



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:45 AM UTC

PDB ID : 1SZ0 / pdb_00001sz0
Title : N-terminal 3 domains of CI-MPR bound to mannose 6-phosphate
Authors : Olson, L.J.; Dahms, N.M.; Kim, J.-J.P.
Deposited on : 2004-04-01
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

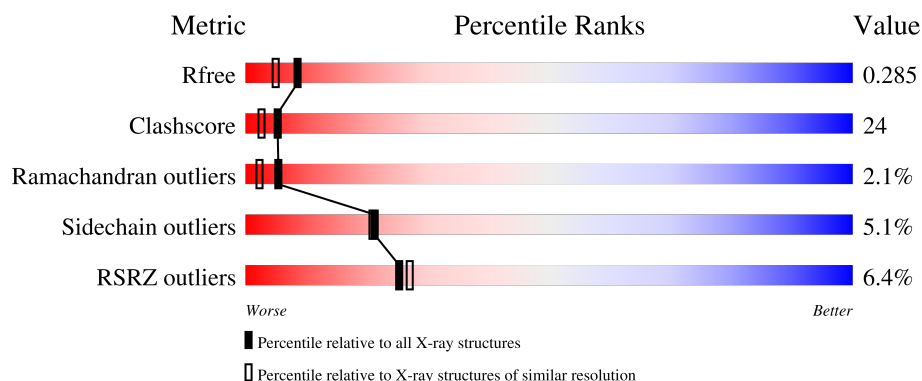
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	432	7% 56% 35% 5% .
1	B	432	5% 57% 34% . . .
2	C	2	50% 50%
3	D	2	50% 50%
3	E	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	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6811 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 cation-independent mannose 6-phosphate receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3218	2011	546	633	28			
1	B	416	Total	C	N	O	S	0	0	0
			3219	2014	548	629	28			

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



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

- Molecule 3 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
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

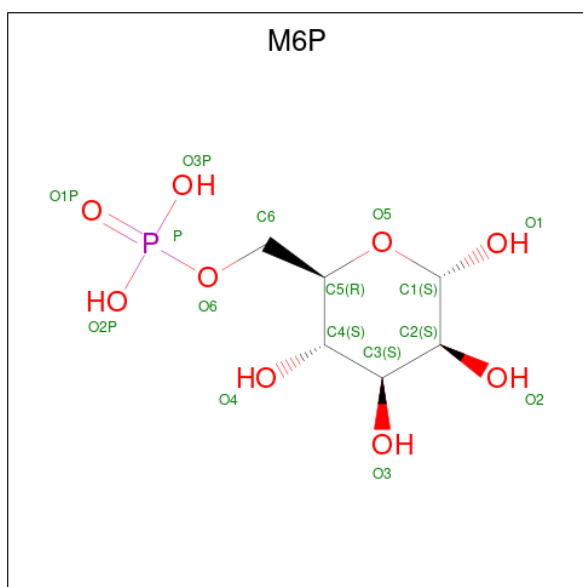


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is OSMIUM ION (CCD ID: OS) (formula: Os).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Os	0	0
			1	1		
5	B	1	Total	Os	0	0
			1	1		

- Molecule 6 is 6-O-phosphono-alpha-D-mannopyranose (CCD ID: M6P) (formula: C₆H₁₃O₉P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	P	0	0
			16	6	9	1		
6	B	1	Total	C	O	P	0	0
			16	6	9	1		

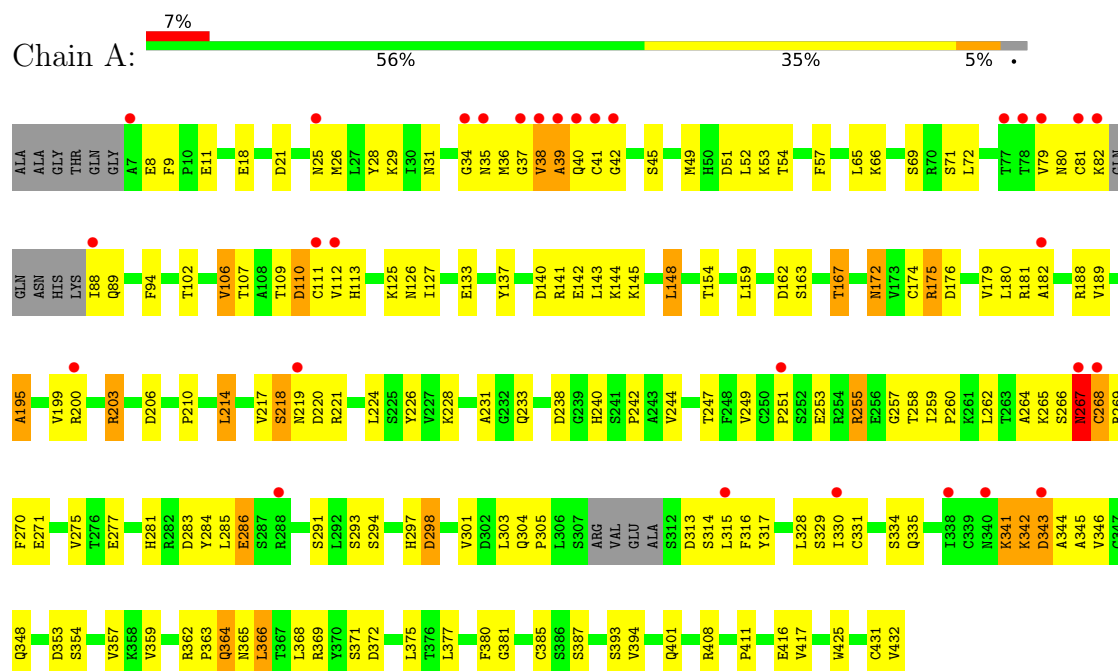
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	98	Total	O	0	0
			98	98		
7	B	144	Total	O	0	0
			144	144		

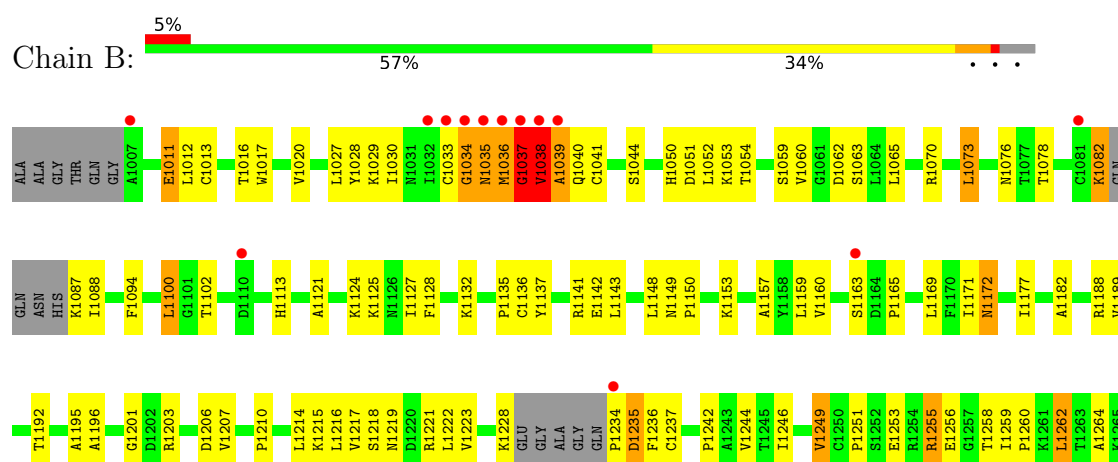
3 Residue-property plots [i](#)

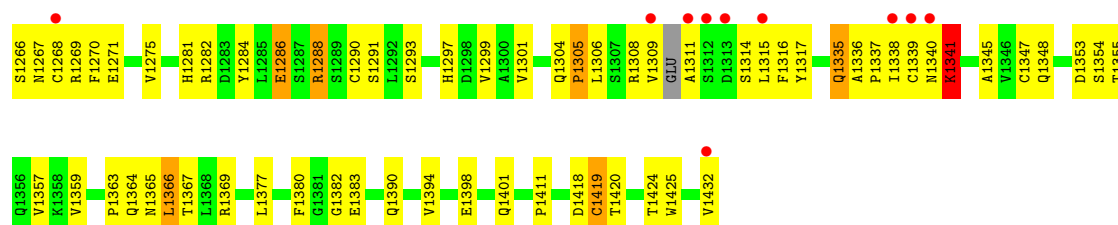
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: cation-independent mannose 6-phosphate receptor



- Molecule 1: cation-independent mannose 6-phosphate receptor





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

Chain C:  50%



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

Chain D:  50%



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

Chain E:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.10Å 86.50Å 84.80Å 90.00° 109.57° 90.00°	Depositor
Resolution (Å)	28.80 – 2.10 28.80 – 2.10	Depositor EDS
% Data completeness (in resolution range)	88.8 (28.80-2.10) 88.8 (28.80-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.287 0.236 , 0.285	Depositor DCC
R_{free} test set	2993 reflections (6.44%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6811	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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: OS, NAG, M6P, NDG

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	0.46	0/3283	0.99	21/4450 (0.5%)
1	B	0.54	4/3283 (0.1%)	1.05	20/4447 (0.4%)
All	All	0.50	4/6566 (0.1%)	1.02	41/8897 (0.5%)

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	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1036	MET	N-CA	-9.33	1.35	1.46
1	B	1036	MET	CA-C	-8.40	1.42	1.53
1	B	1038	VAL	CA-CB	-7.55	1.44	1.54
1	B	1038	VAL	N-CA	-6.06	1.38	1.46

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1036	MET	N-CA-C	11.82	128.23	109.79
1	B	1036	MET	O-C-N	11.77	137.16	121.74
1	B	1038	VAL	N-CA-CB	10.34	128.29	111.23
1	B	1038	VAL	N-CA-C	-9.25	90.10	109.34
1	B	1013	CYS	N-CA-C	7.93	122.22	112.54
1	A	343	ASP	N-CA-CB	7.91	123.64	110.59
1	B	1035	ASN	N-CA-C	-7.84	103.17	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1036	MET	CA-C-O	7.78	131.48	121.67
1	B	1036	MET	CA-C-N	7.22	135.56	121.41
1	B	1036	MET	C-N-CA	7.22	135.56	121.41
1	B	1286	GLU	N-CA-C	7.07	120.48	109.52
1	B	1282	ARG	N-CA-C	6.77	118.66	111.28
1	B	1037	GLY	O-C-N	6.34	130.95	122.70
1	A	345	ALA	N-CA-C	-6.31	104.63	112.90
1	A	203	ARG	CA-C-N	-6.25	113.56	122.94
1	A	203	ARG	C-N-CA	-6.25	113.56	122.94
1	B	1345	ALA	N-CA-C	-6.19	104.08	111.69
1	A	267	ASN	N-CA-C	6.17	119.87	111.17
1	B	1420	THR	N-CA-C	-6.16	98.37	108.41
1	A	9	PHE	CA-C-N	5.96	126.11	119.32
1	A	9	PHE	C-N-CA	5.96	126.11	119.32
1	A	218	SER	N-CA-C	-5.92	101.52	110.28
1	A	267	ASN	CA-C-O	-5.91	115.42	122.27
1	A	238	ASP	N-CA-C	5.78	118.24	111.02
1	A	286	GLU	N-CA-C	5.76	117.94	109.24
1	A	385	CYS	N-CA-C	-5.73	101.98	110.46
1	B	1030	ILE	N-CA-C	5.72	116.12	108.11
1	A	167	THR	N-CA-C	5.67	118.47	109.50
1	B	1172	ASN	N-CA-C	-5.60	101.24	109.81
1	A	267	ASN	CA-C-N	-5.58	114.29	123.05
1	A	267	ASN	C-N-CA	-5.58	114.29	123.05
1	A	42	GLY	CA-C-N	5.35	124.86	119.19
1	A	42	GLY	C-N-CA	5.35	124.86	119.19
1	A	203	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	B	1038	VAL	CA-CB-CG1	-5.26	101.46	110.40
1	A	195	ALA	N-CA-C	-5.16	107.15	113.50
1	A	154	THR	N-CA-C	-5.16	106.99	113.28
1	B	1419	CYS	N-CA-C	5.15	119.51	113.23
1	B	1078	THR	N-CA-C	-5.13	106.71	113.17
1	B	1249	VAL	N-CA-C	5.03	115.15	108.11
1	A	172	ASN	N-CA-C	-5.02	101.74	109.52

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1037	GLY	Mainchain

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	3218	0	3084	167	0
1	B	3219	0	3098	133	0
2	C	28	0	24	3	0
3	D	28	0	25	5	0
3	E	28	0	25	13	0
4	A	14	0	13	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	16	0	11	1	0
6	B	16	0	11	1	0
7	A	98	0	0	2	0
7	B	144	0	0	6	0
All	All	6811	0	6291	313	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (313) 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:267:ASN:HD21	1:A:269:ARG:CG	1.73	1.00
1:A:217:VAL:HG23	1:A:218:SER:H	1.24	0.99
3:D:1:NAG:H5	3:D:2:NAG:H2	1.42	0.97
1:A:342:LYS:NZ	1:A:362:ARG:HH22	1.60	0.97
1:B:1365:ASN:HD21	3:E:1:NAG:C7	1.78	0.97
1:A:221:ARG:HH11	1:A:247:THR:HG21	1.31	0.95
1:B:1365:ASN:HD21	3:E:1:NAG:C2	1.80	0.94
1:A:342:LYS:HZ3	1:A:362:ARG:HH22	1.02	0.94
1:B:1020:VAL:HG12	1:B:1027:LEU:HD13	1.52	0.92
1:A:266:SER:O	1:A:267:ASN:ND2	2.03	0.92
1:A:267:ASN:HD21	1:A:269:ARG:HG3	1.36	0.91
1:A:106:VAL:HG23	1:A:107:THR:HG22	1.52	0.90
1:B:1218:SER:HB3	1:B:1221:ARG:HB2	1.54	0.90
1:B:1365:ASN:ND2	3:E:1:NAG:N2	2.19	0.89
1:B:1299:VAL:HG23	1:B:1432:VAL:HG13	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1207:VAL:HG23	1:B:1242:PRO:HB3	1.57	0.85
1:A:40:GLN:HB3	1:A:57:PHE:HB2	1.61	0.83
1:B:1011:GLU:HG3	7:B:1690:HOH:O	1.78	0.82
1:A:267:ASN:ND2	1:A:269:ARG:CG	2.42	0.82
3:D:1:NAG:H5	3:D:2:NAG:C2	2.10	0.81
1:A:221:ARG:HH11	1:A:247:THR:CG2	1.94	0.79
1:B:1125:LYS:HE3	7:B:1605:HOH:O	1.82	0.79
1:B:1038:VAL:O	1:B:1040:GLN:N	2.17	0.78
1:A:267:ASN:C	1:A:267:ASN:HD22	1.92	0.78
1:A:148:LEU:HD22	1:A:214:LEU:HD11	1.66	0.77
1:A:25:ASN:ND2	1:A:52:LEU:HB2	1.98	0.77
1:A:364:GLN:NE2	1:A:364:GLN:H	1.82	0.77
1:A:285:LEU:HD22	1:A:371:SER:HB2	1.68	0.74
1:A:328:LEU:HD22	1:A:346:VAL:HG22	1.68	0.74
1:A:293:SER:H	1:A:297:HIS:HD2	1.33	0.74
1:A:25:ASN:HD21	1:A:52:LEU:HB2	1.50	0.74
1:B:1308:ARG:HA	1:B:1315:LEU:HD22	1.68	0.74
2:C:1:NDG:H4	2:C:2:NAG:N2	2.03	0.73
1:A:88:ILE:HG12	1:A:111:CYS:HB3	1.71	0.73
1:B:1053:LYS:HE3	1:B:1054:THR:HG23	1.69	0.73
3:D:1:NAG:H3	3:D:2:NAG:O5	1.89	0.73
1:B:1195:ALA:HB2	1:B:1210:PRO:HD3	1.70	0.73
1:B:1365:ASN:ND2	3:E:1:NAG:C2	2.48	0.72
1:A:304:GLN:N	1:A:305:PRO:HD2	2.04	0.72
1:B:1365:ASN:ND2	3:E:1:NAG:C7	2.51	0.72
1:B:1163:SER:O	1:B:1165:PRO:HD3	1.90	0.72
1:B:1214:LEU:HD11	1:B:1222:LEU:HD22	1.72	0.71
1:B:1335:GLN:CD	1:B:1336:ALA:H	1.97	0.71
1:B:1363:PRO:HG2	1:B:1364:GLN:NE2	2.05	0.71
1:A:88:ILE:HA	1:A:111:CYS:O	1.91	0.71
1:A:264:ALA:HB3	1:A:271:GLU:HB2	1.70	0.71
3:E:1:NAG:H61	3:E:2:NAG:H82	1.73	0.70
1:A:195:ALA:HB2	1:A:210:PRO:HD3	1.72	0.70
1:A:175:ARG:HG2	1:A:176:ASP:N	2.07	0.69
1:B:1038:VAL:C	1:B:1040:GLN:H	2.00	0.69
1:A:365:ASN:HD22	1:A:381:GLY:HA3	1.58	0.69
1:A:411:PRO:HG3	1:A:425:TRP:CZ3	2.28	0.69
1:B:1127:ILE:HG23	1:B:1128:PHE:HD1	1.58	0.69
1:A:259:ILE:HG23	1:A:260:PRO:HD2	1.73	0.68
1:A:411:PRO:HG3	1:A:425:TRP:CE3	2.28	0.68
1:B:1020:VAL:HG12	1:B:1027:LEU:CD1	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1038:VAL:C	1:B:1040:GLN:N	2.50	0.68
1:B:1207:VAL:HG21	1:B:1270:PHE:CE1	2.28	0.68
1:B:1251:PRO:HG3	1:B:1255:ARG:HD2	1.76	0.68
1:A:35:ASN:HB2	7:A:701:HOH:O	1.93	0.67
1:A:26:MET:HE3	1:A:49:MET:SD	2.35	0.67
1:B:1206:ASP:OD1	1:B:1228:LYS:HD3	1.95	0.67
1:B:1242:PRO:HA	1:B:1268:CYS:O	1.94	0.67
1:B:1293:SER:H	1:B:1297:HIS:HD2	1.42	0.66
1:A:8:GLU:HG3	1:A:66:LYS:NZ	2.11	0.66
1:A:341:LYS:HE3	1:A:342:LYS:HB2	1.77	0.66
1:B:1366:LEU:HG	1:B:1377:LEU:HD11	1.78	0.65
1:A:221:ARG:NH1	1:A:247:THR:HG21	2.08	0.64
1:A:342:LYS:HZ3	1:A:362:ARG:NH2	1.86	0.64
1:A:343:ASP:C	1:A:343:ASP:OD1	2.42	0.63
1:A:267:ASN:ND2	1:A:269:ARG:HG2	2.13	0.63
1:B:1259:ILE:HG23	1:B:1260:PRO:HD2	1.81	0.63
1:B:1286:GLU:OE1	1:B:1369:ARG:HD3	1.99	0.63
1:A:218:SER:HB3	1:A:221:ARG:CB	2.29	0.63
1:A:267:ASN:ND2	1:A:267:ASN:O	2.31	0.63
1:A:36:MET:SD	1:A:38:VAL:HG22	2.39	0.63
1:B:1365:ASN:HD21	3:E:1:NAG:H2	1.65	0.62
1:B:1337:PRO:HA	1:B:1340:ASN:CG	2.25	0.61
1:B:1033:CYS:O	1:B:1035:ASN:N	2.34	0.61
1:A:218:SER:HB3	1:A:221:ARG:HB3	1.81	0.61
1:B:1341:LYS:HD3	1:B:1341:LYS:N	2.16	0.61
1:A:218:SER:C	1:A:220:ASP:H	2.09	0.60
1:A:217:VAL:HG23	1:A:218:SER:N	2.03	0.60
1:A:21:ASP:HB3	1:A:26:MET:HB2	1.83	0.60
1:B:1264:ALA:HB3	1:B:1271:GLU:HB2	1.83	0.59
1:A:267:ASN:HD21	1:A:269:ARG:CB	2.15	0.59
1:B:1365:ASN:ND2	3:E:1:NAG:O7	2.35	0.59
1:B:1207:VAL:HG22	1:B:1207:VAL:O	2.02	0.59
1:B:1359:VAL:HB	1:B:1383:GLU:HG3	1.85	0.59
1:A:38:VAL:HG23	1:A:38:VAL:O	2.01	0.59
1:B:1182:ALA:HB3	1:B:1188:ARG:HG3	1.84	0.59
1:B:1366:LEU:C	1:B:1366:LEU:HD23	2.27	0.59
1:B:1012:LEU:HD21	1:B:1100:LEU:HD22	1.83	0.59
1:B:1037:GLY:HA2	1:B:1039:ALA:H	1.68	0.59
3:D:2:NAG:O3	3:D:2:NAG:H83	2.03	0.59
1:B:1214:LEU:HD11	1:B:1222:LEU:HB3	1.84	0.58
1:B:1288:ARG:HH21	1:B:1288:ARG:HB3	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:LEU:HD12	1:A:366:LEU:C	2.28	0.58
1:B:1157:ALA:HB1	1:B:1171:ILE:O	2.03	0.58
1:A:365:ASN:HB3	1:A:380:PHE:CD1	2.38	0.58
1:B:1127:ILE:HG23	1:B:1128:PHE:CD1	2.39	0.57
1:A:233:GLN:NE2	1:A:240:HIS:O	2.36	0.57
1:A:341:LYS:H	1:A:341:LYS:HD3	1.68	0.57
1:A:343:ASP:OD1	1:A:363:PRO:CD	2.53	0.57
1:B:1217:VAL:HG23	1:B:1218:SER:H	1.68	0.57
1:B:1051:ASP:OD1	1:B:1053:LYS:HB3	2.05	0.56
1:A:69:SER:OG	1:A:72:LEU:HB3	2.06	0.56
1:B:1309:VAL:HG22	1:B:1317:TYR:CE1	2.41	0.56
1:A:8:GLU:HG3	1:A:66:LYS:HZ1	1.69	0.56
1:A:329:SER:CB	1:A:335:GLN:HE21	2.19	0.56
1:B:1217:VAL:HG23	1:B:1218:SER:N	2.20	0.56
1:A:218:SER:O	1:A:220:ASP:N	2.38	0.56
1:B:1256:GLU:HG2	7:B:1709:HOH:O	2.06	0.56
1:A:125:LYS:C	1:A:127:ILE:H	2.14	0.56
1:B:1304:GLN:C	1:B:1306:LEU:H	2.14	0.56
1:A:31:ASN:ND2	1:A:35:ASN:N	2.54	0.56
1:A:133:GLU:HG3	1:A:175:ARG:HB2	1.87	0.56
1:A:249:VAL:CG2	1:A:275:VAL:HG22	2.36	0.56
1:B:1141:ARG:HH21	1:B:1219:ASN:ND2	2.05	0.55
1:A:416:GLU:HG2	1:A:417:VAL:N	2.22	0.55
1:A:257:GLY:HA3	1:A:372:ASP:HB3	1.87	0.55
1:A:344:ALA:HB2	1:A:359:VAL:HG13	1.88	0.55
1:B:1028:TYR:OH	1:B:1113:HIS:HD2	1.89	0.55
1:A:218:SER:C	1:A:220:ASP:N	2.65	0.54
1:B:1338:ILE:HG23	1:B:1339:CYS:SG	2.46	0.54
1:B:1016:THR:CG2	1:B:1029:LYS:HG3	2.38	0.54
1:A:71:SER:HB3	1:A:94:PHE:O	2.08	0.54
1:A:109:THR:OG1	1:A:112:VAL:HB	2.07	0.54
1:B:1359:VAL:HG23	1:B:1383:GLU:OE2	2.08	0.54
1:A:28:TYR:OH	1:A:113:HIS:HD2	1.91	0.54
1:A:79:VAL:HG12	1:A:80:ASN:N	2.22	0.54
1:A:253:GLU:O	1:A:255:ARG:HG3	2.08	0.54
1:B:1337:PRO:HA	1:B:1340:ASN:OD1	2.07	0.54
1:A:140:ASP:OD2	1:A:144:LYS:HB2	2.09	0.53
1:A:217:VAL:HG23	1:A:221:ARG:HB3	1.91	0.53
1:A:316:PHE:HB3	1:A:334:SER:O	2.08	0.53
1:B:1259:ILE:N	1:B:1259:ILE:HD12	2.23	0.53
1:B:1304:GLN:N	1:B:1305:PRO:HD2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1:NDG:H4	2:C:2:NAG:HN2	1.73	0.53
1:A:255:ARG:HH21	1:A:258:THR:HG23	1.73	0.53
1:B:1364:GLN:H	1:B:1364:GLN:CD	2.17	0.53
1:A:343:ASP:OD1	1:A:363:PRO:HD2	2.08	0.53
1:A:162:ASP:O	1:A:163:SER:HB2	2.08	0.53
1:A:174:CYS:H	1:A:224:LEU:HD21	1.74	0.53
1:B:1172:ASN:HB2	1:B:1177:ILE:HG12	1.92	0.52
1:A:255:ARG:NH2	1:A:258:THR:OG1	2.42	0.52
1:B:1012:LEU:CD2	1:B:1100:LEU:HD22	2.40	0.52
1:B:1214:LEU:HD13	1:B:1215:LYS:N	2.24	0.52
1:B:1215:LYS:HE3	1:B:1223:VAL:HG23	1.92	0.52
3:D:1:NAG:H61	3:D:2:NAG:O7	2.09	0.52
3:E:1:NAG:C6	3:E:2:NAG:H82	2.40	0.52
1:B:1266:SER:O	1:B:1269:ARG:HB3	2.09	0.52
1:A:281:HIS:CE1	1:A:284:TYR:HB2	2.45	0.52
1:A:408:ARG:HB3	1:A:408:ARG:HH11	1.76	0.51
1:A:11:GLU:H	1:A:11:GLU:CD	2.17	0.51
1:B:1338:ILE:O	1:B:1341:LYS:HE2	2.11	0.51
1:A:51:ASP:OD1	1:A:53:LYS:HG2	2.10	0.51
1:A:179:VAL:HG23	1:A:180:LEU:N	2.25	0.51
1:A:341:LYS:HD3	1:A:341:LYS:N	2.25	0.51
1:B:1234:PRO:HB2	1:B:1237:CYS:SG	2.51	0.51
3:E:1:NAG:H5	3:E:2:NAG:H82	1.92	0.51
1:B:1038:VAL:O	1:B:1039:ALA:C	2.54	0.51
1:A:304:GLN:N	1:A:305:PRO:CD	2.73	0.51
1:B:1262:LEU:HD23	1:B:1271:GLU:O	2.11	0.51
1:B:1365:ASN:ND2	3:E:1:NAG:H2	2.22	0.51
1:A:36:MET:SD	1:A:38:VAL:CG2	3.00	0.50
1:B:1070:ARG:NH2	1:B:1124:LYS:HE3	2.26	0.50
1:A:145:LYS:O	1:A:281:HIS:HA	2.12	0.50
1:A:267:ASN:ND2	1:A:269:ARG:HG3	2.12	0.50
1:B:1102:THR:HG22	1:B:1137:TYR:CD2	2.46	0.50
1:A:40:GLN:HB3	1:A:57:PHE:CB	2.39	0.50
1:A:39:ALA:O	1:A:40:GLN:HB2	2.12	0.50
1:A:89:GLN:HG2	1:A:112:VAL:HG22	1.94	0.50
1:A:199:VAL:HA	1:A:203:ARG:O	2.11	0.50
1:A:366:LEU:HD13	1:A:377:LEU:HD11	1.93	0.50
1:B:1380:PHE:HB2	7:B:1651:HOH:O	2.10	0.50
1:A:365:ASN:ND2	1:A:381:GLY:HA3	2.27	0.49
1:B:1311:ALA:N	1:B:1315:LEU:HD21	2.27	0.49
1:B:1041:CYS:HB3	1:B:1059:SER:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLU:OE2	1:A:29:LYS:HE2	2.11	0.49
1:A:365:ASN:HB3	1:A:380:PHE:CE1	2.47	0.49
1:A:342:LYS:NZ	1:A:362:ARG:NH2	2.44	0.49
1:A:65:LEU:HD12	1:A:65:LEU:N	2.27	0.49
1:A:329:SER:HB3	1:A:335:GLN:HE21	1.78	0.49
1:B:1132:LYS:CG	1:B:1210:PRO:HG2	2.43	0.49
1:B:1262:LEU:HD22	1:B:1264:ALA:H	1.78	0.48
1:B:1142:GLU:O	1:B:1143:LEU:HB2	2.13	0.48
1:B:1288:ARG:HB3	1:B:1288:ARG:NH2	2.28	0.48
1:A:82:LYS:HD2	1:A:82:LYS:C	2.39	0.48
1:A:266:SER:C	1:A:267:ASN:ND2	2.72	0.48
1:B:1291:SER:HB2	1:B:1301:VAL:O	2.14	0.48
1:A:189:VAL:HG12	1:A:189:VAL:O	2.14	0.48
1:A:109:THR:O	1:A:111:CYS:N	2.45	0.48
1:A:364:GLN:H	1:A:364:GLN:HE21	1.58	0.48
1:B:1020:VAL:CG1	1:B:1027:LEU:HD13	2.34	0.48
1:B:1065:LEU:HD12	1:B:1065:LEU:N	2.28	0.48
1:B:1034:GLY:HA3	1:B:1063:SER:OG	2.14	0.48
1:B:1215:LYS:HE3	1:B:1223:VAL:CG2	2.44	0.48
1:B:1314:SER:C	1:B:1316:PHE:H	2.22	0.48
1:B:1249:VAL:HG13	1:B:1275:VAL:HA	1.95	0.48
1:B:1304:GLN:O	1:B:1306:LEU:N	2.46	0.48
1:B:1214:LEU:CD1	1:B:1222:LEU:HD22	2.40	0.48
1:A:242:PRO:HA	1:A:268:CYS:O	2.14	0.47
1:B:1073:LEU:HB2	1:B:1094:PHE:HE1	1.79	0.47
1:A:125:LYS:HD2	1:A:387:SER:HA	1.96	0.47
1:A:284:TYR:HE1	1:A:298:ASP:HB2	1.80	0.47
2:C:1:NDG:C4	2:C:2:NAG:N2	2.74	0.47
1:A:167:THR:HG21	1:A:200:ARG:HE	1.78	0.47
1:B:1159:LEU:HD23	1:B:1160:VAL:N	2.29	0.47
1:B:1401:GLN:NE2	1:B:1401:GLN:HA	2.30	0.47
1:A:291:SER:HA	1:A:301:VAL:O	2.15	0.47
1:B:1011:GLU:HG2	1:B:1121:ALA:HB2	1.97	0.47
1:B:1256:GLU:HB3	7:B:1631:HOH:O	2.14	0.47
1:B:1281:HIS:CE1	1:B:1284:TYR:HB2	2.51	0.46
1:B:1050:HIS:O	1:B:1052:LEU:HD12	2.14	0.46
1:A:431:CYS:O	1:A:432:VAL:C	2.58	0.46
1:A:182:ALA:O	1:A:188:ARG:HD2	2.14	0.46
1:B:1353:ASP:C	1:B:1355:THR:H	2.23	0.46
1:A:172:ASN:HB3	1:A:175:ARG:O	2.15	0.46
1:B:1347:CYS:SG	1:B:1357:VAL:HG13	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ILE:HG23	1:A:331:CYS:SG	2.56	0.46
1:B:1237:CYS:SG	1:B:1242:PRO:HG3	2.56	0.46
1:A:125:LYS:O	1:A:127:ILE:N	2.45	0.46
1:A:267:ASN:O	1:A:268:CYS:CB	2.61	0.46
1:B:1290:CYS:SG	1:B:1366:LEU:HD11	2.56	0.46
1:A:37:GLY:O	1:A:38:VAL:C	2.59	0.46
1:A:255:ARG:NH2	1:A:258:THR:HG23	2.31	0.46
1:A:251:PRO:HG2	1:A:277:GLU:HG2	1.97	0.46
1:B:1011:GLU:CD	1:B:1011:GLU:H	2.24	0.46
1:B:1314:SER:HB2	1:B:1316:PHE:CE1	2.51	0.46
1:A:206:ASP:O	1:A:228:LYS:HG3	2.17	0.45
1:A:51:ASP:OD1	1:A:54:THR:HG23	2.17	0.45
3:E:1:NAG:H61	3:E:2:NAG:C8	2.43	0.45
1:A:36:MET:HE3	1:A:45:SER:O	2.17	0.45
1:A:52:LEU:HD11	1:A:143:LEU:HD21	1.98	0.45
1:A:102:THR:HG22	1:A:137:TYR:CD2	2.52	0.45
1:A:255:ARG:HH21	1:A:258:THR:CG2	2.29	0.45
1:A:267:ASN:ND2	1:A:267:ASN:C	2.64	0.45
1:A:226:TYR:HB2	1:A:244:VAL:HB	1.98	0.45
1:B:1149:ASN:N	1:B:1150:PRO:CD	2.79	0.45
1:A:286:GLU:O	1:A:297:HIS:HE1	2.00	0.45
1:A:342:LYS:HD2	1:A:343:ASP:H	1.82	0.45
1:B:1418:ASP:O	1:B:1419:CYS:HB2	2.15	0.45
1:A:8:GLU:HG3	1:A:66:LYS:HZ2	1.82	0.45
1:A:217:VAL:CG2	1:A:218:SER:H	2.09	0.45
1:A:313:ASP:OD1	1:A:314:SER:N	2.50	0.44
1:A:368:LEU:HD11	1:A:375:LEU:HD11	1.98	0.44
1:B:1035:ASN:OD1	1:B:1036:MET:HG2	2.16	0.44
1:A:270:PHE:CD1	1:A:270:PHE:N	2.85	0.44
1:B:1216:LEU:C	1:B:1216:LEU:HD23	2.42	0.44
1:B:1201:GLY:O	1:B:1203:ARG:HG3	2.18	0.44
1:A:303:LEU:C	1:A:305:PRO:HD2	2.43	0.44
1:B:1196:ALA:CB	1:B:1244:VAL:HG21	2.48	0.44
1:A:251:PRO:CG	1:A:255:ARG:HD2	2.47	0.44
1:A:362:ARG:HG2	1:A:362:ARG:HH11	1.83	0.43
1:A:57:PHE:CD1	1:A:57:PHE:N	2.86	0.43
1:B:1011:GLU:CG	1:B:1121:ALA:HB2	2.47	0.43
1:B:1288:ARG:HH21	1:B:1288:ARG:CB	2.29	0.43
1:A:181:ARG:HD3	1:A:181:ARG:N	2.33	0.43
1:B:1053:LYS:HE3	1:B:1054:THR:CG2	2.46	0.43
1:B:1159:LEU:HD23	1:B:1159:LEU:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LYS:HE2	1:A:357:VAL:HG11	2.00	0.43
1:A:218:SER:HB3	1:A:221:ARG:HB2	1.97	0.43
1:A:251:PRO:CB	1:A:255:ARG:HD2	2.49	0.43
1:A:262:LEU:HD13	1:A:262:LEU:C	2.43	0.43
1:B:1153:LYS:HD2	1:B:1157:ALA:HA	1.99	0.43
1:B:1223:VAL:HA	1:B:1246:ILE:O	2.18	0.43
3:E:1:NAG:C5	3:E:2:NAG:H82	2.48	0.43
1:B:1353:ASP:O	1:B:1355:THR:N	2.52	0.43
1:B:1141:ARG:HH21	1:B:1219:ASN:HD22	1.66	0.43
1:B:1235:ASP:O	1:B:1237:CYS:N	2.52	0.43
1:B:1382:GLY:O	1:B:1390:GLN:HG2	2.19	0.42
1:A:82:LYS:HE3	1:A:110:ASP:HB3	2.00	0.42
1:A:294:SER:O	1:A:298:ASP:HA	2.19	0.42
1:B:1411:PRO:HB3	1:B:1425:TRP:CE3	2.55	0.42
1:A:259:ILE:CG2	1:A:260:PRO:HD2	2.47	0.42
1:A:267:ASN:HD21	1:A:269:ARG:HB2	1.83	0.42
1:B:1255:ARG:HH21	1:B:1258:THR:HG23	1.84	0.42
1:A:262:LEU:HD11	1:A:265:LYS:HB2	2.01	0.42
1:A:11:GLU:HG3	7:A:703:HOH:O	2.18	0.42
1:B:1207:VAL:CG2	1:B:1242:PRO:HB3	2.39	0.42
1:A:315:LEU:N	1:A:315:LEU:HD12	2.35	0.42
1:A:317:TYR:CD2	1:A:411:PRO:HD3	2.55	0.42
1:A:257:GLY:CA	1:A:372:ASP:HB3	2.50	0.42
1:B:1082:LYS:N	1:B:1082:LYS:HE3	2.35	0.42
1:A:79:VAL:HG12	1:A:80:ASN:H	1.83	0.42
1:A:401:GLN:HE21	1:A:401:GLN:HA	1.85	0.42
1:B:1366:LEU:HD23	1:B:1367:THR:N	2.35	0.42
1:A:18:GLU:HA	1:A:28:TYR:O	2.20	0.41
1:B:1087:LYS:HE2	7:B:1659:HOH:O	2.20	0.41
1:A:285:LEU:O	1:A:369:ARG:HA	2.20	0.41
1:A:344:ALA:CB	1:A:359:VAL:HG13	2.49	0.41
1:A:142:GLU:O	1:A:143:LEU:HB2	2.20	0.41
1:A:31:ASN:HD22	1:A:34:GLY:C	2.27	0.41
1:A:281:HIS:NE2	1:A:284:TYR:HB2	2.36	0.41
1:A:346:VAL:HG21	1:A:393:SER:CB	2.51	0.41
1:A:110:ASP:O	1:A:111:CYS:HB2	2.20	0.41
1:A:267:ASN:ND2	1:A:269:ARG:CB	2.81	0.41
1:B:1304:GLN:C	1:B:1306:LEU:N	2.77	0.41
1:B:1348:GLN:HE22	6:B:1502:M6P:C2	2.34	0.41
1:B:1017:TRP:CH2	1:B:1135:PRO:HG3	2.56	0.41
1:B:1060:VAL:HG12	1:B:1088:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:HIS:O	1:A:284:TYR:HB3	2.21	0.41
1:A:416:GLU:CG	1:A:417:VAL:N	2.84	0.41
1:B:1044:SER:HB2	1:B:1062:ASP:OD1	2.21	0.41
1:B:1335:GLN:OE1	1:B:1339:CYS:HB2	2.21	0.41
1:A:343:ASP:O	1:A:362:ARG:NH1	2.54	0.41
1:A:113:HIS:ND1	1:A:113:HIS:N	2.69	0.40
1:A:89:GLN:HG3	1:A:112:VAL:HG13	2.04	0.40
1:A:348:GLN:HE22	6:A:603:M6P:C2	2.34	0.40
1:B:1189:VAL:O	1:B:1189:VAL:HG12	2.22	0.40
1:A:38:VAL:O	1:A:38:VAL:CG2	2.69	0.40
1:B:1207:VAL:HG21	1:B:1270:PHE:HE1	1.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/432 (95%)	361 (88%)	41 (10%)	9 (2%)	5	2
1	B	408/432 (94%)	371 (91%)	29 (7%)	8 (2%)	6	2
All	All	819/864 (95%)	732 (89%)	70 (8%)	17 (2%)	5	2

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ALA
1	B	1034	GLY
1	B	1235	ASP
1	A	38	VAL
1	A	126	ASN
1	A	219	ASN
1	A	354	SER

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Mol	Chain	Res	Type
1	B	1039	ALA
1	B	1236	PHE
1	B	1354	SER
1	A	81	CYS
1	A	110	ASP
1	B	1341	LYS
1	B	1267	ASN
1	B	1305	PRO
1	A	231	ALA
1	A	353	ASP

5.3.2 Protein sidechains [i](#)

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	360/370 (97%)	343 (95%)	17 (5%)	23	24
1	B	361/370 (98%)	341 (94%)	20 (6%)	19	18
All	All	721/740 (97%)	684 (95%)	37 (5%)	21	21

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	CYS
1	A	106	VAL
1	A	141	ARG
1	A	148	LEU
1	A	159	LEU
1	A	175	ARG
1	A	214	LEU
1	A	255	ARG
1	A	267	ASN
1	A	268	CYS
1	A	283	ASP
1	A	298	ASP
1	A	341	LYS

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Mol	Chain	Res	Type
1	A	342	LYS
1	A	364	GLN
1	A	366	LEU
1	A	394	VAL
1	B	1011	GLU
1	B	1038	VAL
1	B	1073	LEU
1	B	1076	ASN
1	B	1082	LYS
1	B	1100	LEU
1	B	1136	CYS
1	B	1148	LEU
1	B	1169	LEU
1	B	1192	THR
1	B	1253	GLU
1	B	1255	ARG
1	B	1262	LEU
1	B	1288	ARG
1	B	1335	GLN
1	B	1341	LYS
1	B	1366	LEU
1	B	1394	VAL
1	B	1398	GLU
1	B	1424	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	31	ASN
1	A	58	HIS
1	A	80	ASN
1	A	113	HIS
1	A	131	ASN
1	A	149	ASN
1	A	219	ASN
1	A	233	GLN
1	A	240	HIS
1	A	267	ASN
1	A	297	HIS
1	A	304	GLN
1	A	335	GLN

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Mol	Chain	Res	Type
1	A	348	GLN
1	A	364	GLN
1	A	401	GLN
1	B	1024	ASN
1	B	1040	GLN
1	B	1113	HIS
1	B	1126	ASN
1	B	1131	ASN
1	B	1219	ASN
1	B	1267	ASN
1	B	1297	HIS
1	B	1304	GLN
1	B	1348	GLN
1	B	1365	ASN
1	B	1401	GLN

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 ⓘ

6 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	NDG	C	1	2	14,14,15	0.60	0	17,19,21	0.82	1 (5%)
2	NAG	C	2	2	14,14,15	0.56	0	17,19,21	0.71	0
3	NAG	D	1	1,3	14,14,15	0.85	0	17,19,21	1.22	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	2	3	14,14,15	0.65	0	17,19,21	0.66	0
3	NAG	E	1	3	14,14,15	0.66	0	17,19,21	1.06	1 (5%)
3	NAG	E	2	3	14,14,15	0.46	0	17,19,21	0.78	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
2	NDG	C	1	2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1
3	NAG	E	1	3	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	NAG	C3-C4-C5	3.30	116.21	110.23
2	C	1	NDG	C2-N2-C7	-2.47	119.60	122.90
3	E	1	NAG	C2-N2-C7	-2.22	119.92	122.90
3	D	1	NAG	C2-N2-C7	-2.15	120.02	122.90
3	D	1	NAG	O5-C1-C2	-2.08	108.08	111.29
3	E	2	NAG	C2-N2-C7	-2.00	120.22	122.90

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NDG	C8-C7-N2-C2
2	C	1	NDG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2

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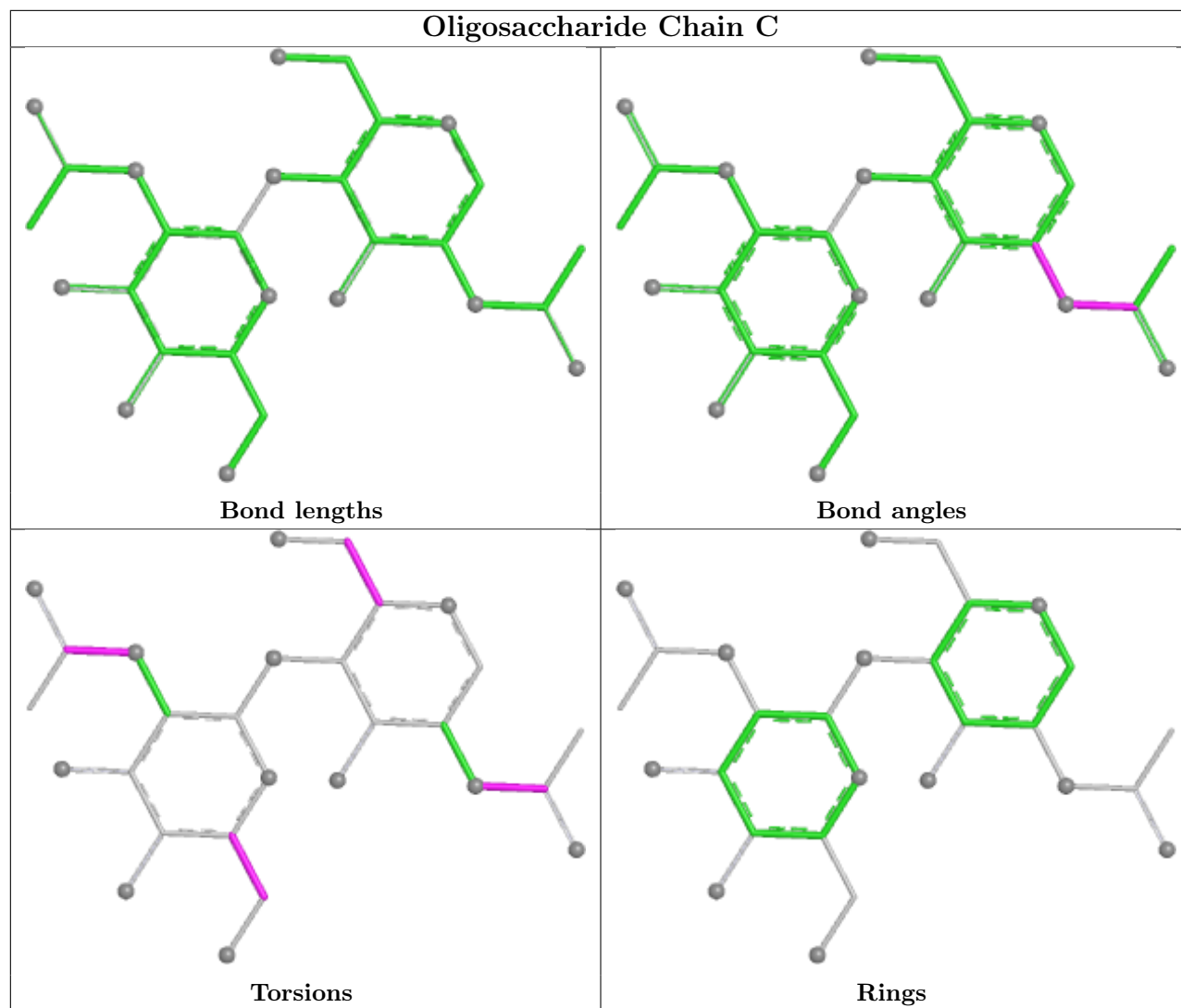
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	O7-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NDG	O5-C5-C6-O6
2	C	1	NDG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6

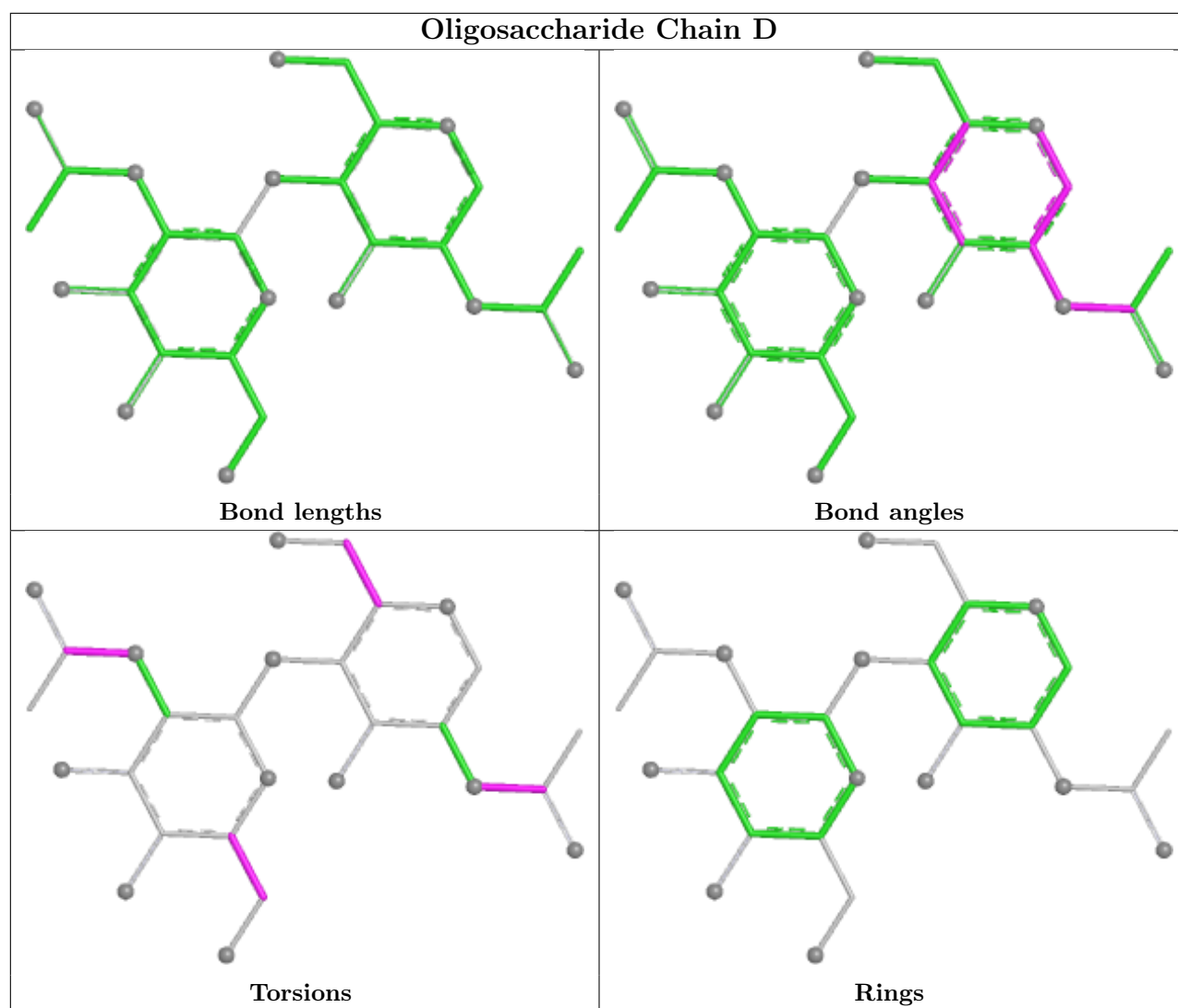
There are no ring outliers.

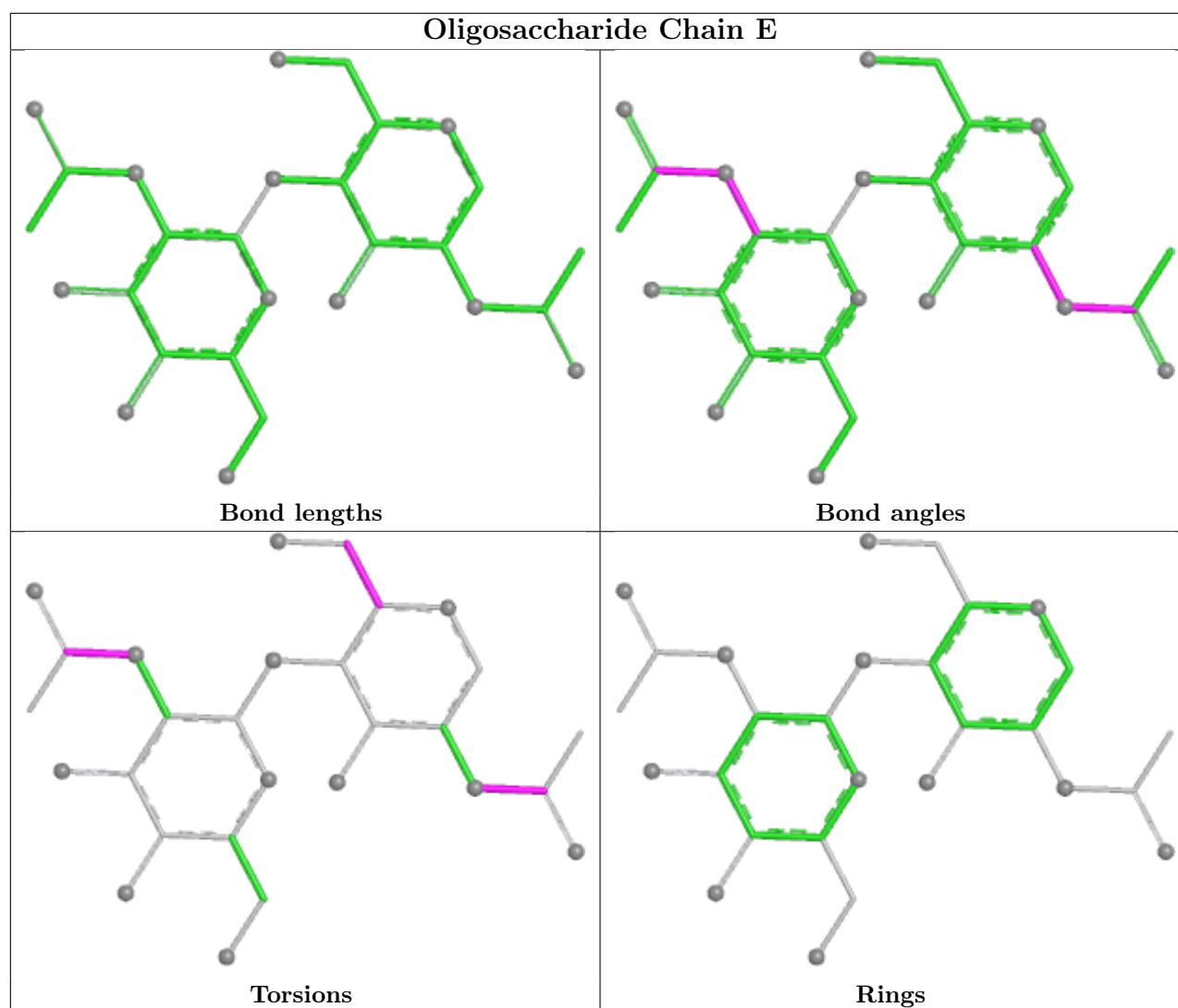
6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	4	0
3	E	1	NAG	13	0
2	C	2	NAG	3	0
2	C	1	NDG	3	0
3	E	2	NAG	5	0
3	D	2	NAG	5	0

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







5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z > 2$
4	NAG	A	601	-	14,14,15	0.62	0	17,19,21	0.71	1 (5%)
6	M6P	B	1502	-	16,16,16	1.61	3 (18%)	23,24,24	0.84	0
6	M6P	A	603	-	16,16,16	1.64	4 (25%)	23,24,24	0.82	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	601	-	-	3/6/23/26	0/1/1/1
6	M6P	B	1502	-	-	0/6/26/26	0/1/1/1
6	M6P	A	603	-	-	0/6/26/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1502	M6P	P-O1P	3.85	1.62	1.50
6	A	603	M6P	P-O1P	3.67	1.61	1.50
6	B	1502	M6P	C3-C2	2.28	1.58	1.52
6	A	603	M6P	C3-C2	2.22	1.58	1.52
6	A	603	M6P	O5-C1	2.19	1.48	1.42
6	A	603	M6P	O1-C1	2.08	1.46	1.39
6	B	1502	M6P	O5-C1	2.05	1.47	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	NAG	C2-N2-C7	-2.12	120.06	122.90

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	C8-C7-N2-C2
4	A	601	NAG	O7-C7-N2-C2
4	A	601	NAG	O5-C5-C6-O6

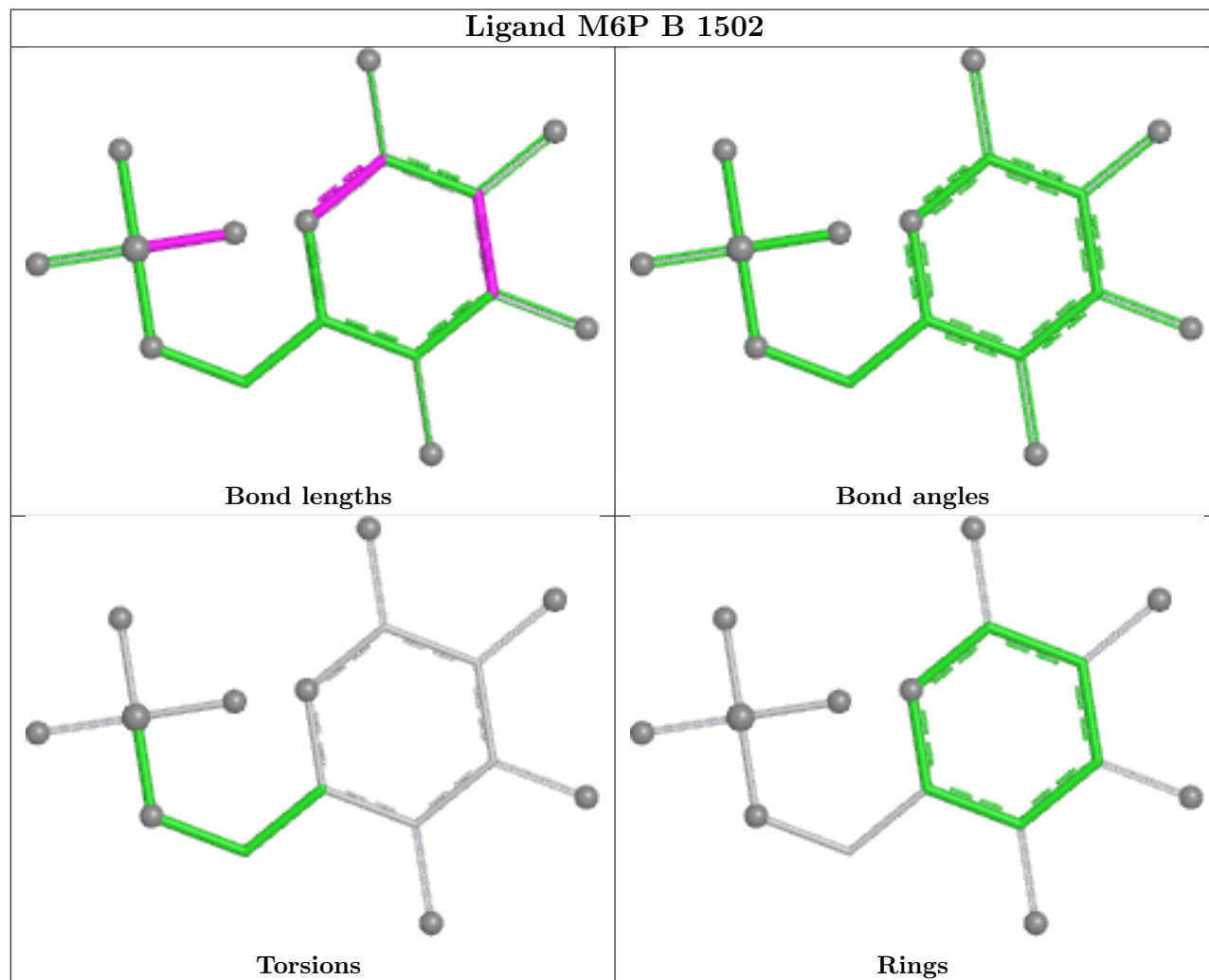
There are no ring outliers.

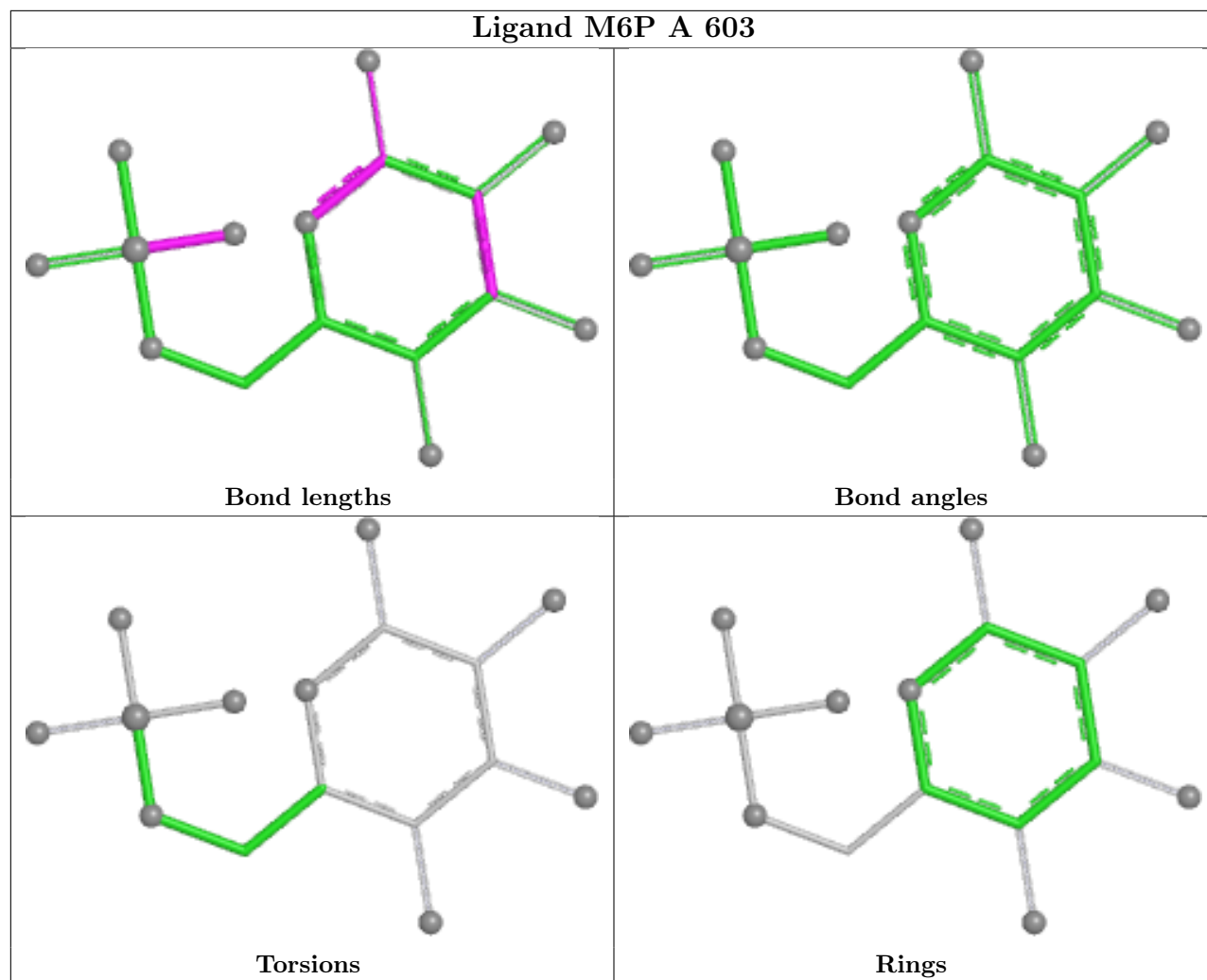
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1502	M6P	1	0
6	A	603	M6P	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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





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	417/432 (96%)	0.66	30 (7%) 21 23	22, 47, 74, 92	0
1	B	416/432 (96%)	0.41	23 (5%) 30 32	17, 39, 76, 93	0
All	All	833/864 (96%)	0.53	53 (6%) 25 27	17, 43, 75, 93	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1038	VAL	7.2
1	B	1037	GLY	6.3
1	B	1034	GLY	4.6
1	A	7	ALA	4.1
1	A	39	ALA	4.0
1	A	37	GLY	3.8
1	B	1039	ALA	3.7
1	A	79	VAL	3.6
1	B	1432	VAL	3.5
1	A	41	CYS	3.4
1	A	268	CYS	3.3
1	A	267	ASN	3.3
1	B	1036	MET	3.3
1	A	38	VAL	3.1
1	A	78	THR	3.1
1	B	1033	CYS	3.0
1	B	1313	ASP	3.0
1	A	40	GLN	2.9
1	B	1340	ASN	2.9
1	A	42	GLY	2.9
1	B	1163	SER	2.8
1	B	1234	PRO	2.7
1	B	1311	ALA	2.6
1	A	219	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	338	ILE	2.6
1	A	82	LYS	2.6
1	A	182	ALA	2.6
1	A	330	ILE	2.5
1	A	251	PRO	2.5
1	B	1339	CYS	2.5
1	A	77	THR	2.5
1	B	1035	ASN	2.5
1	A	112	VAL	2.4
1	A	34	GLY	2.4
1	A	25	ASN	2.4
1	B	1315	LEU	2.4
1	A	88	ILE	2.4
1	B	1268	CYS	2.3
1	A	343	ASP	2.3
1	A	111	CYS	2.3
1	B	1312	SER	2.3
1	A	340	ASN	2.2
1	B	1081	CYS	2.2
1	B	1309	VAL	2.2
1	A	288	ARG	2.2
1	A	315	LEU	2.1
1	A	35	ASN	2.1
1	A	200	ARG	2.1
1	B	1032	ILE	2.1
1	B	1338	ILE	2.1
1	A	81	CYS	2.1
1	B	1110	ASP	2.1
1	B	1007	ALA	2.1

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

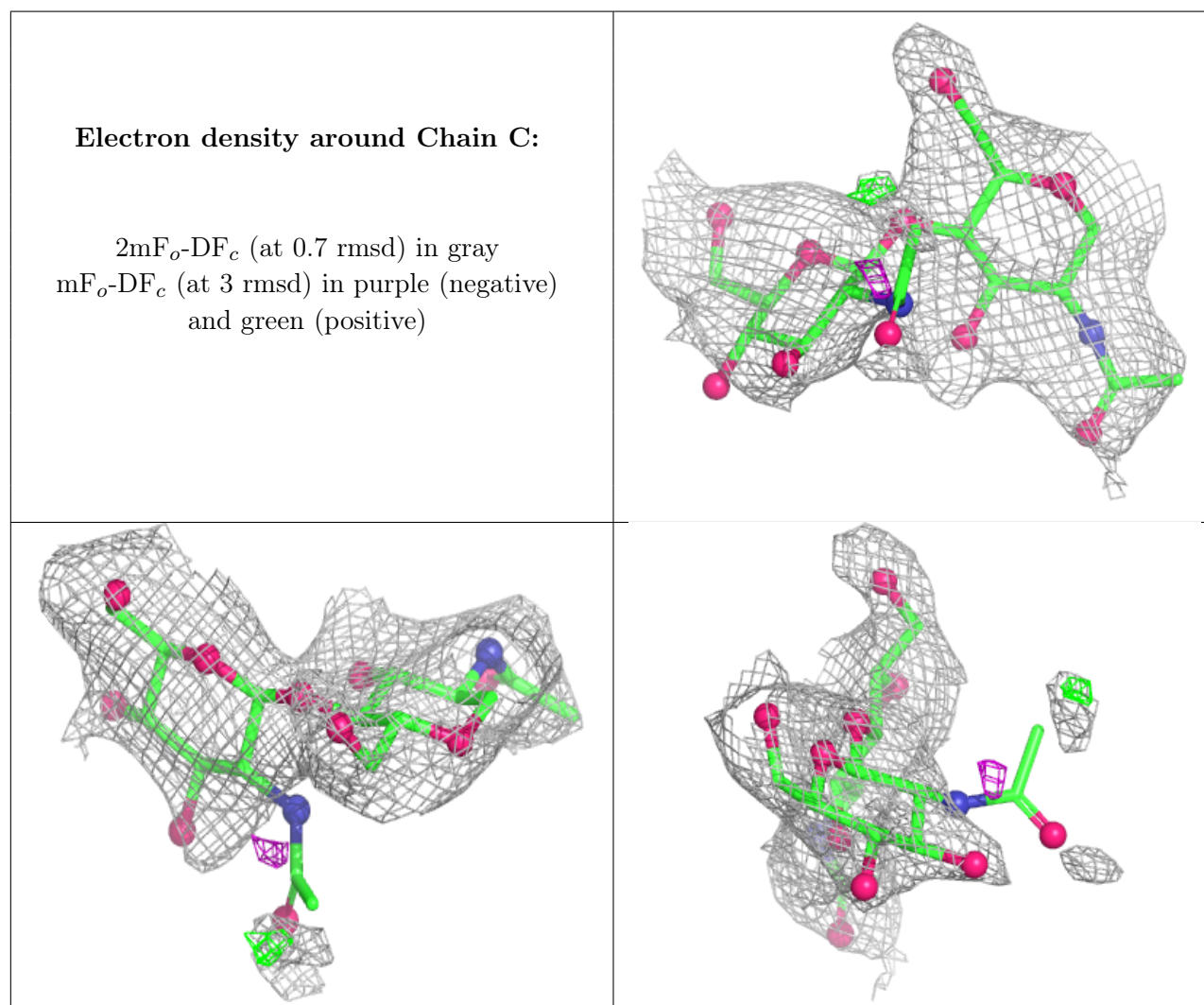
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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

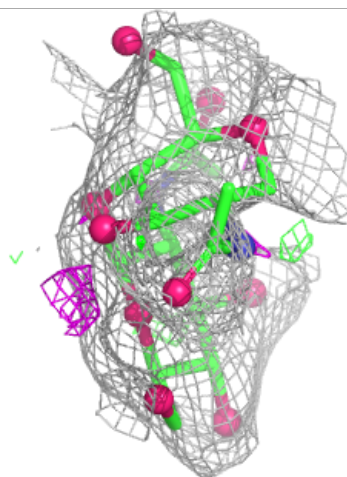
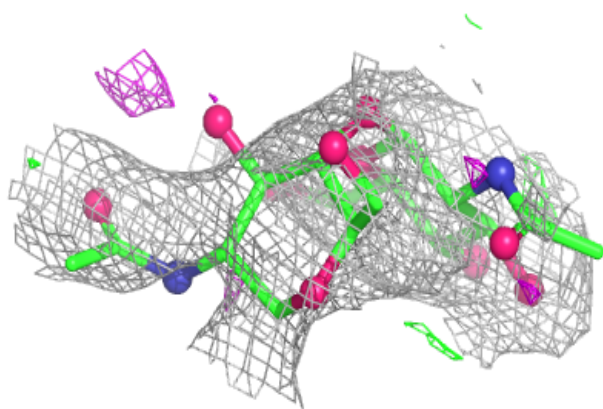
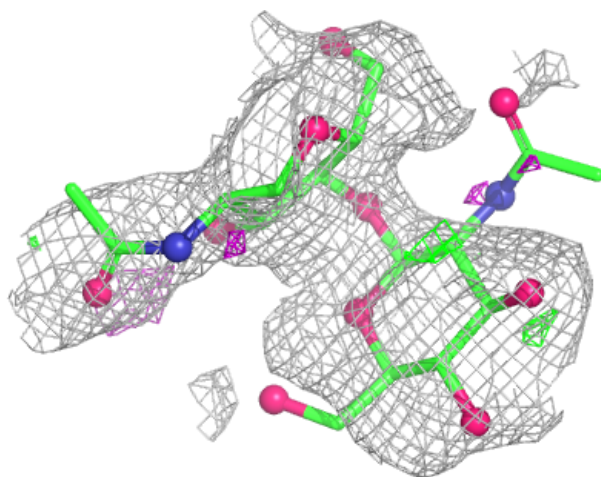
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	C	2	14/15	0.53	0.14	79,80,84,85	0
3	NAG	D	2	14/15	0.56	0.16	90,91,94,94	0
3	NAG	D	1	14/15	0.58	0.15	80,83,87,89	0
3	NAG	E	2	14/15	0.69	0.12	69,71,73,73	0
2	NDG	C	1	14/15	0.72	0.13	68,71,74,77	0
3	NAG	E	1	14/15	0.73	0.12	58,64,69,69	0

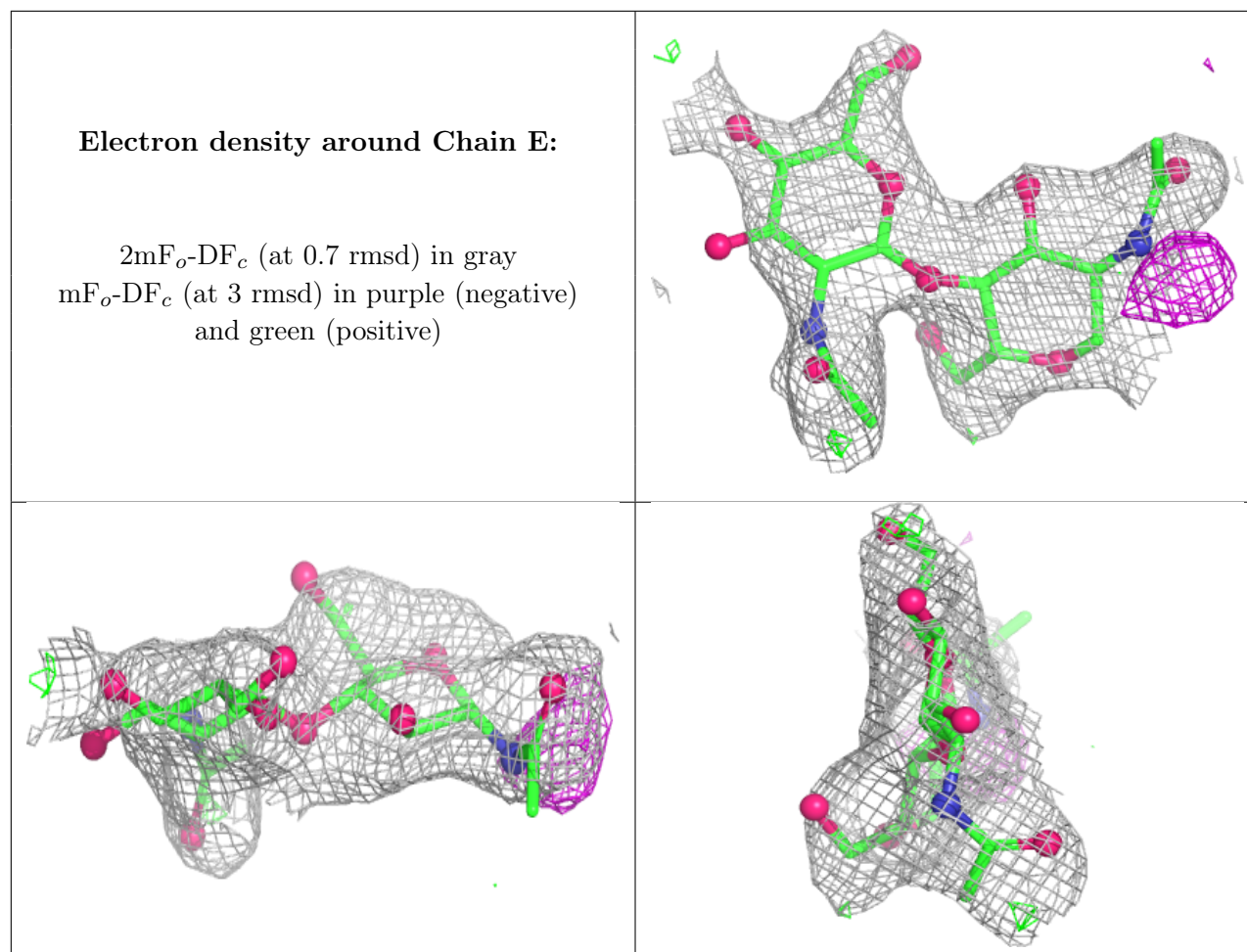
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain D:

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





6.4 Ligands [i](#)

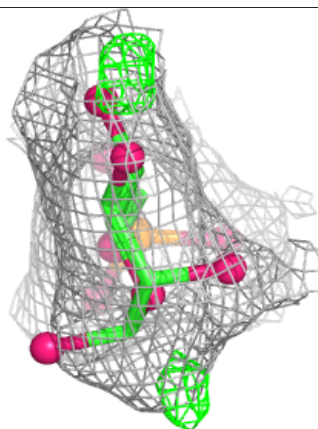
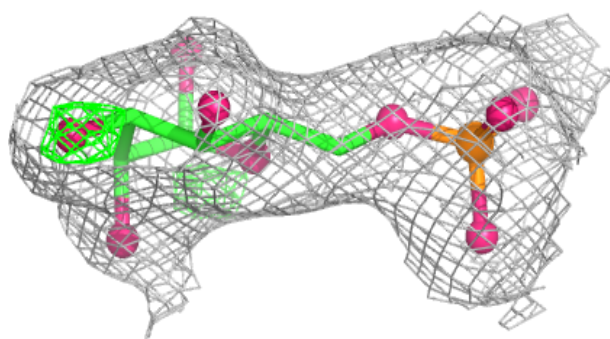
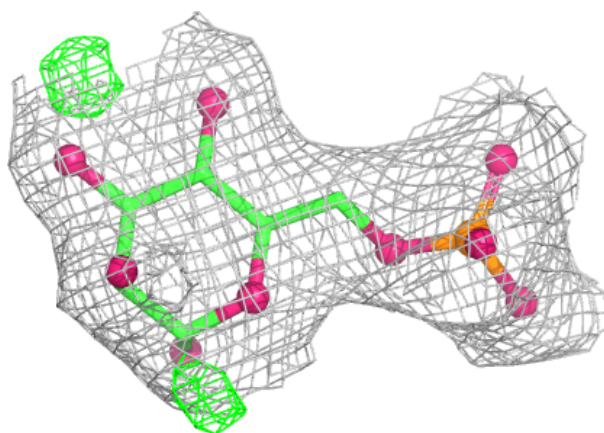
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	A	601	14/15	0.83	0.10	51,53,54,55	0
6	M6P	A	603	16/16	0.90	0.09	40,44,46,49	0
5	OS	B	1501	1/1	0.91	0.09	77,77,77,77	1
6	M6P	B	1502	16/16	0.91	0.09	29,35,37,43	0
5	OS	A	602	1/1	0.98	0.14	61,61,61,61	1

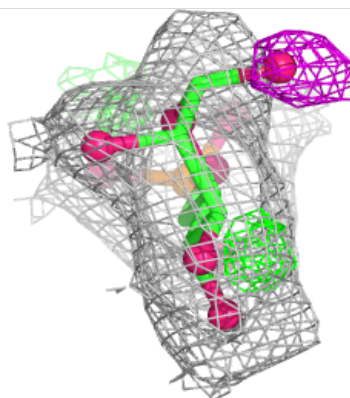
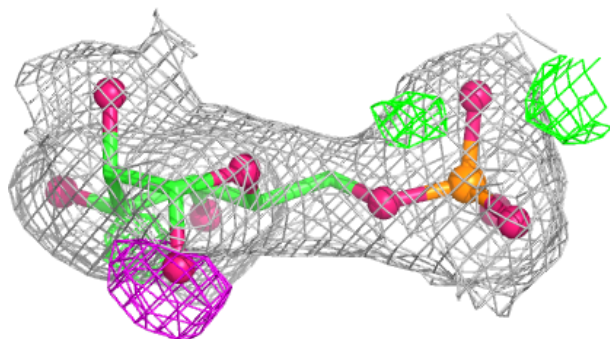
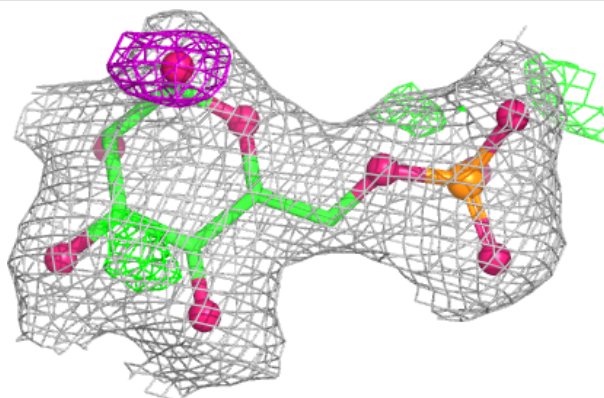
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around M6P A 603:

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

**Electron density around M6P B 1502:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.