



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:56 PM UTC

PDB ID : 1SYO / pdb_00001syo
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 : 2.20 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 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

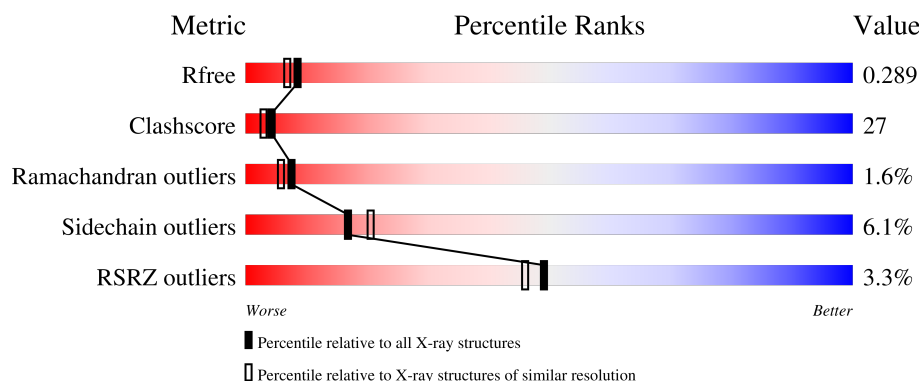
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 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	4% 51% 41% 6%
1	B	432	2% 54% 37% 6%
2	C	3	33% 67%

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
2	NAG	C	2	X	-	-	-
5	GOL	A	603	-	X	-	-
5	GOL	B	1504	-	X	-	-

2 Entry composition [i](#)

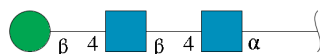
There are 6 unique types of molecules in this entry. The entry contains 6891 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

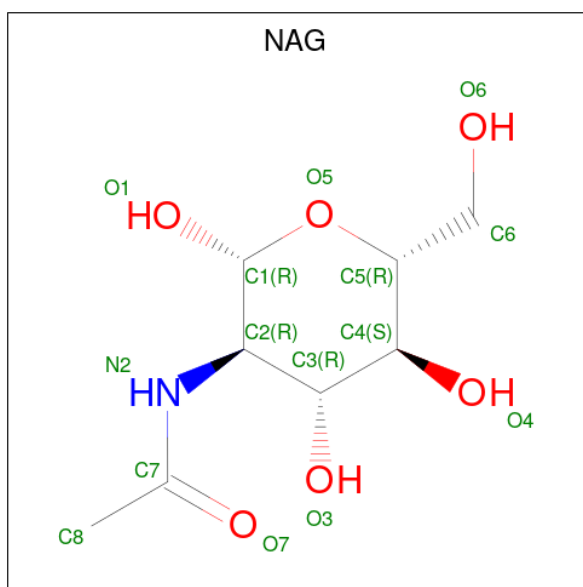
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3268	2040	560	640	28			
1	B	408	Total	C	N	O	S	0	0	0
			3161	1980	538	616	27			

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



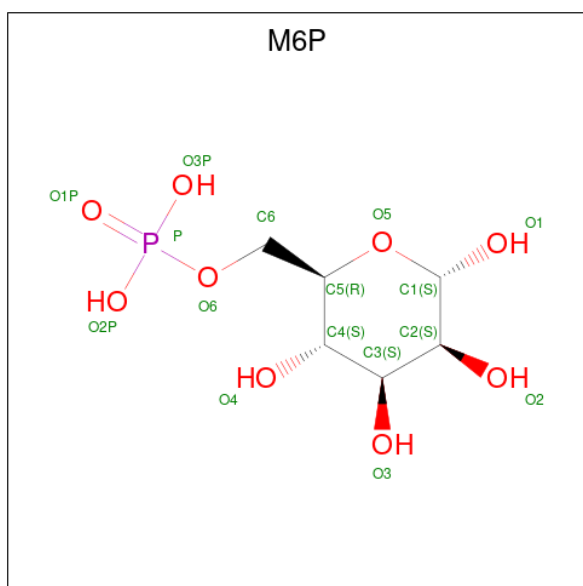
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			40	22	2	16			

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



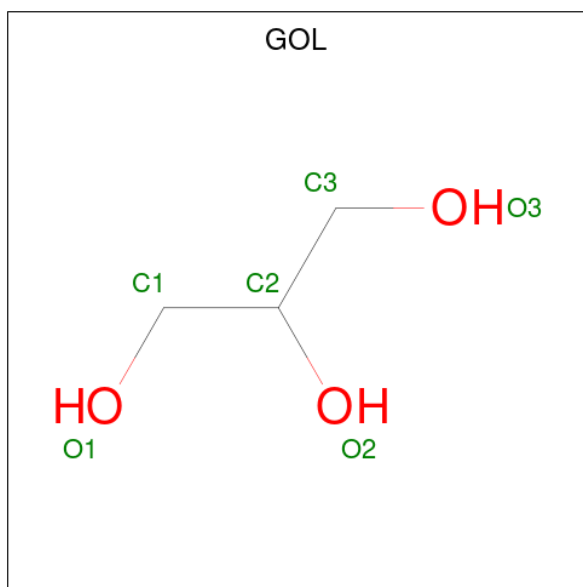
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 6-O-phosphono-alpha-D-mannopyranose (CCD ID: M6P) (formula: $C_6H_{13}O_9P$).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

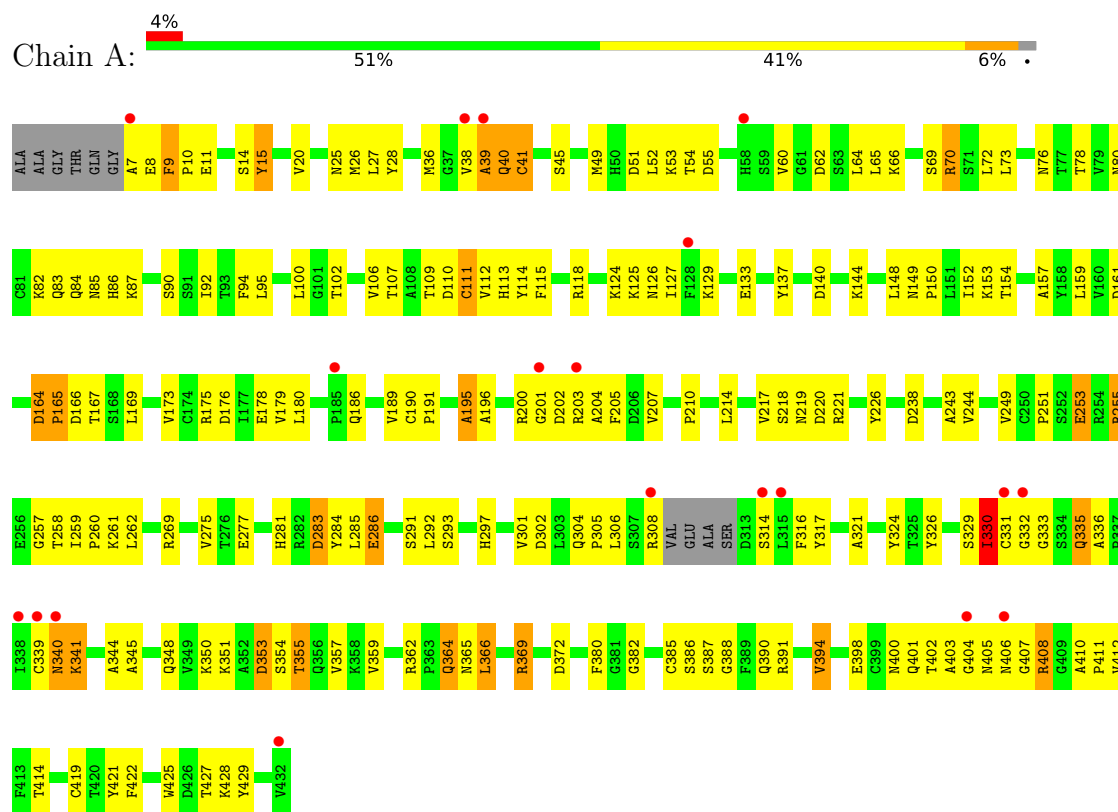
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	150	Total	O	0	0
			150	150		
6	B	186	Total	O	0	0
			186	186		

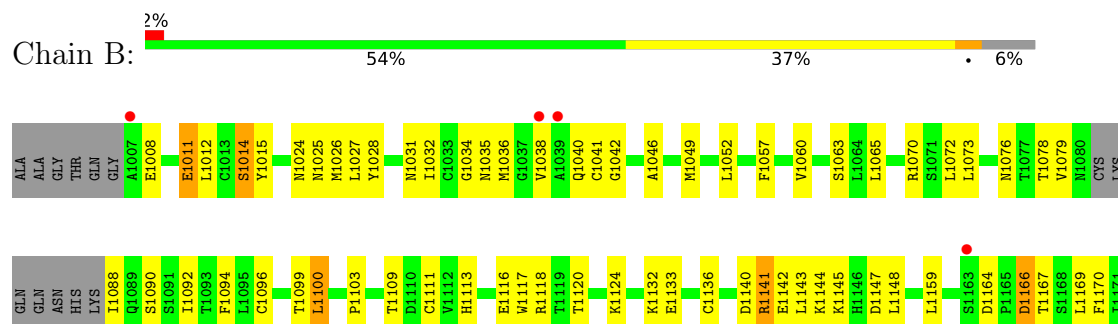
3 Residue-property plots [i](#)

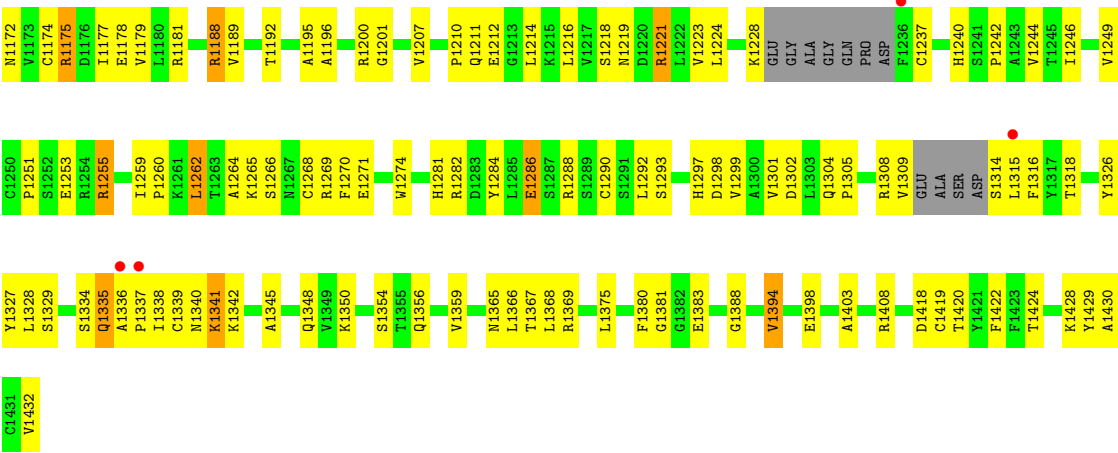
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.40Å 86.40Å 86.90Å 90.00° 108.80° 90.00°	Depositor
Resolution (Å)	29.96 – 2.20 29.96 – 2.20	Depositor EDS
% Data completeness (in resolution range)	88.3 (29.96-2.20) 88.3 (29.96-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.289 0.229 , 0.289	Depositor DCC
R_{free} test set	2600 reflections (6.07%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6891	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDG, NAG, BMA, M6P, GOL

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	0.44	0/3335	1.00	17/4520 (0.4%)
1	B	0.45	0/3224	0.95	7/4369 (0.2%)
All	All	0.45	0/6559	0.97	24/8889 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	VAL	N-CA-C	8.34	118.73	111.56
1	B	1282	ARG	N-CA-C	7.27	119.83	111.11
1	B	1286	GLU	N-CA-C	7.03	120.56	109.81
1	B	1345	ALA	N-CA-C	-6.99	103.09	111.69
1	A	164	ASP	CA-C-N	-6.89	111.22	119.84
1	A	164	ASP	C-N-CA	-6.89	111.22	119.84
1	A	9	PHE	CA-C-N	6.83	126.34	119.24
1	A	9	PHE	C-N-CA	6.83	126.34	119.24
1	A	286	GLU	N-CA-C	6.55	119.67	109.52
1	B	1221	ARG	N-CA-C	6.30	119.00	109.23
1	B	1420	THR	N-CA-C	-6.00	98.74	108.52
1	A	112	VAL	N-CA-C	5.92	116.65	108.12
1	B	1336	ALA	CA-C-N	5.72	125.84	119.32
1	B	1336	ALA	C-N-CA	5.72	125.84	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	VAL	N-CA-C	5.63	116.47	108.42
1	A	419	CYS	N-CA-C	5.57	119.38	112.58
1	A	154	THR	N-CA-C	-5.54	106.48	113.18
1	A	15	TYR	N-CA-C	5.26	117.67	109.52
1	A	408	ARG	N-CA-C	5.22	121.92	110.80
1	A	330	ILE	N-CA-C	5.20	116.78	108.87
1	A	345	ALA	N-CA-C	-5.16	106.67	113.12
1	A	195	ALA	N-CA-C	-5.08	107.21	113.41
1	A	111	CYS	N-CA-C	5.05	120.09	113.88
1	A	78	THR	N-CA-C	-5.01	107.56	113.97

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	369	ARG	Sidechain
1	A	70	ARG	Sidechain

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	3268	0	3134	184	0
1	B	3161	0	3044	156	0
2	C	40	0	34	5	0
3	A	14	0	13	1	0
3	B	28	0	26	0	0
4	A	16	0	11	2	0
4	B	16	0	11	2	0
5	A	6	0	4	0	0
5	B	6	0	4	0	0
6	A	150	0	0	5	0
6	B	186	0	0	6	0
All	All	6891	0	6281	346	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 27.

All (346) 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:B:1341:LYS:HD3	1:B:1341:LYS:H	1.15	1.06
1:B:1031:ASN:ND2	1:B:1035:ASN:H	1.53	1.06
1:A:308:ARG:HD2	1:A:408:ARG:CZ	1.94	0.97
1:B:1299:VAL:HG23	1:B:1432:VAL:HG13	1.47	0.97
1:B:1031:ASN:HD22	1:B:1035:ASN:H	1.18	0.92
1:B:1141:ARG:H	1:B:1141:ARG:HE	1.20	0.90
1:B:1293:SER:H	1:B:1297:HIS:HD2	1.20	0.89
1:A:293:SER:H	1:A:297:HIS:HD2	1.21	0.87
1:B:1308:ARG:HA	1:B:1315:LEU:HD11	1.55	0.87
2:C:1:NDG:O3	2:C:2:NAG:O1	1.92	0.86
1:A:400:ASN:HD22	1:A:403:ALA:HB2	1.41	0.85
1:B:1140:ASP:HB2	1:B:1141:ARG:HH21	1.41	0.85
1:A:308:ARG:HD2	1:A:408:ARG:NH1	1.91	0.84
1:A:124:LYS:HD2	1:A:386:SER:O	1.79	0.83
1:B:1172:ASN:ND2	1:B:1175:ARG:HD2	1.94	0.82
1:B:1167:THR:HG22	1:B:1200:ARG:HB2	1.60	0.82
1:A:62:ASP:HB3	1:A:65:LEU:HD13	1.62	0.81
1:B:1159:LEU:HD23	1:B:1170:PHE:HE2	1.43	0.81
1:B:1365:ASN:HD22	1:B:1381:GLY:HA3	1.46	0.80
1:A:195:ALA:HB2	1:A:210:PRO:HD3	1.64	0.80
1:B:1052:LEU:HD12	1:B:1143:LEU:HD11	1.64	0.79
1:B:1031:ASN:ND2	1:B:1035:ASN:N	2.31	0.78
1:B:1133:GLU:HG3	1:B:1175:ARG:HB3	1.64	0.78
1:B:1341:LYS:HD3	1:B:1341:LYS:N	1.96	0.77
1:B:1207:VAL:HG23	1:B:1242:PRO:HB3	1.66	0.77
1:A:330:ILE:HG23	1:A:331:CYS:SG	2.25	0.77
1:A:80:ASN:HA	1:A:87:LYS:HA	1.66	0.75
1:A:175:ARG:HG2	1:A:176:ASP:N	2.01	0.75
1:A:335:GLN:HE21	1:A:336:ALA:H	1.31	0.75
1:B:1308:ARG:HA	1:B:1315:LEU:CD1	2.17	0.74
1:B:1365:ASN:ND2	1:B:1381:GLY:HA3	2.03	0.74
2:C:1:NDG:C3	2:C:2:NAG:O1	2.35	0.73
1:B:1318:THR:HG22	1:B:1327:TYR:HD1	1.51	0.73
1:B:1288:ARG:HH21	1:B:1366:LEU:H	1.34	0.73
1:B:1142:GLU:HB2	1:B:1144:LYS:HD2	1.69	0.73
1:A:308:ARG:HB2	1:A:408:ARG:NH1	2.04	0.72
1:B:1242:PRO:HA	1:B:1268:CYS:O	1.88	0.72
1:B:1338:ILE:O	1:B:1341:LYS:HE3	1.88	0.72
1:A:196:ALA:CB	1:A:244:VAL:HG21	2.20	0.72
1:A:340:ASN:HB3	6:A:720:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LYS:H	1:A:341:LYS:HD3	1.54	0.71
1:A:251:PRO:HG3	1:A:275:VAL:CG1	2.21	0.70
1:A:28:TYR:OH	1:A:113:HIS:HD2	1.73	0.70
1:B:1140:ASP:CB	1:B:1141:ARG:HH21	2.04	0.70
1:B:1028:TYR:OH	1:B:1113:HIS:HD2	1.73	0.70
1:B:1341:LYS:H	1:B:1341:LYS:CD	2.00	0.70
1:B:1318:THR:HG22	1:B:1327:TYR:CD1	2.27	0.70
2:C:1:NDG:C3	2:C:2:NAG:HO1	2.05	0.69
1:B:1309:VAL:H	1:B:1315:LEU:HD12	1.58	0.69
1:B:1195:ALA:HB2	1:B:1210:PRO:HD3	1.75	0.69
1:A:251:PRO:HG2	1:A:255:ARG:HD2	1.76	0.68
1:B:1339:CYS:HA	1:B:1341:LYS:HZ1	1.56	0.68
1:B:1031:ASN:HD22	1:B:1035:ASN:N	1.89	0.68
1:B:1293:SER:N	1:B:1297:HIS:HD2	1.92	0.67
1:A:411:PRO:HG3	1:A:425:TRP:CZ3	2.30	0.67
1:A:8:GLU:HG3	1:A:66:LYS:NZ	2.10	0.66
1:A:25:ASN:ND2	1:A:52:LEU:HB2	2.11	0.66
1:A:153:LYS:HE3	1:A:157:ALA:O	1.95	0.66
1:A:26:MET:HE3	1:A:49:MET:SD	2.36	0.65
1:B:1070:ARG:NH2	1:B:1124:LYS:HE3	2.10	0.65
1:B:1265:LYS:O	1:B:1265:LYS:HG3	1.98	0.64
1:A:411:PRO:HG3	1:A:425:TRP:CE3	2.32	0.64
1:B:1293:SER:H	1:B:1297:HIS:CD2	2.08	0.64
1:B:1207:VAL:HG21	1:B:1270:PHE:CE1	2.32	0.64
1:B:1337:PRO:HA	1:B:1340:ASN:OD1	1.98	0.63
1:B:1172:ASN:HD21	1:B:1175:ARG:HD2	1.63	0.63
1:A:286:GLU:OE1	1:A:369:ARG:HD3	1.99	0.63
1:B:1145:LYS:HD3	1:B:1147:ASP:HB2	1.81	0.62
1:A:218:SER:HB3	1:A:221:ARG:HD3	1.80	0.62
1:A:76:ASN:ND2	6:A:702:HOH:O	2.32	0.62
1:B:1038:VAL:HG13	1:B:1041:CYS:HB2	1.83	0.61
1:A:51:ASP:OD1	1:A:53:LYS:HG2	2.00	0.61
1:B:1036:MET:HG3	1:B:1038:VAL:HG12	1.81	0.61
1:A:201:GLY:O	1:A:203:ARG:HG3	2.00	0.61
1:B:1040:GLN:HB3	1:B:1057:PHE:HB2	1.81	0.61
1:B:1141:ARG:HH12	1:B:1219:ASN:HA	1.65	0.61
1:B:1281:HIS:CE1	1:B:1284:TYR:HB2	2.36	0.61
1:B:1079:VAL:CG1	1:B:1088:ILE:HD12	2.32	0.60
1:B:1207:VAL:CG2	1:B:1242:PRO:HB3	2.31	0.60
1:B:1286:GLU:OE1	1:B:1369:ARG:NH1	2.29	0.60
1:B:1368:LEU:HD11	1:B:1375:LEU:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1259:ILE:HG23	1:B:1260:PRO:HD2	1.84	0.59
1:A:38:VAL:O	1:A:40:GLN:N	2.35	0.59
1:A:286:GLU:O	1:A:297:HIS:HE1	1.85	0.59
1:B:1326:TYR:CE2	1:B:1348:GLN:HG3	2.37	0.59
1:A:218:SER:O	1:A:219:ASN:HB3	2.02	0.59
2:C:2:NAG:O3	2:C:2:NAG:H83	2.02	0.59
1:A:65:LEU:HD12	1:A:65:LEU:N	2.18	0.59
1:A:8:GLU:HG3	1:A:66:LYS:HZ2	1.66	0.59
1:A:39:ALA:C	1:A:41:CYS:H	2.11	0.58
1:B:1328:LEU:N	1:B:1328:LEU:HD12	2.17	0.58
1:A:38:VAL:O	1:A:38:VAL:HG12	2.04	0.58
1:A:305:PRO:O	1:A:308:ARG:HG3	2.04	0.58
1:A:304:GLN:HA	1:A:304:GLN:HE21	1.67	0.57
1:B:1140:ASP:HB2	1:B:1141:ARG:NH2	2.17	0.57
1:A:364:GLN:NE2	1:A:364:GLN:H	2.02	0.57
1:A:281:HIS:CE1	1:A:284:TYR:HB2	2.40	0.56
1:B:1237:CYS:HB3	1:B:1240:HIS:O	2.05	0.56
1:A:293:SER:H	1:A:297:HIS:CD2	2.13	0.56
1:A:164:ASP:OD1	1:A:165:PRO:N	2.38	0.56
1:A:321:ALA:HB3	1:A:324:TYR:O	2.06	0.56
1:B:1339:CYS:HA	1:B:1341:LYS:NZ	2.21	0.56
1:A:9:PHE:N	1:A:10:PRO:HD3	2.20	0.56
1:B:1116:GLU:OE1	1:B:1118:ARG:NH1	2.38	0.56
1:B:1288:ARG:HH21	1:B:1366:LEU:N	2.01	0.56
1:B:1159:LEU:HD23	1:B:1170:PHE:CE2	2.33	0.56
1:A:133:GLU:HG3	1:A:175:ARG:HB2	1.89	0.55
1:A:335:GLN:HE21	1:A:336:ALA:N	2.04	0.55
1:A:344:ALA:HB2	1:A:359:VAL:HG22	1.87	0.55
1:A:125:LYS:NZ	1:A:386:SER:HB2	2.21	0.55
1:B:1304:GLN:N	1:B:1305:PRO:HD2	2.22	0.55
1:A:255:ARG:HH21	1:A:258:THR:HG23	1.72	0.54
1:B:1394:VAL:HG22	1:B:1422:PHE:CD1	2.42	0.54
1:A:339:CYS:C	1:A:341:LYS:H	2.15	0.54
1:B:1070:ARG:CZ	1:B:1124:LYS:HE3	2.38	0.54
1:B:1350:LYS:HD2	1:B:1356:GLN:CD	2.33	0.54
1:B:1356:GLN:HG2	6:B:1632:HOH:O	2.08	0.54
1:A:412:VAL:O	1:A:414:THR:HG23	2.08	0.53
1:A:153:LYS:HD2	1:A:157:ALA:HA	1.90	0.53
1:A:125:LYS:HZ1	1:A:386:SER:HB2	1.73	0.53
1:A:403:ALA:HB3	1:A:407:GLY:O	2.09	0.53
1:B:1207:VAL:HG22	1:B:1207:VAL:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1012:LEU:HD21	1:B:1100:LEU:HD22	1.91	0.53
1:A:64:LEU:C	1:A:65:LEU:HD12	2.34	0.53
1:A:304:GLN:N	1:A:305:PRO:HD2	2.23	0.53
1:A:365:ASN:N	1:A:365:ASN:HD22	2.07	0.53
1:B:1011:GLU:CD	1:B:1011:GLU:H	2.17	0.53
1:B:1329:SER:OG	1:B:1335:GLN:HG2	2.09	0.53
1:A:82:LYS:HG3	1:A:83:GLN:N	2.24	0.52
1:A:124:LYS:HE2	1:A:388:GLY:HA2	1.92	0.52
1:A:140:ASP:OD2	1:A:144:LYS:HB2	2.08	0.52
1:A:118:ARG:HG3	1:A:118:ARG:HH11	1.74	0.52
1:B:1038:VAL:HG13	1:B:1038:VAL:O	2.10	0.52
1:B:1359:VAL:HB	1:B:1383:GLU:HG3	1.91	0.52
1:B:1366:LEU:HD23	1:B:1367:THR:N	2.24	0.52
1:B:1011:GLU:HG3	6:B:1707:HOH:O	2.10	0.52
1:A:255:ARG:NH2	1:A:258:THR:OG1	2.43	0.52
1:A:366:LEU:HD12	1:A:366:LEU:C	2.34	0.51
1:B:1167:THR:CG2	1:B:1200:ARG:HE	2.23	0.51
1:A:382:GLY:O	1:A:390:GLN:HB3	2.10	0.51
1:B:1079:VAL:HG12	1:B:1088:ILE:HD12	1.92	0.51
1:B:1223:VAL:HA	1:B:1246:ILE:O	2.10	0.51
1:B:1259:ILE:N	1:B:1259:ILE:HD12	2.26	0.51
1:A:73:LEU:HD12	1:A:94:PHE:CE1	2.47	0.50
1:A:178:GLU:OE2	1:A:180:LEU:HB2	2.11	0.50
1:B:1299:VAL:HG23	1:B:1432:VAL:CG1	2.31	0.50
1:A:348:GLN:HE22	4:A:602:M6P:H2	1.76	0.50
1:A:164:ASP:OD1	1:A:166:ASP:N	2.44	0.50
1:A:69:SER:OG	1:A:72:LEU:HB3	2.12	0.50
1:B:1141:ARG:HH12	1:B:1219:ASN:CA	2.24	0.50
1:B:1365:ASN:HB3	1:B:1380:PHE:CE1	2.47	0.50
1:A:102:THR:HG22	1:A:137:TYR:CD2	2.47	0.50
1:A:164:ASP:OD1	1:A:165:PRO:HD2	2.12	0.50
1:A:53:LYS:HG3	1:A:54:THR:HG23	1.94	0.50
1:A:201:GLY:O	1:A:202:ASP:C	2.55	0.50
1:B:1148:LEU:N	1:B:1148:LEU:CD1	2.75	0.50
1:B:1148:LEU:N	1:B:1148:LEU:HD12	2.26	0.50
1:B:1179:VAL:O	1:B:1188:ARG:HG3	2.12	0.50
1:A:302:ASP:OD1	1:A:304:GLN:HB3	2.11	0.49
1:B:1428:LYS:C	1:B:1430:ALA:H	2.19	0.49
1:A:125:LYS:C	1:A:127:ILE:H	2.18	0.49
1:B:1218:SER:HB3	1:B:1221:ARG:HB2	1.95	0.49
1:B:1031:ASN:ND2	1:B:1034:GLY:N	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:SER:HB2	1:A:15:TYR:CE1	2.47	0.49
1:A:7:ALA:HB3	1:A:10:PRO:HG3	1.95	0.49
1:A:218:SER:O	1:A:218:SER:OG	2.29	0.49
1:B:1251:PRO:HG3	1:B:1255:ARG:HD2	1.94	0.49
1:A:329:SER:OG	1:A:335:GLN:HG2	2.12	0.49
1:A:353:ASP:C	1:A:355:THR:H	2.21	0.48
1:A:362:ARG:HG2	1:A:362:ARG:HH11	1.78	0.48
1:A:385:CYS:O	1:A:388:GLY:N	2.41	0.48
1:B:1189:VAL:HG12	1:B:1189:VAL:O	2.12	0.48
1:A:281:HIS:ND1	1:A:283:ASP:OD2	2.47	0.48
1:A:408:ARG:O	1:A:427:THR:HB	2.13	0.48
1:B:1288:ARG:NH2	1:B:1366:LEU:H	2.08	0.48
1:A:255:ARG:NH2	1:A:258:THR:HG23	2.29	0.48
1:B:1196:ALA:CB	1:B:1244:VAL:HG21	2.44	0.48
1:A:106:VAL:O	1:A:107:THR:HB	2.13	0.48
1:A:200:ARG:O	1:A:200:ARG:HG3	2.13	0.48
1:B:1027:LEU:C	1:B:1027:LEU:HD23	2.39	0.48
1:B:1012:LEU:CD2	1:B:1100:LEU:HD22	2.44	0.48
1:B:1038:VAL:CG1	1:B:1041:CYS:HB2	2.43	0.48
1:A:124:LYS:HG3	1:A:387:SER:O	2.13	0.48
1:A:262:LEU:HD13	1:A:262:LEU:C	2.39	0.47
1:A:324:TYR:HA	1:A:351:LYS:HG3	1.96	0.47
1:B:1262:LEU:HD11	1:B:1265:LYS:HE2	1.95	0.47
1:B:1348:GLN:HE22	4:B:1503:M6P:H2	1.79	0.47
1:A:11:GLU:OE2	1:A:129:LYS:HE3	2.14	0.47
1:B:1026:MET:SD	1:B:1049:MET:HE3	2.54	0.47
1:A:152:ILE:HG12	1:A:173:VAL:O	2.14	0.47
1:A:364:GLN:C	1:A:365:ASN:HD22	2.21	0.47
1:B:1132:LYS:HG3	1:B:1210:PRO:HG2	1.95	0.47
1:B:1181:ARG:HD3	1:B:1181:ARG:N	2.29	0.47
1:A:251:PRO:HG3	1:A:275:VAL:HG13	1.94	0.47
1:A:305:PRO:HB2	1:A:429:TYR:CZ	2.49	0.47
1:B:1014:SER:HB2	1:B:1015:TYR:CE1	2.49	0.47
1:A:62:ASP:CB	1:A:65:LEU:HD13	2.38	0.47
1:A:401:GLN:NE2	1:A:401:GLN:HA	2.30	0.47
1:A:164:ASP:OD1	1:A:165:PRO:CD	2.63	0.47
1:B:1286:GLU:OE1	1:B:1369:ARG:HD3	2.15	0.47
1:B:1031:ASN:HD22	1:B:1034:GLY:N	2.13	0.47
1:B:1065:LEU:HB3	1:B:1076:ASN:HB2	1.98	0.46
1:A:106:VAL:HG23	1:A:107:THR:HG22	1.96	0.46
1:B:1096:CYS:HB3	1:B:1388:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1348:GLN:HE22	4:B:1503:M6P:C2	2.28	0.46
1:B:1266:SER:O	1:B:1269:ARG:HB3	2.15	0.46
1:B:1211:GLN:HG2	1:B:1212:GLU:N	2.30	0.46
1:A:291:SER:HA	1:A:301:VAL:O	2.15	0.46
1:B:1350:LYS:HD2	1:B:1356:GLN:NE2	2.31	0.46
1:A:344:ALA:CB	1:A:359:VAL:HG13	2.46	0.46
1:A:195:ALA:HB1	1:A:226:TYR:CE2	2.51	0.46
1:B:1339:CYS:HA	1:B:1341:LYS:HE3	1.98	0.46
1:A:27:LEU:C	1:A:27:LEU:HD23	2.40	0.46
1:B:1408:ARG:HH11	1:B:1408:ARG:HB3	1.80	0.46
1:A:179:VAL:HG23	1:A:180:LEU:N	2.31	0.45
1:A:257:GLY:CA	1:A:372:ASP:HB3	2.46	0.45
1:A:341:LYS:HE2	1:A:357:VAL:HG11	1.98	0.45
1:B:1132:LYS:CG	1:B:1210:PRO:HG2	2.46	0.45
1:A:41:CYS:O	1:A:45:SER:HB2	2.17	0.45
1:A:365:ASN:HB3	1:A:380:PHE:CE1	2.51	0.45
1:A:243:ALA:HB3	1:A:269:ARG:HD3	1.98	0.45
1:A:125:LYS:HZ3	1:A:386:SER:C	2.24	0.45
1:B:1060:VAL:HG23	1:B:1090:SER:OG	2.17	0.45
1:B:1268:CYS:HA	1:B:1270:PHE:CE1	2.52	0.45
1:B:1339:CYS:HA	1:B:1341:LYS:CE	2.47	0.45
1:A:394:VAL:HG22	1:A:422:PHE:CD1	2.52	0.45
1:A:38:VAL:O	1:A:39:ALA:C	2.60	0.45
1:B:1141:ARG:HH22	1:B:1219:ASN:HA	1.81	0.45
1:A:341:LYS:HD3	1:A:341:LYS:N	2.26	0.45
1:A:421:TYR:CD1	1:A:421:TYR:N	2.85	0.45
1:B:1141:ARG:H	1:B:1141:ARG:NE	2.01	0.45
1:B:1147:ASP:C	1:B:1148:LEU:HD12	2.42	0.45
1:A:238:ASP:HA	6:A:730:HOH:O	2.16	0.44
1:A:364:GLN:H	1:A:364:GLN:HE21	1.65	0.44
1:A:400:ASN:ND2	1:A:403:ALA:HB2	2.22	0.44
1:B:1032:ILE:HD12	1:B:1073:LEU:CD1	2.47	0.44
1:B:1072:LEU:HD12	1:B:1092:ILE:O	2.18	0.44
1:B:1270:PHE:CD1	1:B:1270:PHE:N	2.85	0.44
1:B:1024:ASN:O	1:B:1026:MET:HE2	2.17	0.44
1:A:281:HIS:HE1	6:A:785:HOH:O	1.99	0.44
1:A:308:ARG:HB2	1:A:408:ARG:HH12	1.80	0.44
1:A:100:LEU:HG	1:A:133:GLU:HB3	1.99	0.44
1:B:1174:CYS:H	1:B:1224:LEU:HD21	1.82	0.44
1:A:196:ALA:HB3	1:A:244:VAL:HG21	1.99	0.44
1:A:324:TYR:CA	1:A:351:LYS:HG3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1218:SER:O	1:B:1219:ASN:C	2.61	0.44
1:B:1259:ILE:HD12	1:B:1259:ILE:H	1.82	0.44
1:A:365:ASN:HB3	1:A:380:PHE:CD1	2.53	0.44
1:B:1288:ARG:NE	1:B:1366:LEU:O	2.34	0.44
1:A:94:PHE:O	1:A:95:LEU:HD23	2.18	0.43
1:A:149:ASN:N	1:A:150:PRO:CD	2.81	0.43
1:A:255:ARG:HH21	1:A:258:THR:CG2	2.30	0.43
1:B:1103:PRO:HB3	1:B:1117:TRP:CE3	2.53	0.43
1:A:326:TYR:CE2	1:A:348:GLN:HG3	2.53	0.43
1:A:39:ALA:C	1:A:41:CYS:N	2.74	0.43
1:A:186:GLN:O	1:A:189:VAL:HG22	2.17	0.43
1:B:1315:LEU:HD23	1:B:1334:SER:OG	2.19	0.43
1:B:1211:GLN:HB3	6:B:1679:HOH:O	2.18	0.43
1:A:200:ARG:O	1:A:203:ARG:HD2	2.19	0.43
1:A:257:GLY:HA3	1:A:372:ASP:HB3	2.00	0.43
1:A:401:GLN:HA	1:A:401:GLN:HE21	1.83	0.43
1:B:1046:ALA:HB2	1:B:1063:SER:HB3	2.01	0.43
1:B:1365:ASN:HD22	1:B:1381:GLY:CA	2.25	0.43
1:B:1172:ASN:HD22	1:B:1175:ARG:HD2	1.76	0.43
1:B:1200:ARG:O	1:B:1201:GLY:C	2.62	0.43
1:B:1380:PHE:HB2	6:B:1615:HOH:O	2.19	0.43
1:A:124:LYS:HE2	1:A:388:GLY:CA	2.49	0.43
1:A:125:LYS:NZ	1:A:386:SER:CB	2.82	0.43
1:A:394:VAL:O	1:A:394:VAL:CG2	2.67	0.43
1:B:1264:ALA:HB3	1:B:1271:GLU:HB2	2.00	0.43
1:B:1255:ARG:HD3	1:B:1255:ARG:N	2.33	0.43
1:A:348:GLN:HE22	4:A:602:M6P:C2	2.32	0.42
1:A:161:ASP:OD2	1:A:259:ILE:HB	2.19	0.42
1:A:317:TYR:CD2	1:A:411:PRO:HD3	2.54	0.42
1:A:350:LYS:HD3	1:A:353:ASP:HB3	2.01	0.42
1:A:391:ARG:HG3	1:A:391:ARG:HH11	1.84	0.42
1:B:1365:ASN:HB3	1:B:1380:PHE:CD1	2.54	0.42
1:A:86:HIS:HB3	1:A:111:CYS:SG	2.60	0.42
1:A:92:ILE:HG12	1:A:115:PHE:HB2	2.02	0.42
1:B:1418:ASP:O	1:B:1419:CYS:HB2	2.18	0.42
1:A:218:SER:C	1:A:220:ASP:H	2.27	0.42
1:B:1179:VAL:HG22	1:B:1192:THR:HG22	2.00	0.42
1:B:1314:SER:C	1:B:1316:PHE:H	2.27	0.42
1:A:8:GLU:HG3	1:A:66:LYS:HZ1	1.83	0.42
1:A:82:LYS:HG2	1:A:110:ASP:OD2	2.19	0.42
1:B:1299:VAL:HG22	1:B:1301:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:GLN:HA	1:A:304:GLN:NE2	2.33	0.42
1:A:332:GLY:O	1:A:333:GLY:C	2.60	0.42
1:A:339:CYS:HA	1:A:341:LYS:HE2	2.01	0.42
3:A:601:NAG:H2	6:A:820:HOH:O	2.19	0.42
1:A:8:GLU:CG	1:A:66:LYS:HZ1	2.33	0.42
1:A:293:SER:N	1:A:297:HIS:HD2	2.02	0.42
1:A:332:GLY:C	1:A:333:GLY:O	2.58	0.42
1:A:353:ASP:C	1:A:355:THR:N	2.78	0.42
1:B:1088:ILE:HA	1:B:1111:CYS:O	2.20	0.42
1:B:1164:ASP:OD1	1:B:1166:ASP:HB2	2.19	0.42
1:A:203:ARG:HB3	1:A:205:PHE:CE1	2.55	0.42
1:A:306:LEU:HD23	1:A:408:ARG:HG2	2.01	0.42
1:A:54:THR:O	1:A:55:ASP:C	2.63	0.42
1:A:253:GLU:O	1:A:255:ARG:HG3	2.20	0.42
1:B:1341:LYS:HG2	1:B:1342:LYS:HG2	2.02	0.42
1:A:84:GLN:O	1:A:85:ASN:HB2	2.20	0.42
1:A:190:CYS:HA	1:A:191:PRO:HD3	1.92	0.42
1:A:304:GLN:NE2	1:A:304:GLN:CA	2.82	0.42
1:A:405:ASN:O	1:A:406:ASN:C	2.61	0.42
1:B:1008:GLU:HA	6:B:1772:HOH:O	2.20	0.42
1:B:1302:ASP:OD1	1:B:1304:GLN:HB3	2.20	0.42
1:B:1338:ILE:O	1:B:1338:ILE:HG12	2.20	0.42
1:A:94:PHE:C	1:A:95:LEU:HD23	2.44	0.41
1:B:1428:LYS:C	1:B:1430:ALA:N	2.77	0.41
1:A:391:ARG:HG3	1:A:391:ARG:NH1	2.35	0.41
1:B:1042:GLY:HA3	6:B:1646:HOH:O	2.20	0.41
1:B:1099:THR:C	1:B:1120:THR:HG23	2.44	0.41
1:B:1292:LEU:HG	1:B:1368:LEU:HD23	2.02	0.41
1:B:1299:VAL:CG2	1:B:1432:VAL:HG13	2.35	0.41
1:A:362:ARG:HG2	1:A:362:ARG:NH1	2.35	0.41
1:A:410:ALA:HA	1:A:411:PRO:HD3	1.84	0.41
1:A:292:LEU:HB3	1:A:297:HIS:CD2	2.56	0.41
1:A:401:GLN:NE2	1:A:428:LYS:HB2	2.36	0.41
1:A:109:THR:O	1:A:110:ASP:C	2.63	0.41
1:A:207:VAL:O	1:A:244:VAL:HG23	2.20	0.41
1:B:1290:CYS:SG	1:B:1366:LEU:HD11	2.61	0.41
1:A:167:THR:HG22	1:A:200:ARG:CB	2.50	0.41
1:B:1040:GLN:CB	1:B:1057:PHE:HB2	2.49	0.41
1:A:36:MET:HG3	1:A:38:VAL:HG23	2.02	0.41
1:A:106:VAL:CG2	1:A:114:TYR:HB2	2.51	0.41
1:A:106:VAL:HG22	1:A:114:TYR:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:THR:HG22	1:A:200:ARG:HB3	2.03	0.41
1:A:308:ARG:HH12	1:A:406:ASN:HB2	1.85	0.41
1:A:314:SER:C	1:A:316:PHE:H	2.29	0.41
1:B:1073:LEU:HB2	1:B:1094:PHE:HE1	1.86	0.41
1:B:1159:LEU:HD13	1:B:1159:LEU:C	2.46	0.41
1:B:1260:PRO:HB3	1:B:1274:TRP:CD2	2.55	0.41
1:B:1297:HIS:O	1:B:1298:ASP:HB2	2.19	0.41
1:B:1315:LEU:HD23	1:B:1334:SER:H	1.85	0.41
2:C:1:NDG:H3	2:C:2:NAG:O1	2.19	0.41
1:A:259:ILE:HG23	1:A:260:PRO:HD2	2.03	0.41
1:A:218:SER:CB	1:A:220:ASP:OD2	2.69	0.40
1:A:385:CYS:O	1:A:386:SER:C	2.64	0.40
1:A:281:HIS:O	1:A:284:TYR:HB3	2.21	0.40
1:A:401:GLN:HE21	1:A:401:GLN:CA	2.34	0.40
1:A:277:GLU:O	1:A:285:LEU:HD11	2.21	0.40
1:A:365:ASN:N	1:A:365:ASN:ND2	2.67	0.40
1:B:1172:ASN:HB2	1:B:1177:ILE:HG12	2.04	0.40
1:A:60:VAL:HG23	1:A:90:SER:OG	2.21	0.40
1:A:251:PRO:HG3	1:A:275:VAL:HG12	2.00	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	418/432 (97%)	367 (88%)	42 (10%)	9 (2%)	5	3
1	B	400/432 (93%)	360 (90%)	36 (9%)	4 (1%)	12	11
All	All	818/864 (95%)	727 (89%)	78 (10%)	13 (2%)	7	6

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ALA
1	A	204	ALA
1	A	40	GLN
1	A	126	ASN
1	A	165	PRO
1	B	1354	SER
1	A	353	ASP
1	A	354	SER
1	B	1109	THR
1	A	340	ASN
1	B	1403	ALA
1	B	1429	TYR
1	A	404	GLY

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	365/370 (99%)	345 (94%)	20 (6%)	19	24
1	B	354/370 (96%)	330 (93%)	24 (7%)	14	17
All	All	719/740 (97%)	675 (94%)	44 (6%)	17	20

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	CYS
1	A	70	ARG
1	A	148	LEU
1	A	159	LEU
1	A	169	LEU
1	A	214	LEU
1	A	249	VAL
1	A	253	GLU
1	A	255	ARG
1	A	261	LYS
1	A	283	ASP

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Mol	Chain	Res	Type
1	A	330	ILE
1	A	335	GLN
1	A	341	LYS
1	A	355	THR
1	A	364	GLN
1	A	366	LEU
1	A	394	VAL
1	A	398	GLU
1	A	402	THR
1	B	1011	GLU
1	B	1014	SER
1	B	1025	ASN
1	B	1078	THR
1	B	1100	LEU
1	B	1136	CYS
1	B	1141	ARG
1	B	1166	ASP
1	B	1169	LEU
1	B	1175	ARG
1	B	1178	GLU
1	B	1188	ARG
1	B	1214	LEU
1	B	1216	LEU
1	B	1228	LYS
1	B	1249	VAL
1	B	1253	GLU
1	B	1255	ARG
1	B	1262	LEU
1	B	1335	GLN
1	B	1341	LYS
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 (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	80	ASN
1	A	84	GLN
1	A	85	ASN
1	A	113	HIS

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Mol	Chain	Res	Type
1	A	131	ASN
1	A	149	ASN
1	A	233	GLN
1	A	240	HIS
1	A	281	HIS
1	A	297	HIS
1	A	304	GLN
1	A	335	GLN
1	A	348	GLN
1	A	364	GLN
1	A	400	ASN
1	A	401	GLN
1	B	1024	ASN
1	B	1031	ASN
1	B	1058	HIS
1	B	1113	HIS
1	B	1126	ASN
1	B	1186	GLN
1	B	1211	GLN
1	B	1219	ASN
1	B	1281	HIS
1	B	1297	HIS
1	B	1304	GLN
1	B	1348	GLN
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 ⓘ

3 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	0.69	0	17,19,21	1.03	1 (5%)
2	NAG	C	2	2	15,15,15	0.62	0	21,21,21	0.74	1 (4%)
2	BMA	C	3	2	11,11,12	0.53	0	15,15,17	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDG	C	1	2	-	3/6/23/26	0/1/1/1
2	NAG	C	2	2	1/1/6/7	4/6/26/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NDG	C2-N2-C7	-2.77	119.19	122.90
2	C	2	NAG	O1-C1-O5	-2.06	104.29	110.41

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	2	NAG	C1

All (7) torsion outliers are listed below:

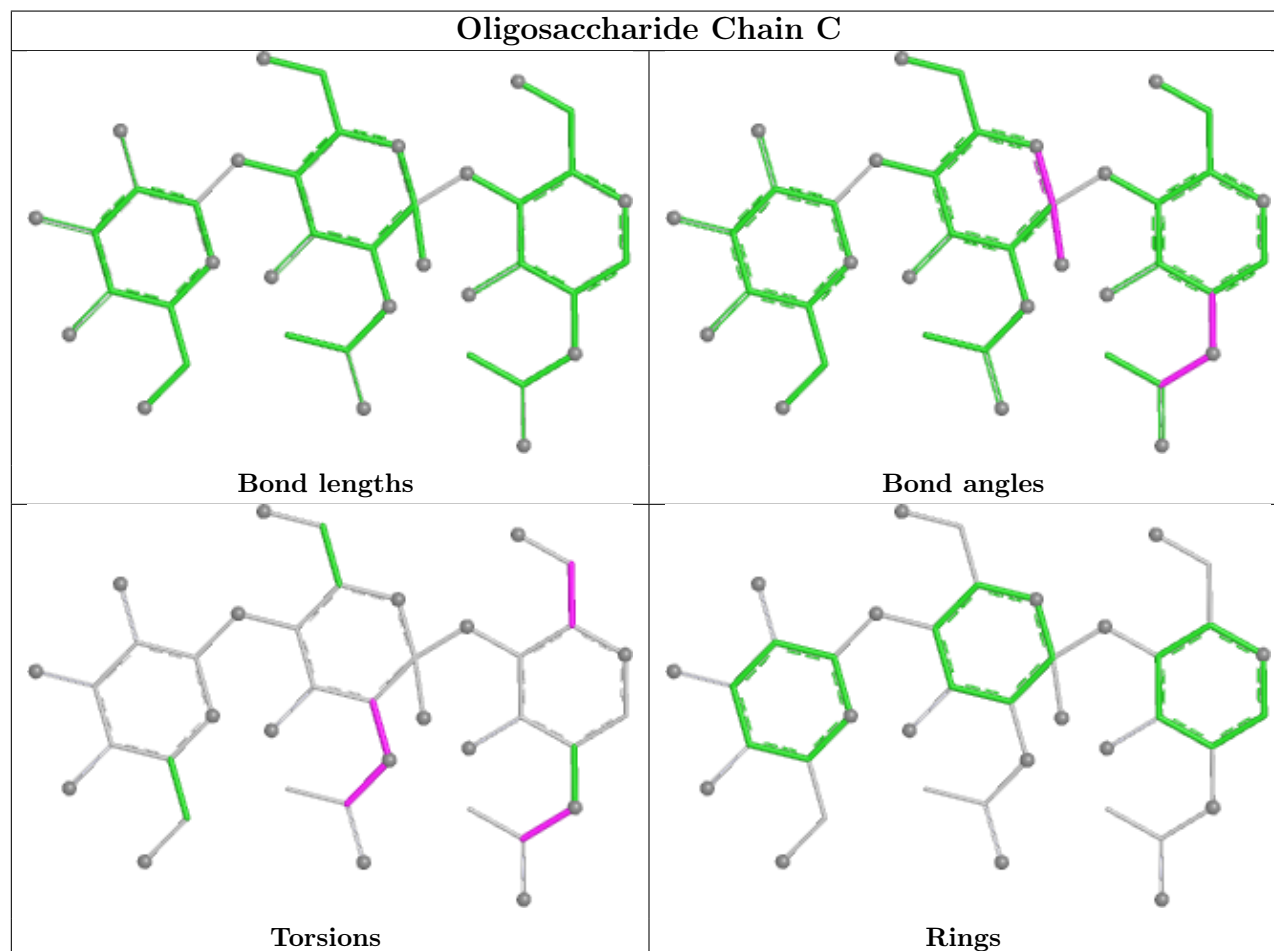
Mol	Chain	Res	Type	Atoms
2	C	1	NDG	C8-C7-N2-C2
2	C	1	NDG	O7-C7-N2-C2
2	C	2	NAG	C1-C2-N2-C7
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	1	NDG	O5-C5-C6-O6
2	C	2	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NDG	4	0
2	C	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](#)

7 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$
5	GOL	A	603	-	5,5,5	4.81	5 (100%)	5,5,5	6.25	3 (60%)
3	NAG	B	1502	-	14,14,15	0.52	0	17,19,21	0.75	1 (5%)
4	M6P	B	1503	-	16,16,16	1.58	4 (25%)	23,24,24	0.90	1 (4%)
3	NAG	A	601	1	14,14,15	0.67	0	17,19,21	0.63	0
4	M6P	A	602	-	16,16,16	1.59	3 (18%)	23,24,24	0.81	0
3	NAG	B	1501	-	14,14,15	0.48	0	17,19,21	0.71	1 (5%)
5	GOL	B	1504	-	5,5,5	4.81	5 (100%)	5,5,5	6.12	3 (60%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	603	-	-	3/4/4/4	-
3	NAG	B	1502	-	-	4/6/23/26	0/1/1/1
4	M6P	B	1503	-	-	0/6/26/26	0/1/1/1
3	NAG	A	601	1	-	4/6/23/26	0/1/1/1
4	M6P	A	602	-	-	0/6/26/26	0/1/1/1
3	NAG	B	1501	-	-	4/6/23/26	0/1/1/1
5	GOL	B	1504	-	-	2/4/4/4	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	603	GOL	C3-C2	-8.17	1.20	1.51
5	B	1504	GOL	C3-C2	-8.05	1.21	1.51
5	B	1504	GOL	O1-C1	4.58	1.61	1.42
5	A	603	GOL	O1-C1	4.31	1.60	1.42
4	A	602	M6P	P-O1P	3.74	1.62	1.50
5	B	1504	GOL	O3-C3	3.52	1.57	1.42
5	A	603	GOL	O3-C3	3.47	1.57	1.42
4	B	1503	M6P	P-O1P	3.47	1.61	1.50
5	A	603	GOL	O2-C2	-3.05	1.34	1.43
5	A	603	GOL	C1-C2	-3.01	1.40	1.51
5	B	1504	GOL	C1-C2	-3.00	1.40	1.51
5	B	1504	GOL	O2-C2	-2.93	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1503	M6P	C3-C2	2.26	1.58	1.52
4	A	602	M6P	C3-C2	2.14	1.57	1.52
4	B	1503	M6P	O5-C5	2.07	1.49	1.44
4	B	1503	M6P	O5-C1	2.03	1.47	1.42
4	A	602	M6P	O5-C5	2.01	1.49	1.44

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	603	GOL	O3-C3-C2	11.40	161.69	110.38
5	B	1504	GOL	O3-C3-C2	10.84	159.18	110.38
5	B	1504	GOL	O2-C2-C3	7.53	140.34	109.18
5	A	603	GOL	O2-C2-C3	7.38	139.74	109.18
5	B	1504	GOL	O1-C1-C2	3.46	125.96	110.38
5	A	603	GOL	O1-C1-C2	3.19	124.75	110.38
3	B	1502	NAG	C2-N2-C7	-2.27	119.86	122.90
3	B	1501	NAG	C2-N2-C7	-2.05	120.15	122.90
4	B	1503	M6P	O3P-P-O6	2.02	111.94	106.67

There are no chirality outliers.

All (17) torsion outliers are listed below:

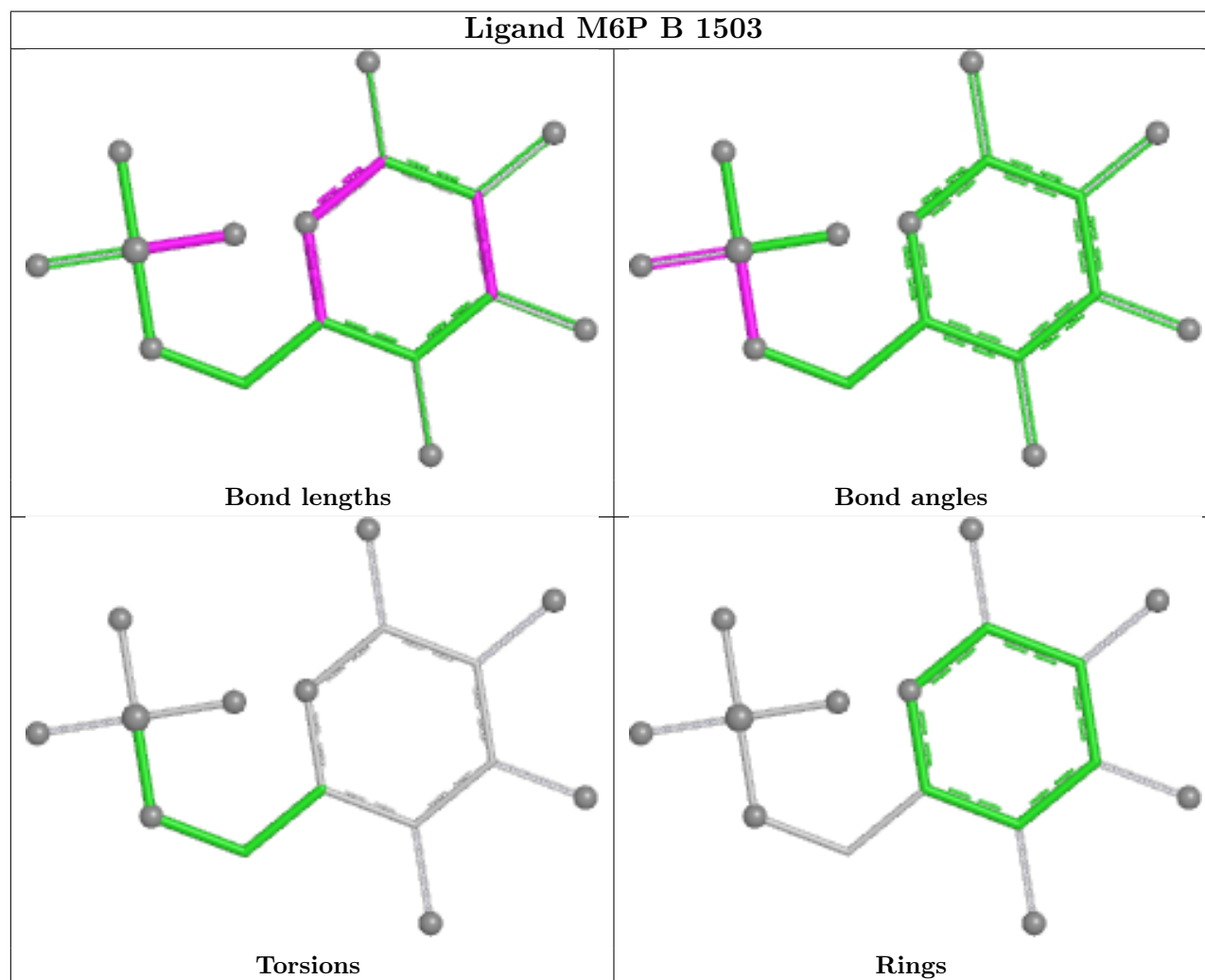
Mol	Chain	Res	Type	Atoms
3	A	601	NAG	C8-C7-N2-C2
3	A	601	NAG	O7-C7-N2-C2
3	B	1501	NAG	C8-C7-N2-C2
3	B	1501	NAG	O7-C7-N2-C2
3	B	1502	NAG	C8-C7-N2-C2
3	B	1502	NAG	O7-C7-N2-C2
5	A	603	GOL	C1-C2-C3-O3
5	B	1504	GOL	O1-C1-C2-C3
5	B	1504	GOL	C1-C2-C3-O3
3	B	1502	NAG	C4-C5-C6-O6
3	B	1502	NAG	O5-C5-C6-O6
5	A	603	GOL	O1-C1-C2-C3
5	A	603	GOL	O1-C1-C2-O2
3	B	1501	NAG	C4-C5-C6-O6
3	A	601	NAG	O5-C5-C6-O6
3	B	1501	NAG	O5-C5-C6-O6
3	A	601	NAG	C3-C2-N2-C7

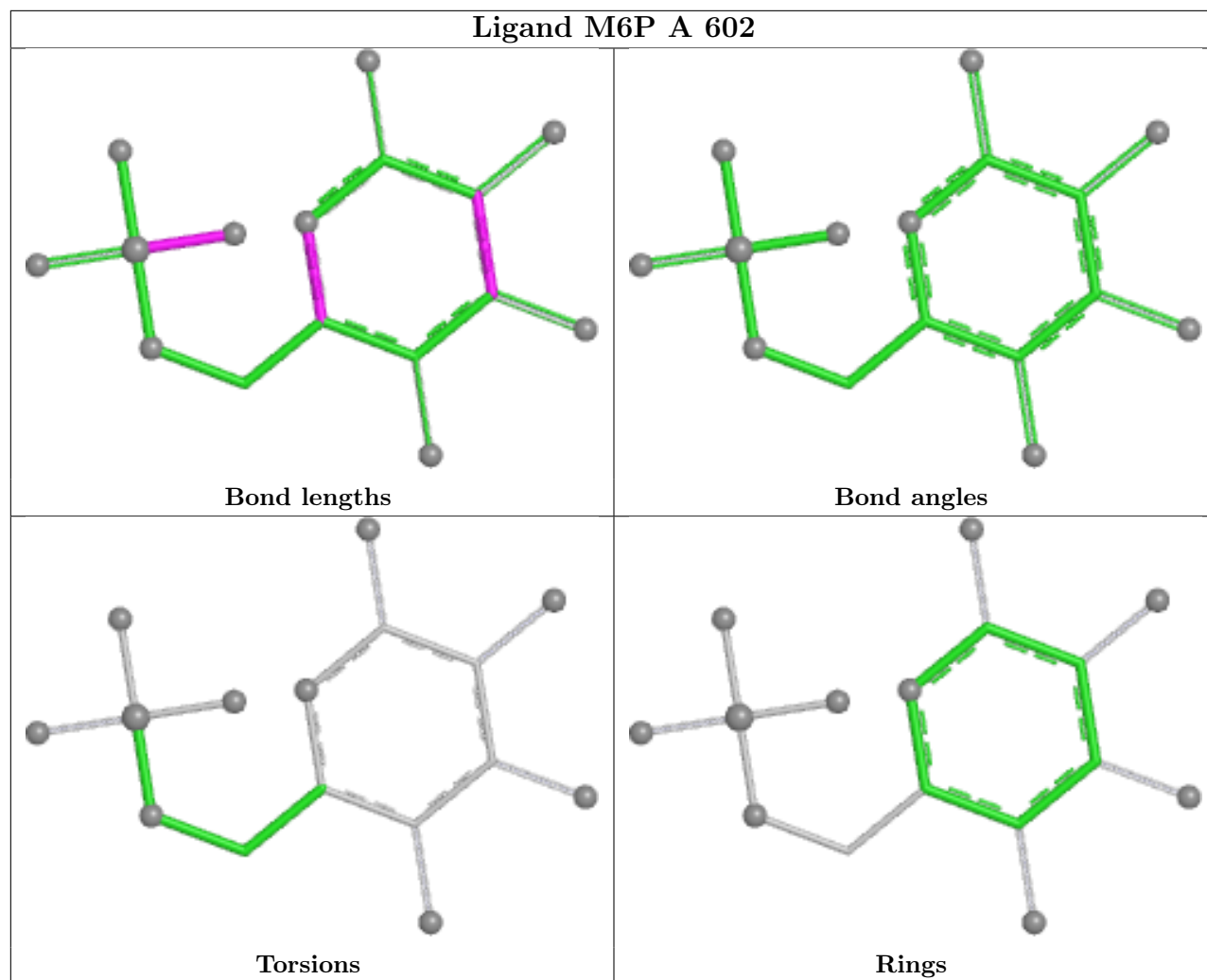
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1503	M6P	2	0
3	A	601	NAG	1	0
4	A	602	M6P	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 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	422/432 (97%)	0.36	19 (4%) 38 35	16, 40, 66, 84	0
1	B	408/432 (94%)	0.13	8 (1%) 65 62	13, 37, 64, 78	0
All	All	830/864 (96%)	0.24	27 (3%) 49 46	13, 38, 65, 84	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	ARG	4.0
1	A	308	ARG	3.7
1	A	338	ILE	3.3
1	B	1236	PHE	3.1
1	A	58	HIS	2.9
1	A	331	CYS	2.8
1	A	185	PRO	2.8
1	B	1336	ALA	2.8
1	B	1007	ALA	2.7
1	B	1039	ALA	2.4
1	B	1038	VAL	2.4
1	A	339	CYS	2.4
1	A	7	ALA	2.3
1	B	1337	PRO	2.3
1	A	201	GLY	2.3
1	A	39	ALA	2.3
1	A	38	VAL	2.3
1	A	340	ASN	2.2
1	A	406	ASN	2.2
1	B	1163	SER	2.2
1	A	404	GLY	2.1
1	A	315	LEU	2.1
1	A	332	GLY	2.1
1	A	314	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	1315	LEU	2.0
1	A	432	VAL	2.0
1	A	128	PHE	2.0

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

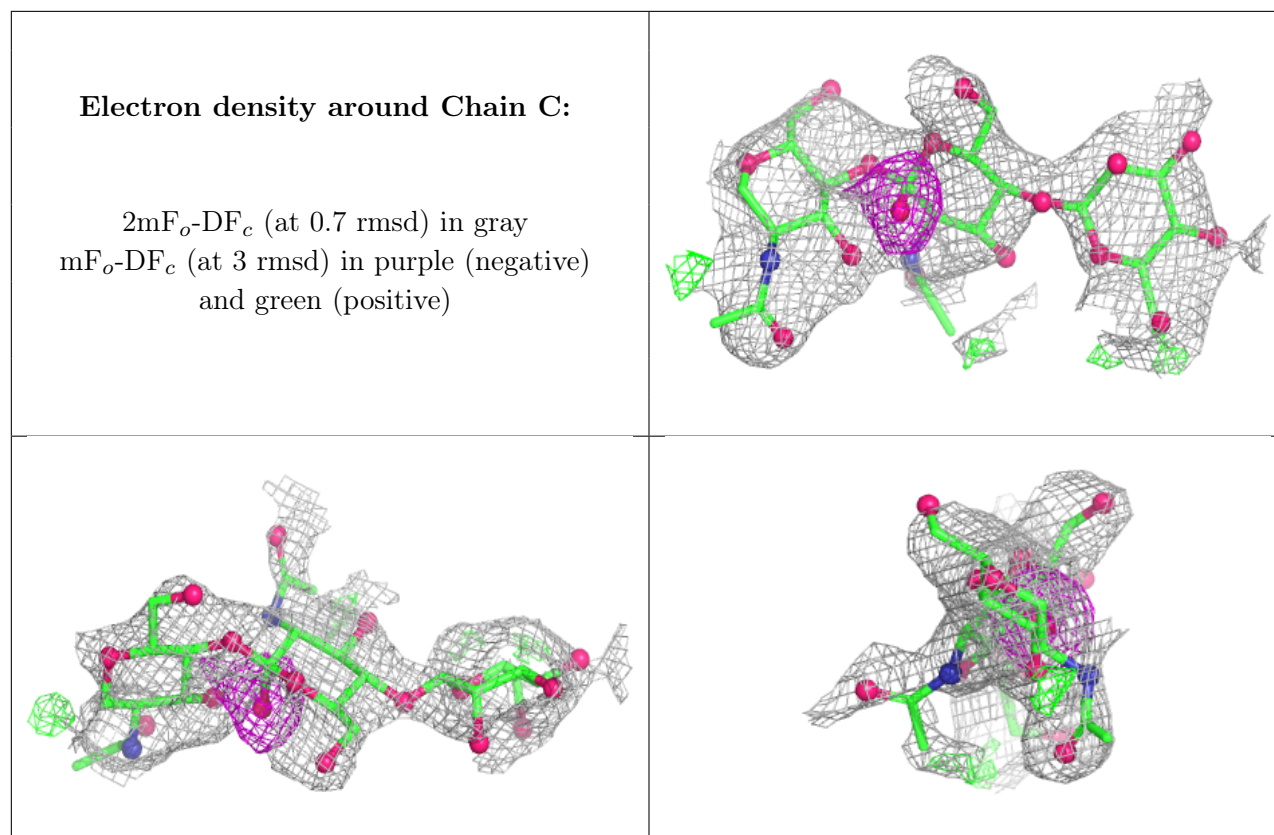
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
2	NAG	C	2	15/15	0.41	0.17	39,86,87,89	0
2	BMA	C	3	11/12	0.44	0.15	90,90,90,91	0
2	NDG	C	1	14/15	0.80	0.14	69,72,76,79	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.



6.4 Ligands [i](#)

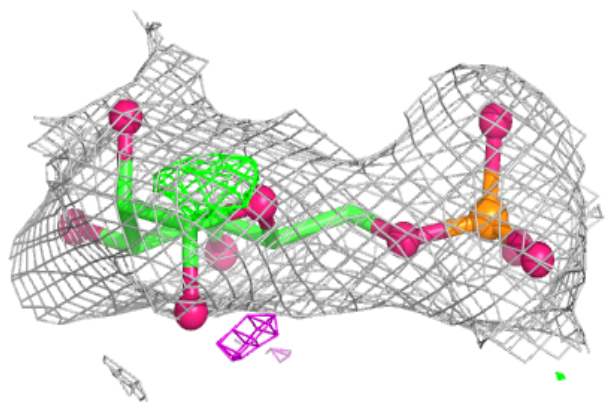
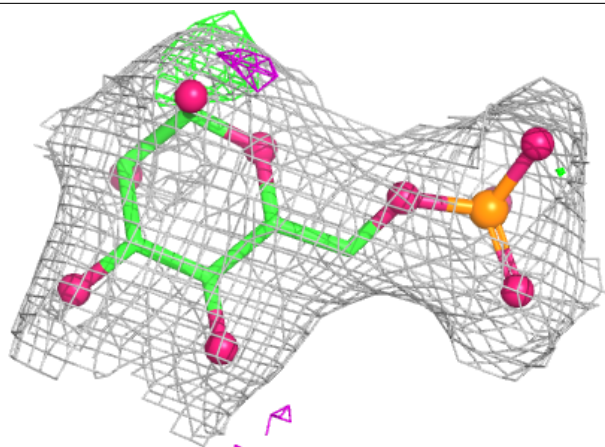
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	NAG	B	1502	14/15	0.68	0.14	52,54,57,62	0
3	NAG	B	1501	14/15	0.70	0.13	61,62,64,65	0
3	NAG	A	601	14/15	0.81	0.10	59,62,64,65	0
5	GOL	B	1504	6/6	0.84	0.14	48,49,49,51	0
5	GOL	A	603	6/6	0.85	0.12	63,66,66,68	0
4	M6P	A	602	16/16	0.87	0.10	42,44,47,47	0
4	M6P	B	1503	16/16	0.90	0.11	34,39,45,48	0

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

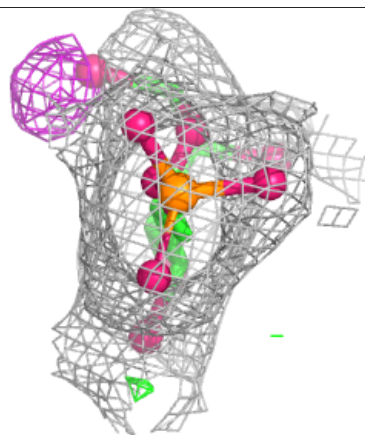
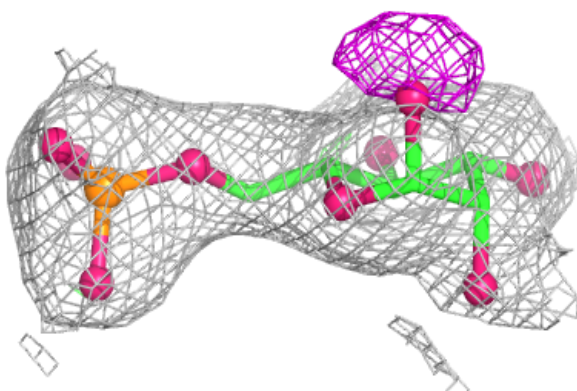
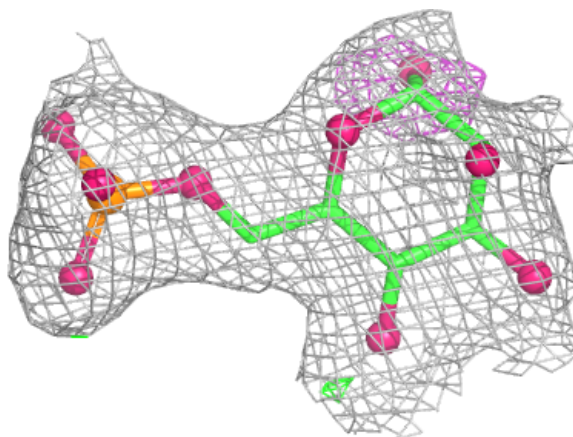
Electron density around M6P A 602:

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



Electron density around M6P B 1503:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.