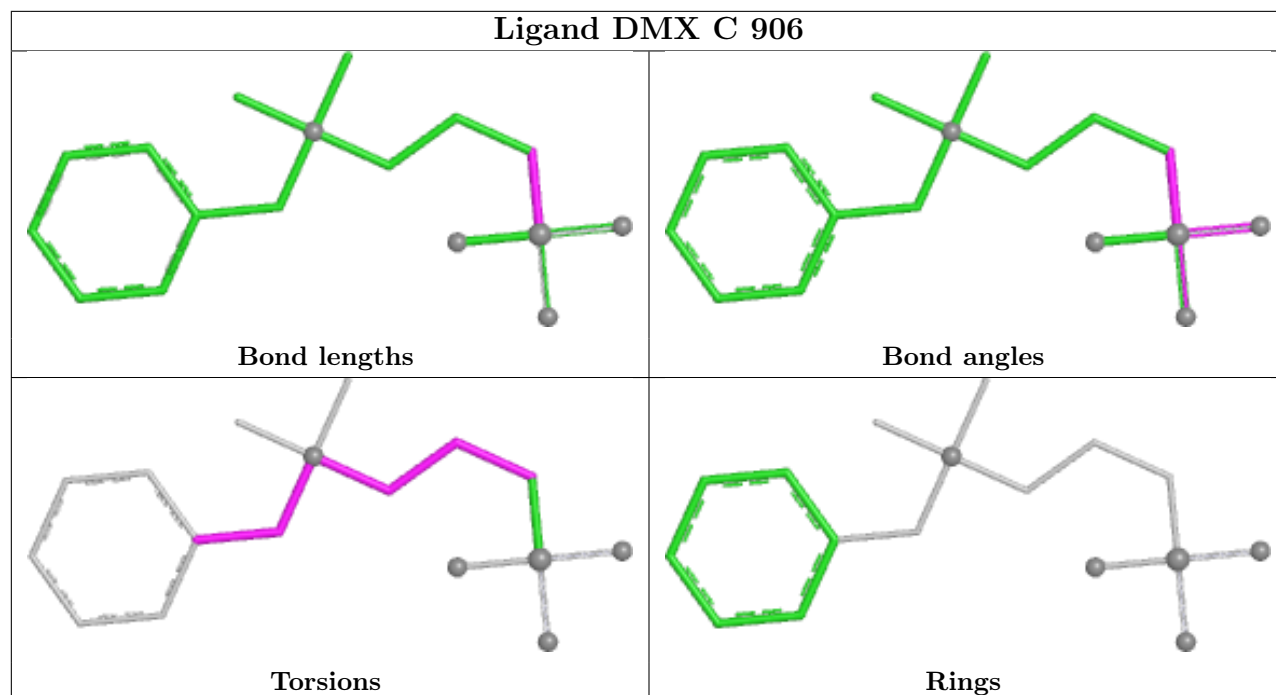
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	905	DMX	5	0
4	A	904	PLM	6	0
3	B	902	NAG	1	0
4	C	907	PLM	4	0
5	B	905	GOL	1	0
5	C	904	GOL	1	0

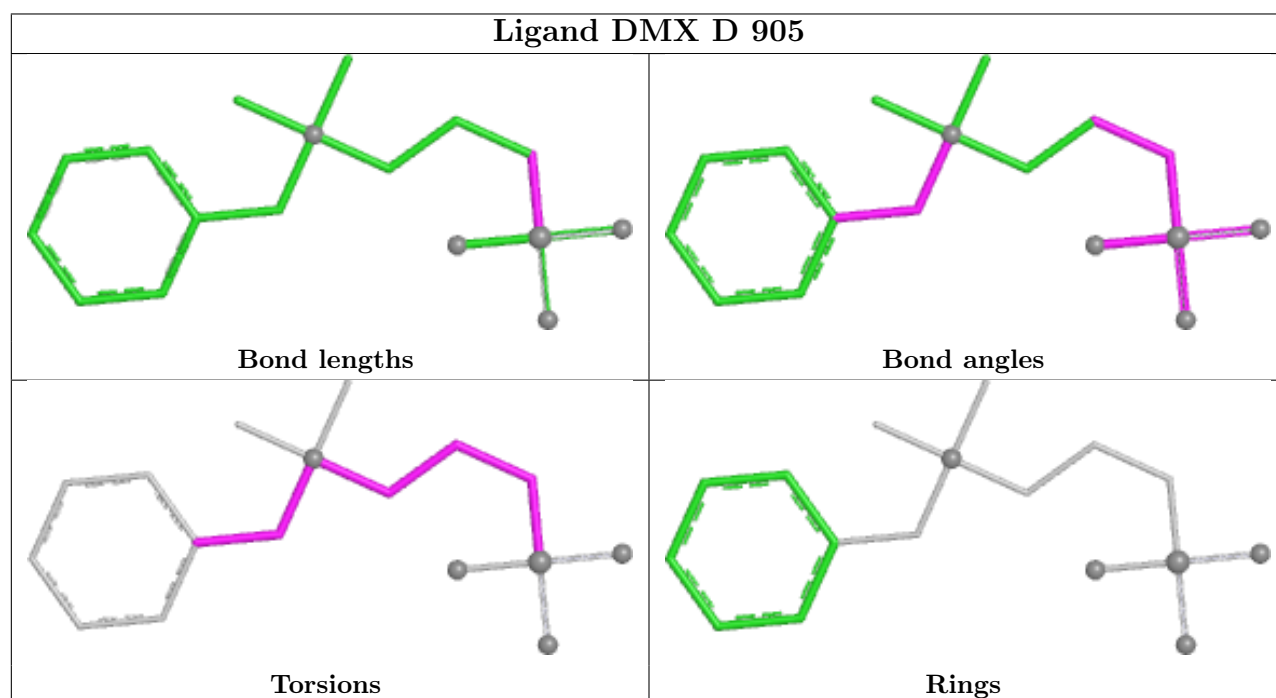
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

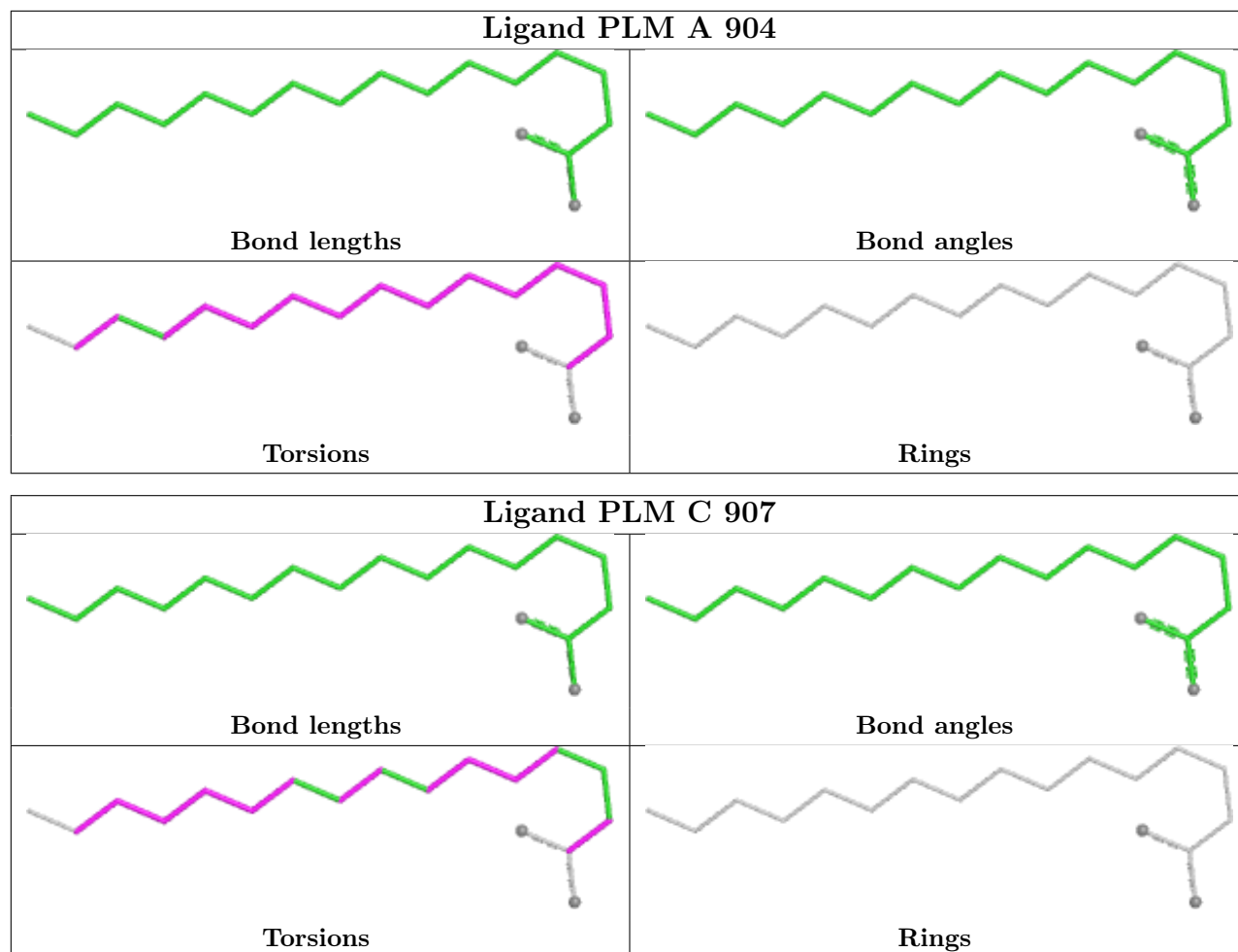


Ligand DMX C 906



Ligand DMX D 905





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	778/818 (95%)	0.55	52 (6%) 24 28	22, 69, 119, 200	3 (0%)
1	B	789/818 (96%)	0.90	87 (11%) 10 12	36, 84, 181, 238	2 (0%)
1	C	782/818 (95%)	0.26	30 (3%) 44 50	29, 58, 102, 185	4 (0%)
1	D	784/818 (95%)	0.13	28 (3%) 46 52	21, 51, 89, 165	6 (0%)
All	All	3133/3272 (95%)	0.46	197 (6%) 26 31	21, 63, 138, 238	15 (0%)

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	744	LEU	8.5
1	C	712	PHE	6.6
1	C	740	LEU	5.5
1	D	718	GLY	4.8
1	D	742	ILE	4.8
1	C	504	PRO	4.3
1	D	633	VAL	4.3
1	B	82	ILE	4.2
1	B	79	LEU	4.0
1	A	547	HIS	3.9
1	A	242	ALA	3.9
1	A	172	PHE	3.8
1	C	395	GLN	3.8
1	C	598[A]	PHE	3.8
1	A	504	PRO	3.8
1	B	141	GLU	3.8
1	B	283	LEU	3.8
1	C	389	GLY	3.8
1	D	632	GLU	3.7
1	C	55	ALA	3.7
1	A	171	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	23	LEU	3.6
1	B	287	LEU	3.5
1	A	505	GLY	3.5
1	D	712	PHE	3.5
1	B	276	LYS	3.4
1	B	8	GLY	3.4
1	A	48	GLU	3.4
1	B	269	ILE	3.3
1	C	242	ALA	3.3
1	C	611	LYS	3.3
1	D	695[A]	HIS	3.3
1	B	274	PRO	3.3
1	A	245	TYR	3.3
1	B	109	TYR	3.2
1	A	503	ALA	3.2
1	B	50	PHE	3.2
1	B	87	ALA	3.2
1	C	503	ALA	3.2
1	C	633	VAL	3.1
1	C	713	SER	3.1
1	B	286	TYR	3.1
1	D	721	GLY	3.1
1	B	55	ALA	3.1
1	B	86	ALA	3.1
1	A	739	ALA	3.1
1	A	397	PRO	3.1
1	C	387	HIS	3.0
1	B	26	VAL	3.0
1	C	742	ILE	3.0
1	B	77	GLY	3.0
1	A	367	ALA	3.0
1	B	272	ALA	3.0
1	A	186	VAL	3.0
1	B	618	LEU	3.0
1	B	302	LEU	2.9
1	B	548	HIS	2.9
1	C	610	PRO	2.9
1	A	366	ALA	2.9
1	B	142	LEU	2.9
1	B	288	LEU	2.9
1	A	357	ARG	2.9
1	B	275	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	53	VAL	2.9
1	A	721	GLY	2.8
1	C	380[A]	HIS	2.8
1	B	395	GLN	2.8
1	B	85	ALA	2.8
1	D	696	MET	2.8
1	A	610	PRO	2.8
1	B	80	ALA	2.8
1	B	63	ILE	2.8
1	B	75	GLN	2.8
1	B	99	ALA	2.8
1	A	332	ILE	2.7
1	B	124	LEU	2.7
1	B	175	ALA	2.7
1	C	523	HIS	2.7
1	C	552	HIS	2.7
1	B	265	LEU	2.7
1	B	11	VAL	2.7
1	B	462	TRP	2.7
1	B	170	TYR	2.7
1	B	633	VAL	2.7
1	A	255	GLY	2.7
1	B	144	ALA	2.6
1	D	5	THR	2.6
1	A	303	GLY	2.6
1	B	333	MET	2.6
1	D	387	HIS	2.6
1	B	290	ASP	2.6
1	B	715	ASN	2.6
1	A	35	GLY	2.6
1	D	610	PRO	2.6
1	A	546	PRO	2.6
1	C	506	GLY	2.6
1	B	111	ILE	2.6
1	D	796	SER	2.6
1	A	552	HIS	2.6
1	B	10	LEU	2.6
1	B	271	ALA	2.6
1	B	97	TRP	2.6
1	A	369	THR	2.6
1	B	185	GLY	2.6
1	A	364	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	759	ARG	2.5
1	B	103	ASN	2.5
1	B	297	ASN	2.5
1	B	88	PHE	2.5
1	D	745	PRO	2.5
1	B	504	PRO	2.5
1	C	505	GLY	2.5
1	B	106	LEU	2.5
1	A	507	PRO	2.5
1	B	610	PRO	2.5
1	D	619	HIS	2.5
1	A	734	THR	2.5
1	B	78	LEU	2.5
1	B	307	LEU	2.5
1	A	115	ALA	2.5
1	B	110	PRO	2.4
1	B	112	ALA	2.4
1	B	334	PRO	2.4
1	C	721	GLY	2.4
1	B	38	VAL	2.4
1	B	243	VAL	2.4
1	B	176	ALA	2.4
1	B	242	ALA	2.4
1	A	758	THR	2.4
1	D	507	PRO	2.3
1	C	739	ALA	2.3
1	B	39	THR	2.3
1	D	548	HIS	2.3
1	B	719	ALA	2.3
1	C	243	VAL	2.3
1	B	60	PRO	2.3
1	A	176	ALA	2.3
1	A	120	TYR	2.3
1	A	321	ALA	2.3
1	A	371	ALA	2.3
1	A	391	ARG	2.3
1	B	52	GLN	2.3
1	C	711	VAL	2.3
1	A	257	PRO	2.2
1	D	389	GLY	2.2
1	B	285	ASN	2.2
1	C	208	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	506	GLY	2.2
1	C	56	THR	2.2
1	A	241	SER	2.2
1	A	545	TYR	2.2
1	B	46	LEU	2.2
1	B	95	PHE	2.2
1	D	626	ARG	2.2
1	B	312	GLU	2.2
1	D	9	LYS	2.2
1	A	179	TYR	2.2
1	D	616	ILE	2.2
1	B	391	ARG	2.2
1	B	396	MET	2.2
1	A	8	GLY	2.2
1	A	181	ILE	2.1
1	B	13	TRP	2.1
1	B	138	LEU	2.1
1	D	618	LEU	2.1
1	D	634	LEU	2.1
1	A	372	ALA	2.1
1	A	124	LEU	2.1
1	B	36	ILE	2.1
1	B	244	ASN	2.1
1	B	113	VAL	2.1
1	A	358	GLN	2.1
1	B	397	PRO	2.1
1	B	718	GLY	2.1
1	D	268	GLY	2.1
1	A	359	THR	2.1
1	B	273	SER	2.1
1	D	722	SER	2.1
1	B	329	LYS	2.1
1	C	291	GLU	2.1
1	A	235	TRP	2.1
1	A	353	ALA	2.1
1	B	54	ALA	2.1
1	C	390	ALA	2.1
1	D	175	ALA	2.1
1	D	719	ALA	2.1
1	A	201	LEU	2.1
1	B	332	ILE	2.1
1	A	199	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	172	PHE	2.1
1	A	573	ARG	2.1
1	D	676	ARG	2.1
1	A	225	THR	2.0
1	C	388	ASN	2.0
1	C	732	THR	2.0
1	B	279	ALA	2.0
1	B	154	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

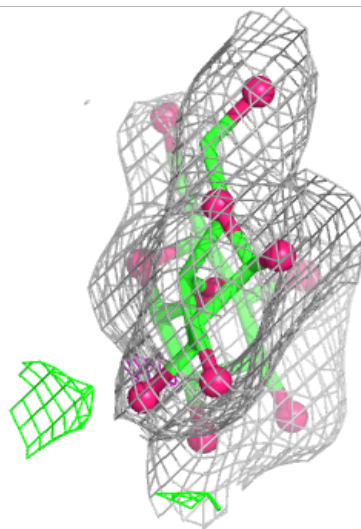
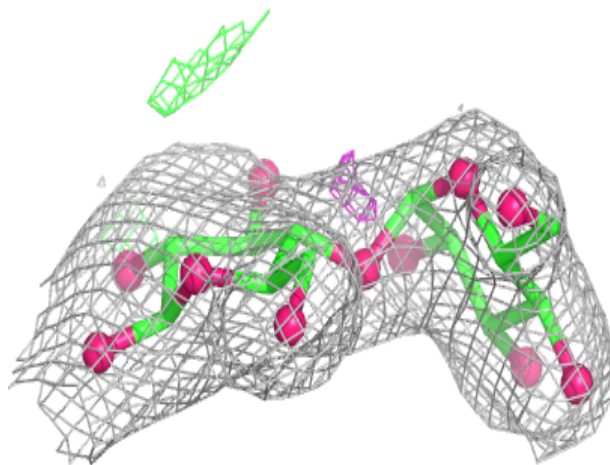
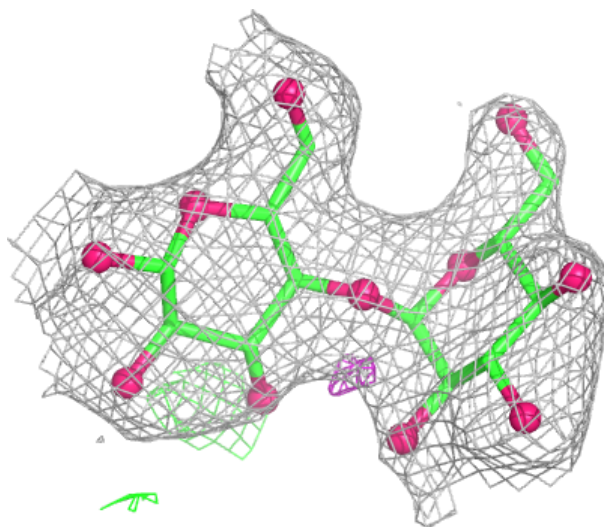
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	F	2	11/12	0.83	0.12	52,65,69,71	0
2	BGC	F	1	12/12	0.85	0.13	48,64,69,73	0
2	BGC	H	1	12/12	0.94	0.08	37,47,53,56	0
2	GLC	G	2	11/12	0.95	0.06	78,95,104,105	0
2	BGC	G	1	12/12	0.95	0.07	76,97,108,113	0
2	GLC	H	2	11/12	0.97	0.06	44,47,51,53	0
2	BGC	I	1	12/12	-	-	34,43,48,52	0
2	GLC	I	2	11/12	-	-	29,33,40,44	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.

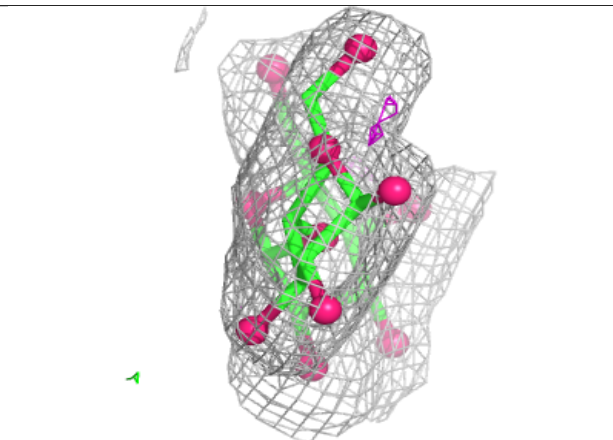
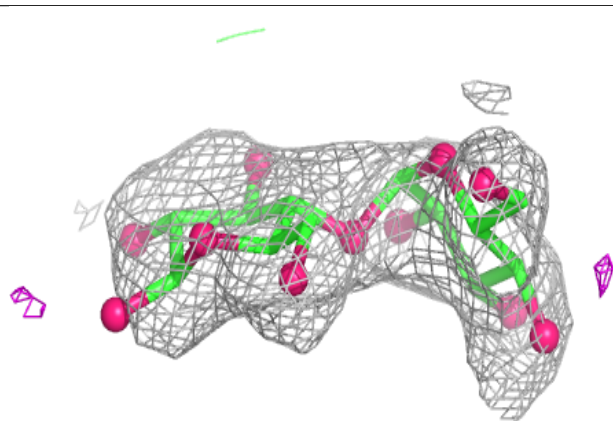
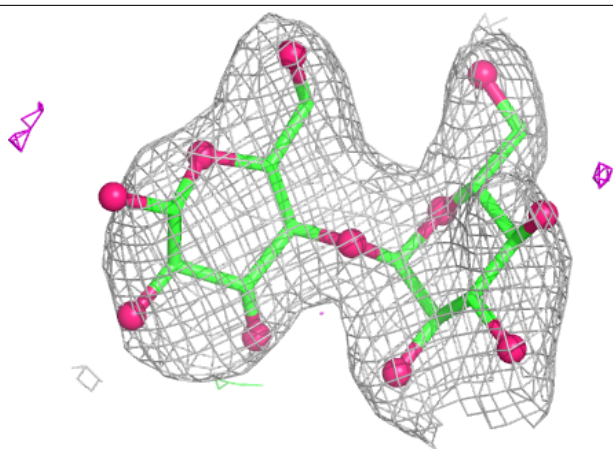
Electron density around Chain F:

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



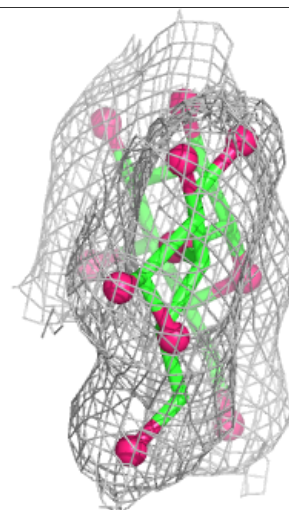
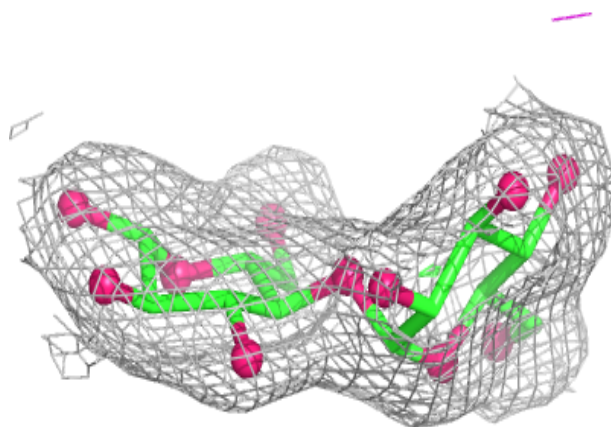
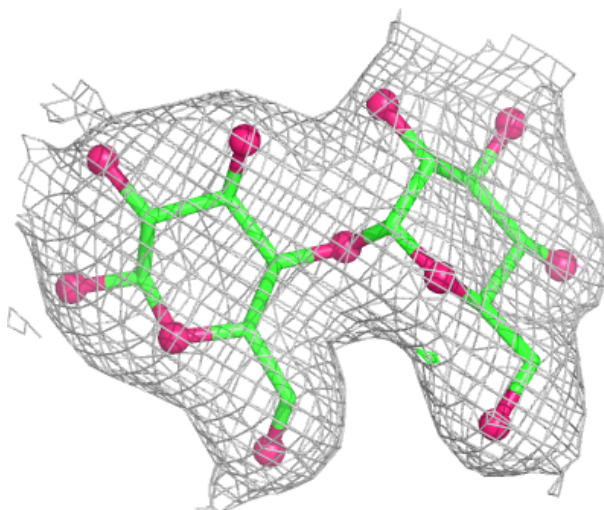
Electron density around Chain G:

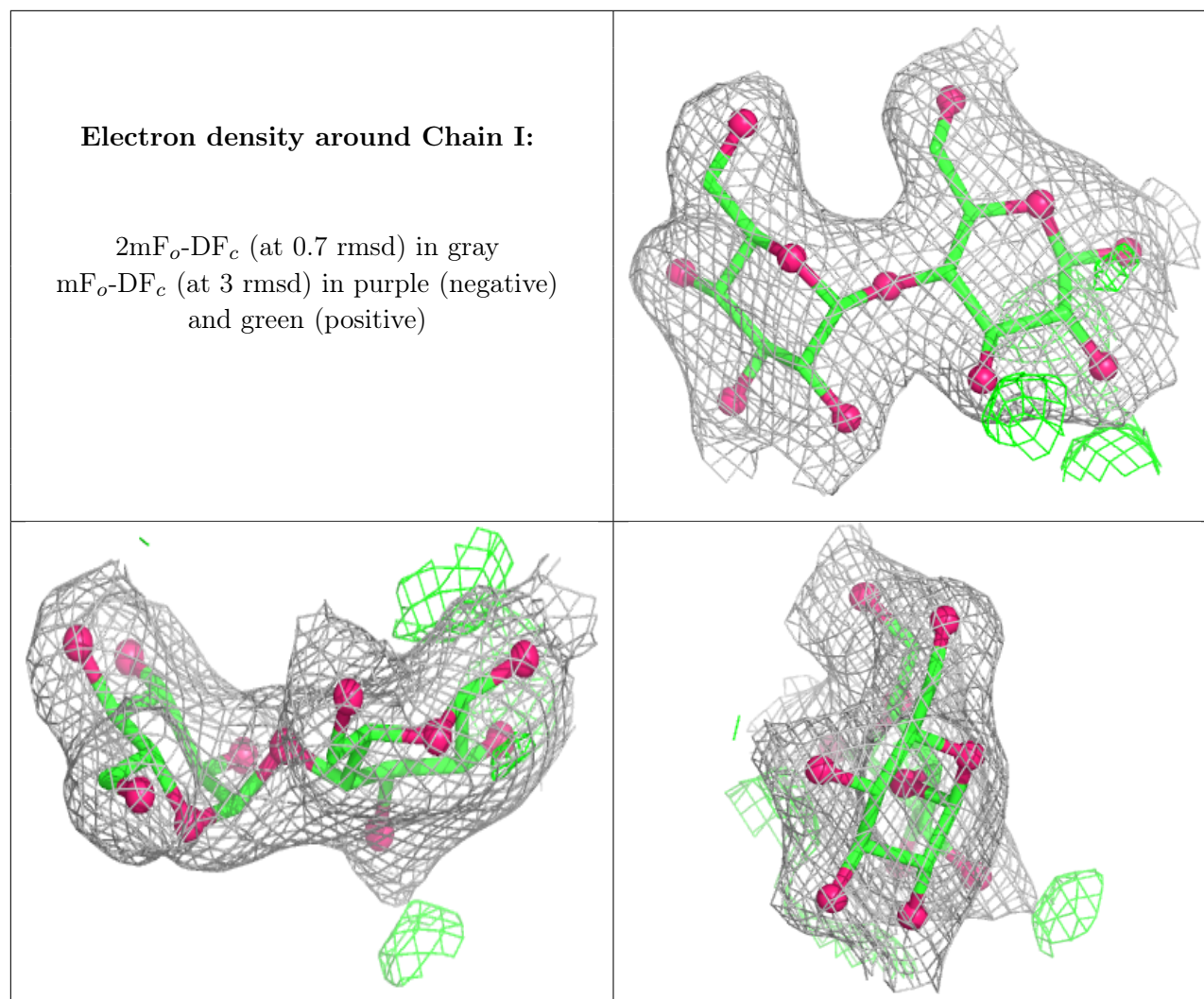
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	DMX	C	906	17/17	0.63	0.21	68,84,120,187	0
3	NAG	A	902	14/15	0.66	0.14	81,93,101,102	0
3	NAG	B	901	14/15	0.70	0.16	74,85,96,98	0
3	NAG	D	901	14/15	0.71	0.18	79,93,100,108	0
3	NAG	D	902	14/15	0.72	0.14	68,87,96,114	0
3	NAG	B	902	14/15	0.73	0.16	82,92,104,106	0
4	PLM	A	904	18/18	0.78	0.21	48,61,75,76	0
7	DMX	C	905	17/17	0.81	0.18	71,93,101,158	0
3	NAG	A	901	14/15	0.81	0.12	55,62,78,79	0

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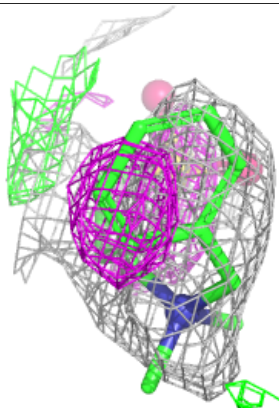
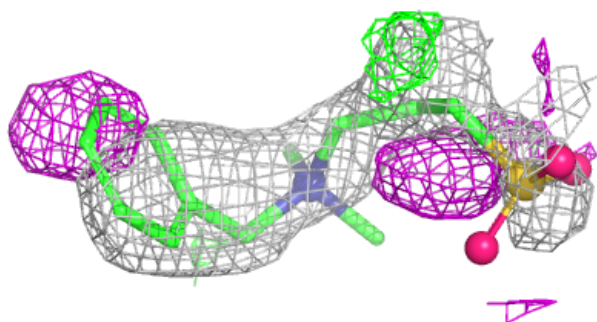
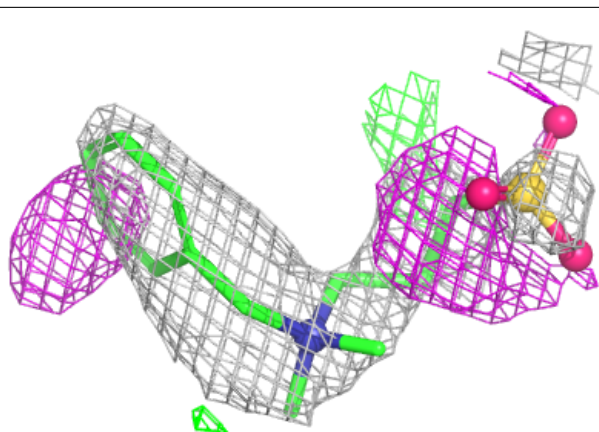
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PLM	C	907	18/18	0.82	0.19	49,63,73,75	0
3	NAG	B	903	14/15	0.83	0.10	79,90,101,106	0
5	GOL	B	905	6/6	0.83	0.11	68,76,80,82	0
7	DMX	D	905	17/17	0.83	0.18	85,120,133,196	0
5	GOL	B	904	6/6	0.84	0.16	67,71,79,82	0
3	NAG	D	903	14/15	0.88	0.09	53,68,81,87	0
3	NAG	A	903	14/15	0.88	0.10	66,77,86,93	0
5	GOL	C	904	6/6	0.89	0.09	64,69,70,78	0
5	GOL	A	905	6/6	0.90	0.12	69,79,83,105	0
3	NAG	C	903	14/15	0.90	0.09	48,53,62,64	0
5	GOL	D	904	6/6	0.90	0.14	64,69,70,70	0
3	NAG	C	902	14/15	0.91	0.09	54,63,76,76	0
6	CL	A	906	1/1	0.92	0.10	82,82,82,82	0
3	NAG	C	901	14/15	0.92	0.09	36,57,63,70	0
6	CL	B	906	1/1	0.93	0.09	68,68,68,68	0
6	CL	D	906	1/1	0.94	0.08	63,63,63,63	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

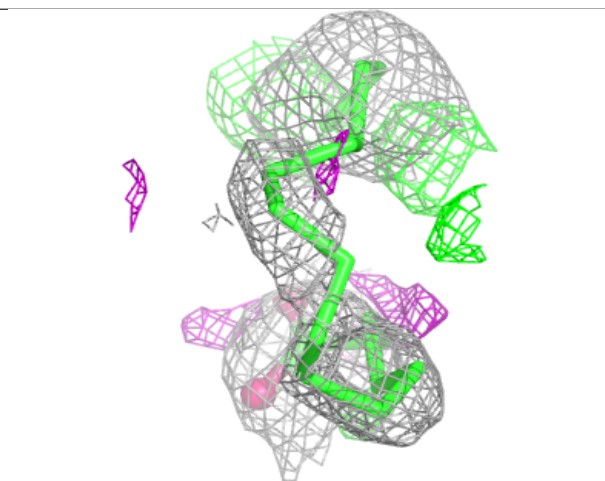
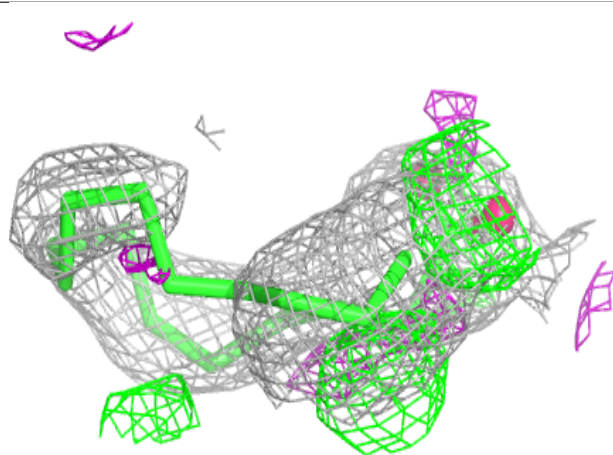
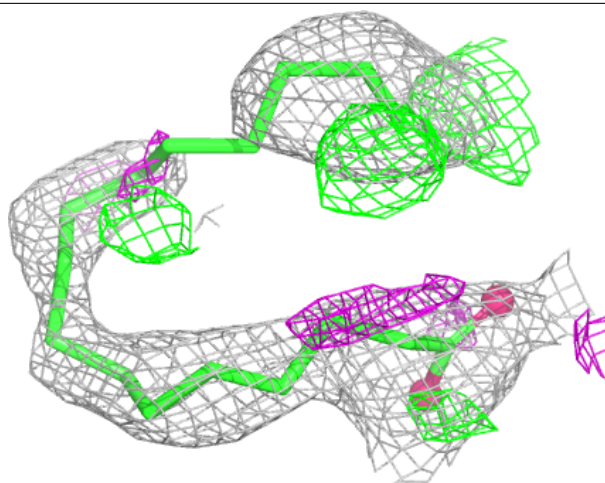
Electron density around DMX C 906:

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



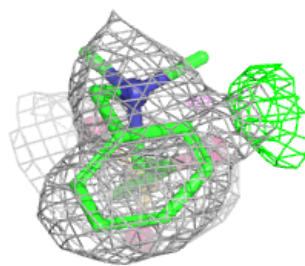
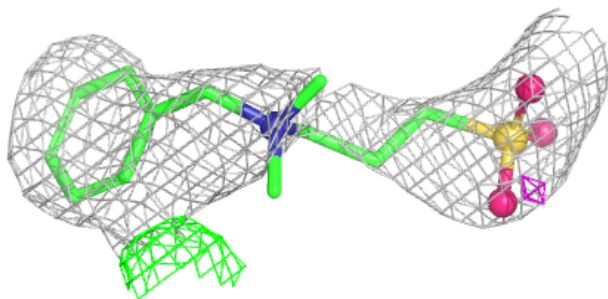
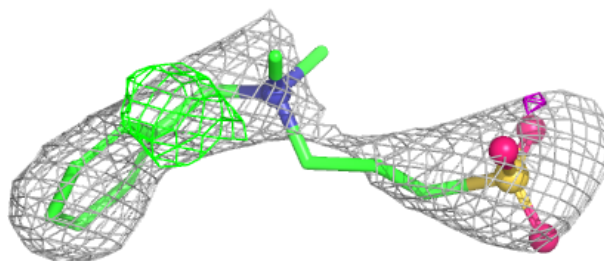
Electron density around PLM A 904:

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



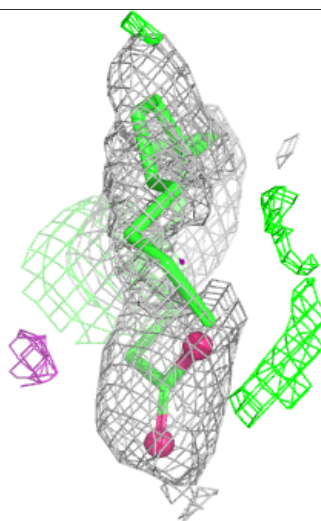
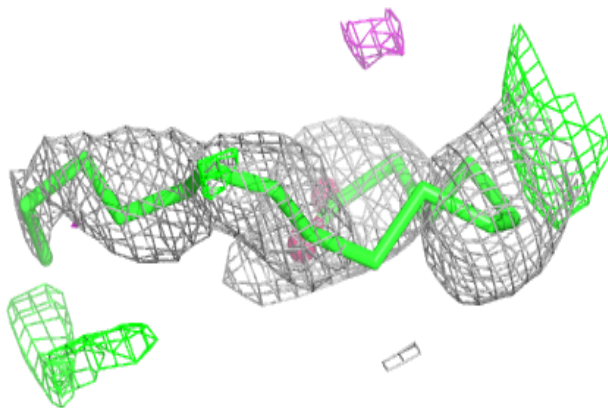
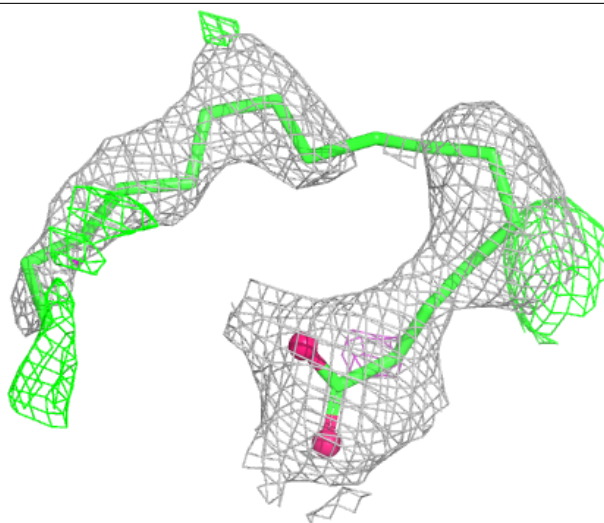
Electron density around DMX C 905:

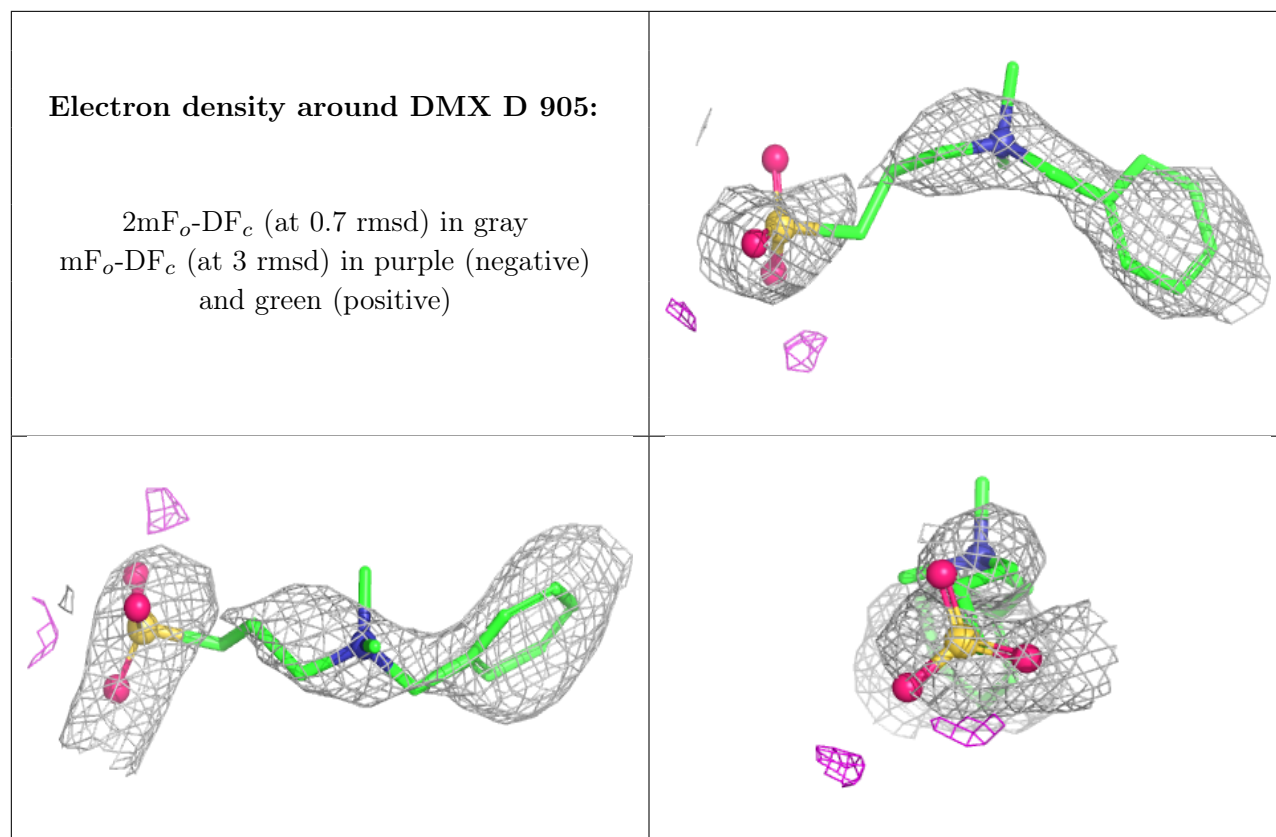
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PLM C 907:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.