



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:27 AM UTC

PDB ID : 2OYE / pdb_00002oye
Title : Indomethacin-(R)-alpha-ethyl-ethanolamide bound to Cyclooxygenase-1
Authors : Harman, C.A.; Garavito, R.M.
Deposited on : 2007-02-21
Resolution : 2.85 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

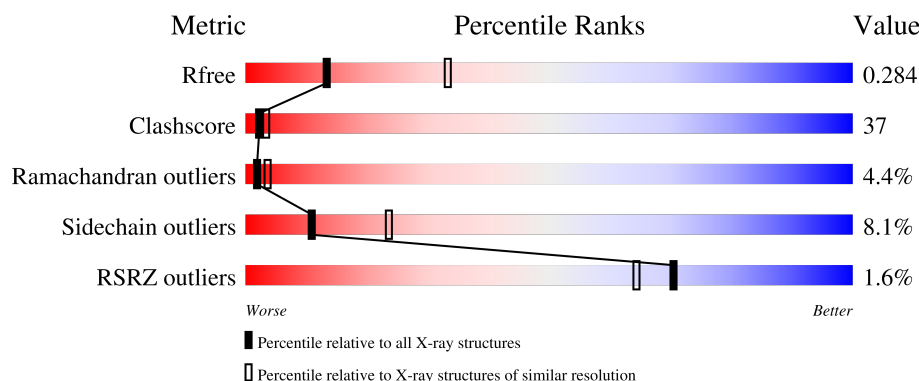
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

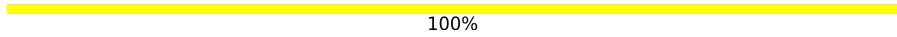
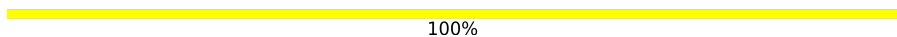
The reported resolution of this entry is 2.85 Å.

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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	P	600	 2% 39% 44% 8% 8%
2	A	2	 100%
3	B	4	 25% 75%
4	C	2	 100%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4605 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 Prostaglandin G/H synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	553	Total	C	N	O	S	0	0	0
			4362	2838	728	768	28			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	92	LEU	MET	SEE REMARK 999	UNP P05979

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



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

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



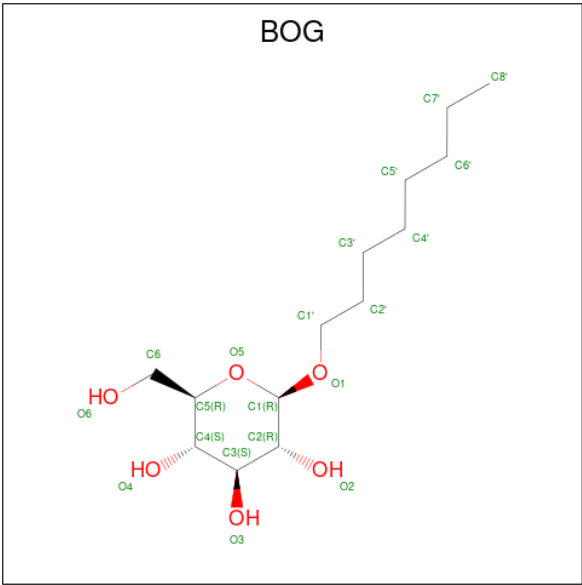
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 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
4	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



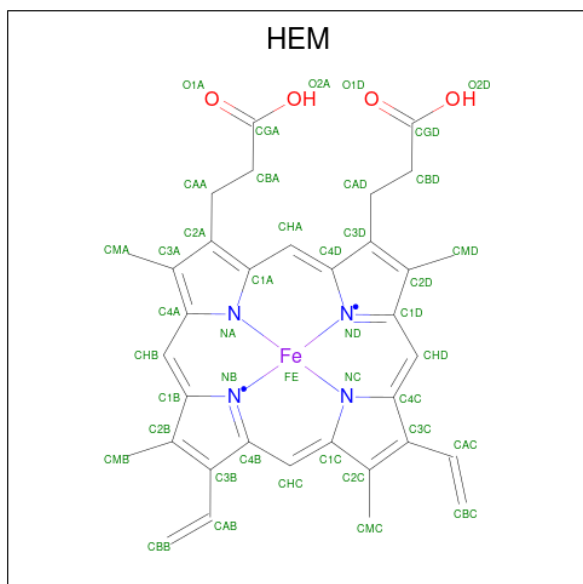
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	P	1	Total	C	O	0	0
			12	6	6		
5	P	1	Total	C	O	0	0
			12	6	6		

- Molecule 6 is CITRATE ANION (CCD ID: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	P	1	Total	C	O	0	0
			13	6	7		

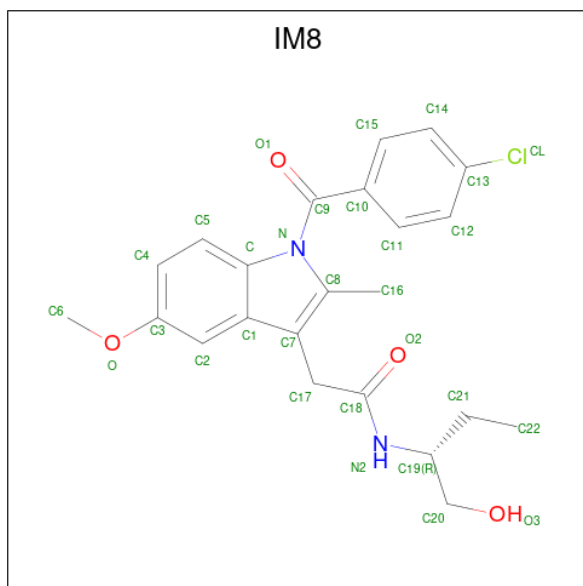
- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 8 is 2-[1-(4-CHLOROBENZOYL)-5-METHOXY-2-METHYL-1H-INDOL-3-YL]-N-[(1R)-1-(HYDROXYMETHYL)PROPYL]ACETAMIDE (CCD ID: IM8) (formula:

$C_{23}H_{25}ClN_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	P	1	Total	C	Cl	N	O	
			30	23	1	2	4	
							0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	P	27	Total	O		
			27	27	0	0

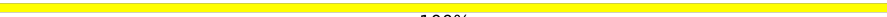
NAG1
NDG2

- Molecule 3: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  25% 75%

NAG1
NAG2
BMA3
BMA4

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

Chain C:  100%

NAG1
NAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	181.72Å 181.72Å 104.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.85 30.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	93.3 (30.00-2.85) 94.9 (30.00-2.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.68Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.292 0.239 , 0.284	Depositor DCC
R_{free} test set	1081 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å ²)	71.8	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4605	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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: IM8, HEM, BOG, NDG, BMA, FLC, 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	P	0.57	0/4501	1.09	33/6136 (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	P	0	1

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	148	TYR	N-CA-C	-8.69	97.66	110.52
1	P	224	LEU	N-CA-C	-8.21	99.47	110.55
1	P	356	PHE	N-CA-C	-7.61	103.79	113.23
1	P	381	PHE	N-CA-C	-7.26	102.97	111.03
1	P	95	HIS	N-CA-C	7.04	122.54	113.18
1	P	417	TYR	N-CA-C	6.75	118.64	111.28
1	P	285	MET	N-CA-C	6.62	120.28	110.48
1	P	357	LEU	N-CA-C	-6.41	100.17	109.59
1	P	519	GLY	N-CA-C	6.32	122.17	112.51
1	P	259	GLY	N-CA-C	-6.13	106.63	115.27
1	P	294	LEU	N-CA-C	6.09	119.54	111.75
1	P	467	ARG	N-CA-C	-6.01	104.42	110.97
1	P	513	HIS	N-CA-C	-5.93	102.30	109.83
1	P	221	THR	N-CA-C	5.92	119.17	108.69
1	P	391	MET	CA-C-N	5.82	127.11	119.84
1	P	391	MET	C-N-CA	5.82	127.11	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	241	GLN	N-CA-C	-5.75	104.93	111.14
1	P	143	SER	N-CA-C	5.74	120.42	112.90
1	P	73	GLU	N-CA-C	-5.70	103.12	110.19
1	P	71	ILE	CA-C-N	5.66	125.59	119.76
1	P	71	ILE	C-N-CA	5.66	125.59	119.76
1	P	247	PHE	N-CA-C	5.58	122.68	110.80
1	P	403	SER	N-CA-C	-5.58	101.72	110.36
1	P	185	ARG	N-CA-C	-5.56	103.05	111.34
1	P	129	THR	N-CA-C	5.52	119.57	111.34
1	P	564	LEU	N-CA-C	-5.43	104.78	111.40
1	P	62	THR	N-CA-C	-5.39	106.75	113.38
1	P	345	ILE	N-CA-C	5.34	115.60	110.74
1	P	447	VAL	N-CA-C	-5.14	104.96	110.36
1	P	101	ASP	N-CA-C	-5.12	105.88	111.82
1	P	425	ALA	N-CA-C	5.08	118.26	111.75
1	P	354	GLY	N-CA-C	-5.05	107.84	115.32
1	P	550	PHE	N-CA-C	-5.04	105.61	112.26

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	147	TYR	Sidechain

5.2 Too-close contacts [\(i\)](#)

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	P	4362	0	4159	321	0
2	A	28	0	24	0	0
3	B	50	0	43	4	0
4	C	28	0	25	0	0
5	P	24	0	22	5	0
6	P	13	0	5	3	0
7	P	43	0	30	6	0
8	P	30	0	25	5	0
9	P	27	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4605	0	4333	327	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 37.

All (327) 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:P:240:ARG:HG3	1:P:271:VAL:HG21	1.34	1.08
1:P:263:PRO:HD2	1:P:285:MET:HE2	1.37	1.03
1:P:151:ILE:HG23	1:P:469:ARG:NH1	1.81	0.95
1:P:339:GLU:HG2	1:P:562:ALA:HB2	1.48	0.95
1:P:202:ALA:O	1:P:206:THR:HG23	1.71	0.90
1:P:387:TRP:HB2	7:P:601:HEM:HBC2	1.53	0.90
1:P:182:LEU:HB3	1:P:440:ILE:HD12	1.55	0.89
1:P:391:MET:HG3	7:P:601:HEM:HAB	1.56	0.86
1:P:120:ARG:NH1	8:P:700:IM8:H201	1.93	0.83
1:P:102:PHE:O	1:P:106:THR:HG23	1.79	0.81
1:P:566:LYS:O	1:P:570:LEU:HB2	1.82	0.79
1:P:582:VAL:HG23	1:P:583:PRO:HD2	1.64	0.78
1:P:272:LEU:HD12	1:P:273:MET:N	1.98	0.78
1:P:243:GLN:HG3	1:P:270:PRO:HG2	1.67	0.76
1:P:344:VAL:O	1:P:348:TYR:HB3	1.85	0.76
1:P:241:GLN:O	1:P:245:ARG:HG3	1.86	0.76
1:P:191:PRO:HB2	1:P:515:ASN:HA	1.69	0.75
1:P:216:MET:HG2	3:B:2:NAG:H82	1.70	0.74
1:P:300:LEU:HD11	1:P:419:VAL:HG13	1.70	0.74
1:P:163:MET:HB3	1:P:462:PRO:HG3	1.70	0.73
1:P:273:MET:HE2	1:P:285:MET:O	1.88	0.73
1:P:388:HIS:HB3	1:P:444:ILE:HD12	1.71	0.73
1:P:137:ILE:HD12	1:P:137:ILE:H	1.53	0.72
1:P:504:TYR:HB3	1:P:505:PRO:HD3	1.70	0.72
1:P:119:VAL:HG12	5:P:751:BOG:H61	1.74	0.70
1:P:208:GLN:NE2	1:P:230:LEU:H	1.89	0.70
1:P:262:TYR:HB3	1:P:285:MET:CE	2.21	0.70
1:P:112:LEU:O	1:P:116:VAL:HG23	1.91	0.70
1:P:326:GLU:OE1	1:P:326:GLU:HA	1.92	0.70
1:P:115:LEU:O	1:P:119:VAL:HG23	1.92	0.69
1:P:530:SER:O	1:P:534:LEU:HD23	1.93	0.69
1:P:208:GLN:HE22	1:P:230:LEU:HD12	1.58	0.69
1:P:237:ASN:ND2	1:P:240:ARG:H	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:239:GLU:H	1:P:239:GLU:CD	2.01	0.68
1:P:171:LEU:HB2	1:P:456:ARG:NH1	2.09	0.68
1:P:323:TRP:CE3	1:P:327:GLN:HG2	2.29	0.67
1:P:291:VAL:HG22	1:P:294:LEU:HD12	1.75	0.67
1:P:263:PRO:HD2	1:P:285:MET:CE	2.20	0.67
1:P:298:LEU:N	1:P:298:LEU:HD12	2.10	0.67
1:P:204:HIS:CD2	1:P:232:HIS:CD2	2.82	0.66
1:P:113:MET:HE2	1:P:117:LEU:HD21	1.78	0.66
1:P:163:MET:HE1	1:P:460:LEU:O	1.95	0.66
1:P:156:PRO:HB2	1:P:159:CYS:SG	2.36	0.65
1:P:183:LEU:HD13	1:P:445:LEU:HD22	1.79	0.65
1:P:287:VAL:HG23	1:P:289:GLN:H	1.62	0.65
1:P:279:ILE:C	1:P:281:PRO:HD2	2.21	0.65
1:P:120:ARG:NH1	8:P:700:IM8:C20	2.60	0.64
1:P:171:LEU:HD12	1:P:456:ARG:HD3	1.77	0.64
1:P:237:ASN:HD21	1:P:240:ARG:H	1.42	0.64
1:P:339:GLU:HG2	1:P:562:ALA:CB	2.26	0.64
1:P:320:HIS:HB3	1:P:323:TRP:CD1	2.33	0.64
1:P:137:ILE:HD12	1:P:137:ILE:N	2.13	0.63
1:P:151:ILE:HG23	1:P:469:ARG:HH11	1.62	0.63
1:P:553:GLU:HG3	1:P:557:ASN:HD21	1.62	0.63
1:P:88:PHE:CE2	1:P:92:LEU:HD11	2.34	0.63
1:P:64:TYR:CE1	1:P:76:THR:HG21	2.34	0.62
1:P:513:HIS:HB2	1:P:516:SER:OG	1.99	0.62
1:P:119:VAL:HG12	5:P:751:BOG:C6	2.29	0.62
1:P:126:SER:HA	1:P:127:PRO:C	2.24	0.62
1:P:279:ILE:HG22	1:P:279:ILE:O	2.00	0.62
1:P:208:GLN:HE21	1:P:230:LEU:H	1.46	0.62
1:P:504:TYR:CZ	1:P:508:LEU:HD11	2.34	0.62
1:P:242:TYR:CD2	1:P:247:PHE:HZ	2.18	0.62
1:P:185:ARG:HD2	1:P:185:ARG:N	2.15	0.62
1:P:282:GLN:O	1:P:283:SER:HB2	1.99	0.61
1:P:43:HIS:O	1:P:44:GLN:HB2	2.00	0.61
1:P:204:HIS:ND1	1:P:301:TYR:HB3	2.16	0.61
1:P:196:LEU:HD11	1:P:392:PRO:HG3	1.83	0.61
1:P:280:PRO:HA	1:P:284:GLN:CG	2.31	0.60
1:P:333:ARG:O	1:P:337:ILE:HG13	2.02	0.60
1:P:134:HIS:HB3	1:P:136:TYR:CE1	2.36	0.60
1:P:260:GLU:CB	1:P:262:TYR:HE1	2.15	0.60
1:P:77:TRP:O	1:P:81:THR:HG23	2.01	0.60
1:P:251:LYS:HB3	1:P:310:ASN:ND2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:263:PRO:HB2	1:P:285:MET:HB3	1.84	0.60
1:P:130:TYR:HB2	1:P:150:ARG:HG3	1.83	0.60
1:P:442:HIS:NE2	1:P:443:HIS:CE1	2.70	0.60
1:P:309:HIS:C	1:P:309:HIS:CD2	2.79	0.59
1:P:483:GLY:N	1:P:511:LYS:HB3	2.17	0.59
1:P:150:ARG:HD3	1:P:152:LEU:O	2.03	0.59
6:P:900:FLC:OA2	6:P:900:FLC:HG2	2.00	0.59
1:P:195:ASN:ND2	1:P:427:SER:HA	2.16	0.59
1:P:279:ILE:C	1:P:281:PRO:CD	2.76	0.59
1:P:564:LEU:HD22	1:P:578:VAL:HG21	1.84	0.59
1:P:40:PRO:O	1:P:68:ASN:HB3	2.03	0.59
1:P:563:THR:HG22	1:P:564:LEU:N	2.18	0.59
1:P:181:PHE:O	1:P:438:ARG:N	2.36	0.59
1:P:213:SER:HA	1:P:222:LYS:HE2	1.84	0.59
1:P:280:PRO:HA	1:P:284:GLN:CD	2.27	0.58
1:P:308:GLU:O	1:P:311:ARG:HB3	2.02	0.58
1:P:93:LEU:CD1	8:P:700:IM8:H222	2.34	0.58
1:P:163:MET:HA	1:P:163:MET:CE	2.33	0.58
1:P:230:LEU:C	1:P:232:HIS:H	2.12	0.58
1:P:275:TYR:CD2	1:P:284:GLN:HG2	2.39	0.58
1:P:388:HIS:HB3	1:P:444:ILE:CD1	2.33	0.58
1:P:344:VAL:HG11	1:P:534:LEU:HD11	1.86	0.57
1:P:96:GLY:O	1:P:97:ARG:C	2.47	0.57
1:P:464:ASN:HB3	9:P:903:HOH:O	2.04	0.57
1:P:295:LEU:CD2	7:P:601:HEM:HBB2	2.35	0.57
1:P:204:HIS:CD2	1:P:232:HIS:HD2	2.22	0.57
1:P:306:LEU:C	1:P:306:LEU:HD23	2.30	0.57
1:P:269:ALA:O	1:P:271:VAL:N	2.35	0.57
1:P:442:HIS:CD2	1:P:443:HIS:N	2.73	0.57
1:P:568:VAL:O	1:P:572:THR:HG23	2.05	0.57
1:P:553:GLU:HG3	1:P:557:ASN:ND2	2.19	0.56
1:P:466:TYR:O	1:P:525:MET:HE2	2.06	0.56
1:P:527:ALA:HB3	1:P:528:PRO:HD3	1.86	0.56
1:P:537:ASN:OD1	1:P:539:ILE:HG23	2.06	0.56
1:P:196:LEU:HD21	1:P:392:PRO:HD3	1.85	0.56
6:P:900:FLC:HA1	7:P:601:HEM:HAA1	1.88	0.56
1:P:577:TYR:CE2	1:P:583:PRO:HD3	2.41	0.56
1:P:246:LEU:HD12	1:P:253:LYS:HG2	1.88	0.56
1:P:97:ARG:O	1:P:101:ASP:OD2	2.24	0.56
1:P:177:LEU:HD12	1:P:181:PHE:CE1	2.41	0.56
1:P:448:ALA:O	1:P:452:ILE:HG13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:900:FLC:CA	7:P:601:HEM:HAA1	2.36	0.56
1:P:237:ASN:OD1	1:P:240:ARG:HB2	2.06	0.56
1:P:263:PRO:CD	1:P:285:MET:HE2	2.25	0.56
1:P:234:TYR:CE2	1:P:333:ARG:HG3	2.41	0.55
1:P:468:LYS:O	1:P:470:PHE:N	2.39	0.55
1:P:245:ARG:NH2	1:P:325:ASP:OD2	2.39	0.55
1:P:103:VAL:HG13	1:P:108:ILE:HB	1.88	0.55
1:P:479:GLN:CB	9:P:923:HOH:O	2.55	0.55
1:P:297:GLY:O	1:P:300:LEU:HB3	2.06	0.55
1:P:564:LEU:HD13	1:P:578:VAL:HG22	1.88	0.55
9:P:925:HOH:O	3:B:3:BMA:H61	2.06	0.55
1:P:120:ARG:HE	5:P:751:BOG:H62	1.71	0.55
1:P:442:HIS:HD2	1:P:443:HIS:N	2.05	0.55
1:P:142:PHE:O	1:P:376:ARG:NH2	2.40	0.55
1:P:327:GLN:O	1:P:329:PHE:N	2.40	0.54
1:P:388:HIS:N	1:P:389:PRO:HD2	2.21	0.54
1:P:172:PRO:HB2	1:P:177:LEU:HD22	1.89	0.54
3:B:3:BMA:O6	3:B:4:BMA:H62	2.07	0.54
1:P:151:ILE:HG23	1:P:469:ARG:HH12	1.71	0.54
1:P:241:GLN:HG2	1:P:245:ARG:CD	2.37	0.54
1:P:380:GLU:HG2	1:P:466:TYR:CZ	2.42	0.54
1:P:433:ARG:HG2	1:P:433:ARG:HH11	1.73	0.54
1:P:152:LEU:HB3	1:P:461:GLN:NE2	2.23	0.54
1:P:478:PHE:CE1	1:P:492:GLU:HA	2.43	0.53
1:P:514:PRO:O	1:P:515:ASN:HB2	2.06	0.53
1:P:51:GLY:N	1:P:54:ARG:HH21	2.06	0.53
1:P:150:ARG:NH1	1:P:154:SER:HA	2.23	0.53
1:P:191:PRO:CB	1:P:515:ASN:HA	2.36	0.53
1:P:49:ARG:HH11	1:P:49:ARG:HB3	1.73	0.53
1:P:517:ILE:HG23	1:P:518:PHE:CD1	2.43	0.53
1:P:157:ARG:HA	1:P:459:ARG:HH11	1.74	0.53
1:P:246:LEU:CD1	1:P:253:LYS:HA	2.39	0.53
1:P:262:TYR:HB3	1:P:285:MET:HE2	1.90	0.53
1:P:327:GLN:O	1:P:328:LEU:C	2.51	0.53
1:P:574:THR:O	1:P:576:PRO:HD3	2.09	0.53
1:P:475:TYR:CD2	1:P:481:LEU:HA	2.44	0.53
1:P:272:LEU:HD12	1:P:272:LEU:C	2.34	0.53
1:P:287:VAL:HG21	1:P:292:PHE:HB2	1.91	0.52
1:P:279:ILE:O	1:P:281:PRO:N	2.43	0.52
1:P:408:LEU:HB3	1:P:409:PHE:CD1	2.43	0.52
1:P:518:PHE:CG	1:P:522:MET:HG2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:234:TYR:OH	1:P:336:LEU:HD12	2.10	0.52
1:P:157:ARG:HA	1:P:459:ARG:NH1	2.25	0.52
1:P:246:LEU:O	1:P:246:LEU:HD23	2.09	0.52
1:P:255:GLN:NE2	1:P:265:SER:N	2.58	0.51
1:P:257:LEU:O	1:P:258:ASN:HB2	2.10	0.51
1:P:266:VAL:C	1:P:268:GLU:H	2.19	0.51
1:P:255:GLN:OE1	1:P:257:LEU:HD21	2.11	0.51
1:P:319:GLU:HB3	1:P:320:HIS:ND1	2.25	0.51
1:P:163:MET:HA	1:P:163:MET:HE2	1.92	0.51
1:P:265:SER:HA	1:P:285:MET:HA	1.91	0.51
1:P:197:MET:HE3	1:P:301:TYR:OH	2.10	0.51
1:P:101:ASP:OD2	1:P:101:ASP:N	2.44	0.51
1:P:331:THR:O	1:P:335:ILE:HG13	2.11	0.51
1:P:373:TYR:CZ	1:P:541:SER:HA	2.46	0.51
1:P:295:LEU:N	1:P:295:LEU:HD12	2.26	0.51
1:P:239:GLU:CD	1:P:239:GLU:N	2.68	0.50
1:P:338:GLY:HA3	1:P:559:VAL:HG13	1.93	0.50
1:P:234:TYR:HE1	1:P:309:HIS:ND1	2.08	0.50
1:P:348:TYR:HA	1:P:580:PHE:CD1	2.46	0.50
1:P:582:VAL:CG2	1:P:583:PRO:HD2	2.37	0.50
1:P:247:PHE:CD1	1:P:247:PHE:N	2.80	0.50
1:P:299:MET:HG3	1:P:414:LEU:CD2	2.42	0.50
1:P:88:PHE:CZ	1:P:92:LEU:HD11	2.47	0.50
1:P:210:PHE:CE1	1:P:382:ASN:HA	2.47	0.50
1:P:389:PRO:HD3	1:P:440:ILE:HG12	1.94	0.50
1:P:501:LEU:HD21	1:P:506:GLY:HA2	1.92	0.50
1:P:444:ILE:O	1:P:447:VAL:HG23	2.11	0.49
1:P:241:GLN:HE21	1:P:245:ARG:HD3	1.76	0.49
1:P:240:ARG:HE	1:P:288:GLY:HA2	1.77	0.49
1:P:171:LEU:CD1	1:P:456:ARG:HD3	2.42	0.49
1:P:60:THR:HG22	1:P:61:ARG:HG3	1.94	0.49
1:P:263:PRO:HG2	1:P:299:MET:SD	2.53	0.49
1:P:44:GLN:HG2	1:P:469:ARG:NE	2.28	0.49
1:P:178:SER:OG	1:P:449:VAL:HG22	2.12	0.49
1:P:296:PRO:HD2	1:P:407:PHE:CE2	2.47	0.49
1:P:408:LEU:HB3	1:P:409:PHE:CE1	2.47	0.49
1:P:475:TYR:CE2	1:P:481:LEU:HA	2.48	0.49
1:P:34:ASN:HB3	1:P:37:CYS:SG	2.53	0.49
1:P:323:TRP:CZ3	1:P:327:GLN:HG2	2.48	0.49
1:P:171:LEU:CB	1:P:456:ARG:NH1	2.75	0.48
1:P:235:GLY:HA3	1:P:240:ARG:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:253:LYS:O	1:P:264:PRO:HD3	2.12	0.48
1:P:276:PRO:O	1:P:278:GLY:N	2.46	0.48
1:P:507:LEU:HD22	1:P:522:MET:SD	2.52	0.48
1:P:74:ILE:CG2	1:P:75:TRP:N	2.76	0.48
1:P:201:PHE:C	1:P:201:PHE:CD2	2.91	0.48
1:P:237:ASN:OD1	1:P:240:ARG:CB	2.61	0.48
1:P:246:LEU:HD13	1:P:253:LYS:HA	1.94	0.48
1:P:38:TYR:O	1:P:39:TYR:HB2	2.14	0.48
1:P:166:LYS:HD2	1:P:499:ASP:HB2	1.94	0.48
1:P:99:LEU:O	1:P:103:VAL:HG23	2.14	0.48
1:P:74:ILE:HG23	1:P:75:TRP:N	2.28	0.48
1:P:152:LEU:HD12	1:P:466:TYR:CE1	2.49	0.48
1:P:524:GLU:OE1	5:P:751:BOG:H2	2.14	0.48
1:P:180:ARG:HA	1:P:180:ARG:NE	2.29	0.47
1:P:204:HIS:HD2	1:P:232:HIS:HD2	1.59	0.47
1:P:280:PRO:HA	1:P:284:GLN:HG3	1.96	0.47
1:P:298:LEU:HD12	1:P:298:LEU:H	1.77	0.47
1:P:418:GLY:O	1:P:419:VAL:C	2.57	0.47
1:P:166:LYS:HD2	1:P:499:ASP:CB	2.45	0.47
1:P:120:ARG:NH1	1:P:120:ARG:HG3	2.29	0.47
1:P:137:ILE:H	1:P:137:ILE:CD1	2.25	0.47
1:P:120:ARG:HE	5:P:751:BOG:C6	2.28	0.47
1:P:261:VAL:HB	1:P:307:ARG:HD3	1.95	0.47
1:P:234:TYR:HE1	1:P:309:HIS:CE1	2.32	0.47
1:P:419:VAL:O	1:P:420:GLU:C	2.57	0.47
1:P:177:LEU:HD21	1:P:495:TYR:OH	2.15	0.47
1:P:193:GLY:O	1:P:582:VAL:HG12	2.15	0.47
1:P:374:ARG:O	1:P:374:ARG:HG2	2.14	0.47
1:P:478:PHE:CE2	1:P:491:LEU:HB3	2.49	0.47
1:P:172:PRO:HG3	1:P:494:LEU:HB3	1.96	0.47
1:P:301:TYR:HA	1:P:304:ILE:HD12	1.97	0.47
1:P:452:ILE:O	1:P:456:ARG:HG3	2.15	0.47
1:P:93:LEU:HD11	8:P:700:IM8:H222	1.96	0.46
1:P:305:TRP:O	1:P:308:GLU:HB3	2.15	0.46
1:P:204:HIS:ND1	1:P:301:TYR:CB	2.78	0.46
1:P:254:TYR:N	1:P:254:TYR:CD2	2.82	0.46
1:P:280:PRO:N	1:P:281:PRO:CD	2.79	0.46
1:P:384:LEU:C	1:P:384:LEU:HD23	2.41	0.46
1:P:459:ARG:HG2	1:P:459:ARG:HH21	1.81	0.46
1:P:33:VAL:HG23	1:P:33:VAL:O	2.15	0.46
1:P:234:TYR:CE1	1:P:309:HIS:ND1	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:478:PHE:CD2	1:P:491:LEU:HB3	2.50	0.46
1:P:209:PHE:HB2	1:P:377:ILE:HG13	1.96	0.46
1:P:320:HIS:O	1:P:323:TRP:HB2	2.15	0.45
1:P:391:MET:CG	7:P:601:HEM:HAB	2.38	0.45
1:P:255:GLN:HG2	1:P:264:PRO:HA	1.98	0.45
1:P:273:MET:HE1	1:P:287:VAL:HG22	1.98	0.45
1:P:289:GLN:HB3	1:P:292:PHE:CD1	2.51	0.45
1:P:303:THR:HG22	1:P:307:ARG:HH21	1.80	0.45
1:P:84:PRO:HB2	1:P:88:PHE:HD1	1.81	0.45
1:P:184:ARG:NH2	1:P:439:ASN:O	2.47	0.45
1:P:291:VAL:HB	9:P:924:HOH:O	2.16	0.45
1:P:306:LEU:HD23	1:P:306:LEU:O	2.15	0.45
1:P:495:TYR:HE2	1:P:502:GLU:HG3	1.82	0.45
1:P:292:PHE:O	1:P:299:MET:HE2	2.16	0.45
1:P:498:ILE:HG23	1:P:499:ASP:N	2.31	0.45
1:P:527:ALA:N	1:P:528:PRO:CD	2.79	0.45
1:P:152:LEU:HD21	1:P:469:ARG:HB2	1.97	0.45
1:P:183:LEU:CD1	1:P:445:LEU:HD22	2.46	0.44
1:P:90:HIS:CE1	1:P:94:THR:HG21	2.53	0.44
1:P:204:HIS:CE1	1:P:301:TYR:HB3	2.53	0.44
1:P:243:GLN:CG	1:P:270:PRO:HG2	2.43	0.44
1:P:43:HIS:O	1:P:44:GLN:CB	2.66	0.44
1:P:196:LEU:HD23	1:P:196:LEU:HA	1.83	0.44
1:P:348:TYR:HA	1:P:580:PHE:CE1	2.53	0.44
1:P:88:PHE:O	1:P:92:LEU:HD13	2.18	0.44
9:P:925:HOH:O	3:B:3:BMA:C6	2.63	0.44
1:P:274:HIS:CD2	1:P:290:GLU:HB2	2.53	0.43
1:P:309:HIS:HB2	1:P:336:LEU:HD11	2.00	0.43
1:P:287:VAL:HG23	1:P:288:GLY:N	2.34	0.43
1:P:577:TYR:CZ	1:P:583:PRO:HB3	2.53	0.43
1:P:34:ASN:HA	1:P:49:ARG:NH2	2.34	0.43
1:P:102:PHE:CE2	1:P:106:THR:HG21	2.54	0.43
1:P:490:GLU:O	1:P:494:LEU:HG	2.19	0.43
1:P:501:LEU:HD12	1:P:502:GLU:H	1.83	0.43
1:P:442:HIS:HD2	1:P:443:HIS:H	1.66	0.43
1:P:241:GLN:HG2	1:P:245:ARG:HG3	1.99	0.43
1:P:344:VAL:CG1	1:P:534:LEU:HD11	2.49	0.43
1:P:204:HIS:HD2	1:P:232:HIS:CD2	2.30	0.43
1:P:239:GLU:O	1:P:242:TYR:N	2.52	0.43
1:P:409:PHE:O	1:P:411:THR:HG23	2.18	0.43
1:P:200:PHE:O	1:P:201:PHE:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:383:GLN:HE22	1:P:455:SER:HB2	1.84	0.43
1:P:149:THR:O	1:P:378:ALA:HA	2.19	0.42
1:P:195:ASN:O	1:P:198:PHE:HB3	2.18	0.42
1:P:255:GLN:HE21	1:P:265:SER:N	2.17	0.42
1:P:117:LEU:O	1:P:118:THR:C	2.62	0.42
1:P:177:LEU:HD12	1:P:181:PHE:CD1	2.54	0.42
1:P:233:ILE:O	1:P:288:GLY:HA3	2.19	0.42
1:P:275:TYR:CG	1:P:284:GLN:HG2	2.54	0.42
1:P:566:LYS:HB3	1:P:566:LYS:HE2	1.84	0.42
1:P:298:LEU:N	1:P:298:LEU:CD1	2.78	0.42
1:P:34:ASN:OD1	1:P:34:ASN:C	2.63	0.42
1:P:155:VAL:O	1:P:156:PRO:C	2.62	0.42
1:P:204:HIS:CD2	1:P:204:HIS:C	2.97	0.42
1:P:230:LEU:C	1:P:232:HIS:N	2.78	0.42
1:P:294:LEU:HB2	1:P:295:LEU:HD12	2.02	0.42
1:P:380:GLU:HG2	1:P:466:TYR:CE1	2.55	0.42
1:P:526:GLY:HA3	8:P:700:IM8:C12	2.49	0.42
1:P:521:SER:O	1:P:525:MET:HB2	2.19	0.42
1:P:178:SER:CB	1:P:449:VAL:HG22	2.50	0.42
1:P:563:THR:HG22	1:P:564:LEU:H	1.81	0.42
1:P:241:GLN:O	1:P:245:ARG:N	2.49	0.41
1:P:505:PRO:O	1:P:509:LEU:HG	2.20	0.41
1:P:204:HIS:NE2	1:P:232:HIS:CD2	2.89	0.41
1:P:466:TYR:C	1:P:525:MET:HE2	2.44	0.41
1:P:556:PHE:CD1	1:P:560:LYS:HE3	2.55	0.41
1:P:233:ILE:C	1:P:235:GLY:H	2.28	0.41
1:P:563:THR:HB	1:P:566:LYS:HG3	2.01	0.41
1:P:564:LEU:HD13	1:P:578:VAL:CG2	2.51	0.41
1:P:388:HIS:N	1:P:389:PRO:CD	2.82	0.41
1:P:577:TYR:HE2	1:P:583:PRO:HD3	1.83	0.41
1:P:327:GLN:C	1:P:329:PHE:N	2.79	0.41
1:P:483:GLY:H	1:P:511:LYS:HB3	1.85	0.41
1:P:32:PRO:O	1:P:33:VAL:C	2.64	0.41
1:P:120:ARG:HG3	1:P:120:ARG:HH11	1.84	0.41
1:P:179:ARG:O	1:P:183:LEU:HB3	2.21	0.41
1:P:241:GLN:O	1:P:245:ARG:CG	2.65	0.41
1:P:254:TYR:HA	1:P:264:PRO:HD3	2.03	0.41
1:P:345:ILE:HG22	1:P:346:GLU:N	2.35	0.41
1:P:575:CYS:HA	1:P:576:PRO:HD2	1.95	0.41
1:P:446:HIS:O	1:P:447:VAL:C	2.65	0.40
1:P:254:TYR:CD1	1:P:261:VAL:HG13	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:136:TYR:C	1:P:136:TYR:CD1	2.99	0.40
1:P:240:ARG:HG3	1:P:271:VAL:CG2	2.26	0.40
1:P:303:THR:CG2	1:P:307:ARG:HH21	2.34	0.40
1:P:190:ASP:HA	1:P:191:PRO:HD2	1.94	0.40
1:P:34:ASN:OD1	1:P:36:CYS:N	2.53	0.40
1:P:253:LYS:CB	1:P:264:PRO:HG3	2.52	0.40
1:P:260:GLU:CB	1:P:262:TYR:CE1	3.02	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	P	551/600 (92%)	446 (81%)	81 (15%)	24 (4%)	2 3

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	117	LEU
1	P	118	THR
1	P	158	ASP
1	P	247	PHE
1	P	277	ARG
1	P	281	PRO
1	P	469	ARG
1	P	328	LEU
1	P	545	TRP
1	P	551	GLY
1	P	327	GLN
1	P	96	GLY
1	P	97	ARG
1	P	204	HIS

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Mol	Chain	Res	Type
1	P	226	HIS
1	P	268	GLU
1	P	270	PRO
1	P	392	PRO
1	P	468	LYS
1	P	484	GLU
1	P	267	GLU
1	P	280	PRO
1	P	290	GLU
1	P	33	VAL

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	P	458/530 (86%)	421 (92%)	37 (8%)	11	23

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

Mol	Chain	Res	Type
1	P	49	ARG
1	P	68	ASN
1	P	70	THR
1	P	74	ILE
1	P	101	ASP
1	P	111	THR
1	P	120	ARG
1	P	163	MET
1	P	209	PHE
1	P	243	GLN
1	P	252	LEU
1	P	257	LEU
1	P	272	LEU
1	P	280	PRO
1	P	281	PRO
1	P	284	GLN

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Mol	Chain	Res	Type
1	P	289	GLN
1	P	290	GLU
1	P	291	VAL
1	P	307	ARG
1	P	322	THR
1	P	326	GLU
1	P	374	ARG
1	P	376	ARG
1	P	384	LEU
1	P	385	TYR
1	P	433	ARG
1	P	484	GLU
1	P	507	LEU
1	P	525	MET
1	P	530	SER
1	P	554	VAL
1	P	556	PHE
1	P	564	LEU
1	P	570	LEU
1	P	574	THR
1	P	579	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	42	GLN
1	P	43	HIS
1	P	56	GLN
1	P	90	HIS
1	P	195	ASN
1	P	203	GLN
1	P	208	GLN
1	P	241	GLN
1	P	274	HIS
1	P	330	GLN
1	P	375	ASN
1	P	383	GLN
1	P	557	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	A	1	2,1	14,14,15	0.79	0	17,19,21	1.29	2 (11%)
2	NDG	A	2	2	14,14,15	0.77	0	17,19,21	1.01	1 (5%)
3	NAG	B	1	3,1	14,14,15	0.87	0	17,19,21	0.88	1 (5%)
3	NAG	B	2	3	14,14,15	1.09	0	17,19,21	1.52	3 (17%)
3	BMA	B	3	3	11,11,12	1.17	1 (9%)	15,15,17	1.38	2 (13%)
3	BMA	B	4	3	11,11,12	0.88	0	15,15,17	0.91	1 (6%)
4	NAG	C	1	4,1	14,14,15	0.70	0	17,19,21	0.79	1 (5%)
4	NAG	C	2	4	14,14,15	0.66	0	17,19,21	1.21	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1	2,1	-	4/6/23/26	0/1/1/1
2	NDG	A	2	2	-	6/6/23/26	0/1/1/1
3	NAG	B	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	B	2	3	-	5/6/23/26	0/1/1/1

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3	BMA	C1-C2	2.44	1.58	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3	BMA	C1-C2-C3	4.23	115.81	109.64
3	B	2	NAG	C4-C3-C2	-3.63	105.70	111.02
3	B	2	NAG	C1-C2-N2	3.52	115.98	110.43
4	C	2	NAG	C2-N2-C7	-3.34	118.43	122.90
3	B	4	BMA	C1-O5-C5	3.03	116.25	112.19
2	A	1	NAG	C4-C3-C2	-3.01	106.61	111.02
4	C	2	NAG	C4-C3-C2	-2.70	107.06	111.02
2	A	1	NAG	C2-N2-C7	-2.68	119.31	122.90
3	B	2	NAG	O5-C1-C2	-2.48	107.45	111.29
3	B	3	BMA	C1-O5-C5	2.39	115.39	112.19
4	C	1	NAG	C2-N2-C7	-2.25	119.88	122.90
2	A	2	NDG	O5-C1-C2	-2.04	108.14	111.29
3	B	1	NAG	C2-N2-C7	-2.03	120.18	122.90

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	NAG	C8-C7-N2-C2
2	A	1	NAG	O7-C7-N2-C2
2	A	2	NDG	C1-C2-N2-C7
3	B	2	NAG	C1-C2-N2-C7
3	B	2	NAG	C8-C7-N2-C2
3	B	2	NAG	O7-C7-N2-C2
4	C	1	NAG	C8-C7-N2-C2
4	C	1	NAG	O7-C7-N2-C2
4	C	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	C	2	NAG	O7-C7-N2-C2
2	A	1	NAG	C4-C5-C6-O6
2	A	2	NDG	O7-C7-N2-C2
3	B	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O7-C7-N2-C2
3	B	3	BMA	C4-C5-C6-O6
3	B	2	NAG	O5-C5-C6-O6
2	A	2	NDG	O5-C5-C6-O6
3	B	4	BMA	O5-C5-C6-O6
2	A	1	NAG	O5-C5-C6-O6
2	A	2	NDG	C8-C7-N2-C2
2	A	2	NDG	C4-C5-C6-O6
3	B	2	NAG	C4-C5-C6-O6
3	B	3	BMA	O5-C5-C6-O6
3	B	4	BMA	C4-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6
2	A	2	NDG	C3-C2-N2-C7

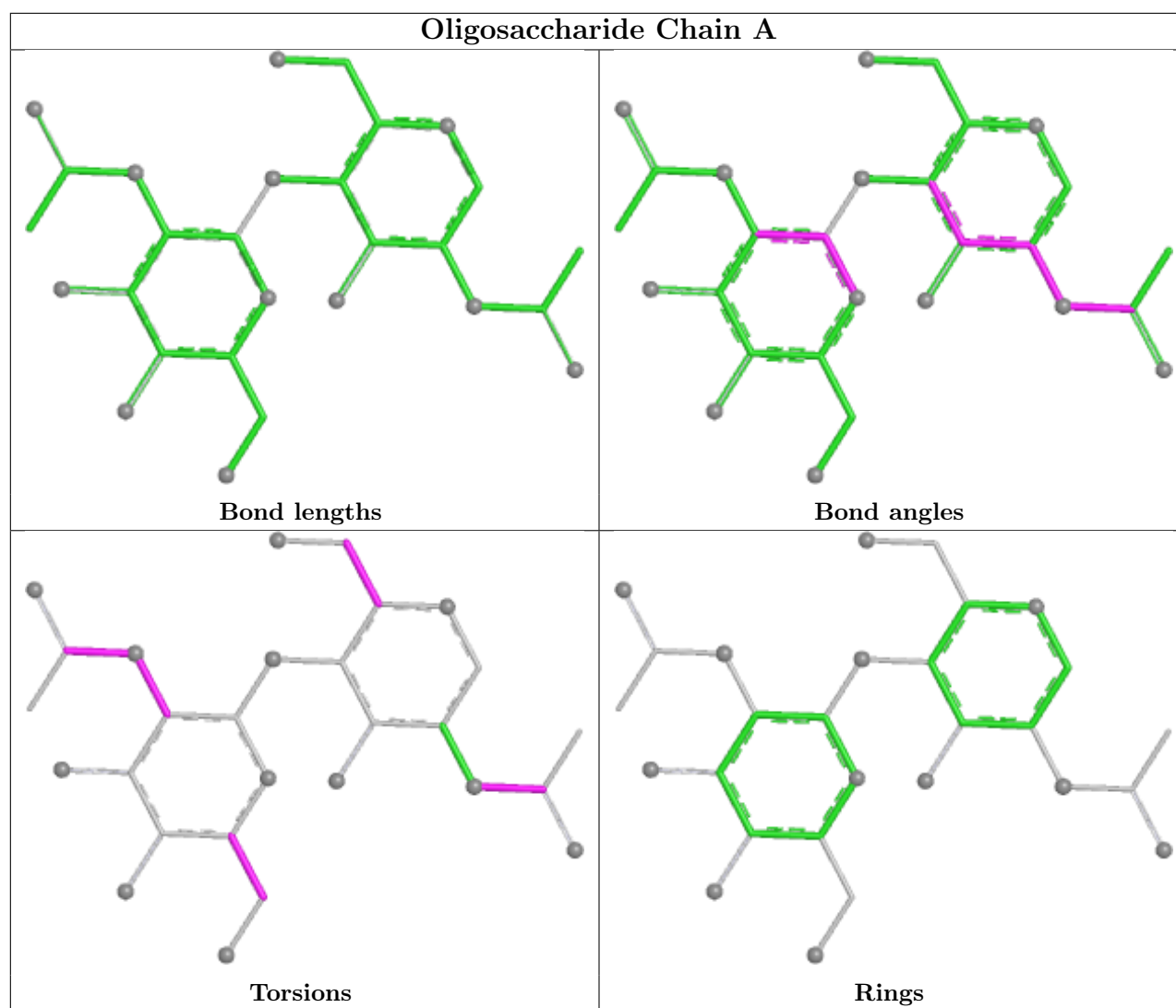
All (1) ring outliers are listed below:

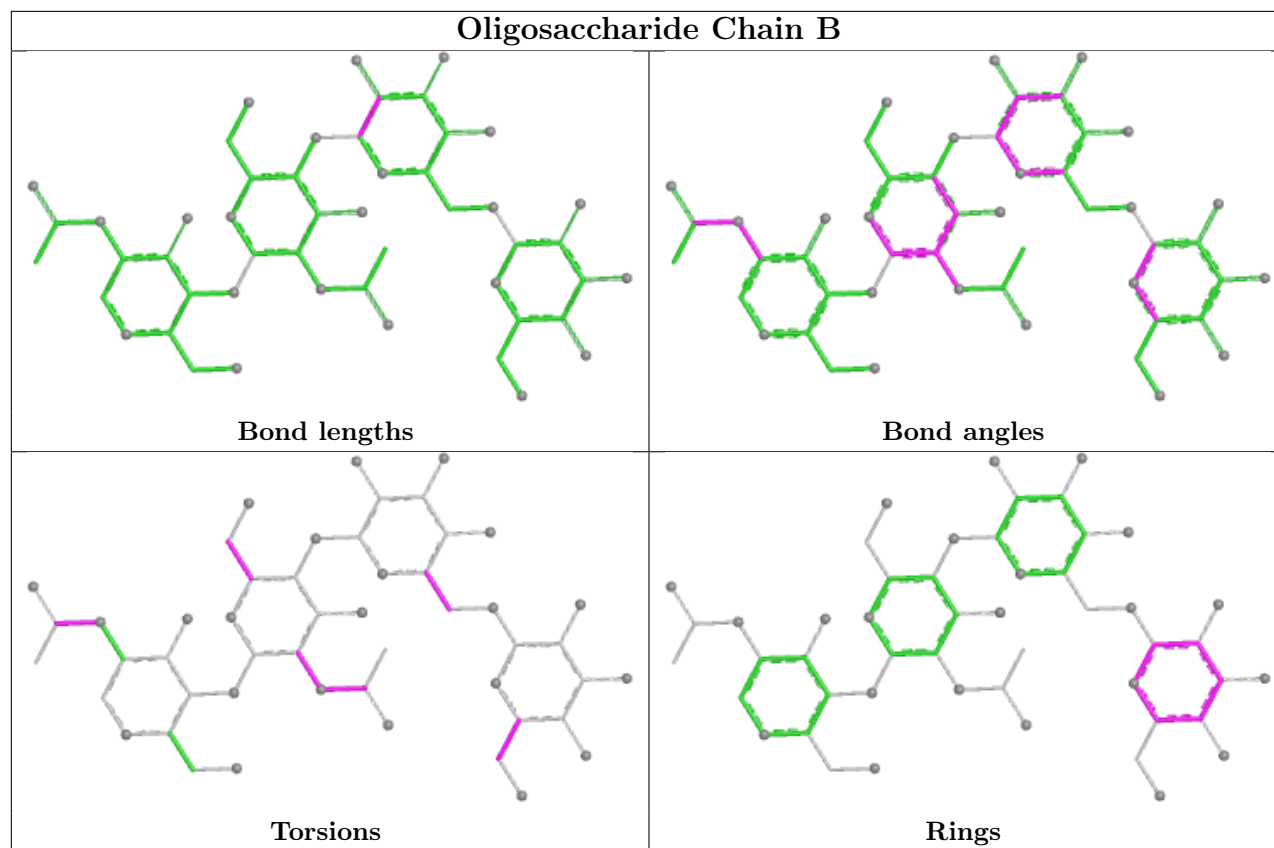
Mol	Chain	Res	Type	Atoms
3	B	4	BMA	C1-C2-C3-C4-C5-O5

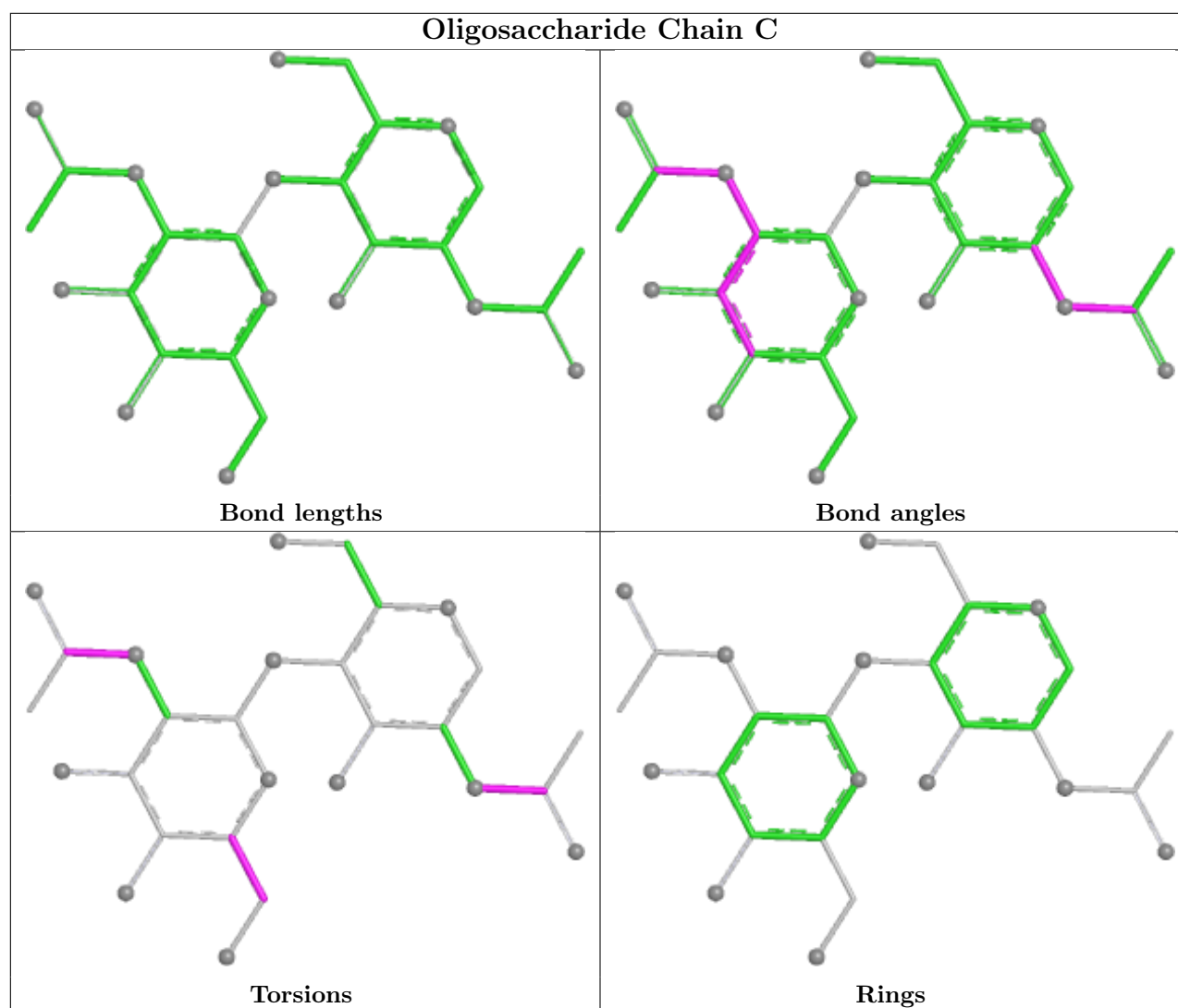
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	4	BMA	1	0
3	B	3	BMA	3	0
3	B	2	NAG	1	0

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







5.6 Ligand geometry [i](#)

5 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	BOG	P	751	-	12,12,20	1.07	1 (8%)	17,17,25	0.88	1 (5%)
6	FLC	P	900	-	12,12,12	1.06	0	17,17,17	2.48	5 (29%)
5	BOG	P	750	-	12,12,20	0.85	0	17,17,25	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	IM8	P	700	-	32,32,32	2.07	12 (37%)	44,45,45	2.34	11 (25%)
7	HEM	P	601	1	50,50,50	1.85	13 (26%)	67,82,82	1.60	15 (22%)

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	BOG	P	751	-	-	0/2/22/31	0/1/1/1
6	FLC	P	900	-	-	8/16/16/16	-
5	BOG	P	750	-	-	0/2/22/31	0/1/1/1
8	IM8	P	700	-	-	3/22/22/22	0/3/3/3
7	HEM	P	601	1	-	8/14/54/54	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	700	IM8	C17-C18	-5.42	1.44	1.51
7	P	601	HEM	C1A-C2A	5.12	1.54	1.44
8	P	700	IM8	C4-C3	4.29	1.46	1.38
7	P	601	HEM	C1D-C2D	4.06	1.52	1.44
7	P	601	HEM	C4A-C3A	3.95	1.52	1.43
8	P	700	IM8	C15-C10	3.51	1.44	1.39
7	P	601	HEM	CAA-C2A	3.43	1.60	1.51
7	P	601	HEM	C4C-NC	-3.19	1.33	1.39
8	P	700	IM8	C2-C3	3.13	1.44	1.39
8	P	700	IM8	C12-C13	3.06	1.43	1.38
7	P	601	HEM	CMC-C2C	2.95	1.56	1.50
7	P	601	HEM	C3C-C4C	-2.89	1.41	1.46
7	P	601	HEM	FE-NC	2.84	2.04	1.95
7	P	601	HEM	CBC-CAC	2.59	1.42	1.30
8	P	700	IM8	O-C3	2.58	1.42	1.37
5	P	751	BOG	C4-C5	2.46	1.58	1.53
8	P	700	IM8	C12-C11	2.46	1.42	1.38
7	P	601	HEM	C4D-ND	2.46	1.44	1.40
8	P	700	IM8	C9-N	-2.36	1.35	1.41
8	P	700	IM8	C14-C13	2.23	1.42	1.38
7	P	601	HEM	CHB-C4A	-2.23	1.34	1.39
7	P	601	HEM	C1D-ND	-2.20	1.34	1.38
8	P	700	IM8	C15-C14	2.20	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	700	IM8	C11-C10	2.15	1.42	1.39
7	P	601	HEM	O2D-CGD	-2.10	1.23	1.30
8	P	700	IM8	C-N	-2.01	1.38	1.41

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	700	IM8	C1-C7-C8	-7.32	101.74	108.13
8	P	700	IM8	C-C1-C7	6.55	113.34	107.38
6	P	900	FLC	OHB-CB-CBC	-6.25	100.10	108.96
8	P	700	IM8	C2-C1-C7	-6.18	122.45	132.81
6	P	900	FLC	CG-CB-CBC	4.60	120.21	110.03
7	P	601	HEM	C3B-C4B-NB	4.43	112.65	109.47
7	P	601	HEM	C2B-C1B-NB	3.76	114.16	109.84
7	P	601	HEM	CAA-C2A-C1A	3.74	132.25	124.94
6	P	900	FLC	OB2-CBC-CB	3.69	120.22	113.14
8	P	700	IM8	C2-C1-C	3.68	124.21	119.82
7	P	601	HEM	C1B-NB-C4B	-3.31	101.29	105.21
8	P	700	IM8	C10-C9-N	3.16	123.99	117.92
8	P	700	IM8	C16-C8-C7	-3.14	123.16	128.07
8	P	700	IM8	C7-C8-N	3.07	111.76	108.85
7	P	601	HEM	C3A-C4A-NA	2.82	114.67	110.14
8	P	700	IM8	C17-C7-C1	2.81	129.62	124.80
6	P	900	FLC	CA-CB-CBC	2.78	116.19	110.03
7	P	601	HEM	CMD-C2D-C3D	2.77	133.64	126.15
8	P	700	IM8	C19-N2-C18	2.75	126.95	122.88
8	P	700	IM8	C1-C-N	-2.69	104.69	107.69
7	P	601	HEM	C1D-C2D-C3D	-2.66	104.19	106.98
7	P	601	HEM	C4A-C3A-C2A	-2.51	103.95	106.82
6	P	900	FLC	OHB-CB-CG	-2.47	103.75	109.38
7	P	601	HEM	CHD-C4C-NC	-2.41	121.83	124.45
7	P	601	HEM	C2D-C1D-ND	2.40	112.68	109.90
7	P	601	HEM	CAA-C2A-C3A	-2.38	121.74	127.07
7	P	601	HEM	C4C-C3C-C2C	-2.28	104.84	106.81
7	P	601	HEM	CBA-CAA-C2A	2.25	118.76	112.53
8	P	700	IM8	C1-C2-C3	-2.24	115.76	119.41
7	P	601	HEM	CHB-C4A-C3A	-2.17	121.12	127.43
5	P	751	BOG	O5-C5-C4	2.03	113.35	109.70
7	P	601	HEM	CHC-C4B-NB	-2.01	122.26	124.42

There are no chirality outliers.

All (19) torsion outliers are listed below:

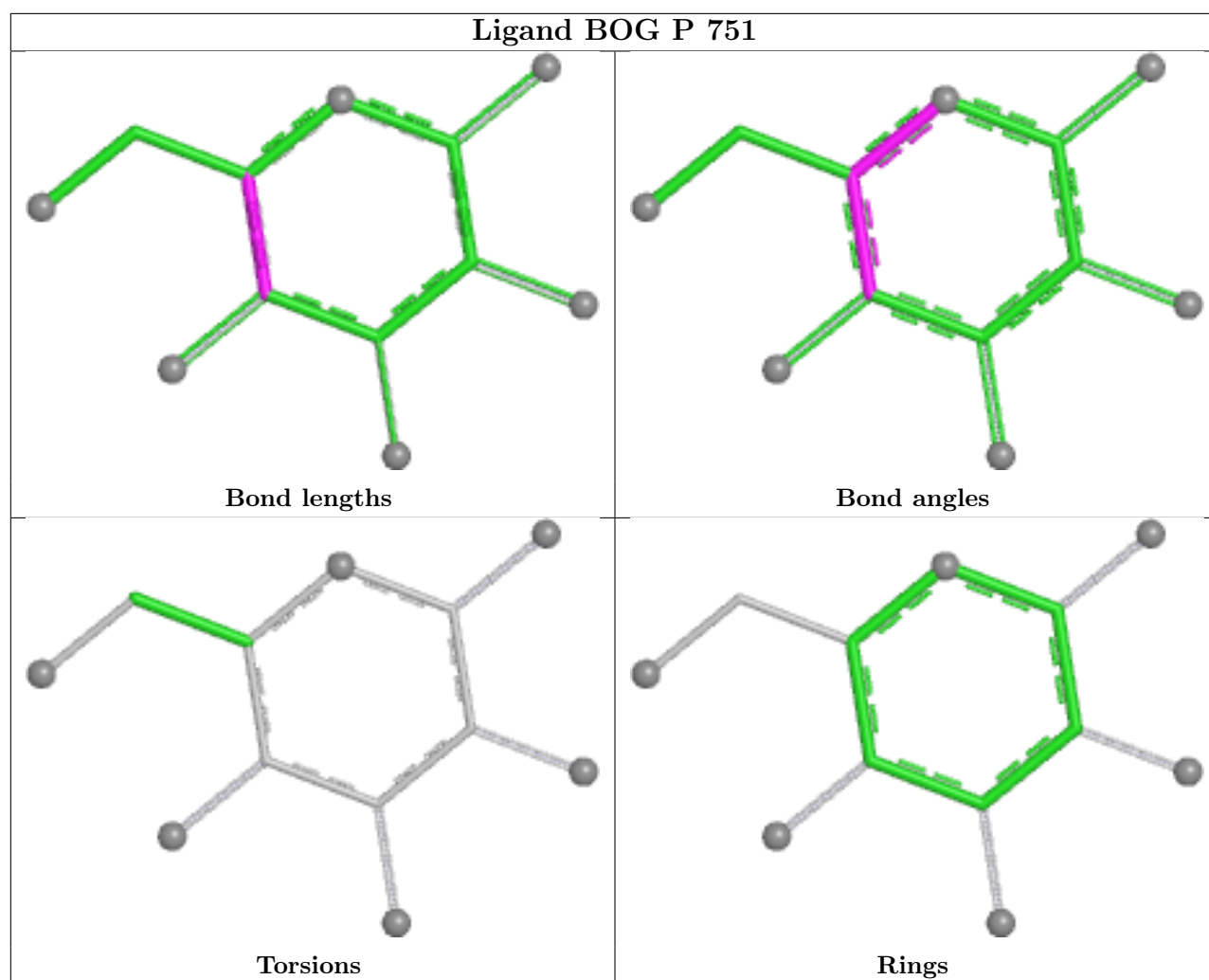
Mol	Chain	Res	Type	Atoms
6	P	900	FLC	CA-CB-CBC-OB1
6	P	900	FLC	CA-CB-CBC-OB2
6	P	900	FLC	CG-CB-CBC-OB2
6	P	900	FLC	OHB-CB-CBC-OB1
6	P	900	FLC	OHB-CB-CBC-OB2
6	P	900	FLC	CG-CB-CBC-OB1
7	P	601	HEM	C2B-C3B-CAB-CBB
6	P	900	FLC	CB-CA-CAC-OA1
6	P	900	FLC	CB-CA-CAC-OA2
8	P	700	IM8	O1-C9-N-C8
7	P	601	HEM	C2C-C3C-CAC-CBC
8	P	700	IM8	C21-C19-N2-C18
7	P	601	HEM	C4B-C3B-CAB-CBB
7	P	601	HEM	C4C-C3C-CAC-CBC
8	P	700	IM8	C20-C19-N2-C18
7	P	601	HEM	CAA-CBA-CGA-O2A
7	P	601	HEM	CAA-CBA-CGA-O1A
7	P	601	HEM	CAD-CBD-CGD-O1D
7	P	601	HEM	CAD-CBD-CGD-O2D

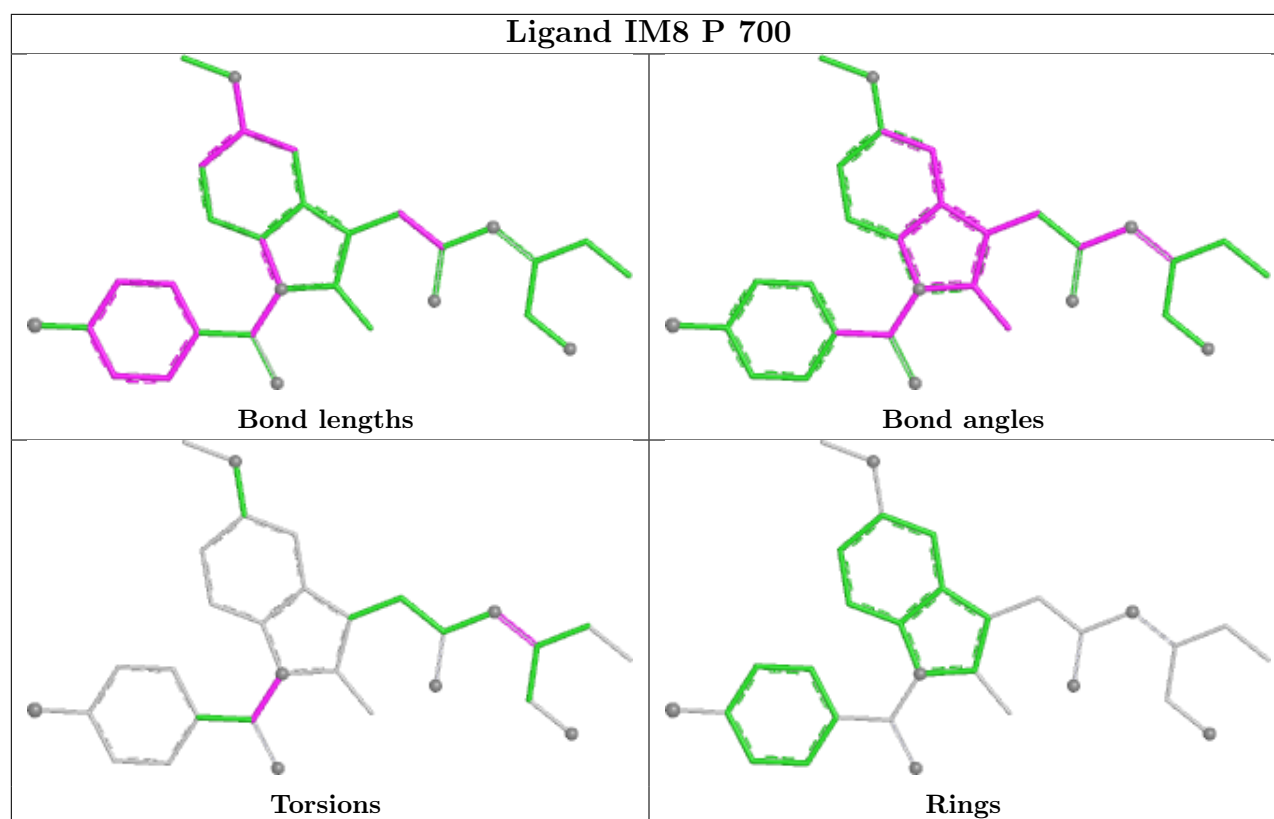
There are no ring outliers.

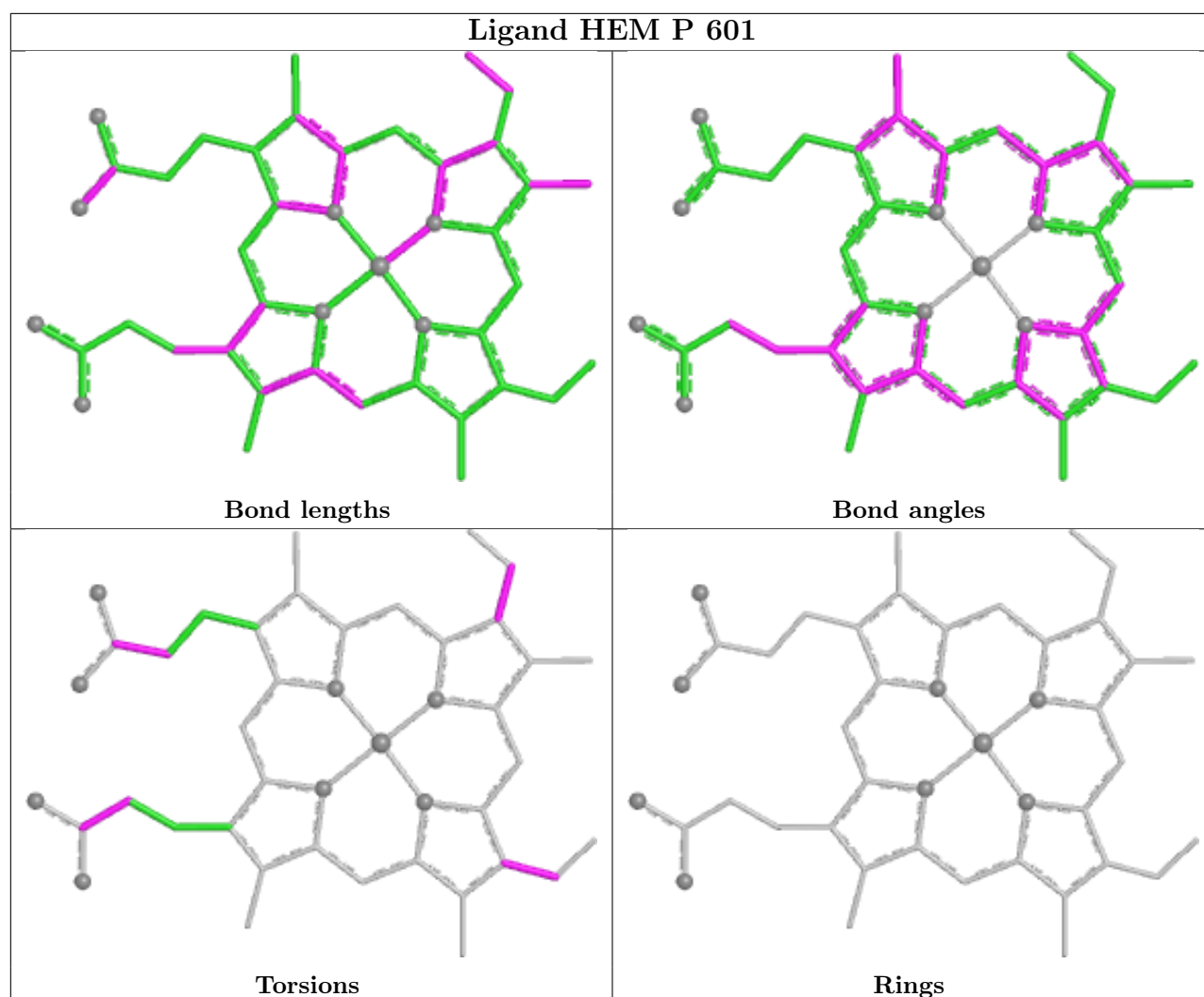
4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	751	BOG	5	0
6	P	900	FLC	3	0
8	P	700	IM8	5	0
7	P	601	HEM	6	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	P	553/600 (92%)	0.09	9 (1%) 70 64	35, 61, 87, 100	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	32	PRO	3.2
1	P	483	GLY	3.2
1	P	280	PRO	3.1
1	P	218	PRO	2.6
1	P	282	GLN	2.6
1	P	59	CYS	2.5
1	P	408	LEU	2.3
1	P	412	SER	2.2
1	P	258	ASN	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.

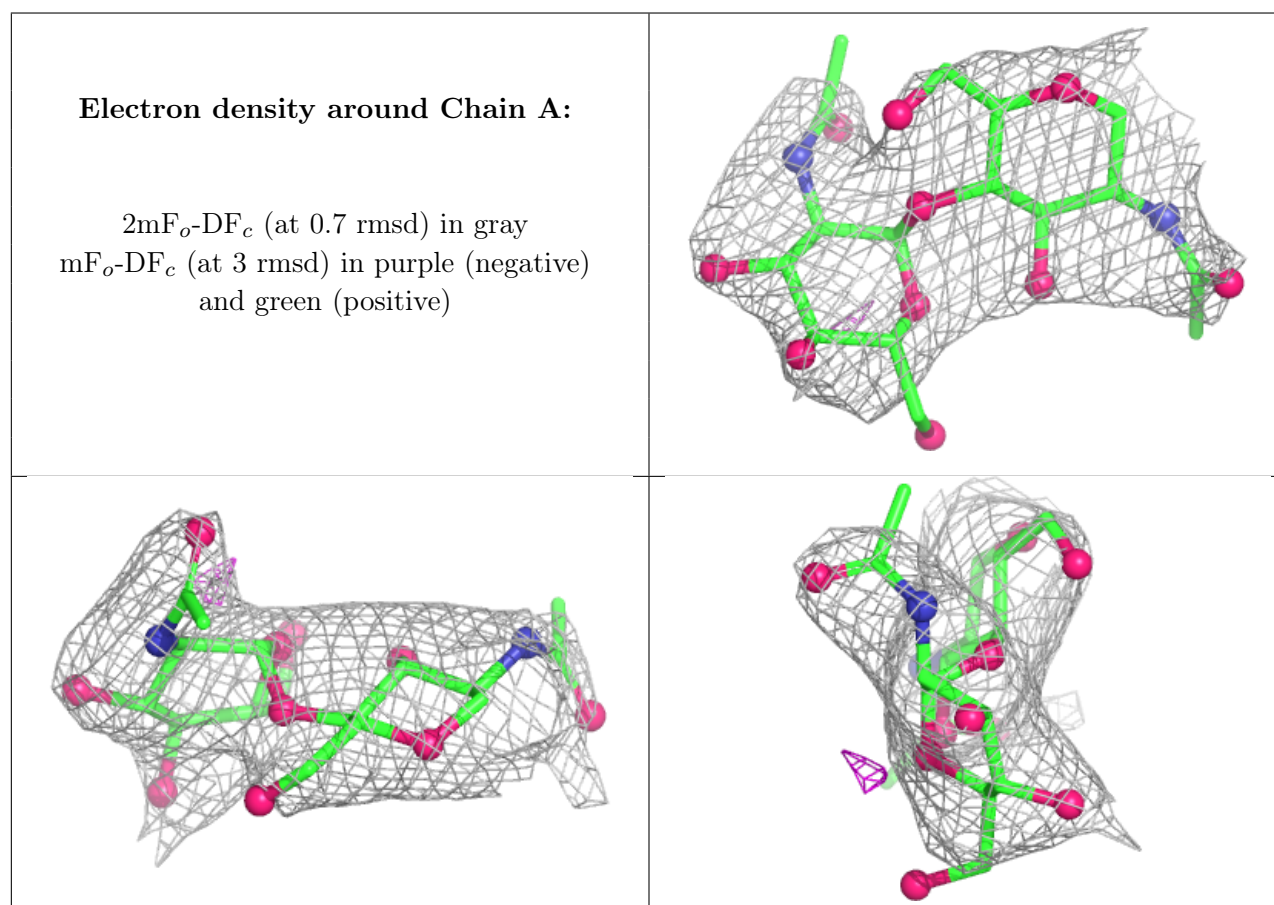
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	1	14/15	-	-	78,78,78,78	0
2	NDG	A	2	14/15	-	-	87,87,87,87	0
4	NAG	C	2	14/15	0.89	0.11	92,92,92,92	0

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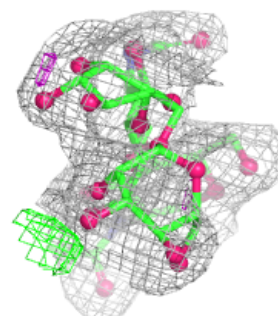
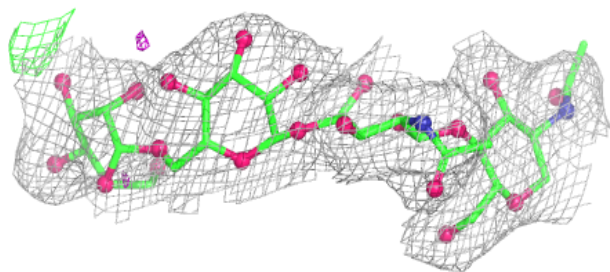
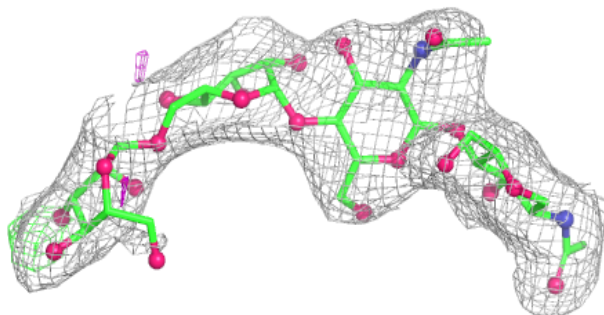
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	B	2	14/15	-	-	78,78,78,78	0
3	BMA	B	3	11/12	-	-	89,89,89,89	0
3	BMA	B	4	11/12	-	-	77,77,77,77	11
3	NAG	B	1	14/15	0.91	0.10	61,61,61,61	0
4	NAG	C	1	14/15	0.93	0.08	77,77,77,77	0

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.

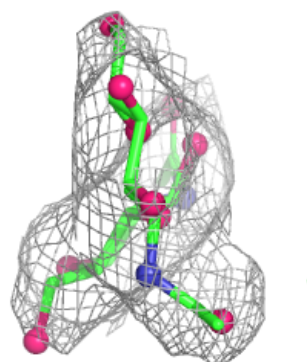
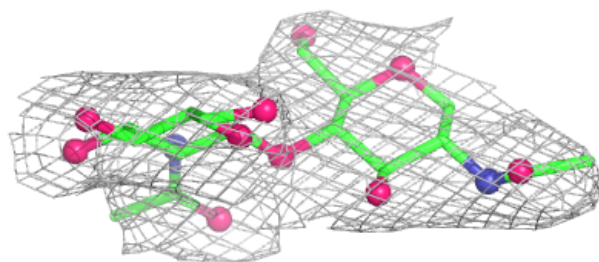
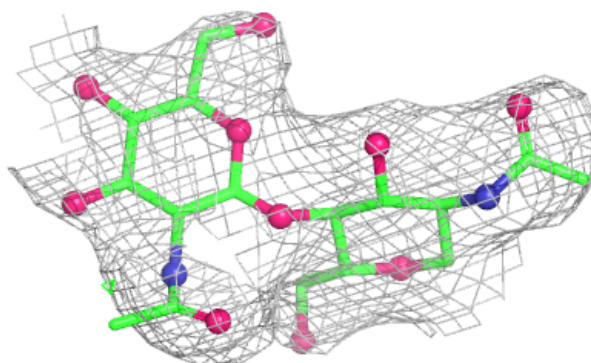


Electron density around Chain B:

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

**Electron density around Chain C:**

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



6.4 Ligands

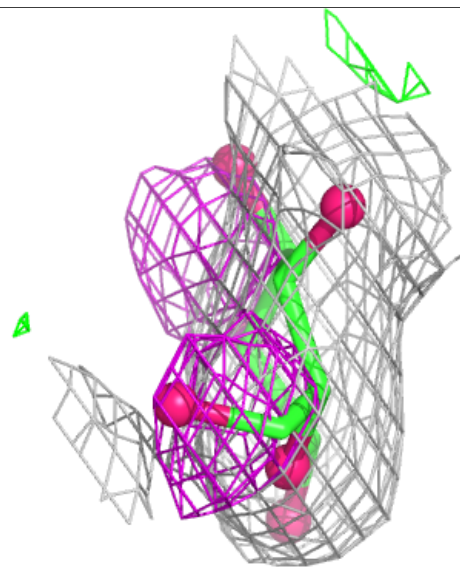
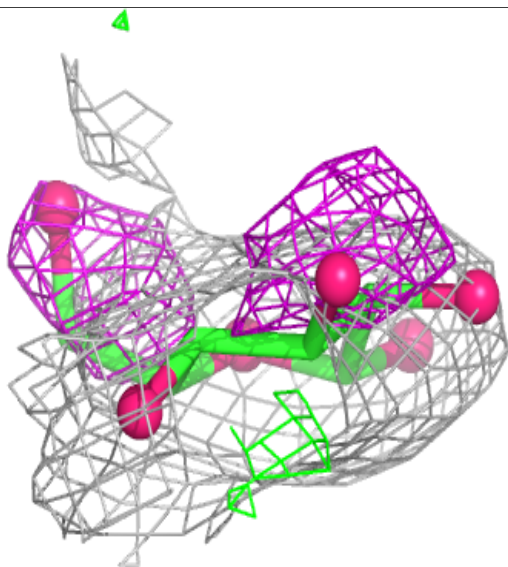
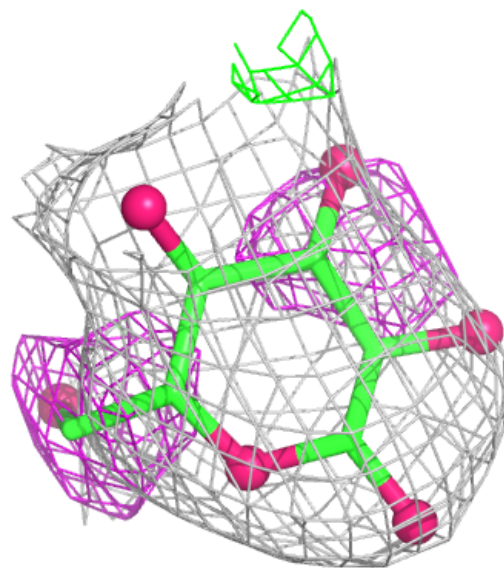
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BOG	P	751	12/20	0.69	0.13	61,61,61,61	0
5	BOG	P	750	12/20	0.75	0.11	61,61,61,61	0
6	FLC	P	900	13/13	0.78	0.15	67,67,67,67	13
8	IM8	P	700	30/30	0.88	0.16	81,81,81,81	0
7	HEM	P	601	43/43	0.96	0.12	73,73,73,73	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.

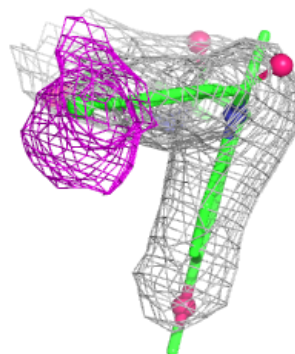
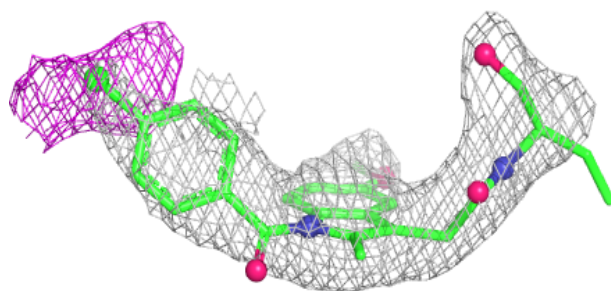
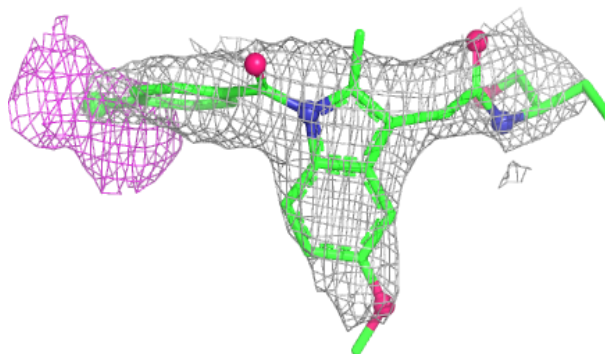
Electron density around BOG P 751:

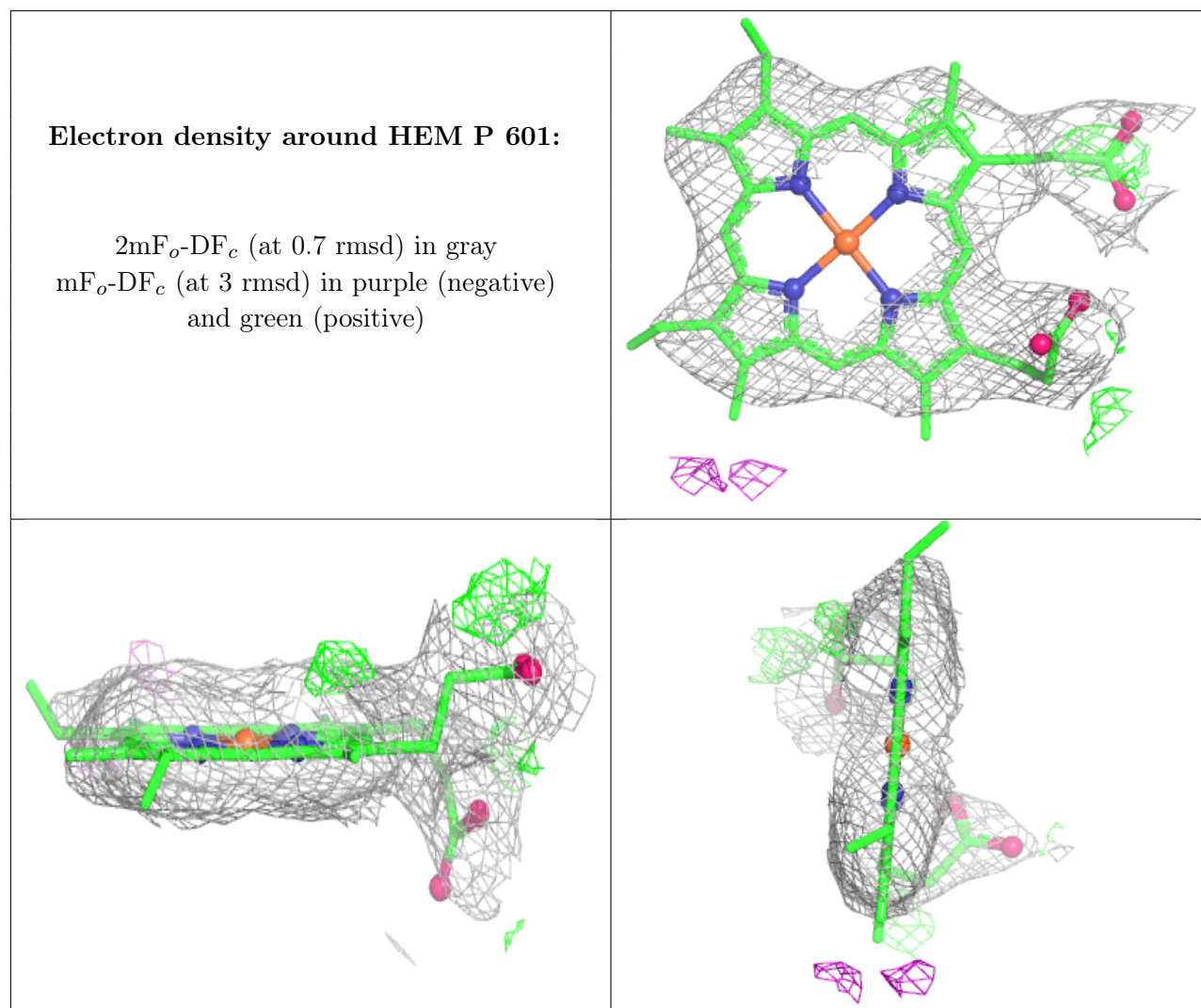
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around IM8 P 700:

$2mF_o-DF_c$ (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.