



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 11:32 AM BST

PDB ID : 4FMF
Title : Crystal structure of human nectin-1 full ectodomain (D1-D3)
Authors : Harrison, O.J.; Brasch, J.; Shapiro, L.
Deposited on : 2012-06-16
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

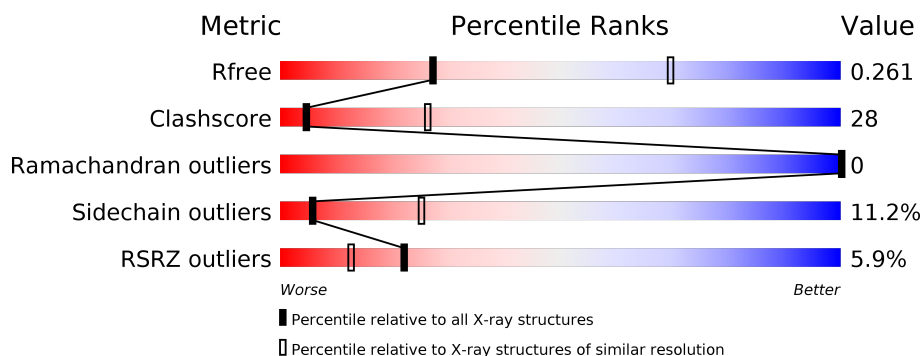
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



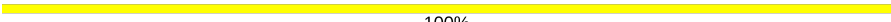

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	313	<div> <div>4%</div> <div> <div></div> <div>59%</div> <div>28%</div> <div>8%</div> <div>• •</div> </div> </div>
1	B	313	<div> <div>10%</div> <div> <div></div> <div>62%</div> <div>27%</div> <div>5%</div> <div>• •</div> </div> </div>
1	C	313	<div> <div>3%</div> <div> <div></div> <div>61%</div> <div>28%</div> <div>6%</div> <div>• •</div> </div> </div>
1	D	313	<div> <div>5%</div> <div> <div></div> <div>65%</div> <div>28%</div> <div>• •</div> </div> </div>
2	E	2	<div> <div></div> <div>100%</div> </div>
2	F	2	<div> <div></div> <div>100%</div> </div>

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9598 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 Poliovirus receptor-related protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2376	1497	410	458	11			
1	B	299	Total	C	N	O	S	0	0	0
			2349	1478	407	453	11			
1	C	301	Total	C	N	O	S	0	0	0
			2369	1492	409	457	11			
1	D	302	Total	C	N	O	S	0	0	0
			2376	1497	410	458	11			

There are 24 discrepancies between the modelled and reference sequences:

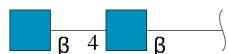
Chain	Residue	Modelled	Actual	Comment	Reference
A	338	HIS	-	expression tag	UNP Q15223
A	339	HIS	-	expression tag	UNP Q15223
A	340	HIS	-	expression tag	UNP Q15223
A	341	HIS	-	expression tag	UNP Q15223
A	342	HIS	-	expression tag	UNP Q15223
A	343	HIS	-	expression tag	UNP Q15223
B	338	HIS	-	expression tag	UNP Q15223
B	339	HIS	-	expression tag	UNP Q15223
B	340	HIS	-	expression tag	UNP Q15223
B	341	HIS	-	expression tag	UNP Q15223
B	342	HIS	-	expression tag	UNP Q15223
B	343	HIS	-	expression tag	UNP Q15223
C	338	HIS	-	expression tag	UNP Q15223
C	339	HIS	-	expression tag	UNP Q15223
C	340	HIS	-	expression tag	UNP Q15223
C	341	HIS	-	expression tag	UNP Q15223
C	342	HIS	-	expression tag	UNP Q15223
C	343	HIS	-	expression tag	UNP Q15223
D	338	HIS	-	expression tag	UNP Q15223
D	339	HIS	-	expression tag	UNP Q15223
D	340	HIS	-	expression tag	UNP Q15223

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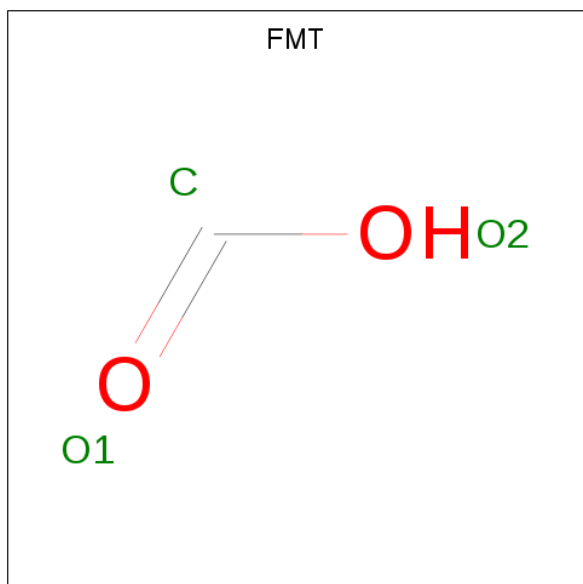
Chain	Residue	Modelled	Actual	Comment	Reference
D	341	HIS	-	expression tag	UNP Q15223
D	342	HIS	-	expression tag	UNP Q15223
D	343	HIS	-	expression tag	UNP Q15223

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			3	1	2		
3	C	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		

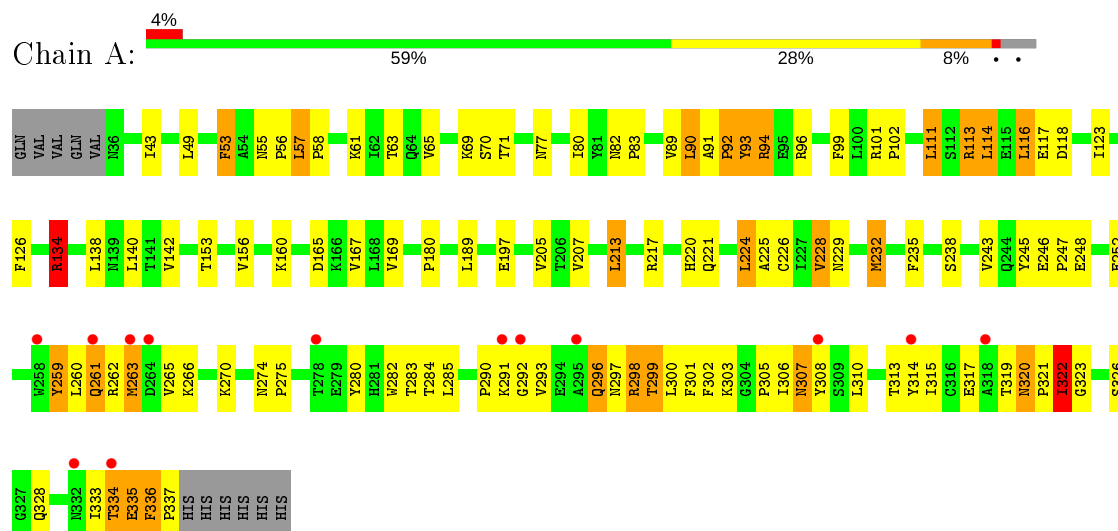
- Molecule 4 is water.

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

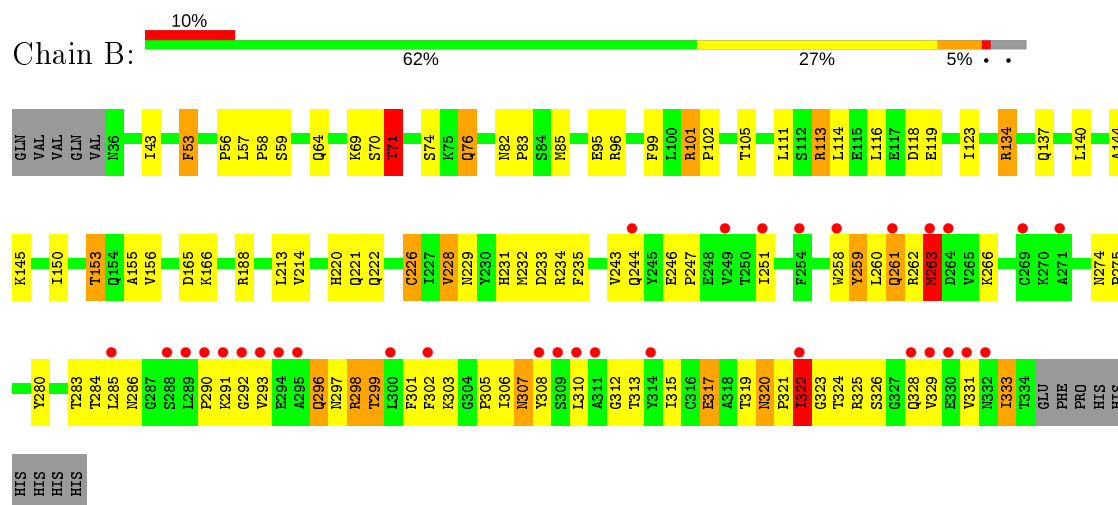
3 Residue-property plots

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

• Molecule 1: Poliovirus receptor-related protein 1

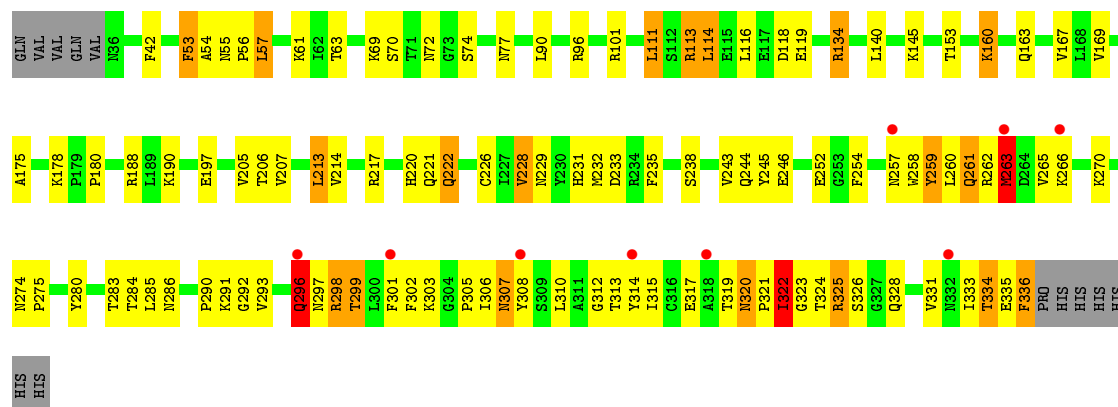


• Molecule 1: Poliovirus receptor-related protein 1

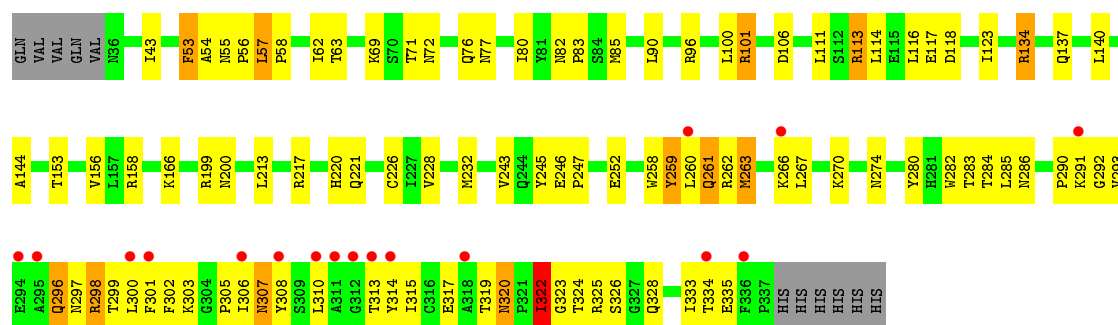


• Molecule 1: Poliovirus receptor-related protein 1





- Molecule 1: Poliovirus receptor-related protein 1



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



MAG1
MAG2

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



MAG1
MAG2

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



MAG1
MAG2

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

Chain H:



MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	106.29Å 106.29Å 334.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.20 38.47 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-3.20) 98.9 (38.47-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.233 , 0.258 0.233 , 0.261	Depositor DCC
R_{free} test set	1749 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	74.6	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.330 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9598	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: FMT, 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	0.80	1/2430 (0.0%)	0.86	5/3308 (0.2%)
1	B	0.74	0/2401	0.81	1/3268 (0.0%)
1	C	0.80	0/2422	0.86	1/3296 (0.0%)
1	D	0.73	1/2430 (0.0%)	0.82	2/3308 (0.1%)
All	All	0.77	2/9683 (0.0%)	0.83	9/13180 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
1	C	0	3
1	D	0	2
All	All	0	12

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	282	TRP	CD2-CE2	5.24	1.47	1.41
1	A	282	TRP	CD2-CE2	5.08	1.47	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	MET	CG-SD-CE	7.19	111.71	100.20
1	C	296	GLN	N-CA-C	-6.82	92.59	111.00
1	A	296	GLN	N-CA-C	-6.36	93.84	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	72	ASN	N-CA-C	5.85	126.80	111.00
1	B	296	GLN	N-CA-C	-5.84	95.24	111.00
1	D	296	GLN	N-CA-C	-5.63	95.80	111.00
1	A	92	PRO	N-CA-C	-5.51	97.78	112.10
1	A	335	GLU	N-CA-C	5.25	125.17	111.00
1	A	134	ARG	NE-CZ-NH1	5.21	122.90	120.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	259	TYR	Peptide
1	A	263	MET	Peptide
1	A	322	ILE	Peptide
1	B	259	TYR	Peptide
1	B	263	MET	Peptide
1	B	322	ILE	Peptide
1	B	71	THR	Peptide
1	C	259	TYR	Peptide
1	C	263	MET	Peptide
1	C	322	ILE	Peptide
1	D	259	TYR	Peptide
1	D	322	ILE	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	2376	0	2324	164	1
1	B	2349	0	2302	129	0
1	C	2369	0	2316	149	0
1	D	2376	0	2324	104	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	24	0	0
2	H	28	0	25	2	0
3	A	3	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	1	0	0
3	C	3	0	1	0	0
3	D	3	0	1	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
All	All	9598	0	9369	533	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (533) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:HD21	1:A:308:TYR:CE1	1.27	1.63
1:C:260:LEU:HD21	1:C:308:TYR:CE1	1.10	1.63
1:C:260:LEU:HD21	1:C:308:TYR:CD1	1.46	1.49
1:C:266:LYS:HE2	1:C:301:PHE:CE1	1.46	1.49
1:B:57:LEU:CD2	1:B:58:PRO:HD2	1.45	1.46
1:C:257:ASN:HB3	1:C:336:PHE:CZ	1.52	1.44
1:C:260:LEU:CD2	1:C:308:TYR:CE1	2.01	1.44
1:C:266:LYS:CE	1:C:301:PHE:HE1	1.27	1.43
1:C:257:ASN:CB	1:C:336:PHE:CZ	2.05	1.38
1:C:266:LYS:CE	1:C:301:PHE:CE1	2.04	1.31
1:A:266:LYS:HE2	1:A:301:PHE:CE1	1.65	1.30
1:A:266:LYS:CE	1:A:301:PHE:HE1	1.44	1.30
1:A:260:LEU:HD21	1:A:308:TYR:CD1	1.68	1.27
1:B:145:LYS:NZ	1:B:235:PHE:HZ	1.30	1.27
1:C:266:LYS:CD	1:C:301:PHE:HE1	1.51	1.24
1:C:257:ASN:HB3	1:C:336:PHE:CE2	1.71	1.23
1:B:260:LEU:HD21	1:B:308:TYR:CD1	1.74	1.22
1:A:260:LEU:CD2	1:A:308:TYR:CE1	2.22	1.20
1:C:260:LEU:CD2	1:C:308:TYR:CD1	2.20	1.20
1:A:246:GLU:HG2	1:A:322:ILE:HG22	1.22	1.19
1:A:266:LYS:CE	1:A:301:PHE:CE1	2.24	1.19
1:C:266:LYS:CD	1:C:301:PHE:CE1	2.25	1.17
1:D:260:LEU:HD21	1:D:308:TYR:CE1	1.78	1.17
1:B:57:LEU:CG	1:B:58:PRO:HD2	1.75	1.16
1:C:266:LYS:HG2	1:C:301:PHE:CD1	1.84	1.12
1:D:266:LYS:HE2	1:D:301:PHE:CE1	1.85	1.12
1:B:246:GLU:HG2	1:B:322:ILE:CG2	1.80	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LEU:HD23	1:B:58:PRO:CD	1.79	1.11
1:A:134:ARG:HH11	1:A:134:ARG:HG3	1.16	1.10
1:C:266:LYS:HE2	1:C:301:PHE:CD1	1.86	1.09
1:B:246:GLU:HG2	1:B:322:ILE:HG22	1.10	1.08
1:D:260:LEU:HD21	1:D:308:TYR:CD1	1.89	1.07
1:B:57:LEU:HD23	1:B:58:PRO:HD2	1.15	1.06
1:A:266:LYS:HE2	1:A:301:PHE:CD1	1.91	1.06
1:C:291:LYS:HD2	1:C:292:GLY:HA2	1.38	1.05
1:B:246:GLU:CG	1:B:322:ILE:CG2	2.33	1.05
1:D:252:GLU:OE2	1:D:270:LYS:HD2	1.57	1.03
1:A:291:LYS:HD2	1:A:292:GLY:HA2	1.40	1.03
1:C:257:ASN:CB	1:C:336:PHE:CE2	2.35	1.01
1:B:260:LEU:HD21	1:B:308:TYR:HD1	1.18	1.01
1:C:266:LYS:HD3	1:C:301:PHE:CE1	1.98	0.99
1:B:134:ARG:HH11	1:B:134:ARG:HG3	1.26	0.98
1:A:71:THR:HG22	1:A:71:THR:O	1.63	0.98
1:B:57:LEU:CD2	1:B:58:PRO:CD	2.37	0.97
1:C:55:ASN:O	1:C:57:LEU:HD23	1.65	0.97
1:A:91:ALA:HA	1:A:92:PRO:C	1.85	0.96
1:B:246:GLU:CG	1:B:322:ILE:HG22	1.94	0.96
1:D:261:GLN:O	1:D:261:GLN:HG3	1.62	0.96
1:A:252:GLU:OE2	1:A:270:LYS:HD2	1.64	0.95
1:A:246:GLU:CG	1:A:322:ILE:CG2	2.44	0.95
1:A:246:GLU:CG	1:A:322:ILE:HG22	1.97	0.95
1:A:61:LYS:HD2	1:B:85:MET:HE1	1.45	0.95
1:C:134:ARG:HG3	1:C:134:ARG:HH11	1.32	0.94
1:C:260:LEU:HD21	1:C:308:TYR:HE1	1.17	0.93
1:C:261:GLN:O	1:C:261:GLN:HG3	1.66	0.93
1:A:43:ILE:HD11	1:A:116:LEU:HD13	1.50	0.93
1:C:257:ASN:CG	1:C:336:PHE:CZ	2.42	0.93
1:B:57:LEU:HG	1:B:58:PRO:HD2	1.48	0.92
1:C:260:LEU:CD2	1:C:308:TYR:HE1	1.68	0.92
1:B:260:LEU:HD21	1:B:308:TYR:CE1	2.04	0.91
1:A:246:GLU:HG2	1:A:322:ILE:CG2	1.99	0.91
1:A:266:LYS:CD	1:A:301:PHE:CE1	2.52	0.91
1:A:93:TYR:N	1:A:93:TYR:HD2	1.68	0.91
1:A:266:LYS:CD	1:A:301:PHE:HE1	1.84	0.91
1:C:260:LEU:CD1	1:C:308:TYR:HE1	1.84	0.91
1:C:260:LEU:HD11	1:C:308:TYR:HE1	1.39	0.88
1:A:260:LEU:HD21	1:A:308:TYR:HE1	1.05	0.88
1:C:260:LEU:CG	1:C:308:TYR:HE1	1.87	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LYS:HG2	1:A:301:PHE:CD1	2.09	0.87
1:B:263:MET:SD	1:B:263:MET:N	2.48	0.86
1:A:260:LEU:CD2	1:A:308:TYR:CD1	2.49	0.86
1:A:261:GLN:HG3	1:A:261:GLN:O	1.75	0.86
1:B:246:GLU:HG3	1:B:322:ILE:CG2	2.07	0.85
1:D:266:LYS:HE2	1:D:301:PHE:CZ	2.12	0.85
1:B:261:GLN:O	1:B:261:GLN:HG3	1.75	0.84
1:C:336:PHE:CD1	1:C:336:PHE:C	2.47	0.84
1:B:57:LEU:HG	1:B:58:PRO:CD	2.07	0.84
1:A:260:LEU:CD2	1:A:308:TYR:HE1	1.76	0.84
1:C:266:LYS:HG2	1:C:301:PHE:HD1	1.42	0.83
1:A:92:PRO:C	1:A:93:TYR:HD2	1.81	0.83
1:B:113:ARG:HG2	1:B:113:ARG:HH11	1.43	0.83
1:D:263:MET:SD	1:D:263:MET:N	2.51	0.83
1:C:257:ASN:HB2	1:C:336:PHE:CZ	2.15	0.82
1:A:246:GLU:HG3	1:A:322:ILE:CG2	2.08	0.82
1:C:101:ARG:HG3	1:C:101:ARG:O	1.79	0.81
1:C:113:ARG:HH11	1:C:113:ARG:HG2	1.46	0.81
1:C:134:ARG:HG3	1:C:134:ARG:NH1	1.95	0.80
1:D:57:LEU:HB3	1:D:58:PRO:HD2	1.64	0.80
1:A:93:TYR:N	1:A:93:TYR:CD2	2.38	0.80
1:A:91:ALA:HB2	1:A:94:ARG:HG3	1.62	0.79
1:C:315:ILE:HG22	1:C:328:GLN:HG2	1.64	0.79
1:A:296:GLN:O	1:A:299:THR:O	2.00	0.79
1:B:246:GLU:CG	1:B:322:ILE:HG21	2.12	0.79
1:B:134:ARG:HG3	1:B:134:ARG:NH1	1.87	0.79
1:D:56:PRO:O	1:D:57:LEU:HD23	1.82	0.79
1:C:296:GLN:O	1:C:299:THR:O	2.01	0.79
1:C:266:LYS:CG	1:C:301:PHE:CD1	2.64	0.79
1:A:298:ARG:CG	1:A:298:ARG:HH11	1.95	0.78
1:B:246:GLU:HG3	1:B:322:ILE:HG21	1.66	0.78
1:C:260:LEU:HD11	1:C:308:TYR:CE1	2.18	0.78
1:B:57:LEU:CG	1:B:58:PRO:CD	2.58	0.78
1:D:296:GLN:O	1:D:299:THR:O	2.02	0.78
1:A:336:PHE:CD1	1:A:337:PRO:N	2.52	0.77
1:C:257:ASN:HB2	1:C:336:PHE:CE2	2.18	0.77
1:C:298:ARG:CG	1:C:298:ARG:HH11	1.97	0.77
1:D:298:ARG:HH11	1:D:298:ARG:CG	1.98	0.77
1:C:217:ARG:HG2	1:C:245:TYR:CD2	2.20	0.77
1:B:145:LYS:NZ	1:B:235:PHE:CZ	2.19	0.77
1:B:296:GLN:O	1:B:299:THR:O	2.04	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:ASN:HB3	1:C:336:PHE:HZ	1.44	0.76
1:C:260:LEU:CG	1:C:308:TYR:CE1	2.66	0.76
1:C:257:ASN:ND2	1:C:336:PHE:CZ	2.53	0.76
1:A:61:LYS:HD3	1:B:85:MET:HE3	1.68	0.76
1:A:56:PRO:O	1:A:57:LEU:HD23	1.85	0.76
1:B:298:ARG:HH11	1:B:298:ARG:CG	1.99	0.75
1:C:220:HIS:HD2	1:C:243:VAL:H	1.32	0.75
1:A:91:ALA:CA	1:A:92:PRO:O	2.34	0.75
1:D:113:ARG:HH11	1:D:113:ARG:HG2	1.51	0.75
1:A:228:VAL:HG13	1:A:235:PHE:HD1	1.52	0.75
1:A:266:LYS:HD3	1:A:301:PHE:CE1	2.22	0.75
1:A:315:ILE:HG22	1:A:328:GLN:HG2	1.68	0.75
1:D:56:PRO:C	1:D:57:LEU:HD23	2.07	0.75
1:A:91:ALA:CA	1:A:92:PRO:C	2.53	0.74
1:C:291:LYS:HD2	1:C:292:GLY:CA	2.17	0.74
1:A:220:HIS:HD2	1:A:243:VAL:H	1.34	0.74
1:C:190:LYS:HG3	1:C:190:LYS:O	1.88	0.74
1:A:92:PRO:C	1:A:93:TYR:CD2	2.60	0.74
1:D:220:HIS:HD2	1:D:243:VAL:H	1.33	0.73
1:D:298:ARG:HH11	1:D:298:ARG:HG3	1.52	0.73
1:A:291:LYS:HD2	1:A:292:GLY:CA	2.16	0.73
1:A:71:THR:O	1:A:71:THR:CG2	2.37	0.73
1:A:113:ARG:HG2	1:A:113:ARG:HH11	1.53	0.73
1:A:101:ARG:HG3	1:A:101:ARG:O	1.86	0.73
1:C:298:ARG:HG2	1:C:298:ARG:HH11	1.54	0.72
1:A:61:LYS:CD	1:B:85:MET:HE1	2.19	0.72
1:C:257:ASN:CG	1:C:336:PHE:CE1	2.63	0.72
1:B:43:ILE:HD12	1:B:144:ALA:HB2	1.71	0.72
1:B:43:ILE:CD1	1:B:144:ALA:HB2	2.20	0.72
1:D:113:ARG:CG	1:D:113:ARG:HH11	2.01	0.72
1:A:61:LYS:CD	1:B:85:MET:CE	2.68	0.71
1:B:315:ILE:HG22	1:B:328:GLN:HG2	1.70	0.71
1:A:336:PHE:CE1	1:A:337:PRO:C	2.64	0.71
1:C:113:ARG:HH11	1:C:113:ARG:CG	2.04	0.71
1:A:61:LYS:HD2	1:B:85:MET:CE	2.19	0.71
1:A:134:ARG:HG3	1:A:134:ARG:NH1	1.90	0.70
1:B:220:HIS:HD2	1:B:243:VAL:H	1.37	0.70
1:A:56:PRO:C	1:A:57:LEU:HD23	2.11	0.70
1:D:43:ILE:HD11	1:D:144:ALA:HB2	1.73	0.69
1:B:260:LEU:CD2	1:B:308:TYR:HD1	2.00	0.69
1:C:134:ARG:CG	1:C:134:ARG:HH11	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:TYR:HE2	1:A:337:PRO:HB3	1.58	0.69
1:C:260:LEU:HD22	1:C:308:TYR:CD1	2.25	0.69
1:A:89:VAL:HG12	1:A:90:LEU:O	1.93	0.68
1:D:200:ASN:HB3	2:H:1:NAG:H62	1.75	0.68
1:B:145:LYS:CE	1:B:235:PHE:HZ	2.06	0.68
1:D:260:LEU:HD21	1:D:308:TYR:HE1	1.48	0.68
1:C:262:ARG:HH12	1:C:265:VAL:HG23	1.57	0.68
1:A:262:ARG:HH12	1:A:265:VAL:HG23	1.59	0.68
1:B:317:GLU:HG2	1:B:326:SER:HB3	1.74	0.68
1:A:228:VAL:HG13	1:A:235:PHE:CD1	2.29	0.68
1:C:257:ASN:ND2	1:C:336:PHE:HZ	1.92	0.67
1:A:266:LYS:NZ	1:A:301:PHE:HE1	1.92	0.67
1:C:217:ARG:HG2	1:C:245:TYR:CG	2.29	0.67
1:C:266:LYS:CG	1:C:301:PHE:CE1	2.77	0.67
1:D:315:ILE:HG22	1:D:328:GLN:HG2	1.76	0.67
1:B:260:LEU:CD2	1:B:308:TYR:CD1	2.66	0.66
1:B:113:ARG:CG	1:B:113:ARG:HH11	2.07	0.66
1:D:134:ARG:HH11	1:D:134:ARG:HG3	1.61	0.66
1:D:43:ILE:CD1	1:D:144:ALA:HB2	2.25	0.66
1:D:55:ASN:O	1:D:57:LEU:HD23	1.95	0.66
1:B:228:VAL:O	1:B:228:VAL:HG22	1.97	0.65
1:C:252:GLU:OE2	1:C:270:LYS:HD2	1.97	0.65
1:D:298:ARG:HG3	1:D:298:ARG:NH1	2.09	0.64
1:A:246:GLU:HG3	1:A:322:ILE:HG21	1.78	0.64
1:A:91:ALA:HB1	1:A:94:ARG:HH11	1.63	0.64
1:B:134:ARG:HH11	1:B:134:ARG:CG	2.04	0.64
1:A:91:ALA:C	1:A:92:PRO:O	2.31	0.64
1:C:280:TYR:CD1	1:C:298:ARG:HB2	2.33	0.64
1:A:220:HIS:NE2	1:A:274:ASN:ND2	2.47	0.63
1:A:298:ARG:HG3	1:A:298:ARG:HH11	1.62	0.63
1:C:307:ASN:HD21	1:C:310:LEU:HG	1.62	0.63
1:C:336:PHE:HD1	1:C:336:PHE:C	2.00	0.63
1:D:324:THR:O	1:D:325:ARG:HG2	1.98	0.63
1:C:231:HIS:O	1:C:232:MET:HB2	1.97	0.63
1:A:77:ASN:HB2	1:A:90:LEU:HD23	1.80	0.62
1:D:53:PHE:CE1	1:D:134:ARG:NH2	2.68	0.62
1:A:113:ARG:HH11	1:A:113:ARG:CG	2.12	0.62
1:D:306:ILE:HG23	1:D:310:LEU:HD12	1.81	0.62
1:A:228:VAL:HG22	1:A:228:VAL:O	1.99	0.62
1:D:134:ARG:HG3	1:D:134:ARG:NH1	2.15	0.62
1:A:225:ALA:HB2	1:A:238:SER:CB	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LEU:HD23	1:B:59:SER:H	1.65	0.62
1:A:180:PRO:HG3	1:A:205:VAL:HG21	1.82	0.61
1:A:336:PHE:HD1	1:A:337:PRO:N	1.94	0.61
1:A:55:ASN:O	1:A:57:LEU:HD23	2.00	0.61
1:C:260:LEU:CD2	1:C:308:TYR:HD1	2.02	0.61
1:D:260:LEU:CD2	1:D:308:TYR:CD1	2.76	0.61
1:C:197:GLU:HG2	1:C:207:VAL:HG22	1.81	0.61
1:C:312:GLY:O	1:C:331:VAL:HG12	2.01	0.61
1:A:280:TYR:CD1	1:A:298:ARG:HB2	2.36	0.61
1:A:61:LYS:HD3	1:B:85:MET:CE	2.30	0.61
1:B:285:LEU:HB2	1:B:313:THR:HB	1.82	0.61
1:B:301:PHE:HE2	1:B:303:LYS:CG	2.13	0.61
1:C:175:ALA:HA	1:C:206:THR:HG23	1.83	0.61
1:A:246:GLU:CG	1:A:322:ILE:HG21	2.30	0.60
1:B:43:ILE:HD12	1:B:144:ALA:CB	2.30	0.60
1:A:259:TYR:CE2	1:A:337:PRO:HB3	2.36	0.60
1:D:101:ARG:O	1:D:101:ARG:CG	2.50	0.60
1:D:293:VAL:HG12	1:D:302:PHE:HD1	1.66	0.60
1:B:101:ARG:O	1:B:101:ARG:CG	2.50	0.60
1:D:220:HIS:CE1	1:D:221:GLN:HG3	2.36	0.60
1:A:246:GLU:N	1:A:322:ILE:HG21	2.17	0.59
1:A:260:LEU:CG	1:A:308:TYR:HE1	2.15	0.59
1:A:298:ARG:HG3	1:A:298:ARG:NH1	2.15	0.59
1:B:280:TYR:CD1	1:B:298:ARG:HB2	2.37	0.59
1:B:312:GLY:O	1:B:331:VAL:HG12	2.02	0.59
1:B:53:PHE:CE1	1:B:134:ARG:NH2	2.70	0.59
1:C:257:ASN:CB	1:C:336:PHE:CE1	2.79	0.59
1:A:224:LEU:HG	1:A:224:LEU:O	2.02	0.59
1:D:220:HIS:NE2	1:D:274:ASN:ND2	2.50	0.59
1:B:306:ILE:HG23	1:B:310:LEU:HD12	1.85	0.58
1:A:263:MET:SD	1:A:263:MET:N	2.76	0.58
1:A:303:LYS:O	1:A:305:PRO:HD2	2.02	0.58
1:C:257:ASN:HD22	1:C:336:PHE:HZ	1.50	0.58
1:D:200:ASN:CB	2:H:1:NAG:H62	2.33	0.58
1:C:220:HIS:CE1	1:C:221:GLN:HG3	2.39	0.58
1:D:317:GLU:HG2	1:D:326:SER:HB3	1.85	0.58
1:D:307:ASN:HD21	1:D:310:LEU:HG	1.69	0.58
1:A:334:THR:HG22	1:A:335:GLU:H	1.68	0.57
1:B:303:LYS:O	1:B:305:PRO:HD2	2.05	0.57
1:C:307:ASN:ND2	1:C:310:LEU:HG	2.18	0.57
1:A:317:GLU:HG2	1:A:326:SER:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:PRO:HG3	1:C:205:VAL:HG21	1.87	0.57
1:B:307:ASN:HD21	1:B:310:LEU:HG	1.69	0.57
1:B:145:LYS:CE	1:B:235:PHE:CZ	2.85	0.57
1:B:229:ASN:HD21	1:B:234:ARG:CG	2.18	0.57
1:B:298:ARG:HG3	1:B:298:ARG:NH1	2.20	0.57
1:D:290:PRO:O	1:D:293:VAL:HG13	2.05	0.57
1:A:220:HIS:CE1	1:A:221:GLN:HG3	2.40	0.57
1:A:306:ILE:HG23	1:A:310:LEU:HD12	1.85	0.57
1:B:298:ARG:HG3	1:B:298:ARG:HH11	1.67	0.57
1:B:246:GLU:N	1:B:322:ILE:HG21	2.20	0.57
1:C:220:HIS:NE2	1:C:274:ASN:ND2	2.52	0.56
1:C:252:GLU:OE1	1:C:270:LYS:HD2	2.05	0.56
1:C:56:PRO:C	1:C:57:LEU:HD23	2.26	0.56
1:C:260:LEU:HD22	1:C:308:TYR:HD1	1.68	0.56
1:A:91:ALA:HB2	1:A:94:ARG:CG	2.34	0.55
1:C:252:GLU:CD	1:C:270:LYS:HD2	2.26	0.55
1:C:77:ASN:HB2	1:C:90:LEU:HD12	1.86	0.55
1:C:77:ASN:HB2	1:C:90:LEU:CD1	2.36	0.55
1:C:263:MET:SD	1:C:263:MET:N	2.80	0.55
1:C:63:THR:HG21	1:D:63:THR:HG22	1.88	0.55
1:A:262:ARG:NH1	1:A:265:VAL:HG23	2.21	0.55
1:C:119:GLU:OE2	1:C:178:LYS:NZ	2.29	0.55
1:C:260:LEU:CD1	1:C:308:TYR:CE1	2.76	0.55
1:D:293:VAL:HG12	1:D:302:PHE:CD1	2.40	0.55
1:C:285:LEU:HD23	1:C:285:LEU:O	2.06	0.55
1:D:246:GLU:N	1:D:322:ILE:HG21	2.22	0.55
1:D:280:TYR:CD1	1:D:298:ARG:HB2	2.42	0.55
1:D:55:ASN:O	1:D:57:LEU:CD2	2.55	0.55
1:B:220:HIS:CE1	1:B:221:GLN:HG3	2.41	0.54
1:A:260:LEU:HD11	1:A:308:TYR:HE1	1.71	0.54
1:A:91:ALA:HB2	1:A:94:ARG:HD3	1.88	0.54
1:C:246:GLU:N	1:C:322:ILE:HG21	2.22	0.54
1:B:259:TYR:HB3	1:B:260:LEU:O	2.06	0.54
1:C:293:VAL:HG12	1:C:302:PHE:HD1	1.72	0.54
1:D:283:THR:HG22	1:D:284:THR:N	2.22	0.54
1:A:298:ARG:CG	1:A:298:ARG:NH1	2.61	0.54
1:C:101:ARG:O	1:C:101:ARG:CG	2.54	0.54
1:A:96:ARG:NH2	1:A:118:ASP:OD2	2.33	0.54
1:C:275:PRO:HG2	1:C:321:PRO:HG2	1.90	0.54
1:C:55:ASN:O	1:C:57:LEU:CD2	2.50	0.53
1:D:266:LYS:HG2	1:D:267:LEU:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ASN:HD21	1:A:310:LEU:HG	1.72	0.53
1:C:298:ARG:CG	1:C:298:ARG:NH1	2.62	0.53
1:C:266:LYS:NZ	1:C:301:PHE:HE1	2.01	0.53
1:C:285:LEU:HB2	1:C:313:THR:HB	1.89	0.53
1:B:101:ARG:O	1:B:101:ARG:HG3	2.09	0.53
1:A:298:ARG:HG2	1:A:298:ARG:HH11	1.74	0.53
1:A:69:LYS:NZ	1:A:117:GLU:O	2.42	0.53
1:C:283:THR:HG22	1:C:284:THR:N	2.23	0.53
1:D:261:GLN:CG	1:D:261:GLN:O	2.47	0.53
1:C:266:LYS:NZ	1:C:301:PHE:CE1	2.74	0.53
1:C:96:ARG:NH2	1:C:118:ASP:OD2	2.33	0.53
1:C:290:PRO:O	1:C:293:VAL:HG13	2.09	0.53
1:C:306:ILE:HG23	1:C:310:LEU:HD12	1.91	0.53
1:B:301:PHE:HE2	1:B:303:LYS:HG2	1.73	0.53
1:A:336:PHE:C	1:A:336:PHE:CD1	2.80	0.53
1:C:190:LYS:CG	1:C:190:LYS:O	2.55	0.52
1:C:160:LYS:HB3	1:C:163:GLN:CG	2.39	0.52
1:D:113:ARG:HH11	1:D:113:ARG:CB	2.21	0.52
1:A:260:LEU:CD1	1:A:308:TYR:HE1	2.22	0.52
1:A:293:VAL:HG12	1:A:302:PHE:HD1	1.74	0.52
1:A:63:THR:HG21	1:B:64:GLN:OE1	2.10	0.52
1:A:225:ALA:HB2	1:A:238:SER:OG	2.10	0.52
1:D:113:ARG:CG	1:D:113:ARG:NH1	2.70	0.52
1:B:307:ASN:ND2	1:B:310:LEU:HG	2.24	0.52
1:C:229:ASN:HA	1:C:233:ASP:O	2.09	0.52
1:D:101:ARG:O	1:D:101:ARG:HG3	2.10	0.52
1:B:285:LEU:CB	1:B:313:THR:HB	2.39	0.52
1:D:69:LYS:NZ	1:D:117:GLU:O	2.43	0.52
1:A:91:ALA:CB	1:A:94:ARG:HH11	2.22	0.52
1:C:61:LYS:HD2	1:D:85:MET:CE	2.41	0.51
1:D:307:ASN:ND2	1:D:310:LEU:HG	2.24	0.51
1:D:320:ASN:O	1:D:323:GLY:N	2.40	0.51
1:B:57:LEU:HD21	1:B:58:PRO:HD2	1.74	0.51
1:A:217:ARG:CZ	1:A:248:GLU:OE1	2.59	0.51
1:A:307:ASN:ND2	1:A:310:LEU:HG	2.25	0.51
1:A:259:TYR:HB3	1:A:260:LEU:O	2.10	0.51
1:A:228:VAL:CG1	1:A:235:PHE:HD1	2.21	0.51
1:C:303:LYS:O	1:C:305:PRO:HD2	2.09	0.51
1:A:134:ARG:HH11	1:A:134:ARG:CG	2.06	0.51
1:C:317:GLU:HG2	1:C:326:SER:HB3	1.92	0.51
1:A:299:THR:HB	1:A:301:PHE:CE2	2.47	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:HIS:NE2	1:B:274:ASN:ND2	2.59	0.50
1:B:57:LEU:HD23	1:B:58:PRO:N	2.24	0.50
1:A:266:LYS:HG2	1:A:301:PHE:HD1	1.72	0.50
1:A:197:GLU:HG2	1:A:207:VAL:HG22	1.93	0.50
1:B:43:ILE:HD11	1:B:144:ALA:HB2	1.94	0.50
1:A:262:ARG:NH1	1:A:265:VAL:CG2	2.74	0.50
1:C:111:LEU:HD13	1:C:114:LEU:CD1	2.41	0.50
1:A:225:ALA:HA	1:A:238:SER:HA	1.93	0.50
1:A:89:VAL:CG1	1:A:90:LEU:O	2.59	0.50
1:A:53:PHE:CE1	1:A:134:ARG:NH2	2.79	0.50
1:A:43:ILE:HD13	1:A:142:VAL:CG1	2.41	0.50
1:D:62:ILE:N	1:D:62:ILE:HD12	2.27	0.50
1:B:53:PHE:C	1:B:53:PHE:CD1	2.85	0.50
1:C:70:SER:HA	1:C:74:SER:O	2.12	0.50
1:A:266:LYS:NZ	1:A:301:PHE:CE1	2.75	0.49
1:B:266:LYS:HG2	1:B:301:PHE:HD1	1.77	0.49
1:B:283:THR:HG22	1:B:284:THR:N	2.26	0.49
1:C:53:PHE:C	1:C:53:PHE:CD1	2.86	0.49
1:C:293:VAL:HG23	1:C:293:VAL:O	2.12	0.49
1:B:320:ASN:O	1:B:323:GLY:N	2.42	0.49
1:D:298:ARG:NH1	1:D:298:ARG:CG	2.64	0.49
1:D:43:ILE:HD12	1:D:144:ALA:CB	2.41	0.49
1:B:229:ASN:HD21	1:B:234:ARG:HD2	1.78	0.49
1:B:251:ILE:HB	1:B:329:VAL:HG23	1.93	0.49
1:C:262:ARG:NH1	1:C:265:VAL:CG2	2.76	0.49
1:D:77:ASN:HB2	1:D:90:LEU:HD11	1.95	0.49
1:A:220:HIS:CD2	1:A:274:ASN:HD22	2.31	0.48
1:A:290:PRO:O	1:A:293:VAL:HG13	2.13	0.48
1:C:262:ARG:NH1	1:C:265:VAL:HG23	2.26	0.48
1:D:96:ARG:NH2	1:D:118:ASP:OD2	2.39	0.48
1:C:220:HIS:CD2	1:C:274:ASN:ND2	2.82	0.48
1:A:225:ALA:CB	1:A:238:SER:HA	2.43	0.48
1:A:228:VAL:O	1:A:228:VAL:CG2	2.60	0.48
1:B:290:PRO:O	1:B:293:VAL:HG13	2.12	0.48
1:A:53:PHE:CD1	1:A:53:PHE:C	2.86	0.48
1:D:220:HIS:CD2	1:D:243:VAL:H	2.23	0.48
1:D:56:PRO:O	1:D:57:LEU:CD2	2.60	0.48
1:B:293:VAL:HG12	1:B:302:PHE:HD1	1.78	0.48
1:A:283:THR:HG22	1:A:284:THR:N	2.28	0.48
1:B:96:ARG:NH2	1:B:118:ASP:OD2	2.39	0.48
1:A:77:ASN:CB	1:A:90:LEU:HD23	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:LYS:HB3	1:C:163:GLN:HG3	1.95	0.48
1:D:315:ILE:HG13	1:D:315:ILE:O	2.14	0.48
1:C:220:HIS:CD2	1:C:274:ASN:HD22	2.31	0.48
1:C:69:LYS:HE3	1:C:119:GLU:O	2.14	0.48
1:B:222:GLN:HE21	1:B:222:GLN:CA	2.27	0.47
1:A:228:VAL:CG1	1:A:235:PHE:CD1	2.95	0.47
1:B:222:GLN:HA	1:B:222:GLN:NE2	2.29	0.47
1:B:298:ARG:HG2	1:B:298:ARG:HH11	1.77	0.47
1:C:299:THR:HB	1:C:301:PHE:CE2	2.49	0.47
1:A:90:LEU:HD12	1:A:90:LEU:HA	1.63	0.47
1:D:113:ARG:HB2	1:D:113:ARG:NH1	2.30	0.47
1:D:220:HIS:CD2	1:D:274:ASN:HD22	2.31	0.47
1:A:90:LEU:C	1:A:92:PRO:O	2.53	0.47
1:D:299:THR:HG1	1:D:301:PHE:HE2	1.62	0.47
1:B:266:LYS:HE2	1:B:301:PHE:CD1	2.50	0.47
1:B:275:PRO:HG2	1:B:321:PRO:HG2	1.97	0.47
1:B:320:ASN:OD1	1:B:320:ASN:C	2.53	0.47
1:B:53:PHE:C	1:B:53:PHE:HD1	2.18	0.47
1:C:262:ARG:HH12	1:C:265:VAL:CG2	2.25	0.47
1:A:266:LYS:CG	1:A:301:PHE:CD1	2.89	0.47
1:B:229:ASN:ND2	1:B:234:ARG:CB	2.77	0.47
1:C:274:ASN:HA	1:C:275:PRO:C	2.36	0.47
1:A:65:VAL:HG22	1:A:126:PHE:CD1	2.49	0.47
1:C:54:ALA:H	1:C:134:ARG:HH21	1.62	0.47
1:D:297:ASN:O	1:D:298:ARG:HB3	2.15	0.47
1:B:123:ILE:HG13	1:B:137:GLN:HG2	1.97	0.47
1:B:71:THR:O	1:B:74:SER:OG	2.17	0.47
1:B:222:GLN:HE21	1:B:222:GLN:HA	1.81	0.46
1:A:293:VAL:O	1:A:293:VAL:HG23	2.15	0.46
1:A:320:ASN:O	1:A:323:GLY:N	2.40	0.46
1:C:266:LYS:CE	1:C:301:PHE:CD1	2.66	0.46
1:D:320:ASN:C	1:D:320:ASN:OD1	2.53	0.46
1:B:57:LEU:HG	1:B:58:PRO:HD3	1.95	0.46
1:C:63:THR:CG2	1:D:63:THR:CG2	2.93	0.46
1:A:320:ASN:C	1:A:320:ASN:OD1	2.54	0.46
1:D:113:ARG:NH1	1:D:113:ARG:CB	2.78	0.46
1:B:229:ASN:ND2	1:B:234:ARG:HB2	2.31	0.46
1:B:70:SER:HA	1:B:74:SER:O	2.15	0.46
1:D:43:ILE:CD1	1:D:144:ALA:CB	2.93	0.46
1:B:280:TYR:CG	1:B:298:ARG:HB2	2.51	0.46
1:B:315:ILE:HG13	1:B:315:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASN:O	1:A:57:LEU:CD2	2.64	0.46
1:B:301:PHE:CE2	1:B:303:LYS:HG3	2.50	0.46
1:C:220:HIS:CD2	1:C:243:VAL:H	2.22	0.46
1:A:336:PHE:HD1	1:A:337:PRO:CD	2.29	0.46
1:A:117:GLU:HG3	1:A:117:GLU:O	2.16	0.45
1:A:285:LEU:HB2	1:A:313:THR:HB	1.98	0.45
1:B:297:ASN:O	1:B:298:ARG:HB3	2.14	0.45
1:C:324:THR:O	1:C:325:ARG:HG2	2.16	0.45
1:C:284:THR:HG23	1:C:286:ASN:H	1.80	0.45
1:C:285:LEU:CB	1:C:313:THR:HB	2.45	0.45
1:D:284:THR:HG23	1:D:286:ASN:H	1.81	0.45
1:A:225:ALA:HB2	1:A:238:SER:CA	2.46	0.45
1:A:156:VAL:O	1:A:156:VAL:HG23	2.16	0.45
1:C:293:VAL:HG12	1:C:302:PHE:CD1	2.51	0.45
1:D:217:ARG:HG2	1:D:245:TYR:CD2	2.51	0.45
1:A:70:SER:HB3	1:A:123:ILE:HD11	1.99	0.45
1:A:94:ARG:HB2	1:A:94:ARG:CZ	2.46	0.45
1:C:261:GLN:CG	1:C:261:GLN:O	2.48	0.45
1:D:134:ARG:HH11	1:D:134:ARG:CG	2.28	0.45
1:D:285:LEU:HB2	1:D:313:THR:HB	1.98	0.45
1:A:92:PRO:CB	1:A:93:TYR:HA	2.46	0.45
1:B:301:PHE:CE2	1:B:303:LYS:CG	2.97	0.45
1:B:324:THR:O	1:B:325:ARG:HG2	2.17	0.45
1:C:61:LYS:HD2	1:D:85:MET:HE1	1.98	0.45
1:D:247:PRO:HD3	1:D:320:ASN:ND2	2.32	0.45
1:A:99:PHE:HB2	1:A:102:PRO:HG3	1.99	0.45
1:C:254:PHE:HE2	1:C:331:VAL:HG23	1.82	0.45
1:C:63:THR:HG22	1:D:63:THR:HG21	1.98	0.45
1:B:56:PRO:HG3	1:B:105:THR:HG21	1.99	0.45
1:B:284:THR:HG23	1:B:286:ASN:H	1.81	0.44
1:C:314:TYR:O	1:C:328:GLN:HA	2.17	0.44
1:C:257:ASN:ND2	1:C:336:PHE:CE1	2.85	0.44
1:D:266:LYS:CE	1:D:301:PHE:CE1	2.77	0.44
1:C:63:THR:HG22	1:D:63:THR:CG2	2.46	0.44
1:D:291:LYS:HA	1:D:292:GLY:HA2	1.70	0.44
1:A:280:TYR:CG	1:A:298:ARG:HB2	2.51	0.44
1:C:169:VAL:HG21	1:C:213:LEU:CD2	2.48	0.44
1:C:53:PHE:C	1:C:53:PHE:HD1	2.19	0.44
1:A:53:PHE:C	1:A:53:PHE:HD1	2.21	0.44
1:B:247:PRO:HG3	1:B:320:ASN:HD22	1.83	0.44
1:A:111:LEU:HD13	1:A:114:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:TYR:CD1	1:A:262:ARG:HB2	2.52	0.44
1:A:91:ALA:HB2	1:A:94:ARG:CD	2.47	0.44
1:B:229:ASN:ND2	1:B:234:ARG:CG	2.80	0.44
1:B:99:PHE:HB2	1:B:102:PRO:HG3	1.99	0.44
1:C:320:ASN:C	1:C:320:ASN:OD1	2.56	0.44
1:D:53:PHE:CD1	1:D:53:PHE:C	2.90	0.44
1:C:291:LYS:HA	1:C:292:GLY:HA2	1.77	0.44
1:D:156:VAL:HG21	1:D:158:ARG:NH2	2.32	0.44
1:A:80:ILE:N	1:A:80:ILE:HD12	2.32	0.44
1:B:258:TRP:HB3	1:B:333:ILE:HG22	2.00	0.44
1:D:280:TYR:CG	1:D:298:ARG:HB2	2.53	0.44
1:A:225:ALA:HB2	1:A:238:SER:HA	1.99	0.43
1:B:69:LYS:HE3	1:B:119:GLU:O	2.18	0.43
1:C:261:GLN:HA	1:C:306:ILE:H	1.84	0.43
1:D:258:TRP:CD1	1:D:262:ARG:NH1	2.86	0.43
1:B:231:HIS:O	1:B:231:HIS:CG	2.70	0.43
1:D:293:VAL:HG23	1:D:293:VAL:O	2.17	0.43
1:A:274:ASN:HA	1:A:275:PRO:C	2.38	0.43
1:A:57:LEU:HB3	1:A:58:PRO:HD2	2.00	0.43
1:B:229:ASN:ND2	1:B:234:ARG:HG3	2.33	0.43
1:C:244:GLN:HG2	1:C:275:PRO:HD3	2.00	0.43
1:C:266:LYS:CG	1:C:301:PHE:HD1	2.20	0.43
1:D:259:TYR:CD1	1:D:262:ARG:HB2	2.53	0.43
1:A:247:PRO:HG3	1:A:320:ASN:HD22	1.83	0.43
1:B:298:ARG:NH1	1:B:298:ARG:CG	2.65	0.43
1:C:228:VAL:HG13	1:C:235:PHE:CD1	2.53	0.43
1:D:100:LEU:HA	1:D:100:LEU:HD23	1.75	0.43
1:A:56:PRO:O	1:A:57:LEU:CD2	2.61	0.43
1:C:298:ARG:HG3	1:C:298:ARG:NH1	2.34	0.43
1:B:293:VAL:CG1	1:B:302:PHE:HD1	2.31	0.43
1:C:320:ASN:O	1:C:323:GLY:N	2.45	0.43
1:D:283:THR:HG22	1:D:284:THR:H	1.83	0.43
1:A:291:LYS:HA	1:A:292:GLY:HA2	1.73	0.43
1:A:91:ALA:N	1:A:92:PRO:O	2.52	0.43
1:B:113:ARG:CG	1:B:113:ARG:NH1	2.74	0.43
1:B:228:VAL:CG2	1:B:228:VAL:O	2.60	0.43
1:D:77:ASN:HB2	1:D:90:LEU:CD1	2.49	0.43
1:D:53:PHE:HD1	1:D:54:ALA:N	2.17	0.43
1:A:90:LEU:O	1:A:92:PRO:O	2.36	0.43
1:B:220:HIS:CD2	1:B:243:VAL:H	2.27	0.43
1:D:259:TYR:HB3	1:D:260:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:PRO:HG2	1:A:321:PRO:HG2	2.01	0.42
1:B:82:ASN:HA	1:B:83:PRO:HD2	1.84	0.42
1:A:189:LEU:HD12	1:A:224:LEU:HB2	2.01	0.42
1:D:156:VAL:HG21	1:D:158:ARG:HH21	1.82	0.42
1:D:53:PHE:C	1:D:53:PHE:HD1	2.22	0.42
1:C:42:PHE:CE1	1:C:145:LYS:HG3	2.55	0.42
1:D:123:ILE:HG13	1:D:137:GLN:HG2	2.01	0.42
1:A:262:ARG:HH12	1:A:265:VAL:CG2	2.30	0.42
1:B:301:PHE:CE2	1:B:303:LYS:HA	2.54	0.42
1:D:57:LEU:HB3	1:D:58:PRO:CD	2.42	0.42
1:D:69:LYS:HD3	1:D:76:GLN:NE2	2.34	0.42
1:C:334:THR:HG22	1:C:335:GLU:H	1.84	0.42
1:A:169:VAL:HG11	1:A:213:LEU:CD2	2.49	0.42
1:C:257:ASN:O	1:C:258:TRP:HD1	2.03	0.42
1:D:260:LEU:HD21	1:D:308:TYR:HD1	1.68	0.42
1:A:266:LYS:CG	1:A:301:PHE:CE1	3.03	0.42
1:B:229:ASN:HA	1:B:233:ASP:O	2.20	0.42
1:C:222:GLN:HE21	1:C:222:GLN:CA	2.32	0.42
1:A:314:TYR:O	1:A:328:GLN:HA	2.19	0.42
1:C:228:VAL:HG13	1:C:235:PHE:HD1	1.85	0.42
1:C:259:TYR:HB3	1:C:260:LEU:O	2.20	0.42
1:A:220:HIS:CD2	1:A:243:VAL:H	2.25	0.42
1:B:76:GLN:HE21	1:B:76:GLN:HB2	1.66	0.42
1:B:260:LEU:CD2	1:B:308:TYR:CE1	2.89	0.41
1:A:297:ASN:O	1:A:298:ARG:HB3	2.19	0.41
1:B:166:LYS:HG3	1:B:214:VAL:HG13	2.01	0.41
1:B:244:GLN:HG2	1:B:275:PRO:HD3	2.01	0.41
1:B:259:TYR:CD1	1:B:262:ARG:HB2	2.55	0.41
1:A:82:ASN:HA	1:A:83:PRO:HD2	1.88	0.41
1:B:150:ILE:HD12	1:B:226:CYS:HB3	2.01	0.41
1:D:220:HIS:O	1:D:221:GLN:HB2	2.21	0.41
1:D:261:GLN:HA	1:D:306:ILE:H	1.86	0.41
1:B:229:ASN:HD21	1:B:234:ARG:CD	2.33	0.41
1:B:291:LYS:HA	1:B:292:GLY:HA2	1.67	0.41
1:D:82:ASN:HA	1:D:83:PRO:HD2	1.83	0.41
1:B:274:ASN:HA	1:B:275:PRO:C	2.41	0.41
1:B:259:TYR:CB	1:B:260:LEU:O	2.69	0.41
1:C:280:TYR:CG	1:C:298:ARG:HB2	2.55	0.41
1:C:220:HIS:HD2	1:C:243:VAL:N	2.07	0.41
1:D:166:LYS:HE3	1:D:166:LYS:HB2	1.99	0.40
1:D:314:TYR:O	1:D:328:GLN:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:HG3	1:A:245:TYR:CE2	2.56	0.40
1:A:285:LEU:CB	1:A:313:THR:HB	2.51	0.40
1:B:145:LYS:HE2	1:B:235:PHE:CZ	2.55	0.40
1:C:53:PHE:CE1	1:C:134:ARG:NH2	2.89	0.40
1:D:101:ARG:HD2	1:D:106:ASP:OD2	2.21	0.40
1:D:266:LYS:HD3	1:D:299:THR:HB	2.03	0.40
1:D:303:LYS:O	1:D:305:PRO:HD2	2.22	0.40
1:A:49:LEU:HD22	1:A:138:LEU:HD11	2.03	0.40
1:A:220:HIS:CD2	1:A:274:ASN:ND2	2.89	0.40
1:B:153:THR:HB	1:B:155:ALA:H	1.85	0.40
1:C:297:ASN:O	1:C:298:ARG:HB3	2.20	0.40
1:C:160:LYS:HB3	1:C:163:GLN:HG2	2.03	0.40
1:C:259:TYR:CD1	1:C:262:ARG:HB2	2.57	0.40
1:D:80:ILE:N	1:D:80:ILE:HD12	2.36	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ASN:OD1	1:A:232:MET:CE[3_565]	2.01	0.19

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	300/313 (96%)	286 (95%)	14 (5%)	0	100	100
1	B	297/313 (95%)	287 (97%)	10 (3%)	0	100	100
1	C	299/313 (96%)	288 (96%)	11 (4%)	0	100	100
1	D	300/313 (96%)	293 (98%)	7 (2%)	0	100	100
All	All	1196/1252 (96%)	1154 (96%)	42 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	264/275 (96%)	234 (89%)	30 (11%)	5	24
1	B	261/275 (95%)	232 (89%)	29 (11%)	6	25
1	C	263/275 (96%)	231 (88%)	32 (12%)	5	22
1	D	264/275 (96%)	237 (90%)	27 (10%)	7	29
All	All	1052/1100 (96%)	934 (89%)	118 (11%)	6	25

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	PHE
1	A	57	LEU
1	A	90	LEU
1	A	93	TYR
1	A	94	ARG
1	A	111	LEU
1	A	113	ARG
1	A	114	LEU
1	A	116	LEU
1	A	134	ARG
1	A	140	LEU
1	A	153	THR
1	A	160	LYS
1	A	165	ASP
1	A	167	VAL
1	A	213	LEU
1	A	224	LEU
1	A	226	CYS
1	A	228	VAL
1	A	261	GLN
1	A	298	ARG
1	A	299	THR

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Mol	Chain	Res	Type
1	A	300	LEU
1	A	307	ASN
1	A	319	THR
1	A	320	ASN
1	A	322	ILE
1	A	333	ILE
1	A	334	THR
1	A	336	PHE
1	B	53	PHE
1	B	71	THR
1	B	76	GLN
1	B	95	GLU
1	B	101	ARG
1	B	111	LEU
1	B	113	ARG
1	B	114	LEU
1	B	116	LEU
1	B	134	ARG
1	B	140	LEU
1	B	153	THR
1	B	156	VAL
1	B	165	ASP
1	B	188	ARG
1	B	213	LEU
1	B	226	CYS
1	B	228	VAL
1	B	232	MET
1	B	261	GLN
1	B	263	MET
1	B	298	ARG
1	B	299	THR
1	B	307	ASN
1	B	317	GLU
1	B	319	THR
1	B	320	ASN
1	B	322	ILE
1	B	333	ILE
1	C	53	PHE
1	C	57	LEU
1	C	72	ASN
1	C	111	LEU
1	C	113	ARG

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Mol	Chain	Res	Type
1	C	114	LEU
1	C	116	LEU
1	C	134	ARG
1	C	140	LEU
1	C	153	THR
1	C	160	LYS
1	C	167	VAL
1	C	188	ARG
1	C	213	LEU
1	C	214	VAL
1	C	222	GLN
1	C	226	CYS
1	C	228	VAL
1	C	238	SER
1	C	261	GLN
1	C	263	MET
1	C	296	GLN
1	C	298	ARG
1	C	299	THR
1	C	307	ASN
1	C	319	THR
1	C	320	ASN
1	C	322	ILE
1	C	325	ARG
1	C	333	ILE
1	C	334	THR
1	C	336	PHE
1	D	53	PHE
1	D	57	LEU
1	D	71	THR
1	D	101	ARG
1	D	111	LEU
1	D	113	ARG
1	D	114	LEU
1	D	116	LEU
1	D	134	ARG
1	D	140	LEU
1	D	153	THR
1	D	199	ARG
1	D	213	LEU
1	D	226	CYS
1	D	228	VAL

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Mol	Chain	Res	Type
1	D	232	MET
1	D	261	GLN
1	D	263	MET
1	D	298	ARG
1	D	300	LEU
1	D	307	ASN
1	D	319	THR
1	D	320	ASN
1	D	322	ILE
1	D	333	ILE
1	D	334	THR
1	D	335	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	222	GLN
1	A	261	GLN
1	A	307	ASN
1	B	72	ASN
1	B	76	GLN
1	B	139	ASN
1	B	163	GLN
1	B	222	GLN
1	B	229	ASN
1	B	307	ASN
1	C	76	GLN
1	C	220	HIS
1	C	222	GLN
1	C	307	ASN
1	D	222	GLN
1	D	261	GLN
1	D	307	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	NAG	E	1	1,2	14,14,15	0.85	0	17,19,21	1.86	6 (35%)
2	NAG	E	2	2	14,14,15	0.82	0	17,19,21	2.03	3 (17%)
2	NAG	F	1	1,2	14,14,15	0.65	0	17,19,21	1.35	2 (11%)
2	NAG	F	2	2	14,14,15	0.77	0	17,19,21	2.07	5 (29%)
2	NAG	G	1	1,2	14,14,15	0.97	1 (7%)	17,19,21	2.29	6 (35%)
2	NAG	G	2	2	14,14,15	0.76	0	17,19,21	2.14	5 (29%)
2	NAG	H	1	1,2	14,14,15	1.59	1 (7%)	17,19,21	1.86	3 (17%)
2	NAG	H	2	2	14,14,15	0.86	1 (7%)	17,19,21	2.39	4 (23%)

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	NAG	E	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	3/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	NAG	O5-C1	-5.28	1.35	1.43
2	H	2	NAG	C1-C2	2.28	1.55	1.52
2	G	1	NAG	C1-C2	-2.17	1.49	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	NAG	C1-O5-C5	5.70	119.91	112.19
2	G	1	NAG	O7-C7-N2	-5.34	112.13	121.95
2	E	2	NAG	C4-C3-C2	-5.14	103.48	111.02
2	G	2	NAG	C4-C3-C2	-4.85	103.92	111.02
2	H	1	NAG	C4-C3-C2	4.63	117.80	111.02
2	H	2	NAG	C4-C3-C2	-4.26	104.77	111.02
2	F	2	NAG	C2-N2-C7	4.16	128.82	122.90
2	G	1	NAG	C8-C7-N2	4.04	122.95	116.10
2	E	2	NAG	C2-N2-C7	4.02	128.63	122.90
2	G	1	NAG	C4-C3-C2	4.02	116.91	111.02
2	H	2	NAG	C1-C2-N2	4.02	117.35	110.49
2	H	2	NAG	C2-N2-C7	3.93	128.50	122.90
2	F	2	NAG	C1-O5-C5	3.91	117.49	112.19
2	E	1	NAG	C8-C7-N2	3.79	122.51	116.10
2	G	2	NAG	C3-C4-C5	-3.78	103.50	110.24
2	G	2	NAG	C2-N2-C7	3.64	128.08	122.90
2	H	1	NAG	C8-C7-N2	3.55	122.11	116.10
2	F	1	NAG	C4-C3-C2	3.40	116.00	111.02
2	E	1	NAG	O7-C7-N2	-3.38	115.74	121.95
2	F	2	NAG	C4-C3-C2	-3.35	106.11	111.02
2	F	2	NAG	O5-C1-C2	-3.30	106.08	111.29
2	E	1	NAG	C1-O5-C5	3.23	116.57	112.19
2	E	2	NAG	O5-C1-C2	-3.21	106.22	111.29
2	F	1	NAG	O4-C4-C3	-2.48	104.60	110.35
2	H	1	NAG	C2-N2-C7	2.48	126.44	122.90
2	E	1	NAG	O5-C1-C2	-2.45	107.42	111.29
2	F	2	NAG	C1-C2-N2	2.37	114.53	110.49
2	E	1	NAG	C1-C2-N2	-2.36	106.45	110.49
2	G	2	NAG	O4-C4-C5	2.31	115.04	109.30
2	E	1	NAG	O4-C4-C3	-2.29	105.05	110.35
2	G	1	NAG	C1-C2-N2	-2.27	106.60	110.49
2	G	1	NAG	O4-C4-C3	-2.18	105.32	110.35
2	G	1	NAG	C2-N2-C7	2.13	125.93	122.90
2	G	2	NAG	O5-C1-C2	-2.04	108.07	111.29

There are no chirality outliers.

All (21) torsion outliers are listed below:

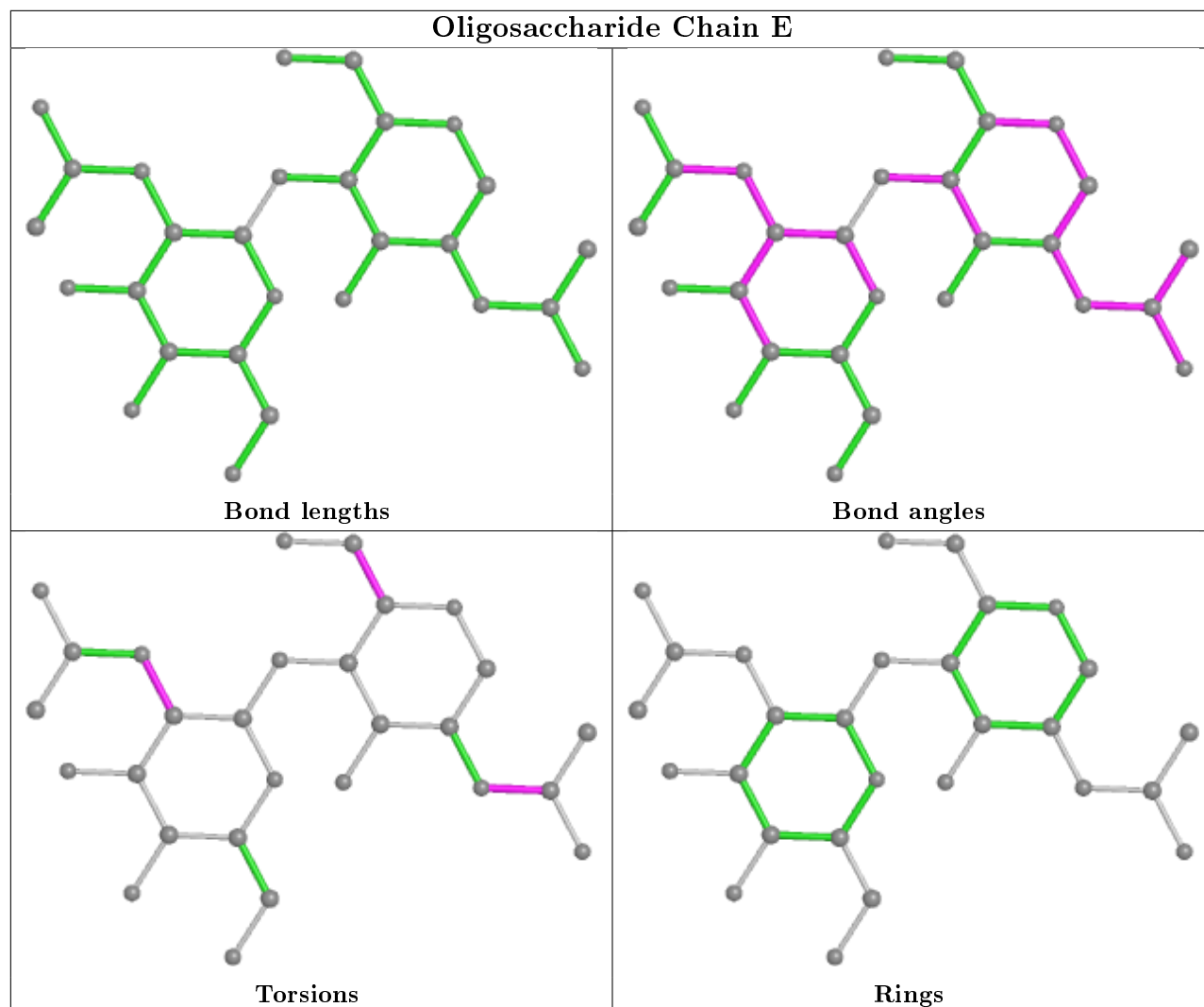
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	G	2	NAG	C3-C2-N2-C7
2	H	2	NAG	C3-C2-N2-C7
2	E	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6

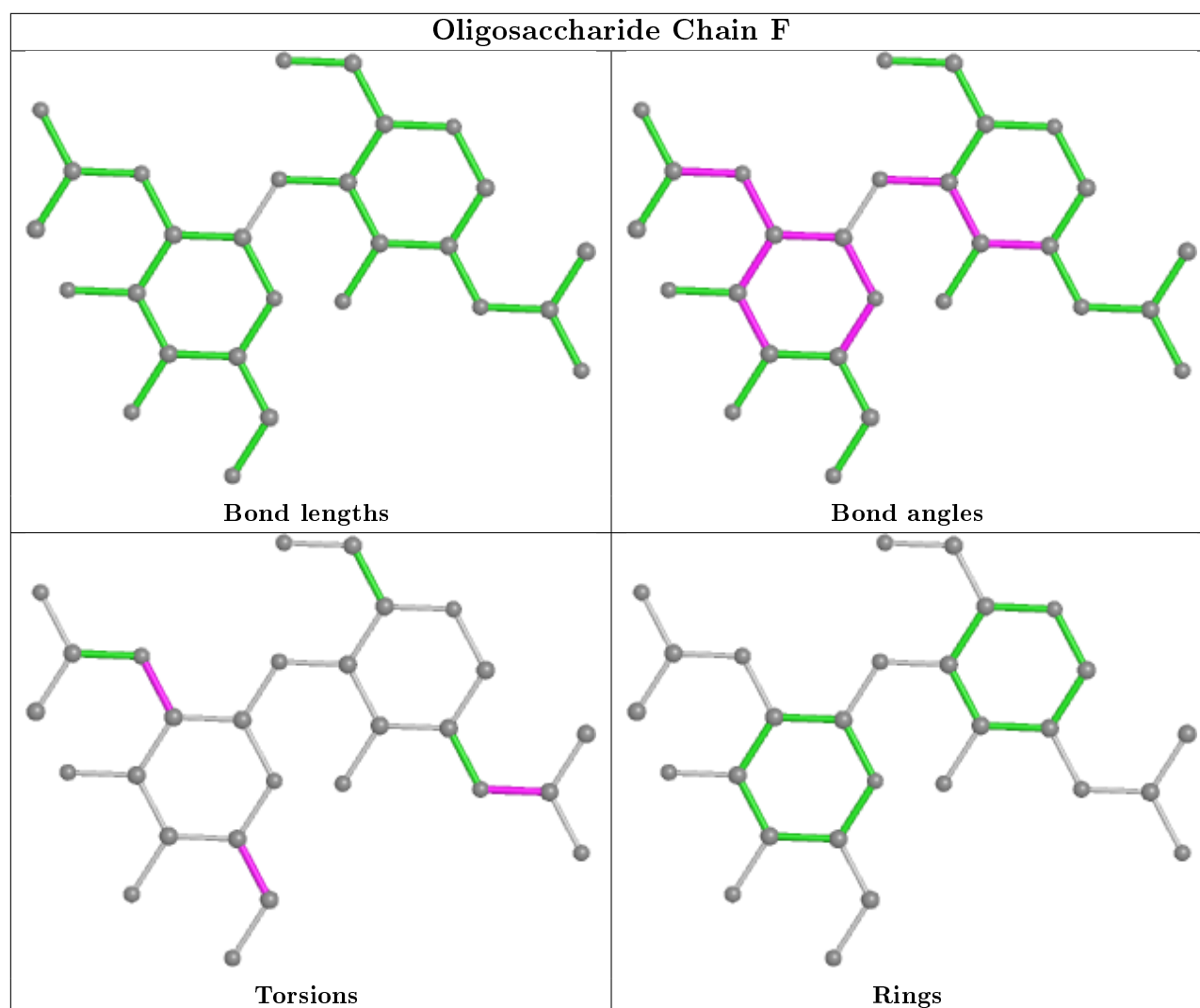
There are no ring outliers.

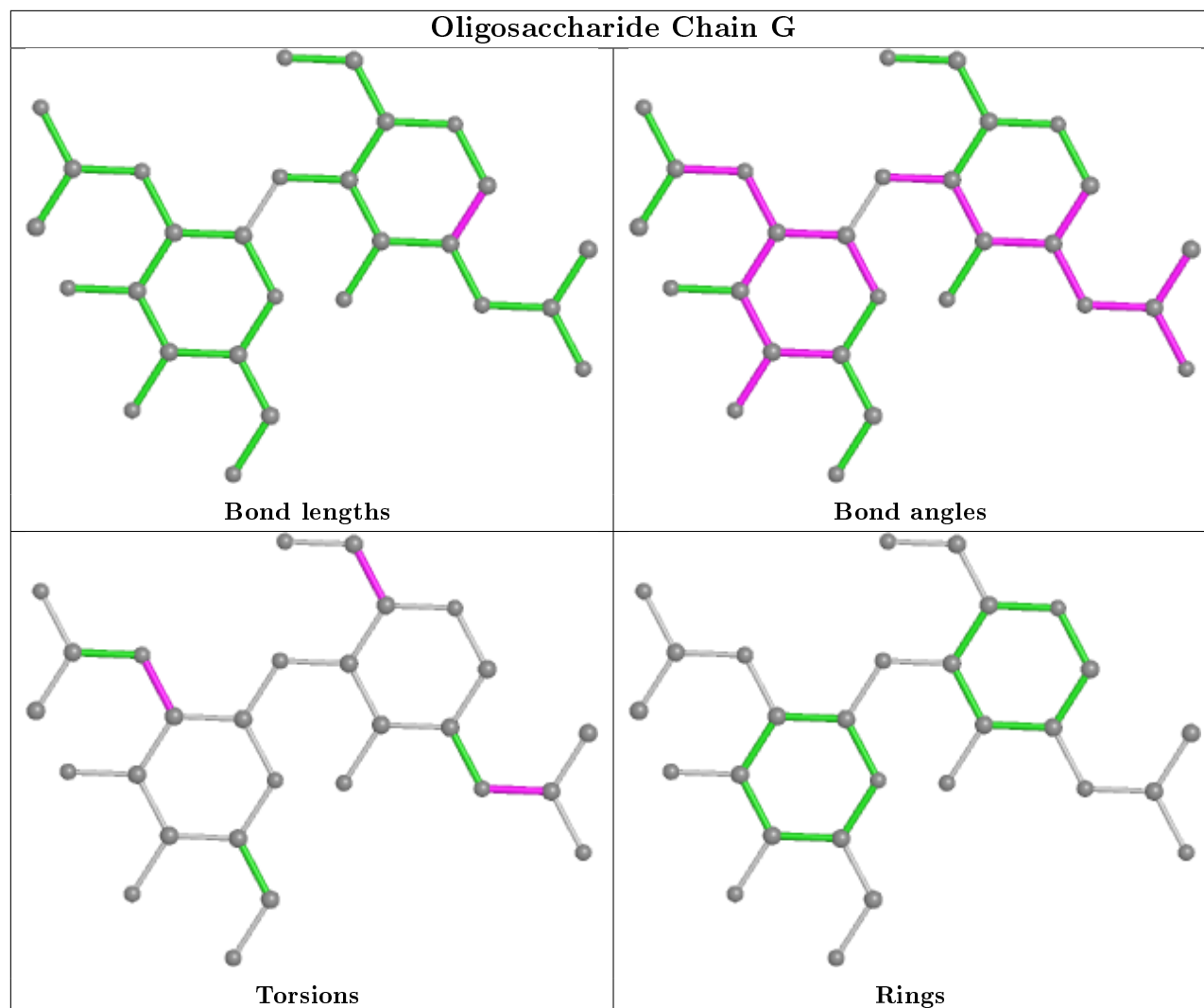
1 monomer is involved in 2 short contacts:

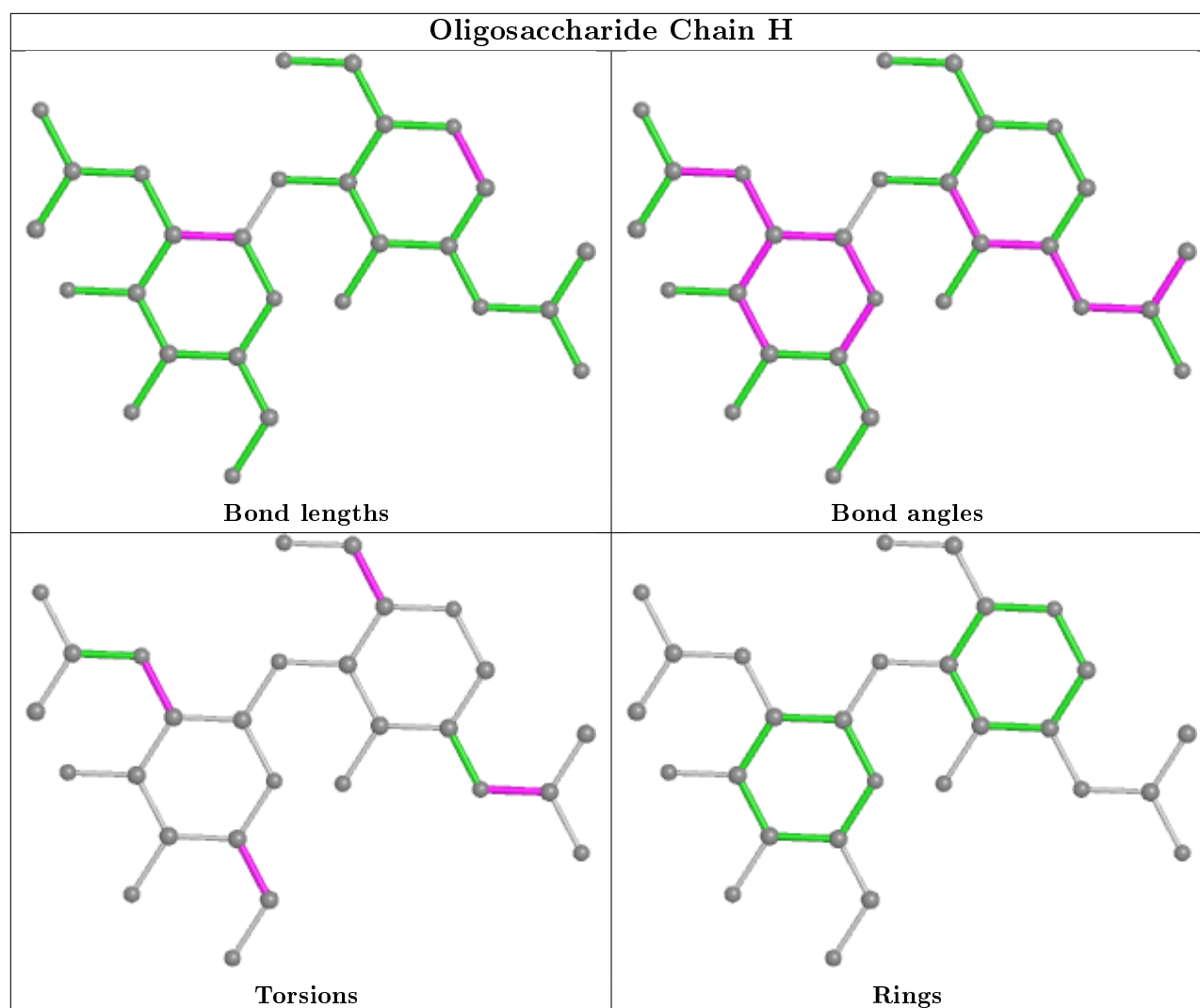
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	2	0

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









5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	FMT	D	403	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	403	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	403	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	403	-	0,2,2	0.00	-	0,1,1	0.00	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	302/313 (96%)	0.35	13 (4%) 35 22	48, 67, 183, 204	0
1	B	299/313 (95%)	0.66	32 (10%) 6 3	48, 78, 230, 255	0
1	C	301/313 (96%)	0.26	9 (2%) 50 34	46, 66, 152, 178	0
1	D	302/313 (96%)	0.34	17 (5%) 24 13	50, 81, 159, 181	0
All	All	1204/1252 (96%)	0.40	71 (5%) 22 13	46, 73, 201, 255	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	310	LEU	8.2
1	B	261	GLN	7.8
1	B	311	ALA	7.4
1	B	289	LEU	7.3
1	B	300	LEU	7.2
1	B	258	TRP	7.0
1	B	295	ALA	6.6
1	A	261	GLN	5.8
1	B	254	PHE	5.7
1	A	291	LYS	5.5
1	A	308	TYR	5.0
1	D	311	ALA	4.8
1	B	291	LYS	4.5
1	B	332	ASN	4.3
1	B	309	SER	4.2
1	A	264	ASP	4.2
1	B	328	GLN	3.8
1	D	266	LYS	3.7
1	D	300	LEU	3.6
1	C	266	LYS	3.5
1	D	301	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	260	LEU	3.4
1	D	314	TYR	3.4
1	A	292	GLY	3.4
1	D	312	GLY	3.3
1	C	301	PHE	3.3
1	B	294	GLU	3.3
1	B	308	TYR	3.3
1	B	302	PHE	3.2
1	B	322	ILE	3.1
1	B	314	TYR	3.1
1	A	334	THR	3.1
1	D	313	THR	3.0
1	B	329	VAL	3.0
1	A	263	MET	2.9
1	B	290	PRO	2.9
1	C	308	TYR	2.9
1	B	293	VAL	2.9
1	B	244	GLN	2.8
1	B	330	GLU	2.8
1	C	263	MET	2.7
1	D	318	ALA	2.7
1	B	263	MET	2.7
1	C	257	ASN	2.6
1	A	314	TYR	2.5
1	B	269	CYS	2.5
1	C	314	TYR	2.5
1	D	295	ALA	2.5
1	D	291	LYS	2.5
1	A	278	THR	2.5
1	B	285	LEU	2.5
1	B	292	GLY	2.4
1	A	332	ASN	2.3
1	A	318	ALA	2.3
1	D	334	THR	2.3
1	B	288	SER	2.3
1	A	295	ALA	2.3
1	D	308	TYR	2.3
1	B	271	ALA	2.3
1	D	310	LEU	2.2
1	B	264	ASP	2.2
1	B	249	VAL	2.2
1	C	332	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	336	PHE	2.1
1	D	294	GLU	2.1
1	B	251	ILE	2.1
1	A	258	TRP	2.0
1	C	318	ALA	2.0
1	B	331	VAL	2.0
1	D	306	ILE	2.0
1	C	296	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

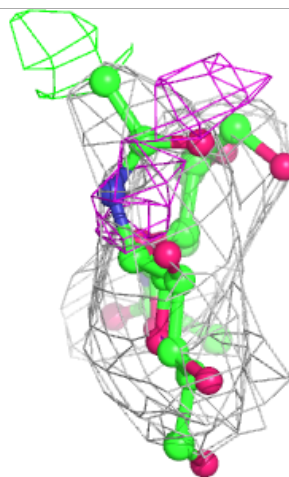
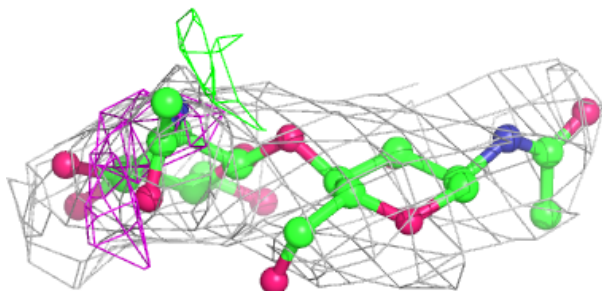
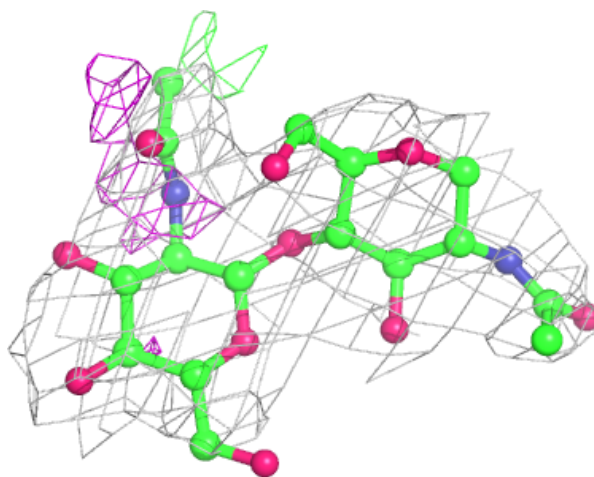
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	H	2	14/15	0.79	0.23	93,105,111,116	0
2	NAG	G	2	14/15	0.81	0.25	85,98,109,114	0
2	NAG	H	1	14/15	0.86	0.23	90,95,105,107	0
2	NAG	E	2	14/15	0.89	0.32	81,90,98,101	0
2	NAG	G	1	14/15	0.89	0.21	75,79,88,92	0
2	NAG	F	2	14/15	0.90	0.24	86,96,106,110	0
2	NAG	F	1	14/15	0.91	0.22	75,80,86,91	0
2	NAG	E	1	14/15	0.92	0.27	73,78,82,89	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.

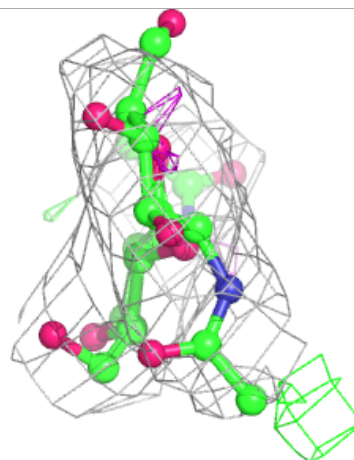
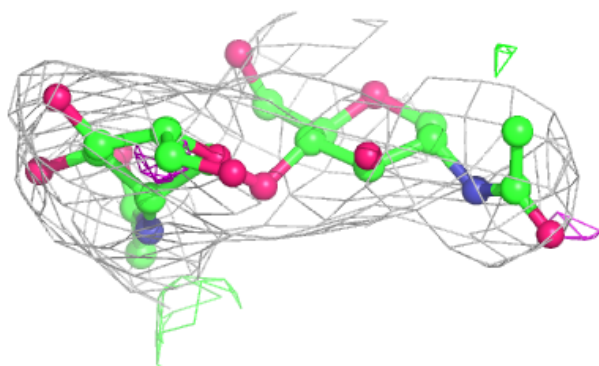
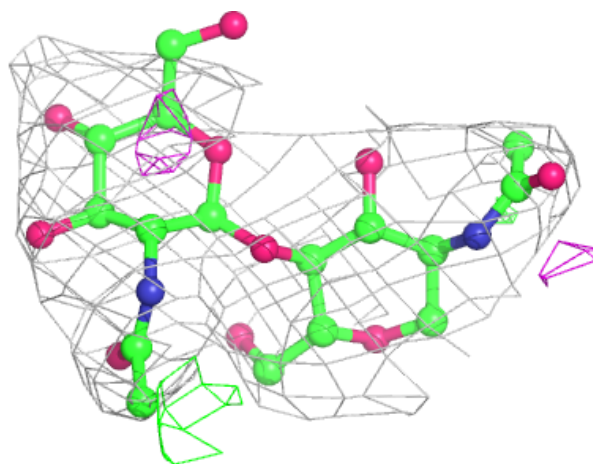
Electron density around Chain E:

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



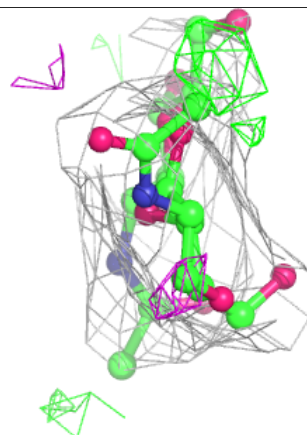
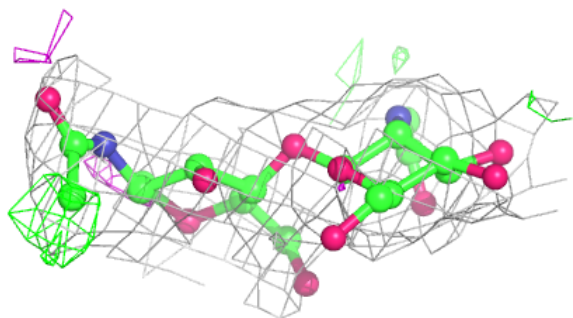
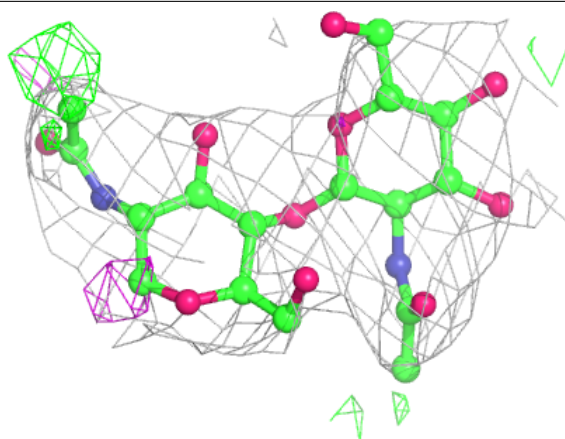
Electron density around Chain F:

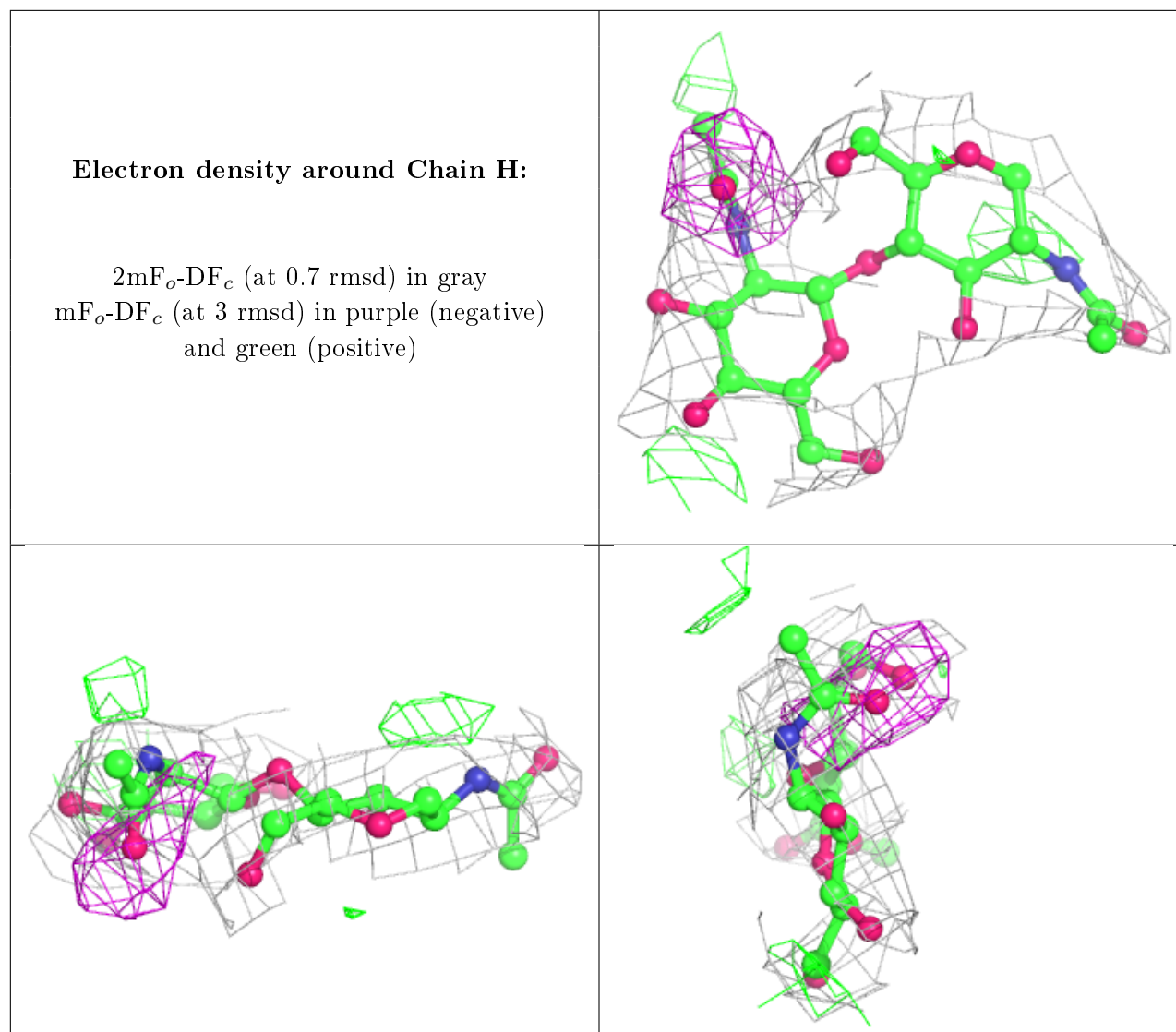
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

$2mF_o - DF_c$ (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
3	FMT	A	403	3/3	0.85	0.22	32,32,34,35	0
3	FMT	C	403	3/3	0.89	0.24	44,44,44,45	0
3	FMT	D	403	3/3	0.92	0.17	57,57,60,60	0
3	FMT	B	403	3/3	0.94	0.27	60,60,63,64	0

6.5 Other polymers

There are no such residues in this entry.