



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 07:36 AM EDT

PDB ID : 1MOX
Title : Crystal Structure of Human Epidermal Growth Factor Receptor (residues 1-501) in complex with TGF-alpha
Authors : Garrett, T.P.J.; McKern, N.M.; Lou, M.; Elleman, T.C.; Adams, T.E.; Lovrecz, G.O.; Zhu, H.-J.; Walker, F.; Frenkel, M.J.; Hoyne, P.A.; Jorissen, R.N.; Nice, E.C.; Burgess, A.W.; Ward, C.W.
Deposited on : 2002-09-10
Resolution : 2.50 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

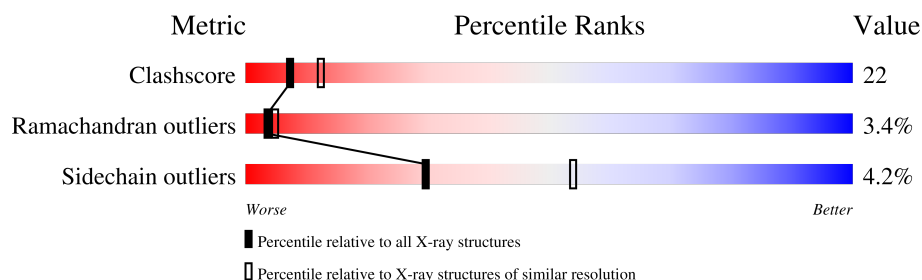
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	501	63% 32% .
1	B	501	66% 30% .
2	C	50	62% 32% . .
2	D	50	52% 34% 8% . .
3	E	3	33% 67%
4	F	4	25% 50% 25%
5	G	4	50% 50%
6	H	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	E	1	-	-	X	-
7	PT	B	702	-	-	X	-
9	CL	A	737	-	-	X	-
9	CL	A	739	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 8686 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.

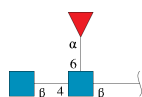
- Molecule 1 is a protein called Epidermal Growth Factor Receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			3820	2369	674	735	42			
1	B	501	Total	C	N	O	S	0	0	0
			3844	2381	682	739	42			

- Molecule 2 is a protein called Transforming Growth Factor alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	49	Total	C	N	O	S	0	0	0
			377	232	69	70	6			
2	D	48	Total	C	N	O	S	0	0	0
			365	225	66	68	6			

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



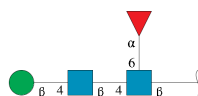
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O		0	0	0
			38	22	2	14				

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 6 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
6	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	Pt	0	0
			3	3		
7	B	4	Total	Pt	0	0
			4	4		

- Molecule 8 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total	Cd	0	0
			4	4		
8	B	5	Total	Cd	0	0
			5	5		

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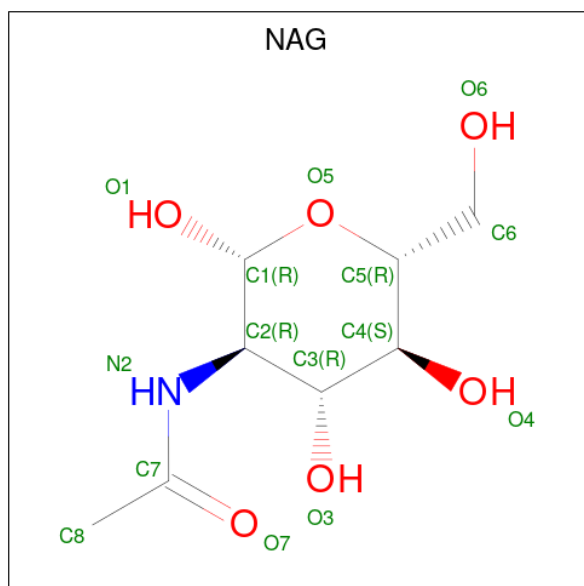
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Cd	0	0
			1	1		
8	D	1	Total	Cd	0	0
			1	1		

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	3	Total	Cl	0	0
			3	3		
9	B	1	Total	Cl	0	0
			1	1		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	29	Total	O	0	0
			29	29		

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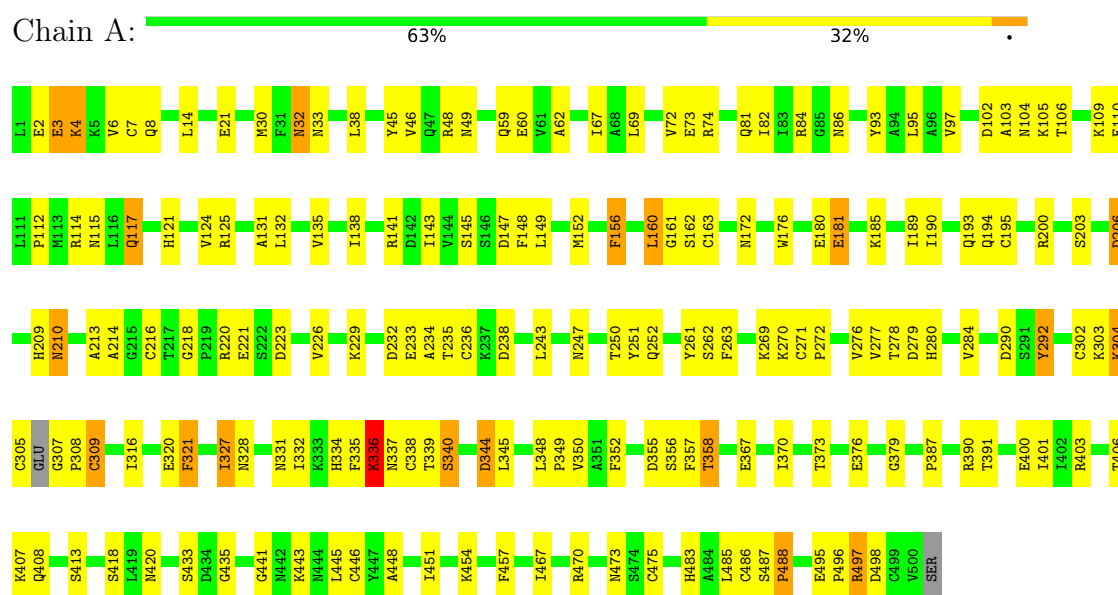
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	39	Total 39	O 39	0	0
11	C	6	Total 6	O 6	0	0
11	D	5	Total 5	O 5	0	0

3 Residue-property plots

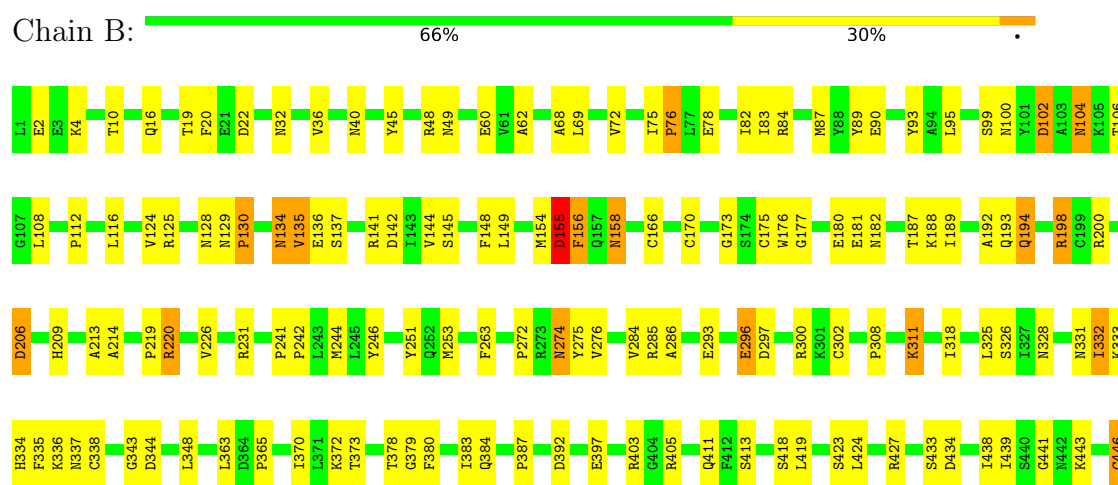
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: Epidermal Growth Factor Receptor



• Molecule 1: Epidermal Growth Factor Receptor





- Molecule 2: Transforming Growth Factor alpha



- Molecule 2: Transforming Growth Factor alpha



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



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



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.59Å 198.71Å 78.90Å 90.00° 102.03° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.237 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8686	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, FUC, PT, MAN, CL, CD, 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	0.39	1/3889 (0.0%)	0.69	2/5259 (0.0%)
1	B	0.39	1/3914 (0.0%)	0.70	2/5291 (0.0%)
2	C	0.44	0/388	0.77	0/524
2	D	0.41	0/375	0.69	0/506
All	All	0.39	2/8566 (0.0%)	0.70	4/11580 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	296	GLU	CB-CG	-5.29	1.42	1.52
1	A	2	GLU	CB-CG	-5.25	1.42	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	308	PRO	N-CA-CB	5.87	110.35	103.30
1	A	308	PRO	N-CA-CB	5.38	109.76	103.30
1	A	327	ILE	N-CA-C	-5.14	97.11	111.00
1	B	446	CYS	N-CA-C	5.08	124.72	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3820	0	3676	176	5
1	B	3844	0	3705	161	4
2	C	377	0	323	21	0
2	D	365	0	311	14	0
3	E	38	0	34	8	0
4	F	50	0	43	4	0
5	G	49	0	43	1	0
6	H	28	0	25	4	0
7	A	3	0	0	0	0
7	B	4	0	0	2	0
8	A	4	0	0	0	1
8	B	5	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	3	0	0	4	0
9	B	1	0	0	0	0
10	B	14	0	13	0	0
11	A	29	0	0	6	0
11	B	39	0	0	0	0
11	C	6	0	0	0	0
11	D	5	0	0	0	0
All	All	8686	0	8173	372	5

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 22.

All (372) 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:141:ARG:HH21	1:A:189:ILE:HD11	1.16	1.05
3:E:1:NAG:H62	3:E:3:FUC:H3	1.53	0.90
1:A:496:PRO:HD2	1:A:497:ARG:NH2	1.87	0.88
1:B:158:ASN:H	1:B:158:ASN:HD22	1.21	0.88
4:F:3:BMA:H3	4:F:4:MAN:H3	1.56	0.87
1:A:446:CYS:SG	1:A:470:ARG:HG2	2.15	0.86
1:A:213:ALA:HB3	1:A:226:VAL:HG23	1.58	0.85
2:C:6:ASN:ND2	2:C:7:ASP:H	1.73	0.84
2:C:6:ASN:HD22	2:C:7:ASP:H	1.24	0.83
1:B:418:SER:HA	1:B:441:GLY:O	1.77	0.82
1:A:3:GLU:O	1:A:4:LYS:HB2	1.78	0.82
1:A:496:PRO:HD2	1:A:497:ARG:CZ	2.09	0.82
1:B:311:LYS:HD2	1:B:338:CYS:HA	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:26:GLN:HE21	2:D:26:GLN:HA	1.46	0.81
1:A:486:CYS:C	1:A:488:PRO:HD2	2.03	0.79
1:B:244:MET:CE	7:B:702:PT:PT	1.52	0.78
1:B:274:ASN:ND2	1:B:434:ASP:HB2	1.98	0.78
1:A:487:SER:N	1:A:488:PRO:HD2	2.00	0.76
1:B:284:VAL:HG12	1:B:286:ALA:H	1.50	0.76
1:A:145:SER:HB2	1:A:148:PHE:HD1	1.51	0.75
1:A:74:ARG:HG3	1:A:110:GLU:HG3	1.71	0.73
1:A:292:TYR:CE2	1:A:303:LYS:HB3	2.24	0.73
1:A:334:HIS:HD2	9:A:737:CL:CL	2.08	0.73
1:A:420:ASN:OD1	1:A:443:LYS:HE2	1.88	0.73
1:A:336:LYS:HG3	1:A:337:ASN:H	1.52	0.73
2:C:24:LEU:HD11	2:C:27:GLU:HB2	1.69	0.73
1:B:102:ASP:OD2	1:B:106:THR:HB	1.88	0.72
1:A:292:TYR:HE2	1:A:303:LYS:HB3	1.53	0.72
1:B:158:ASN:HD22	1:B:158:ASN:N	1.88	0.71
1:B:325:LEU:H	6:H:1:NAG:H83	1.54	0.71
1:A:60:GLU:HG2	1:A:82:ILE:CG2	2.20	0.71
1:B:486:CYS:C	1:B:488:PRO:HD2	2.10	0.71
3:E:1:NAG:H61	3:E:3:FUC:H5	1.72	0.71
1:A:280:HIS:NE2	1:B:244:MET:SD	2.64	0.71
1:A:332:ILE:HG21	1:A:367:GLU:HG2	1.72	0.71
1:A:141:ARG:HH21	1:A:189:ILE:CD1	2.00	0.70
1:A:269:LYS:H	1:A:269:LYS:HD3	1.55	0.70
1:A:220:ARG:HB2	1:A:223:ASP:OD2	1.92	0.70
1:B:363:LEU:O	1:B:365:PRO:HD3	1.91	0.69
1:A:276:VAL:HG11	1:A:302:CYS:SG	2.32	0.69
1:B:213:ALA:HB3	1:B:226:VAL:HG13	1.75	0.69
1:B:336:LYS:HD3	1:B:337:ASN:N	2.08	0.69
1:B:343:GLY:H	1:B:378:THR:HB	1.58	0.69
1:B:141:ARG:HG2	1:B:189:ILE:HD11	1.74	0.68
1:B:128:ASN:C	1:B:130:PRO:HD3	2.14	0.68
1:A:344:ASP:OD2	1:A:379:GLY:HA3	1.94	0.67
1:A:14:LEU:HD13	2:C:24:LEU:HD21	1.78	0.66
1:A:327:ILE:HD11	1:A:345:LEU:HD22	1.78	0.66
1:B:333:LYS:HE3	1:B:334:HIS:NE2	2.10	0.66
2:C:6:ASN:HD22	2:C:7:ASP:N	1.94	0.66
1:A:334:HIS:C	1:A:336:LYS:H	1.99	0.66
1:A:81:GLN:HA	1:A:115:ASN:O	1.96	0.66
1:B:136:GLU:HB3	1:B:156:PHE:HB2	1.77	0.65
1:A:48:ARG:NH1	1:A:73:GLU:HB2	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:HIS:ND1	1:A:221:GLU:HG2	2.11	0.65
1:B:137:SER:HB2	1:B:173:GLY:O	1.96	0.65
1:A:328:ASN:HB2	11:A:751:HOH:O	1.96	0.64
1:B:336:LYS:HD3	1:B:337:ASN:H	1.62	0.64
1:A:105:LYS:HG2	1:A:106:THR:HG23	1.78	0.64
2:C:6:ASN:ND2	2:C:7:ASP:N	2.44	0.64
2:C:21:CYS:SG	2:C:22:ARG:N	2.71	0.64
1:A:145:SER:HB2	1:A:148:PHE:CD1	2.31	0.63
1:A:200:ARG:HD2	1:A:218:GLY:H	1.62	0.63
1:B:411:GLN:OE1	2:D:49:LEU:HD21	1.98	0.63
2:D:6:ASN:HB3	2:D:23:PHE:HB3	1.80	0.63
2:D:13:THR:O	2:D:14:GLN:HB3	1.99	0.63
1:A:95:LEU:HB3	1:A:124:VAL:HG22	1.80	0.63
1:B:200:ARG:HG2	1:B:206:ASP:O	1.99	0.62
1:A:141:ARG:NH2	1:A:189:ILE:HD11	2.01	0.62
1:B:452:ASN:ND2	1:B:455:LYS:HB2	2.13	0.62
4:F:3:BMA:H3	4:F:4:MAN:C3	2.28	0.62
1:A:117:GLN:HE21	1:A:185:LYS:HB2	1.64	0.62
1:B:274:ASN:HD21	1:B:434:ASP:HB2	1.64	0.62
1:A:348:LEU:HB3	1:A:349:PRO:HD2	1.82	0.61
1:A:400:GLU:CB	1:A:401:ILE:HD12	2.29	0.61
1:B:450:THR:HB	1:B:490:GLY:HA2	1.83	0.61
1:B:112:PRO:HA	1:B:176:TRP:HB3	1.83	0.61
1:A:181:GLU:OE1	1:A:181:GLU:N	2.34	0.61
1:A:251:TYR:HB2	1:B:285:ARG:HG3	1.82	0.60
1:A:209:HIS:CE1	1:A:221:GLU:HG2	2.36	0.60
1:B:486:CYS:O	1:B:488:PRO:N	2.35	0.60
9:A:737:CL:CL	9:A:739:CL:CL	2.94	0.60
1:A:358:THR:HG21	4:F:1:NAG:HN2	1.68	0.59
1:B:246:TYR:CB	1:B:253:MET:HE1	2.31	0.59
1:B:284:VAL:CG1	1:B:286:ALA:H	2.15	0.59
2:C:4:HIS:HE1	2:C:26:GLN:HE22	1.50	0.59
2:D:26:GLN:HA	2:D:26:GLN:NE2	2.16	0.59
1:A:495:GLU:O	1:A:498:ASP:HB2	2.02	0.59
1:A:149:LEU:HG	1:A:152:MET:HE1	1.85	0.58
1:A:45:TYR:HA	1:A:69:LEU:O	2.03	0.58
1:A:269:LYS:HD3	1:A:269:LYS:N	2.18	0.58
1:B:284:VAL:HG12	1:B:286:ALA:N	2.17	0.58
1:A:117:GLN:HA	11:A:780:HOH:O	2.03	0.58
1:A:103:ALA:O	1:A:105:LYS:N	2.37	0.58
1:A:149:LEU:HG	1:A:152:MET:CE	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1:NAG:H62	3:E:3:FUC:C3	2.30	0.58
1:B:483:HIS:ND1	1:B:484:ALA:N	2.51	0.58
1:A:334:HIS:CD2	9:A:737:CL:CL	2.93	0.57
3:E:1:NAG:C6	3:E:3:FUC:H5	2.32	0.57
1:B:331:ASN:O	1:B:333:LYS:N	2.38	0.57
1:B:483:HIS:CD2	1:B:496:PRO:HG3	2.39	0.57
1:B:144:VAL:HG12	1:B:145:SER:N	2.19	0.57
1:B:246:TYR:HA	1:B:253:MET:HE1	1.85	0.57
1:B:338:CYS:O	1:B:373:THR:HG23	2.05	0.57
1:B:89:TYR:CE2	1:B:90:GLU:HG2	2.40	0.57
1:A:161:GLY:C	1:A:163:CYS:H	2.08	0.57
1:A:413:SER:HB2	1:A:435:GLY:HA3	1.86	0.57
1:A:156:PHE:CD1	1:A:156:PHE:N	2.73	0.56
1:B:275:TYR:OH	1:B:285:ARG:NH1	2.38	0.56
1:B:325:LEU:H	6:H:1:NAG:C8	2.18	0.56
1:A:332:ILE:HG12	1:A:370:ILE:HD12	1.87	0.56
1:A:403:ARG:HA	1:A:433:SER:HB2	1.87	0.56
1:B:192:ALA:O	1:B:194:GLN:N	2.38	0.56
1:B:452:ASN:HD22	1:B:455:LYS:HB2	1.70	0.56
1:A:320:GLU:HG3	1:A:321:PHE:CE1	2.41	0.56
2:C:4:HIS:CE1	2:C:26:GLN:HE22	2.23	0.56
1:A:132:LEU:HD21	1:A:135:VAL:HG21	1.87	0.55
1:B:128:ASN:N	1:B:128:ASN:HD22	2.05	0.55
1:A:121:HIS:HD1	1:A:148:PHE:HZ	1.54	0.55
1:B:246:TYR:CA	1:B:253:MET:HE1	2.36	0.55
1:A:62:ALA:HB1	1:A:86:ASN:ND2	2.22	0.55
1:A:336:LYS:HG3	1:A:337:ASN:N	2.20	0.55
1:B:141:ARG:HA	1:B:149:LEU:HD21	1.89	0.55
2:D:48:LEU:O	2:D:50:ALA:N	2.39	0.55
1:A:117:GLN:HE22	1:A:185:LYS:HD2	1.72	0.55
1:B:486:CYS:O	1:B:487:SER:C	2.45	0.55
1:A:200:ARG:HD2	1:A:218:GLY:N	2.20	0.55
1:A:445:LEU:O	1:A:470:ARG:HB3	2.06	0.55
1:A:487:SER:N	1:A:488:PRO:CD	2.69	0.55
1:B:246:TYR:HD1	1:B:253:MET:CE	2.20	0.55
1:A:400:GLU:HB3	1:A:401:ILE:HD12	1.89	0.55
1:A:252:GLN:HA	1:B:284:VAL:HG22	1.89	0.55
1:B:145:SER:HB3	1:B:148:PHE:HD1	1.71	0.54
1:B:69:LEU:N	1:B:69:LEU:HD12	2.22	0.54
1:B:134:ASN:ND2	1:B:177:GLY:HA2	2.23	0.54
1:B:75:ILE:HG13	1:B:108:LEU:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:CYS:C	1:A:488:PRO:CD	2.75	0.54
1:A:321:PHE:HE2	1:A:331:ASN:HB2	1.72	0.54
1:B:93:TYR:CE2	1:B:125:ARG:HB2	2.43	0.54
1:B:104:ASN:HD22	1:B:104:ASN:N	2.04	0.53
1:A:467:ILE:C	1:A:467:ILE:HD12	2.28	0.53
1:B:244:MET:HE1	7:B:702:PT:PT	1.28	0.53
1:A:46:VAL:HG12	1:A:72:VAL:HB	1.90	0.53
5:G:2:NAG:H83	5:G:2:NAG:O3	2.07	0.53
1:B:380:PHE:CB	1:B:413:SER:HA	2.38	0.53
1:A:269:LYS:H	1:A:269:LYS:CD	2.19	0.53
1:A:102:ASP:CG	1:A:103:ALA:H	2.12	0.53
1:A:278:THR:HG22	1:A:279:ASP:H	1.73	0.53
1:A:203:SER:HB3	1:A:206:ASP:OD1	2.09	0.53
1:A:497:ARG:NE	1:A:497:ARG:H	2.06	0.53
1:A:321:PHE:CE2	1:A:331:ASN:HB2	2.44	0.53
1:B:272:PRO:HB2	1:B:275:TYR:HD1	1.74	0.52
1:A:470:ARG:HG2	1:A:475:CYS:SG	2.49	0.52
1:A:355:ASP:OD2	1:A:358:THR:HB	2.10	0.52
1:B:285:ARG:HH11	1:B:285:ARG:HG2	1.75	0.52
1:B:36:VAL:HG22	1:B:60:GLU:HG2	1.91	0.52
2:D:49:LEU:O	2:D:50:ALA:CB	2.57	0.52
1:B:142:ASP:OD1	1:B:142:ASP:O	2.28	0.52
1:B:246:TYR:CD1	1:B:253:MET:HE1	2.45	0.52
1:B:486:CYS:C	1:B:488:PRO:CD	2.77	0.52
2:D:6:ASN:OD1	2:D:7:ASP:N	2.43	0.51
1:B:296:GLU:O	1:B:297:ASP:HB3	2.10	0.51
2:C:19:GLY:HA3	2:C:34:CYS:HA	1.92	0.51
2:D:49:LEU:O	2:D:50:ALA:HB2	2.10	0.51
1:A:403:ARG:O	1:A:433:SER:HB2	2.10	0.51
1:B:187:THR:OG1	1:B:198:ARG:HD2	2.10	0.51
1:A:485:LEU:C	1:A:486:CYS:SG	2.88	0.51
1:A:262:SER:HB3	1:B:246:TYR:CD2	2.45	0.51
1:B:188:LYS:HD2	1:B:198:ARG:NH1	2.26	0.51
1:A:400:GLU:C	1:A:401:ILE:HD12	2.31	0.51
1:A:213:ALA:O	1:A:214:ALA:HB3	2.10	0.51
1:A:483:HIS:CD2	1:A:485:LEU:HD13	2.46	0.51
1:A:45:TYR:CZ	1:A:69:LEU:HD13	2.46	0.51
1:B:2:GLU:HA	1:B:231:ARG:NH1	2.26	0.51
1:B:311:LYS:CD	1:B:338:CYS:HA	2.39	0.51
1:A:114:ARG:HA	1:A:176:TRP:CD1	2.46	0.50
1:A:181:GLU:CD	1:A:181:GLU:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ASP:HB3	1:A:358:THR:HG22	1.94	0.50
1:A:387:PRO:HB2	1:A:390:ARG:HG3	1.94	0.50
1:B:102:ASP:CG	1:B:106:THR:HB	2.32	0.50
1:B:104:ASN:N	1:B:104:ASN:ND2	2.60	0.50
1:A:263:PHE:CZ	1:A:272:PRO:HG2	2.47	0.50
1:B:48:ARG:O	1:B:49:ASN:HB2	2.12	0.50
1:B:293:GLU:OE1	1:B:300:ARG:HD3	2.12	0.50
1:B:158:ASN:N	1:B:158:ASN:ND2	2.58	0.50
1:B:246:TYR:HD1	1:B:253:MET:HE1	1.75	0.50
1:B:328:ASN:H	1:B:331:ASN:HB2	1.76	0.50
1:A:229:LYS:HD2	1:A:238:ASP:OD1	2.11	0.50
2:D:19:GLY:HA2	2:D:35:HIS:CE1	2.47	0.50
1:A:30:MET:CE	11:A:805:HOH:O	2.59	0.50
1:B:209:HIS:HB2	1:B:220:ARG:O	2.12	0.50
1:B:246:TYR:HB2	1:B:253:MET:HE1	1.93	0.50
1:B:372:LYS:HD2	1:B:397:GLU:HG2	1.94	0.49
1:B:372:LYS:HD2	1:B:397:GLU:OE1	2.12	0.49
2:C:47:ASP:OD1	2:C:47:ASP:O	2.29	0.49
1:A:189:ILE:HG23	1:A:190:ILE:HG23	1.95	0.49
1:A:247:ASN:HB3	1:A:250:THR:HB	1.93	0.49
1:B:497:ARG:HG3	1:B:497:ARG:HH11	1.77	0.49
1:B:76:PRO:C	1:B:78:GLU:H	2.16	0.49
2:D:19:GLY:HA3	2:D:33:VAL:O	2.12	0.49
1:A:62:ALA:HA	1:A:84:ARG:HD2	1.94	0.49
1:A:408:GLN:OE1	1:A:408:GLN:HA	2.11	0.49
1:A:316:ILE:HD11	1:A:327:ILE:HD13	1.93	0.49
1:A:305:CYS:HB3	1:A:307:GLY:N	2.28	0.49
1:A:84:ARG:HG2	1:A:84:ARG:HH11	1.77	0.49
1:B:488:PRO:HB3	1:B:501:SER:HB2	1.94	0.49
1:B:104:ASN:ND2	1:B:104:ASN:H	2.11	0.48
1:A:418:SER:HA	1:A:441:GLY:O	2.13	0.48
1:A:473:ASN:HB2	11:A:784:HOH:O	2.13	0.48
1:B:4:LYS:NZ	1:B:60:GLU:OE1	2.45	0.48
1:B:326:SER:HB2	1:B:348:LEU:HG	1.95	0.48
1:A:336:LYS:CG	1:A:337:ASN:H	2.22	0.48
1:B:465:LYS:NZ	1:B:467:ILE:HD11	2.29	0.48
1:A:235:THR:HG22	1:A:236:CYS:N	2.27	0.48
1:A:210:ASN:N	1:A:210:ASN:HD22	2.12	0.48
1:B:443:LYS:O	1:B:470:ARG:HB2	2.13	0.48
1:A:4:LYS:HE3	1:A:59:GLN:OE1	2.14	0.48
1:B:68:ALA:HB1	1:B:69:LEU:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:VAL:HG12	1:B:156:PHE:CE2	2.49	0.48
1:B:380:PHE:HB2	1:B:413:SER:HA	1.95	0.48
1:A:32:ASN:ND2	3:E:1:NAG:C7	2.77	0.48
1:B:198:ARG:HG2	1:B:198:ARG:HH11	1.78	0.48
1:B:284:VAL:CG1	1:B:285:ARG:N	2.77	0.48
1:A:292:TYR:HD2	1:A:292:TYR:N	2.11	0.48
1:A:292:TYR:N	1:A:292:TYR:CD2	2.82	0.47
1:A:320:GLU:OE2	9:A:739:CL:CL	2.69	0.47
1:A:209:HIS:CD2	1:A:210:ASN:HD22	2.32	0.47
1:A:350:VAL:CG2	1:A:355:ASP:HB2	2.44	0.47
1:B:500:VAL:HG23	1:B:501:SER:N	2.29	0.47
1:A:290:ASP:O	1:A:309:CYS:SG	2.72	0.47
1:A:340:SER:HB2	1:A:376:GLU:HG2	1.95	0.47
1:B:424:LEU:HD11	1:B:439:ILE:HD13	1.95	0.47
1:B:188:LYS:HB2	1:B:198:ARG:HD3	1.97	0.47
1:A:407:LYS:HD3	1:A:435:GLY:CA	2.44	0.47
1:B:68:ALA:HB1	1:B:69:LEU:HD13	1.97	0.47
1:A:4:LYS:O	1:A:6:VAL:HG23	2.15	0.47
1:A:367:GLU:O	1:A:370:ILE:HG13	2.15	0.47
1:B:213:ALA:O	1:B:214:ALA:HB3	2.15	0.47
1:A:3:GLU:O	1:A:4:LYS:CB	2.54	0.47
1:B:285:ARG:O	1:B:405:ARG:NH1	2.46	0.47
1:B:370:ILE:O	1:B:373:THR:HG22	2.15	0.47
1:A:30:MET:HE2	11:A:805:HOH:O	2.15	0.47
1:B:455:LYS:HD3	1:B:455:LYS:C	2.35	0.47
1:A:45:TYR:CE2	1:A:69:LEU:HD13	2.50	0.47
1:A:145:SER:HB3	1:A:147:ASP:OD1	2.13	0.47
1:B:128:ASN:O	1:B:130:PRO:HD3	2.15	0.47
1:A:203:SER:HB3	1:A:206:ASP:CG	2.35	0.46
1:B:134:ASN:O	1:B:136:GLU:N	2.47	0.46
1:A:243:LEU:HD11	1:A:261:TYR:CE2	2.50	0.46
1:B:89:TYR:CD2	1:B:90:GLU:HG2	2.51	0.46
1:A:73:GLU:CG	1:A:109:LYS:HE3	2.45	0.46
1:A:232:ASP:O	1:A:234:ALA:N	2.49	0.46
1:B:99:SER:OG	2:D:26:GLN:HG2	2.16	0.46
1:B:446:CYS:SG	1:B:470:ARG:HD3	2.56	0.46
1:B:497:ARG:HH11	1:B:497:ARG:CG	2.29	0.46
1:B:89:TYR:O	1:B:90:GLU:HB2	2.16	0.46
1:A:93:TYR:CE2	1:A:125:ARG:HB2	2.51	0.46
1:B:69:LEU:N	1:B:69:LEU:CD1	2.79	0.46
1:A:284:VAL:HA	1:B:251:TYR:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:SER:HB3	1:B:488:PRO:HD3	1.97	0.45
1:A:74:ARG:CZ	1:A:112:PRO:HG3	2.47	0.45
2:C:24:LEU:HD11	2:C:27:GLU:CB	2.42	0.45
1:A:408:GLN:HG2	2:C:48:LEU:HD11	1.97	0.45
1:B:365:PRO:HB3	1:B:387:PRO:HB3	1.99	0.45
1:A:250:THR:HG22	1:A:252:GLN:HB2	1.99	0.45
1:B:383:ILE:HG22	1:B:419:LEU:HD11	1.98	0.45
3:E:1:NAG:C6	3:E:3:FUC:C5	2.94	0.45
1:A:74:ARG:HD2	1:A:110:GLU:OE2	2.17	0.45
1:B:156:PHE:CD1	1:B:156:PHE:N	2.85	0.45
1:A:290:ASP:O	1:A:305:CYS:N	2.47	0.45
1:B:36:VAL:HG13	1:B:60:GLU:HG3	1.99	0.45
1:A:117:GLN:NE2	1:A:185:LYS:HD2	2.32	0.45
1:A:271:CYS:SG	1:A:277:VAL:HG22	2.58	0.44
1:A:278:THR:HG22	1:A:279:ASP:N	2.33	0.44
1:A:334:HIS:C	1:A:336:LYS:N	2.69	0.44
1:B:69:LEU:HA	1:B:99:SER:O	2.17	0.44
1:B:170:CYS:SG	1:B:175:CYS:HB3	2.56	0.44
1:B:383:ILE:CG2	1:B:419:LEU:HD11	2.48	0.44
1:B:443:LYS:HA	1:B:443:LYS:HE2	1.99	0.44
1:B:451:ILE:HD11	1:B:491:CYS:O	2.17	0.44
1:A:74:ARG:CG	1:A:110:GLU:HG3	2.42	0.44
1:A:263:PHE:CE2	1:A:272:PRO:HG2	2.53	0.44
1:B:95:LEU:HD23	1:B:124:VAL:HG13	1.99	0.44
1:B:470:ARG:NH2	1:B:478:THR:OG1	2.51	0.44
1:A:352:PHE:CE2	1:A:387:PRO:HG3	2.53	0.44
1:B:263:PHE:CZ	1:B:272:PRO:HG2	2.52	0.44
1:B:331:ASN:O	1:B:332:ILE:C	2.55	0.44
1:A:303:LYS:O	1:A:304:LYS:HB2	2.18	0.43
1:B:144:VAL:CG1	1:B:145:SER:N	2.81	0.43
1:A:216:CYS:HB2	1:A:223:ASP:O	2.19	0.43
1:B:403:ARG:O	1:B:433:SER:HB2	2.18	0.43
6:H:1:NAG:O3	6:H:1:NAG:H82	2.18	0.43
1:A:32:ASN:HD22	3:E:1:NAG:C7	2.31	0.43
1:B:272:PRO:HB2	1:B:275:TYR:CD1	2.52	0.43
1:B:378:THR:O	1:B:403:ARG:HB2	2.18	0.43
1:A:103:ALA:C	1:A:105:LYS:N	2.72	0.43
1:B:325:LEU:HB2	6:H:1:NAG:H81	2.01	0.43
1:B:372:LYS:HD2	1:B:397:GLU:CG	2.48	0.43
2:C:35:HIS:O	2:C:36:SER:C	2.56	0.43
1:A:33:ASN:HD21	3:E:1:NAG:C6	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:THR:CG2	1:A:236:CYS:N	2.82	0.43
1:B:62:ALA:HA	1:B:84:ARG:HB2	2.01	0.43
1:B:392:ASP:HA	1:B:423:SER:O	2.18	0.43
2:C:24:LEU:HD12	2:C:27:GLU:H	1.84	0.43
1:B:16:GLN:OE1	1:B:20:PHE:HE2	2.02	0.43
1:A:149:LEU:HD23	1:A:149:LEU:C	2.39	0.43
1:A:339:THR:HA	1:A:373:THR:O	2.18	0.43
1:B:68:ALA:HA	1:B:100:ASN:OD1	2.18	0.43
1:B:348:LEU:HD22	1:B:384:GLN:NE2	2.34	0.43
2:C:47:ASP:C	2:C:49:LEU:N	2.71	0.43
1:A:221:GLU:H	1:A:221:GLU:HG3	1.66	0.43
1:A:485:LEU:HD12	1:A:485:LEU:N	2.33	0.43
1:A:38:LEU:O	1:A:62:ALA:HB3	2.18	0.42
1:A:161:GLY:O	1:A:163:CYS:N	2.44	0.42
1:B:241:PRO:HA	1:B:242:PRO:HD3	1.86	0.42
2:C:24:LEU:CD1	2:C:27:GLU:HB2	2.44	0.42
1:A:6:VAL:HG12	1:A:7:CYS:N	2.34	0.42
1:A:209:HIS:NE2	1:A:210:ASN:ND2	2.67	0.42
1:B:180:GLU:O	1:B:182:ASN:N	2.52	0.42
1:B:451:ILE:HG12	1:B:492:TRP:CH2	2.55	0.42
1:A:131:ALA:HA	1:A:160:LEU:HB2	2.01	0.42
1:A:161:GLY:C	1:A:163:CYS:N	2.72	0.42
1:A:143:ILE:HD11	11:A:776:HOH:O	2.20	0.42
1:A:448:ALA:O	1:A:451:ILE:HD12	2.20	0.42
1:A:141:ARG:HG2	1:A:141:ARG:O	2.20	0.42
1:B:455:LYS:HD3	1:B:456:LEU:HD23	2.01	0.42
1:B:10:THR:O	1:B:40:ASN:HB2	2.19	0.42
1:B:344:ASP:OD2	1:B:379:GLY:HA3	2.19	0.42
2:C:4:HIS:CE1	2:C:26:GLN:NE2	2.87	0.42
1:A:407:LYS:HD3	1:A:435:GLY:HA2	2.01	0.42
1:B:129:ASN:N	1:B:130:PRO:HD3	2.34	0.42
1:A:269:LYS:O	1:A:270:LYS:HD2	2.20	0.42
1:B:75:ILE:HG13	1:B:108:LEU:HD11	2.00	0.42
1:A:67:ILE:O	1:A:97:VAL:HA	2.20	0.42
1:A:292:TYR:HD2	1:A:292:TYR:H	1.68	0.41
4:F:3:BMA:C3	4:F:4:MAN:H3	2.38	0.41
1:A:408:GLN:HG2	2:C:48:LEU:CD1	2.51	0.41
1:B:496:PRO:O	1:B:499:CYS:SG	2.78	0.41
1:B:335:PHE:HA	1:B:338:CYS:SG	2.61	0.41
2:D:10:ASP:C	2:D:12:HIS:H	2.24	0.41
1:A:138:ILE:HD13	1:A:138:ILE:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ILE:HD12	1:A:401:ILE:N	2.36	0.41
1:B:427:ARG:HD3	1:B:498:ASP:OD1	2.21	0.41
1:A:454:LYS:HA	1:A:457:PHE:CD2	2.56	0.41
1:B:155:ASP:C	1:B:156:PHE:CG	2.93	0.41
1:B:332:ILE:HD13	1:B:332:ILE:HA	1.95	0.41
1:A:74:ARG:NH2	1:A:112:PRO:HG3	2.35	0.41
1:B:48:ARG:HA	1:B:72:VAL:HA	2.02	0.41
1:B:134:ASN:O	1:B:135:VAL:C	2.59	0.41
2:D:8:CYS:HA	2:D:9:PRO:HD3	1.78	0.41
1:A:209:HIS:CD2	1:A:210:ASN:ND2	2.89	0.41
1:A:335:PHE:HA	1:A:338:CYS:SG	2.61	0.41
1:A:348:LEU:HB2	1:A:350:VAL:HG12	2.03	0.41
1:B:128:ASN:N	1:B:128:ASN:ND2	2.68	0.41
1:B:500:VAL:CG2	1:B:501:SER:N	2.83	0.41
1:A:193:GLN:C	1:A:195:CYS:H	2.24	0.41
1:A:200:ARG:HB2	1:A:206:ASP:HB3	2.02	0.41
1:B:19:THR:O	1:B:22:ASP:N	2.54	0.41
1:B:82:ILE:HG12	1:B:83:ILE:N	2.34	0.41
2:C:48:LEU:C	2:C:50:ALA:H	2.24	0.41
1:B:276:VAL:HG11	1:B:302:CYS:SG	2.61	0.41
1:A:336:LYS:CG	1:A:337:ASN:N	2.83	0.40
1:B:19:THR:O	1:B:20:PHE:C	2.58	0.40
1:B:451:ILE:HG12	1:B:492:TRP:CZ2	2.56	0.40
1:A:73:GLU:HG3	1:A:109:LYS:HE3	2.02	0.40
1:A:221:GLU:C	1:A:223:ASP:H	2.24	0.40
1:A:356:SER:CB	2:C:13:THR:OG1	2.69	0.40
1:A:483:HIS:HD2	1:A:485:LEU:HD13	1.83	0.40
1:B:438:ILE:HG13	1:B:465:LYS:HB3	2.02	0.40
1:B:488:PRO:CB	1:B:501:SER:HB2	2.51	0.40
1:B:45:TYR:HA	1:B:69:LEU:O	2.22	0.40
1:B:145:SER:HB3	1:B:148:PHE:CD1	2.55	0.40

All (5) 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:180:GLU:OE1	8:A:730:CD:CD[1_554]	1.40	0.80
1:A:21:GLU:CD	1:B:474:SER:OG[2_546]	1.55	0.65
1:A:21:GLU:OE1	1:B:474:SER:OG[2_546]	1.75	0.45
1:A:49:ASN:O	1:B:477:ALA:O[2_546]	2.03	0.17
1:A:21:GLU:OE2	1:B:474:SER:OG[2_546]	2.10	0.10

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	495/501 (99%)	417 (84%)	66 (13%)	12 (2%)	6	9
1	B	499/501 (100%)	420 (84%)	62 (12%)	17 (3%)	3	5
2	C	47/50 (94%)	38 (81%)	8 (17%)	1 (2%)	7	11
2	D	46/50 (92%)	32 (70%)	7 (15%)	7 (15%)	0	0
All	All	1087/1102 (99%)	907 (83%)	143 (13%)	37 (3%)	3	5

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	4	LYS
1	A	104	ASN
1	A	488	PRO
1	B	166	CYS
1	B	193	GLN
1	B	332	ILE
1	B	488	PRO
2	D	9	PRO
2	D	10	ASP
2	D	14	GLN
1	A	336	LYS
1	B	102	ASP
1	B	135	VAL
1	B	155	ASP
1	B	181	GLU
2	D	26	GLN
1	A	8	GLN
1	A	32	ASN
1	A	233	GLU
1	A	357	PHE
1	B	134	ASN

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Mol	Chain	Res	Type
1	B	198	ARG
2	C	7	ASP
2	D	11	SER
1	A	162	SER
1	A	194	GLN
1	A	304	LYS
1	B	32	ASN
1	B	130	PRO
1	B	220	ARG
1	B	487	SER
2	D	49	LEU
1	B	116	LEU
2	D	27	GLU
1	B	219	PRO
1	B	76	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/440 (97%)	409 (96%)	17 (4%)	31	56
1	B	429/440 (98%)	414 (96%)	15 (4%)	36	62
2	C	40/43 (93%)	38 (95%)	2 (5%)	24	46
2	D	38/43 (88%)	33 (87%)	5 (13%)	4	7
All	All	933/966 (97%)	894 (96%)	39 (4%)	30	54

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	156	PHE
1	A	160	LEU
1	A	172	ASN
1	A	181	GLU
1	A	206	ASP

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Mol	Chain	Res	Type
1	A	210	ASN
1	A	292	TYR
1	A	309	CYS
1	A	321	PHE
1	A	336	LYS
1	A	340	SER
1	A	344	ASP
1	A	358	THR
1	A	391	THR
1	A	406	THR
1	A	497	ARG
1	B	87	MET
1	B	104	ASN
1	B	154	MET
1	B	155	ASP
1	B	156	PHE
1	B	158	ASN
1	B	194	GLN
1	B	206	ASP
1	B	274	ASN
1	B	311	LYS
1	B	318	ILE
1	B	455	LYS
1	B	478	THR
1	B	488	PRO
1	B	497	ARG
2	C	5	PHE
2	C	6	ASN
2	D	4	HIS
2	D	5	PHE
2	D	22	ARG
2	D	26	GLN
2	D	29	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	86	ASN
1	A	91	ASN
1	A	115	ASN
1	A	117	GLN

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Mol	Chain	Res	Type
1	A	151	ASN
1	A	164	GLN
1	A	210	ASN
1	A	211	GLN
1	A	334	HIS
1	A	346	HIS
1	A	394	HIS
1	A	452	ASN
1	A	483	HIS
1	B	33	ASN
1	B	49	ASN
1	B	104	ASN
1	B	117	GLN
1	B	134	ASN
1	B	151	ASN
1	B	158	ASN
1	B	193	GLN
1	B	210	ASN
1	B	331	ASN
1	B	389	ASN
1	B	452	ASN
1	B	480	GLN
2	C	6	ASN
2	C	26	GLN
2	D	35	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

13 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
3	NAG	E	1	3,1	14,14,15	0.68	0	17,19,21	0.88	0
3	NAG	E	2	3	14,14,15	0.47	0	17,19,21	0.66	0
3	FUC	E	3	3	10,10,11	0.55	0	14,14,16	0.60	0
4	NAG	F	1	1,4	14,14,15	0.54	0	17,19,21	0.67	0
4	NAG	F	2	4	14,14,15	0.59	0	17,19,21	0.68	0
4	BMA	F	3	4	11,11,12	0.68	0	15,15,17	0.44	0
4	MAN	F	4	4	11,11,12	0.56	0	15,15,17	0.87	1 (6%)
5	NAG	G	1	1,5	14,14,15	0.53	0	17,19,21	0.83	1 (5%)
5	NAG	G	2	5	14,14,15	0.62	0	17,19,21	0.64	0
5	BMA	G	3	5	11,11,12	0.51	0	15,15,17	0.25	0
5	FUC	G	4	5	10,10,11	0.48	0	14,14,16	0.42	0
6	NAG	H	1	6,1	14,14,15	0.68	0	17,19,21	0.64	0
6	NAG	H	2	6	14,14,15	0.50	0	17,19,21	0.75	1 (5%)

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	E	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	FUC	E	3	3	-	-	0/1/1/1
4	NAG	F	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	F	2	4	-	3/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
4	MAN	F	4	4	-	2/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	4/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	FUC	G	4	5	-	-	0/1/1/1
6	NAG	H	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	4	MAN	C1-O5-C5	2.80	115.98	112.19
5	G	1	NAG	C2-N2-C7	-2.41	119.47	122.90
6	H	2	NAG	C2-N2-C7	-2.23	119.73	122.90

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
6	H	1	NAG	C8-C7-N2-C2
6	H	1	NAG	O7-C7-N2-C2
5	G	2	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
4	F	4	MAN	C4-C5-C6-O6
4	F	4	MAN	O5-C5-C6-O6
4	F	2	NAG	C8-C7-N2-C2
6	H	2	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
6	H	2	NAG	C8-C7-N2-C2
4	F	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	F	3	BMA	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
6	H	2	NAG	O7-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2

There are no ring outliers.

7 monomers are involved in 17 short contacts:

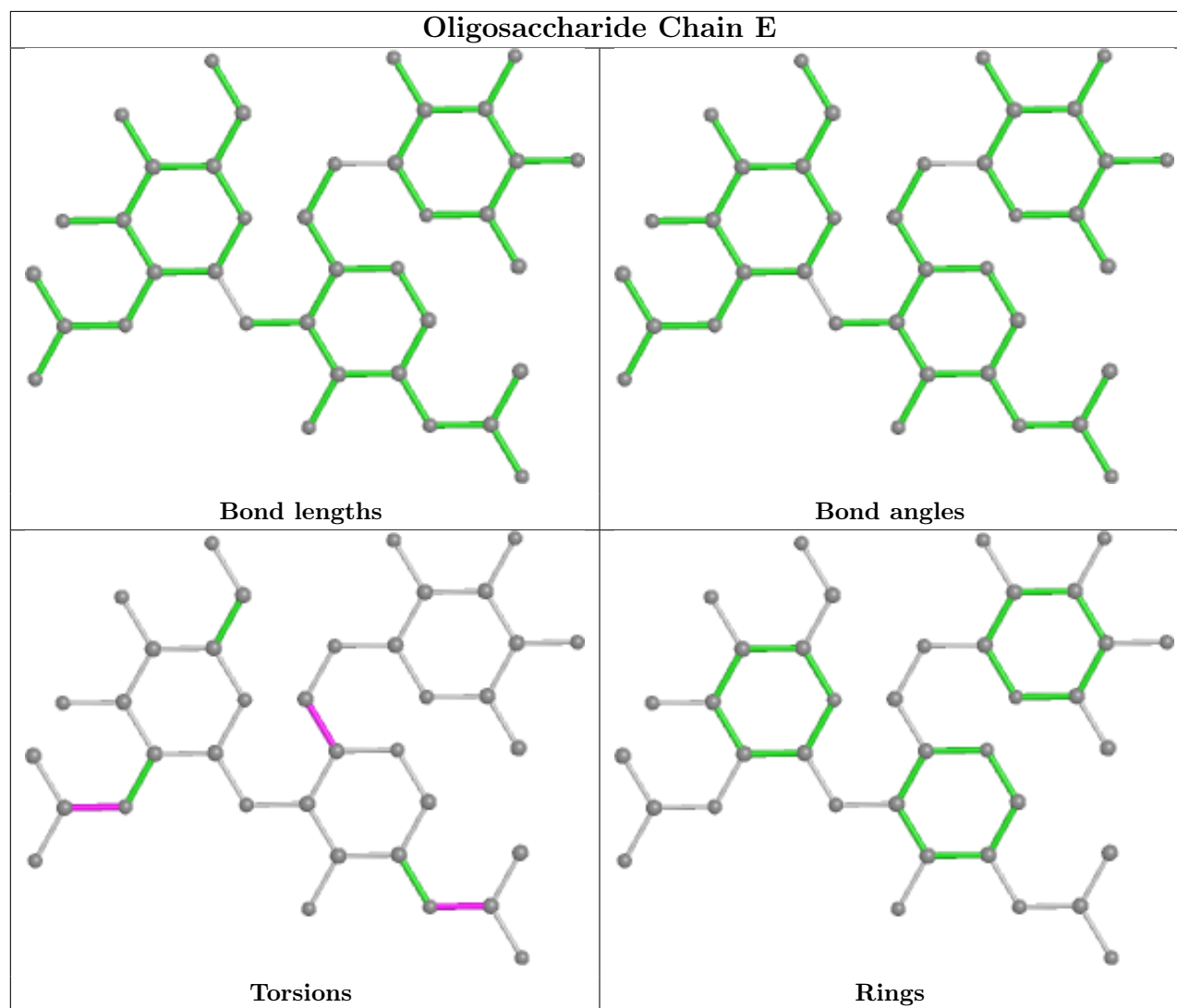
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	3	BMA	3	0

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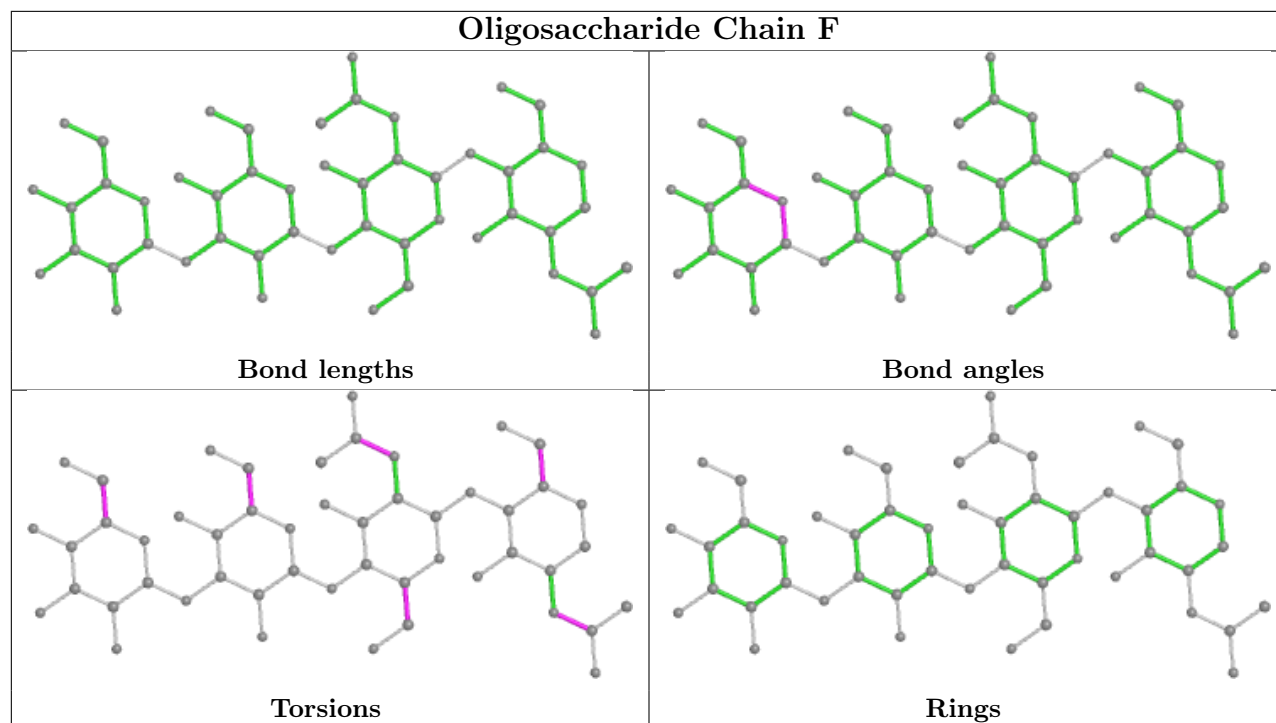
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	2	NAG	1	0
4	F	4	MAN	3	0
3	E	3	FUC	5	0
4	F	1	NAG	1	0
3	E	1	NAG	8	0
6	H	1	NAG	4	0

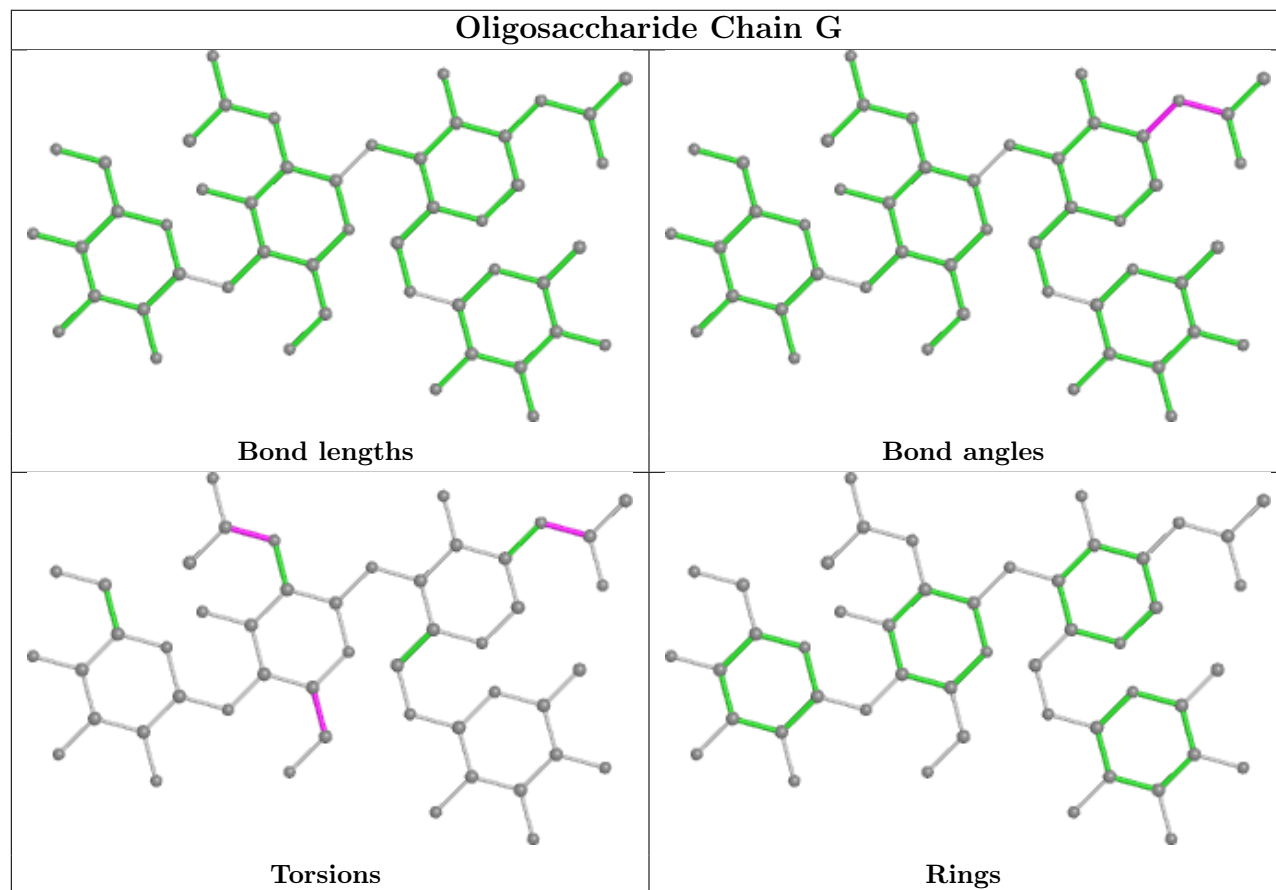
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

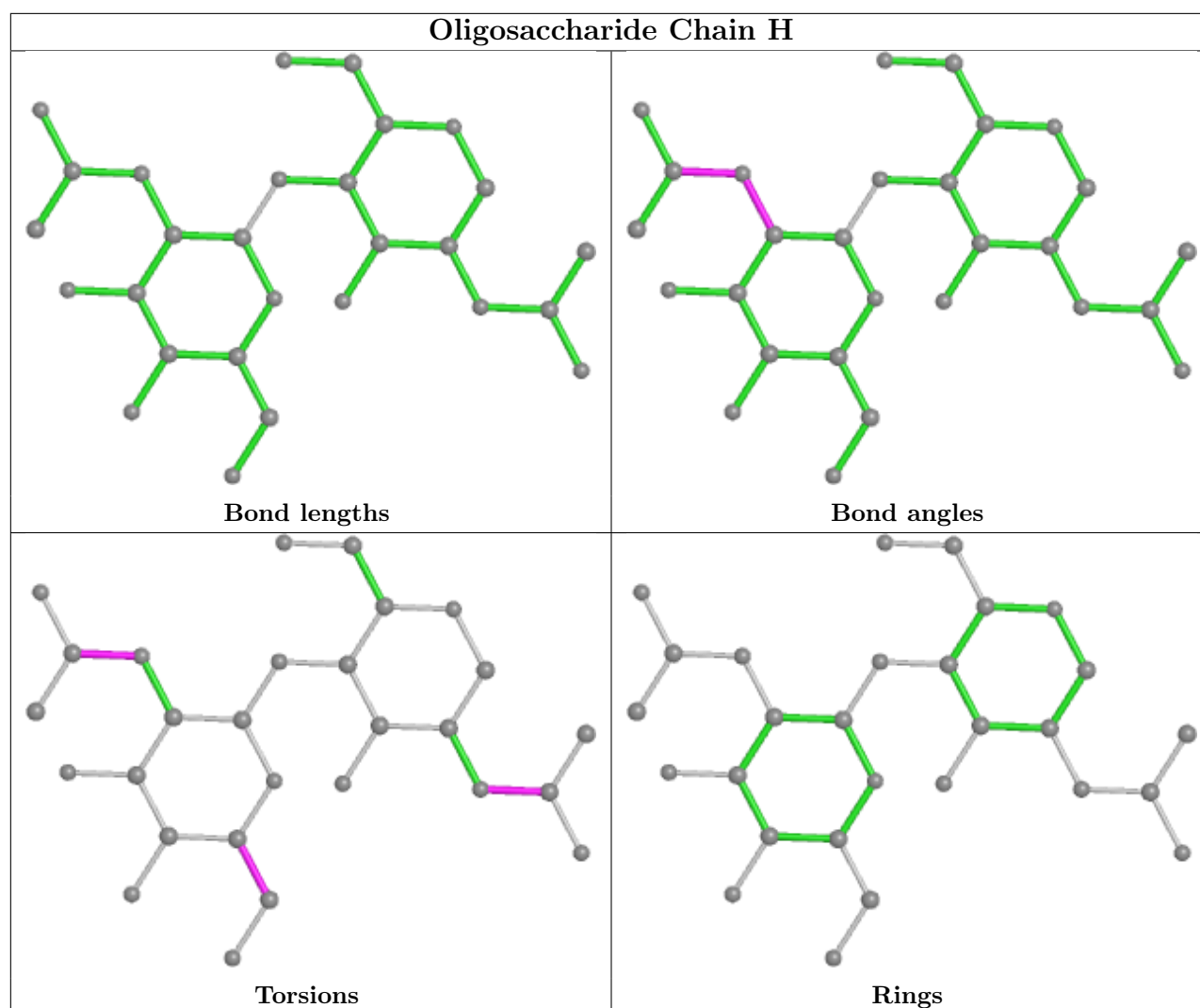


Oligosaccharide Chain F



Oligosaccharide Chain G





5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 22 are monoatomic - leaving 1 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	$\# Z > 2$
10	NAG	B	630	1	14,14,15	0.53	0	17,19,21	0.63	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	B	630	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	630	NAG	C8-C7-N2-C2
10	B	630	NAG	O7-C7-N2-C2
10	B	630	NAG	C4-C5-C6-O6
10	B	630	NAG	O5-C5-C6-O6

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.