



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:59 AM UTC

PDB ID : 3RLF / pdb_00003rlf
Title : Crystal structure of the maltose-binding protein/maltose transporter complex
in an outward-facing conformation bound to MgAMPPNP
Authors : Oldham, M.L.; Chen, J.
Deposited on : 2011-04-19
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:

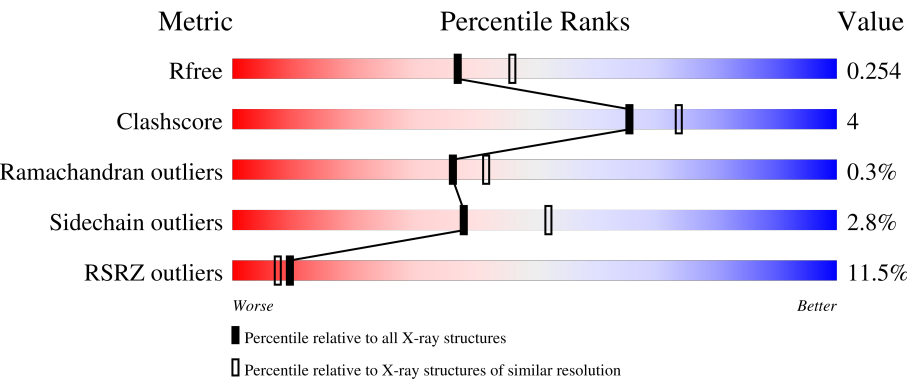
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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.



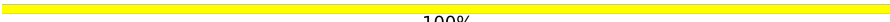
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	E	380	14% 89%9%..
2	F	514	22% 85%9%5%
3	G	296	5% 90%6%..
4	A	381	3% 85%12%..
4	B	381	7% 85%11%..

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Mol	Chain	Length	Quality of chain
5	C	2	 100%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 15268 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 Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	374	Total	C	N	O	S	0	2	0
			2914	1875	476	557	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	371	ALA	-	expression tag	UNP P0AEX9
E	372	SER	-	expression tag	UNP P0AEX9
E	373	ALA	-	expression tag	UNP P0AEX9
E	374	SER	-	expression tag	UNP P0AEX9
E	375	HIS	-	expression tag	UNP P0AEX9
E	376	HIS	-	expression tag	UNP P0AEX9
E	377	HIS	-	expression tag	UNP P0AEX9
E	378	HIS	-	expression tag	UNP P0AEX9
E	379	HIS	-	expression tag	UNP P0AEX9
E	380	HIS	-	expression tag	UNP P0AEX9

- Molecule 2 is a protein called Maltose transport system permease protein malF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	490	Total	C	N	O	S	0	1	0
			3832	2517	612	686	17			

- Molecule 3 is a protein called Maltose transport system permease protein malG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	286	Total	C	N	O	S	0	2	0
			2214	1484	352	370	8			

- Molecule 4 is a protein called Maltose/maltodextrin import ATP-binding protein MalK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	371	Total	C	N	O	S	0	0	0
			2876	1819	515	529	13			
4	B	371	Total	C	N	O	S	0	1	0
			2881	1822	515	531	13			

There are 20 discrepancies between the modelled and reference sequences:

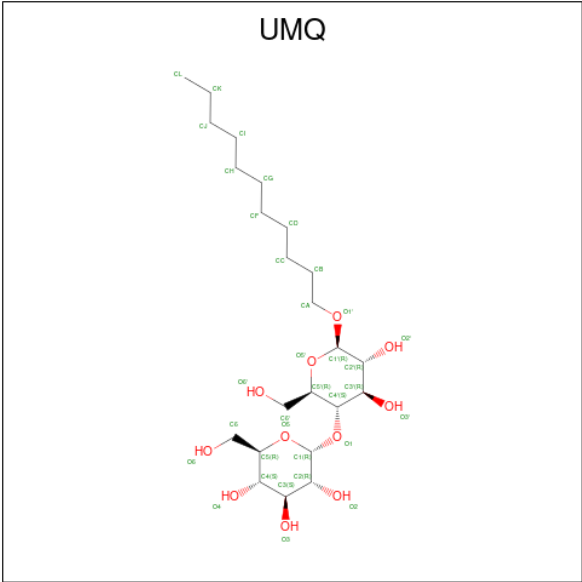
Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	-	expression tag	UNP P68187
A	373	SER	-	expression tag	UNP P68187
A	374	ALA	-	expression tag	UNP P68187
A	375	SER	-	expression tag	UNP P68187
A	376	HIS	-	expression tag	UNP P68187
A	377	HIS	-	expression tag	UNP P68187
A	378	HIS	-	expression tag	UNP P68187
A	379	HIS	-	expression tag	UNP P68187
A	380	HIS	-	expression tag	UNP P68187
A	381	HIS	-	expression tag	UNP P68187
B	372	ALA	-	expression tag	UNP P68187
B	373	SER	-	expression tag	UNP P68187
B	374	ALA	-	expression tag	UNP P68187
B	375	SER	-	expression tag	UNP P68187
B	376	HIS	-	expression tag	UNP P68187
B	377	HIS	-	expression tag	UNP P68187
B	378	HIS	-	expression tag	UNP P68187
B	379	HIS	-	expression tag	UNP P68187
B	380	HIS	-	expression tag	UNP P68187
B	381	HIS	-	expression tag	UNP P68187

- Molecule 5 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



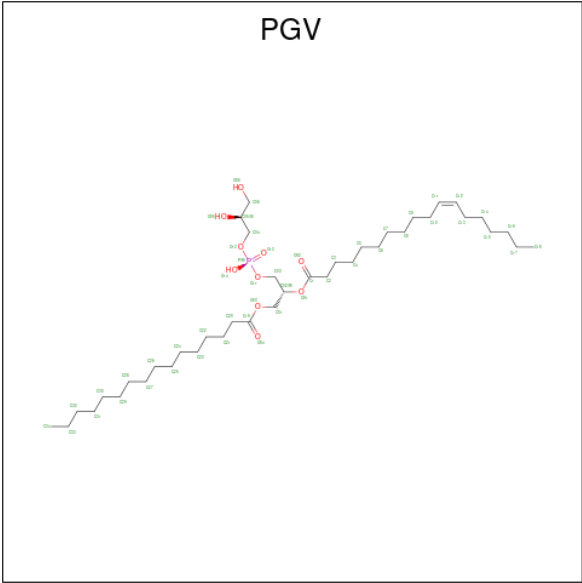
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	C	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 6 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: C₂₃H₄₄O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			34	23	11		

- Molecule 7 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	F	1	Total	C	O	P	0	0
			51	40	10	1		
7	F	1	Total		C	0		
			14		14			

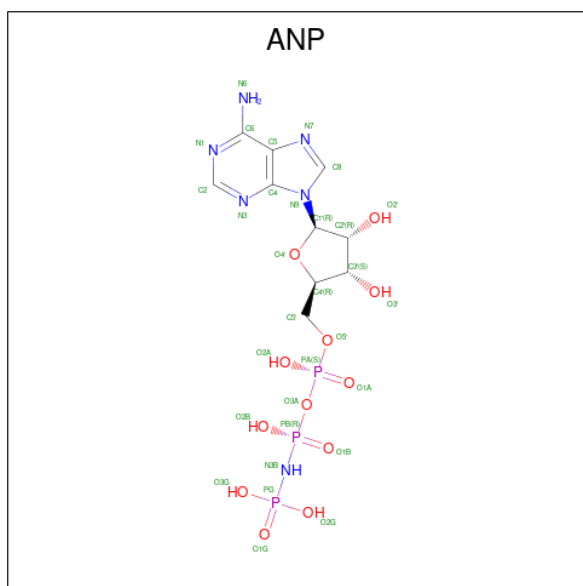
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	C	0	0
			14	14		
7	G	1	Total	C	0	0
			12	12		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		

- Molecule 9 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
9	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

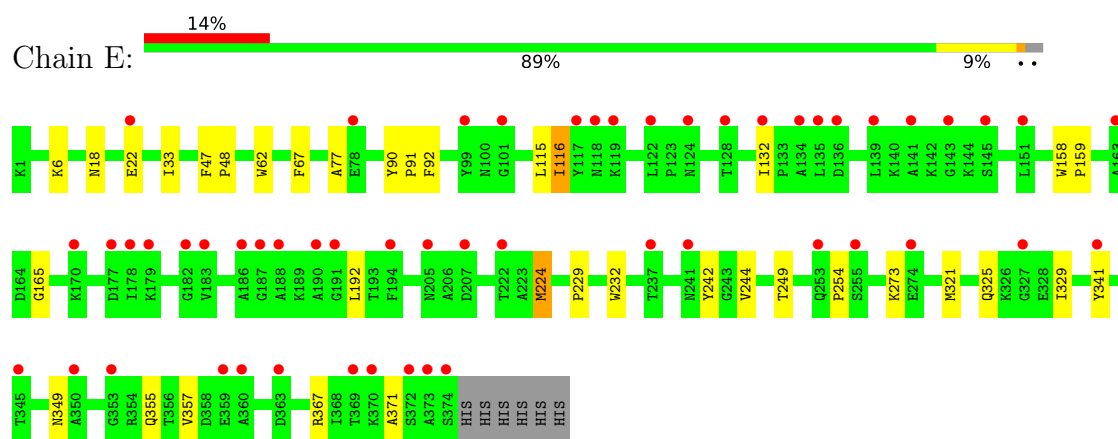
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	E	62	Total 62	O 62	0	0
10	F	63	Total 63	O 63	0	0
10	G	59	Total 59	O 59	0	0
10	A	81	Total 81	O 81	0	0
10	B	74	Total 74	O 74	0	0

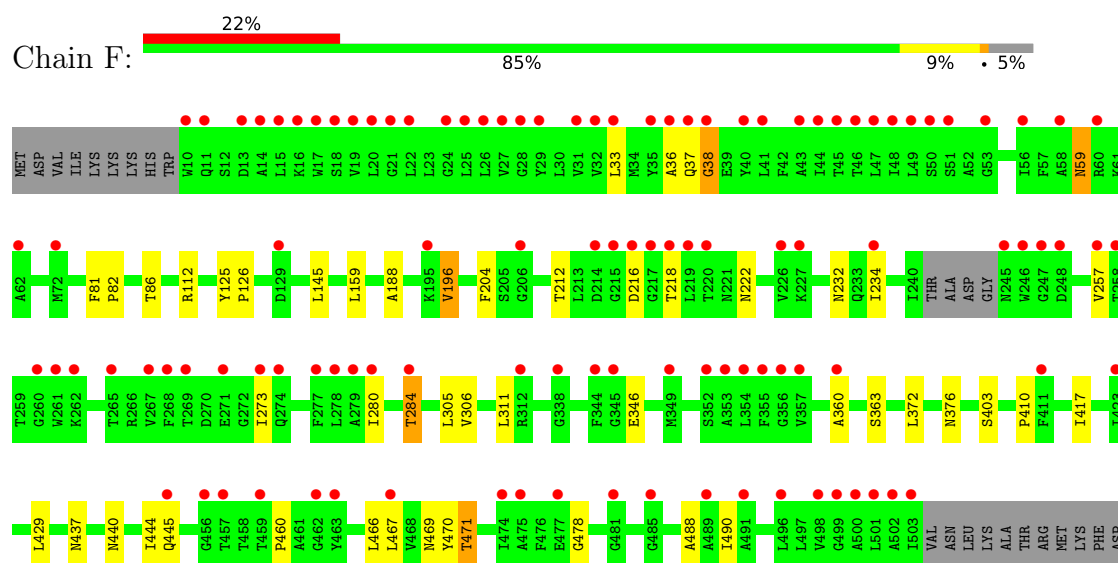
3 Residue-property plots [i](#)

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: Maltose-binding periplasmic protein

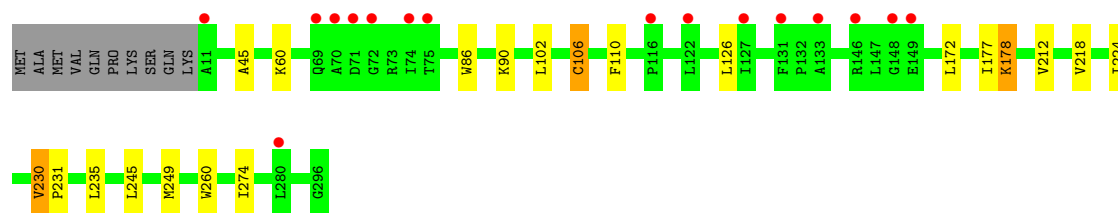


- Molecule 2: Maltose transport system permease protein malF

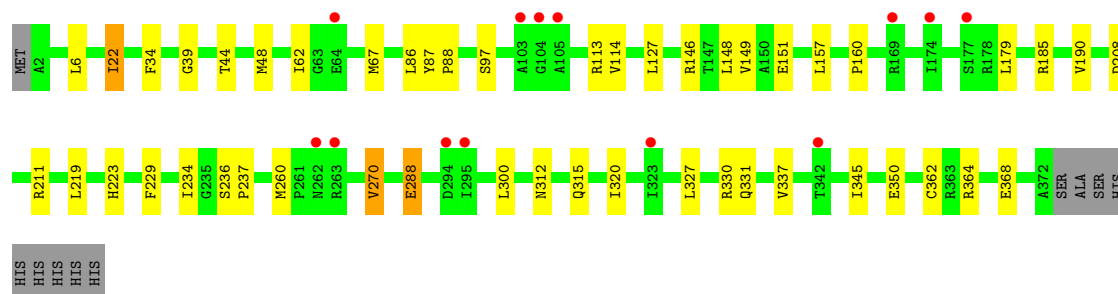
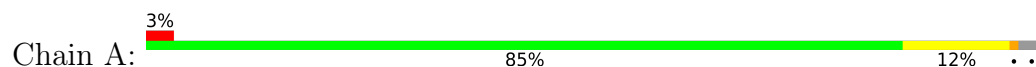


- Molecule 3: Maltose transport system permease protein malG

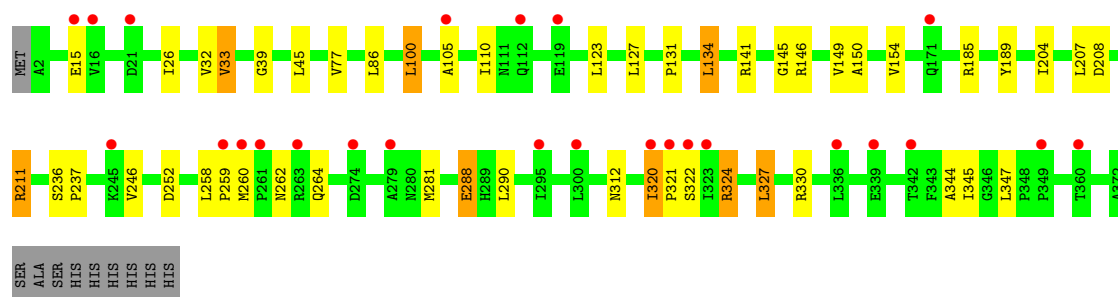
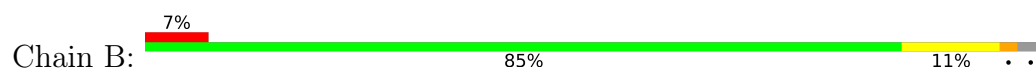




• Molecule 4: Maltose/maltodextrin import ATP-binding protein MalK



• Molecule 4: Maltose/maltodextrin import ATP-binding protein MalK



• Molecule 5: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.10Å 95.81Å 109.98Å 86.70° 82.68° 76.40°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	86.3 (20.00-2.20) 86.2 (20.00-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.223 , 0.254 0.223 , 0.254	Depositor DCC
R_{free} test set	6209 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15268	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: MG, PGV, UMQ, ANP, GLC

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	E	0.46	1/2983 (0.0%)	0.80	0/4048
2	F	0.46	0/3927	0.79	0/5344
3	G	0.50	0/2278	0.83	0/3115
4	A	0.47	0/2926	0.78	0/3968
4	B	0.48	0/2932	0.77	0/3974
All	All	0.47	1/15046 (0.0%)	0.79	0/20449

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	132	ILE	CA-CB	6.22	1.57	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	E	2914	0	2888	22	0
2	F	3832	0	3861	32	0
3	G	2214	0	2302	10	0
4	A	2876	0	2941	28	0
4	B	2881	0	2942	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	23	0	21	0	0
6	E	34	0	44	0	0
7	F	65	0	100	2	0
7	G	26	0	44	1	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	31	0	13	2	0
9	B	31	0	13	2	0
10	A	81	0	0	1	0
10	B	74	0	0	2	0
10	E	62	0	0	0	0
10	F	63	0	0	0	0
10	G	59	0	0	0	0
All	All	15268	0	15169	115	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 4.

All (115) 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)
2:F:471:THR:HG21	2:F:490:ILE:HG21	1.42	1.01
4:A:39:GLY:H	9:A:2501:ANP:HNB1	1.16	0.94
4:B:39:GLY:H	9:B:2502:ANP:HNB1	1.18	0.88
4:A:223:HIS:CE1	4:A:368:GLU:HG2	2.12	0.85
4:B:344:ALA:CB	4:B:344:ALA:C	2.51	0.83
4:B:344:ALA:CB	4:B:344:ALA:N	2.45	0.80
4:B:141:ARG:NH1	10:B:455:HOH:O	2.05	0.78
1:E:116:ILE:HD11	1:E:242:TYR:HD2	1.51	0.76
2:F:196:VAL:HG13	2:F:204:PHE:HB3	1.69	0.75
2:F:471:THR:CG2	2:F:490:ILE:HG21	2.16	0.75
4:A:288:GLU:HG2	4:B:312:ASN:HB2	1.70	0.73
2:F:159:LEU:HD11	2:F:188:ALA:HB1	1.70	0.73
4:B:344:ALA:C	4:B:344:ALA:N	2.47	0.72
4:A:39:GLY:N	9:A:2501:ANP:HNB1	1.88	0.70
1:E:116:ILE:HD11	1:E:242:TYR:CD2	2.27	0.69
3:G:86:TRP:CE2	3:G:90:LYS:HD2	2.29	0.68
4:B:39:GLY:N	9:B:2502:ANP:HNB1	1.93	0.66
2:F:196:VAL:CG1	2:F:204:PHE:HB3	2.27	0.65
4:A:6:LEU:HD22	4:A:22:ILE:HD11	1.78	0.65
2:F:471:THR:HG21	2:F:490:ILE:CG2	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:320:ILE:HD11	4:B:327:LEU:HB2	1.80	0.63
4:A:208:ASP:O	4:A:211:ARG:HG2	2.02	0.59
1:E:367:ARG:HD2	2:F:460:PRO:HG3	1.84	0.59
2:F:280:ILE:O	2:F:284:THR:HG23	2.02	0.59
4:A:312:ASN:HB2	4:B:288:GLU:HG2	1.85	0.59
2:F:444:ILE:HG13	2:F:466:LEU:HG	1.85	0.57
4:B:324:ARG:HD3	4:B:324:ARG:H	1.70	0.57
2:F:471:THR:HG23	2:F:490:ILE:HD13	1.88	0.56
2:F:36:ALA:O	2:F:38:GLY:N	2.37	0.56
2:F:59:ASN:HD22	2:F:59:ASN:H	1.54	0.56
2:F:360:ALA:HB1	2:F:363:SER:HB2	1.90	0.54
4:A:223:HIS:ND1	4:A:368:GLU:HG2	2.22	0.54
2:F:212:THR:HG23	2:F:222:ASN:HD21	1.72	0.54
3:G:45:ALA:HB2	3:G:260:TRP:CE2	2.43	0.54
4:A:44:THR:HG22	4:A:48:MET:HE2	1.91	0.53
4:B:246:VAL:HG23	4:B:281:MET:HG3	1.91	0.53
4:B:288:GLU:HG3	4:B:330:ARG:HD3	1.91	0.52
4:A:97:SER:HB3	4:A:114:VAL:HG21	1.91	0.52
1:E:321:MET:HE2	1:E:325:GLN:HG3	1.91	0.52
4:B:236:SER:HA	4:B:237:PRO:C	2.35	0.51
4:A:270:VAL:HG13	4:A:362:CYS:HB3	1.92	0.51
4:A:208:ASP:HB2	4:A:229:PHE:CE2	2.46	0.51
4:A:86:LEU:HA	4:A:146:ARG:NH2	2.25	0.50
3:G:110:PHE:HB3	3:G:178:LYS:HD2	1.93	0.50
4:B:26:ILE:HG12	4:B:32:VAL:HG21	1.93	0.50
4:A:288:GLU:HG3	4:A:330:ARG:HD3	1.94	0.50
3:G:60:LYS:HE2	7:G:4006:PGV:H201	1.94	0.50
3:G:224:ILE:HG12	3:G:274[A]:ILE:HD12	1.94	0.50
1:E:321:MET:HE3	1:E:321:MET:HA	1.94	0.49
4:B:146:ARG:HD2	10:B:393:HOH:O	2.12	0.49
4:B:208:ASP:O	4:B:211:ARG:HG3	2.13	0.49
4:B:290:LEU:HD22	4:B:345:ILE:HD13	1.94	0.48
3:G:230:VAL:HB	3:G:231:PRO:HD3	1.95	0.48
1:E:116:ILE:HG12	1:E:244:VAL:HG22	1.95	0.48
2:F:445:GLN:HG2	2:F:469:ASN:HD22	1.79	0.47
1:E:62:TRP:HB3	1:E:67:PHE:HE1	1.79	0.47
2:F:403:SER:HB3	2:F:417:ILE:HD11	1.96	0.46
1:E:115:LEU:HD21	1:E:224:MET:HE3	1.97	0.46
2:F:86:THR:O	2:F:488:ALA:HB1	2.14	0.46
4:B:145:GLY:O	4:B:149:VAL:HG23	2.16	0.46
4:A:62:ILE:HB	4:A:67:MET:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:273:ILE:HA	2:F:470:TYR:OH	2.15	0.46
2:F:376:ASN:HD21	2:F:437:ASN:ND2	2.14	0.46
1:E:6:LYS:HA	1:E:33:ILE:HG23	1.98	0.46
4:A:157:LEU:HB3	4:A:160:PRO:HG3	1.96	0.46
2:F:372:LEU:HD21	2:F:444:ILE:HD12	1.98	0.46
4:B:33:VAL:HG22	4:B:204:ILE:HG12	1.97	0.46
4:A:260:MET:HE2	4:A:300:LEU:HD22	1.97	0.46
4:A:260:MET:CE	4:A:300:LEU:HD22	2.46	0.45
4:A:236:SER:HA	4:A:237:PRO:C	2.40	0.45
4:B:86:LEU:HA	4:B:146:ARG:NH2	2.31	0.45
3:G:245:LEU:HG	3:G:249:MET:CE	2.47	0.45
4:B:77:VAL:HG12	4:B:154:VAL:HB	1.99	0.45
2:F:284:THR:HG21	2:F:467:LEU:H	1.80	0.45
4:B:100:LEU:HB3	4:B:110:ILE:HG12	1.98	0.45
4:B:131:PRO:HA	4:B:134:LEU:HD22	1.99	0.45
2:F:125:TYR:HA	2:F:126:PRO:HD2	1.89	0.44
4:A:34:PHE:HB2	4:A:190:VAL:HG22	1.98	0.44
4:A:86:LEU:HA	4:A:146:ARG:HH22	1.82	0.44
2:F:429:LEU:HD23	3:G:172:LEU:HD22	2.00	0.44
1:E:18:ASN:O	1:E:22:GLU:HG2	2.18	0.44
4:B:321:PRO:O	4:B:322:SER:HB3	2.17	0.44
1:E:192:LEU:HD23	1:E:357:VAL:HG13	1.98	0.44
4:B:262:ASN:ND2	4:B:264:GLN:HB2	2.33	0.44
2:F:305:LEU:O	2:F:311:LEU:HD12	2.18	0.44
2:F:216:ASP:OD1	2:F:218:THR:HG22	2.18	0.43
2:F:305:LEU:HD23	7:F:4001:PGV:H011	2.00	0.43
2:F:410:PRO:HB3	7:F:4001:PGV:H02	1.99	0.43
4:A:113:ARG:HG3	4:A:149:VAL:HG13	2.01	0.43
4:B:45:LEU:HD12	4:B:207:LEU:HD11	2.00	0.43
1:E:92:PHE:HD1	1:E:329:ILE:HD11	1.83	0.43
2:F:232:ASN:O	2:F:257:VAL:HG21	2.18	0.43
2:F:284:THR:HG22	2:F:466:LEU:HA	2.01	0.43
1:E:371:ALA:HB1	2:F:478:GLY:O	2.19	0.42
1:E:77:ALA:HB2	1:E:273:LYS:HE3	2.01	0.42
1:E:229:PRO:HA	1:E:232:TRP:CE2	2.54	0.42
1:E:349:ASN:HB3	1:E:355:GLN:HB2	2.02	0.42
4:A:315:GLN:HG2	4:A:330:ARG:HG2	2.01	0.42
4:B:33:VAL:HA	4:B:189:TYR:O	2.19	0.42
4:B:259:PRO:HD2	4:B:260:MET:HE3	2.00	0.42
4:A:151:GLU:O	4:A:185:ARG:NH2	2.52	0.42
1:E:90:TYR:HA	1:E:91:PRO:HD3	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:100:LEU:HD13	4:B:150:ALA:HA	2.00	0.42
1:E:158:TRP:N	1:E:159:PRO:CD	2.82	0.41
4:A:364:ARG:HD2	10:A:423:HOH:O	2.18	0.41
1:E:249:THR:HG22	1:E:254:PRO:HA	2.02	0.41
1:E:47:PHE:HB3	1:E:48:PRO:HD3	2.02	0.41
4:A:260:MET:HE3	4:A:320:ILE:HG21	2.02	0.41
1:E:92:PHE:HZ	1:E:321:MET:HE1	1.85	0.41
1:E:341:TYR:CE2	2:F:460:PRO:HB2	2.56	0.41
4:A:148:LEU:HD22	4:A:179:LEU:HD22	2.02	0.41
2:F:81:PHE:HB3	2:F:82:PRO:HD3	2.02	0.40
3:G:102:LEU:O	3:G:106:CYS:HB2	2.21	0.40
4:A:87:TYR:HA	4:A:88:PRO:HD3	1.87	0.40
3:G:177:ILE:HD11	3:G:218:VAL:HG21	2.02	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	E	374/380 (98%)	364 (97%)	9 (2%)	1 (0%)	36	42
2	F	487/514 (95%)	471 (97%)	14 (3%)	2 (0%)	30	34
3	G	286/296 (97%)	283 (99%)	2 (1%)	1 (0%)	36	42
4	A	369/381 (97%)	360 (98%)	9 (2%)	0	100	100
4	B	369/381 (97%)	360 (98%)	8 (2%)	1 (0%)	36	42
All	All	1885/1952 (97%)	1838 (98%)	42 (2%)	5 (0%)	36	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	37	GLN

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Mol	Chain	Res	Type
2	F	38	GLY
1	E	165	GLY
4	B	105	ALA
3	G	230	VAL

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	E	299/305 (98%)	297 (99%)	2 (1%)	76	87
2	F	403/424 (95%)	392 (97%)	11 (3%)	39	53
3	G	230/237 (97%)	225 (98%)	5 (2%)	45	61
4	A	314/323 (97%)	303 (96%)	11 (4%)	32	43
4	B	315/323 (98%)	300 (95%)	15 (5%)	23	30
All	All	1561/1612 (97%)	1517 (97%)	44 (3%)	38	52

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

Mol	Chain	Res	Type
1	E	116	ILE
1	E	224	MET
2	F	33	LEU
2	F	59	ASN
2	F	112	ARG
2	F	145	LEU
2	F	196	VAL
2	F	234	ILE
2	F	284	THR
2	F	306	VAL
2	F	346	GLU
2	F	440	ASN
2	F	471	THR
3	G	106	CYS
3	G	126	LEU

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Mol	Chain	Res	Type
3	G	178	LYS
3	G	212	VAL
3	G	235	LEU
4	A	22	ILE
4	A	127	LEU
4	A	219	LEU
4	A	234	ILE
4	A	270	VAL
4	A	288	GLU
4	A	327	LEU
4	A	331	GLN
4	A	337	VAL
4	A	345	ILE
4	A	350	GLU
4	B	15	GLU
4	B	33	VAL
4	B	100	LEU
4	B	123	LEU
4	B	127	LEU
4	B	134	LEU
4	B	185	ARG
4	B	211	ARG
4	B	252	ASP
4	B	258	LEU
4	B	288	GLU
4	B	320	ILE
4	B	324	ARG
4	B	327	LEU
4	B	347	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	349	ASN
1	E	355	GLN
2	F	59	ASN
2	F	98	ASN
2	F	165	GLN
2	F	222	ASN
2	F	232	ASN
2	F	437	ASN
2	F	440	ASN

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Mol	Chain	Res	Type
3	G	69	GLN
3	G	241	ASN
4	A	27	HIS
4	A	122	GLN
4	A	280	ASN
4	A	305	GLN
4	A	319	GLN
4	A	331	GLN
4	B	7	GLN
4	B	111	ASN
4	B	122	GLN
4	B	180	HIS
4	B	317	HIS

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 ⓘ

2 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	$\# Z > 2$
5	GLC	C	1	5	12,12,12	0.51	0	17,17,17	1.07	1 (5%)
5	GLC	C	2	5	11,11,12	0.35	0	15,15,17	0.92	1 (6%)

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	GLC	C	1	5	-	0/2/22/22	0/1/1/1
5	GLC	C	2	5	-	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(°)
5	C	1	GLC	C1-O5-C5	3.01	119.48	113.65
5	C	2	GLC	C1-O5-C5	3.00	116.21	112.19

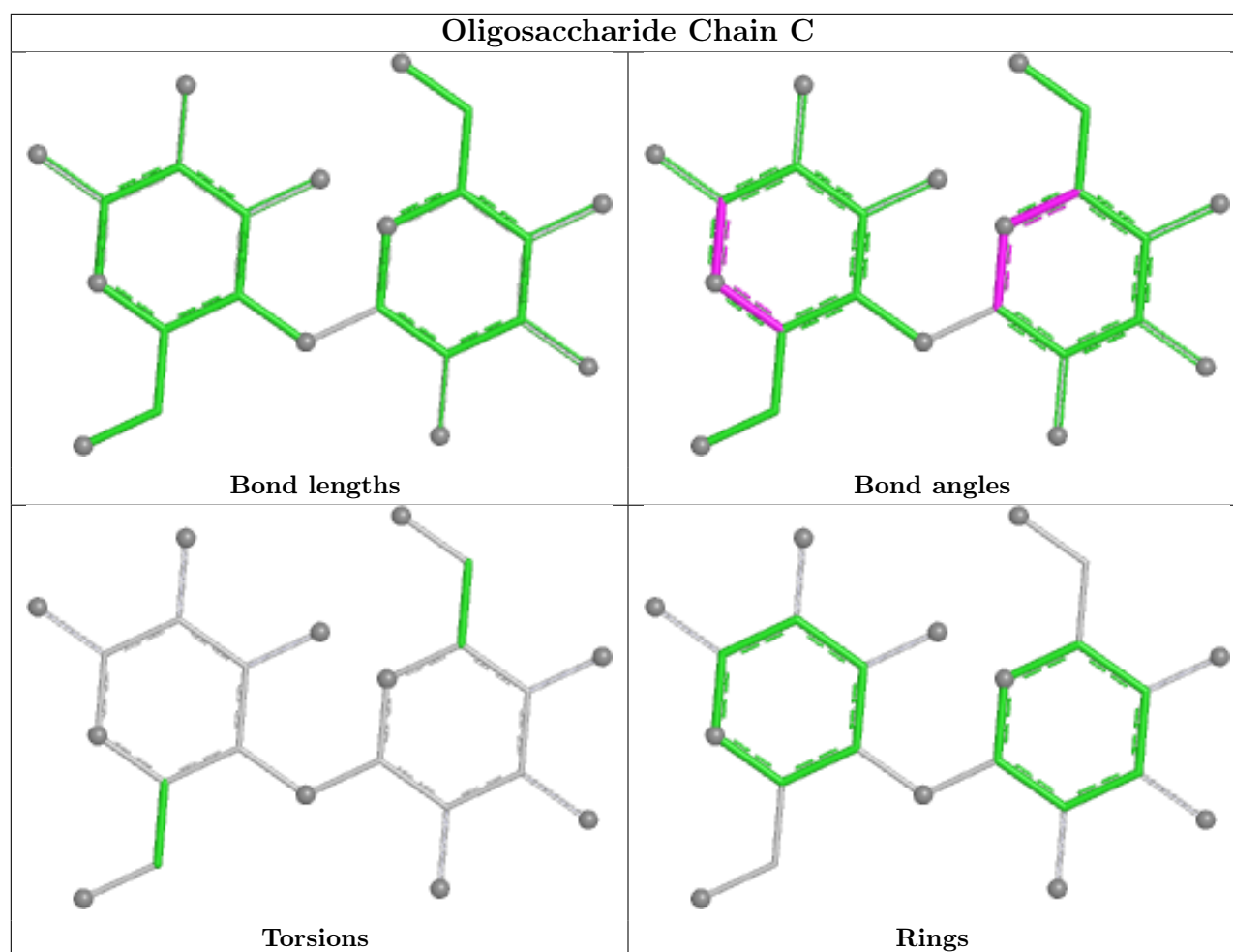
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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
9	ANP	A	2501	8	33,33,33	2.07	13 (39%)	45,52,52	2.29	14 (31%)
7	PGV	G	4006	-	13,13,50	0.27	0	12,12,56	0.54	0
9	ANP	B	2502	8	33,33,33	2.00	11 (33%)	45,52,52	2.11	13 (28%)
7	PGV	F	4001	-	50,50,50	1.09	3 (6%)	53,56,56	1.03	3 (5%)
7	PGV	F	4002	-	13,13,50	0.28	0	12,12,56	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	UMQ	E	5004	-	35,35,35	0.44	0	46,46,46	0.85	2 (4%)
7	PGV	G	4009	-	11,11,50	0.27	0	10,10,56	0.53	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
9	ANP	A	2501	8	-	3/18/38/38	0/3/3/3
7	PGV	G	4006	-	-	3/11/11/55	-
9	ANP	B	2502	8	-	3/18/38/38	0/3/3/3
7	PGV	F	4001	-	-	27/55/55/55	-
7	PGV	F	4002	-	-	9/11/11/55	-
6	UMQ	E	5004	-	-	10/20/60/60	0/2/2/2
7	PGV	G	4009	-	-	7/9/9/55	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2501	ANP	C5-C4	4.79	1.47	1.39
9	B	2502	ANP	C5-C4	4.64	1.47	1.39
9	A	2501	ANP	PB-N3B	4.41	1.74	1.63
7	F	4001	PGV	O03-C19	4.39	1.46	1.33
9	A	2501	ANP	PG-N3B	4.36	1.74	1.63
7	F	4001	PGV	O01-C1	4.29	1.46	1.34
9	B	2502	ANP	PB-N3B	4.25	1.74	1.63
9	B	2502	ANP	PG-N3B	4.16	1.74	1.63
7	F	4001	PGV	C12-C11	3.72	1.52	1.31
9	B	2502	ANP	PB-O1B	3.60	1.51	1.46
9	B	2502	ANP	PG-O1G	3.51	1.51	1.46
9	A	2501	ANP	PB-O1B	3.50	1.51	1.46
9	A	2501	ANP	PG-O1G	3.46	1.51	1.46
9	B	2502	ANP	C5-C6	2.77	1.48	1.41
9	A	2501	ANP	C5-C6	2.76	1.48	1.41
9	A	2501	ANP	PB-O3A	2.58	1.62	1.59
9	B	2502	ANP	PG-O3G	-2.43	1.50	1.56
9	A	2501	ANP	PG-O2G	-2.40	1.50	1.56
9	A	2501	ANP	C8-N7	2.36	1.36	1.31
9	B	2502	ANP	C5-N7	-2.35	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2501	ANP	PB-O2B	-2.27	1.50	1.56
9	B	2502	ANP	PG-O2G	-2.15	1.51	1.56
9	B	2502	ANP	C8-N7	2.15	1.35	1.31
9	A	2501	ANP	C5-N7	-2.14	1.35	1.39
9	B	2502	ANP	PB-O2B	-2.06	1.51	1.56
9	A	2501	ANP	PG-O3G	-2.05	1.51	1.56
9	A	2501	ANP	PA-O3A	2.03	1.61	1.59

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2501	ANP	O1G-PG-N3B	-7.95	100.06	111.77
9	B	2502	ANP	O1G-PG-N3B	-5.91	103.07	111.77
9	A	2501	ANP	C5-C4-N3	-5.48	119.17	126.72
9	B	2502	ANP	C5-C4-N3	-5.38	119.31	126.72
9	A	2501	ANP	O2B-PB-O1B	4.60	119.74	109.87
9	A	2501	ANP	N3-C4-N9	4.56	134.92	127.17
9	B	2502	ANP	N3-C4-N9	4.49	134.80	127.17
7	F	4001	PGV	O01-C1-C2	4.16	120.48	111.48
9	B	2502	ANP	O2B-PB-O1B	4.09	118.64	109.87
9	A	2501	ANP	C2-N3-C4	3.69	120.85	111.83
9	A	2501	ANP	O1B-PB-N3B	-3.61	106.45	111.77
9	B	2502	ANP	C2-N3-C4	3.59	120.60	111.83
9	A	2501	ANP	N3-C2-N1	-3.55	123.21	128.58
9	B	2502	ANP	N3-C2-N1	-3.44	123.38	128.58
9	B	2502	ANP	C4-C5-N7	-3.21	106.91	110.58
9	A	2501	ANP	C4-C5-N7	-3.17	106.96	110.58
9	B	2502	ANP	O1B-PB-N3B	-3.10	107.20	111.77
9	A	2501	ANP	C4-N9-C8	3.08	108.97	105.74
9	B	2502	ANP	C4-N9-C8	2.99	108.88	105.74
9	B	2502	ANP	O2G-PG-O3G	2.72	114.89	107.59
7	F	4001	PGV	O03-C19-C20	2.61	119.80	111.83
9	B	2502	ANP	C5-N7-C8	2.58	107.50	103.45
9	A	2501	ANP	C5-N7-C8	2.53	107.42	103.45
6	E	5004	UMQ	C3'-C4'-C5'	2.35	116.14	110.93
9	A	2501	ANP	N9-C8-N7	-2.26	110.73	113.94
9	A	2501	ANP	O2G-PG-O3G	2.25	113.64	107.59
6	E	5004	UMQ	C2'-C3'-C4'	2.24	114.77	109.68
7	F	4001	PGV	O01-C1-O02	-2.23	118.50	123.70
9	B	2502	ANP	N9-C8-N7	-2.19	110.82	113.94
9	B	2502	ANP	C6-C5-N7	2.11	136.15	132.09
9	A	2501	ANP	C6-C5-N7	2.08	136.10	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2501	ANP	C2-N1-C6	2.00	122.02	118.73

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	4001	PGV	C03-O11-P-O12
7	F	4001	PGV	C03-O11-P-O13
7	F	4001	PGV	C03-O11-P-O14
7	F	4001	PGV	C04-C05-C06-O06
7	F	4001	PGV	C2-C1-O01-C02
9	A	2501	ANP	PG-N3B-PB-O1B
9	A	2501	ANP	PA-O3A-PB-O2B
9	B	2502	ANP	PB-N3B-PG-O1G
9	B	2502	ANP	PG-N3B-PB-O1B
9	B	2502	ANP	PA-O3A-PB-O2B
7	F	4001	PGV	O02-C1-O01-C02
7	F	4001	PGV	C10-C11-C12-C13
7	F	4001	PGV	C20-C19-O03-C01
7	F	4001	PGV	O04-C19-O03-C01
6	E	5004	UMQ	C2'-C1'-O1'-CA
6	E	5004	UMQ	O5'-C5'-C6'-O6'
7	F	4001	PGV	C1-C2-C3-C4
6	E	5004	UMQ	O5'-C1'-O1'-CA
7	F	4001	PGV	C23-C24-C25-C26
7	F	4001	PGV	C25-C26-C27-C28
7	G	4009	PGV	C23-C24-C25-C26
6	E	5004	UMQ	CC-CD-CF-CG
7	G	4006	PGV	C22-C23-C24-C25
7	F	4001	PGV	C6-C7-C8-C9
7	F	4001	PGV	C22-C23-C24-C25
7	F	4001	PGV	C21-C22-C23-C24
7	F	4001	PGV	C26-C27-C28-C29
7	F	4001	PGV	C4-C5-C6-C7
7	F	4001	PGV	C20-C21-C22-C23
6	E	5004	UMQ	CG-CH-CI-CJ
7	F	4001	PGV	C29-C30-C31-C32
7	F	4001	PGV	C11-C10-C9-C8
7	G	4009	PGV	C20-C21-C22-C23
7	F	4001	PGV	C19-C20-C21-C22
7	F	4001	PGV	O05-C05-C06-O06
7	F	4001	PGV	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
7	F	4001	PGV	C2-C3-C4-C5
7	F	4002	PGV	C20-C21-C22-C23
7	G	4009	PGV	C26-C27-C28-C29
7	F	4002	PGV	C28-C29-C30-C31
7	F	4002	PGV	C22-C23-C24-C25
7	G	4009	PGV	C25-C26-C27-C28
7	F	4002	PGV	C27-C28-C29-C30
7	F	4001	PGV	O03-C01-C02-C03
7	F	4001	PGV	C14-C15-C16-C17
7	G	4009	PGV	C27-C28-C29-C30
7	F	4002	PGV	C21-C22-C23-C24
6	E	5004	UMQ	CI-CJ-CK-CL
7	G	4009	PGV	C21-C22-C23-C24
7	F	4001	PGV	O03-C01-C02-O01
7	G	4009	PGV	C19-C20-C21-C22
6	E	5004	UMQ	CD-CF-CG-CH
7	F	4002	PGV	C19-C20-C21-C22
7	G	4006	PGV	C23-C24-C25-C26
6	E	5004	UMQ	CB-CC-CD-CF
7	F	4002	PGV	C25-C26-C27-C28
7	F	4002	PGV	C23-C24-C25-C26
6	E	5004	UMQ	CH-CI-CJ-CK
7	G	4006	PGV	C21-C22-C23-C24
7	F	4002	PGV	C26-C27-C28-C29
6	E	5004	UMQ	CA-CB-CC-CD
9	A	2501	ANP	PB-N3B-PG-O1G

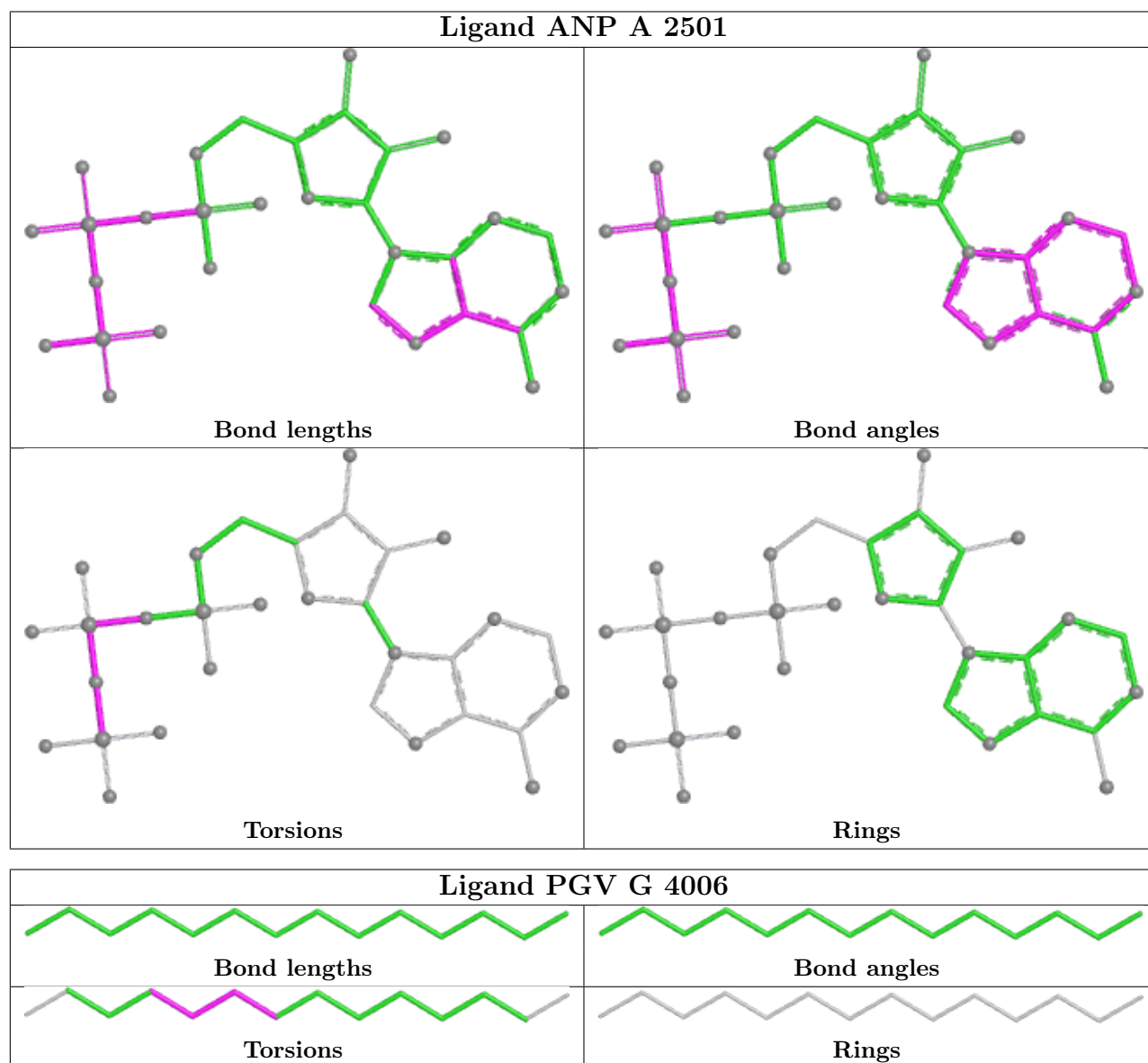
There are no ring outliers.

4 monomers are involved in 7 short contacts:

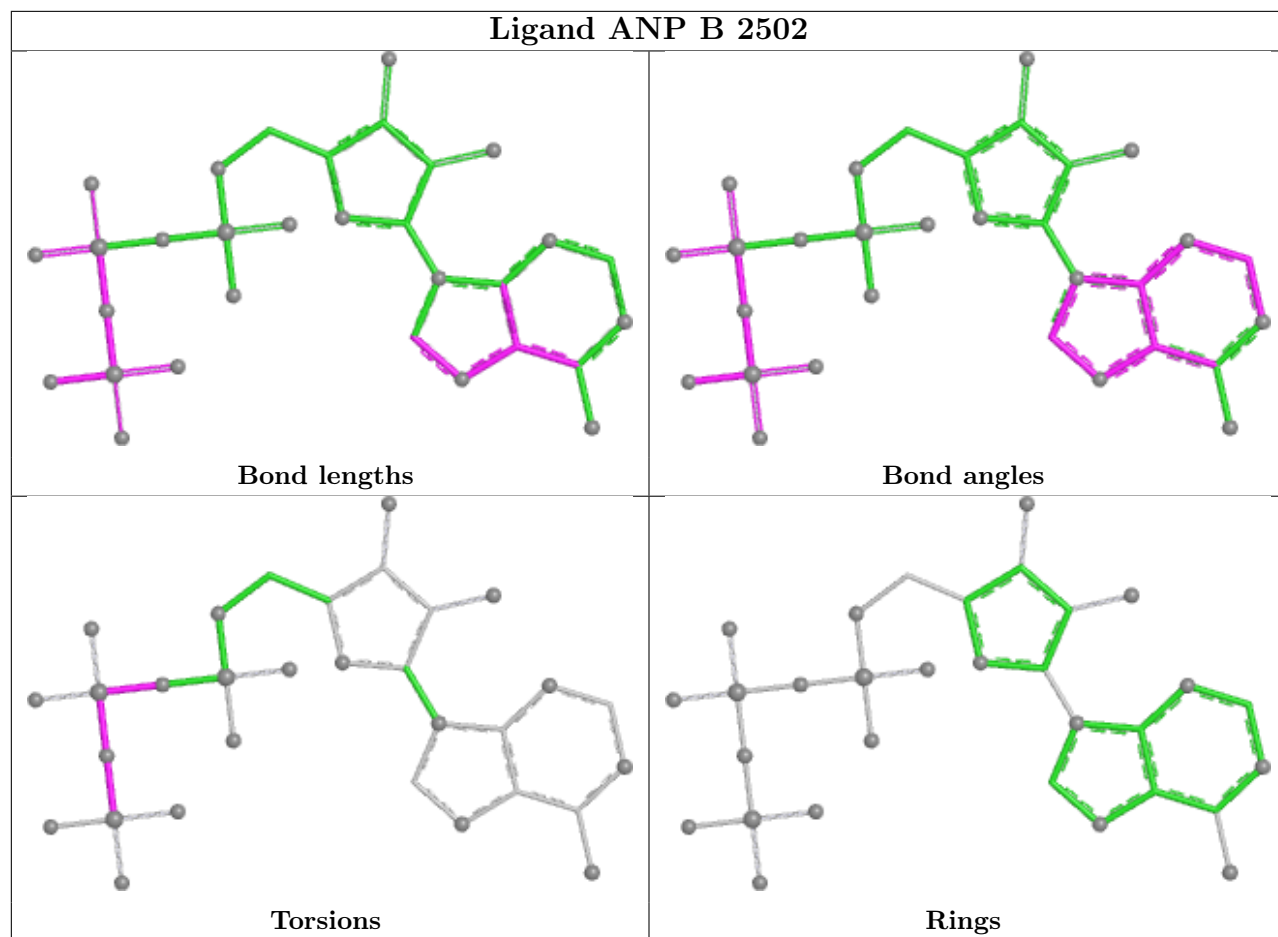
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2501	ANP	2	0
7	G	4006	PGV	1	0
9	B	2502	ANP	2	0
7	F	4001	PGV	2	0

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

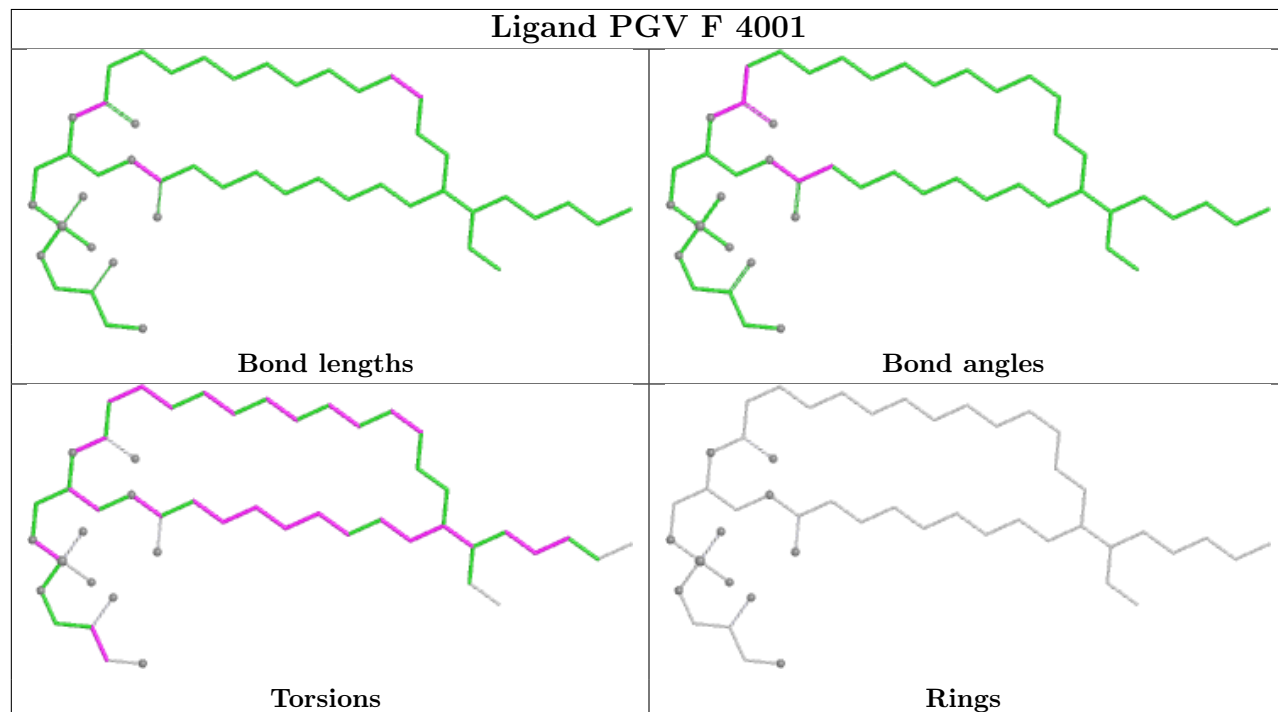
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



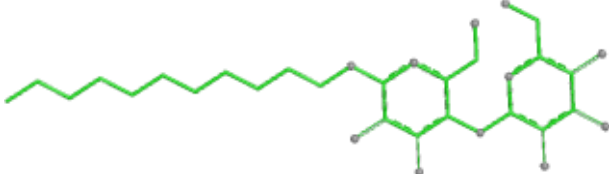
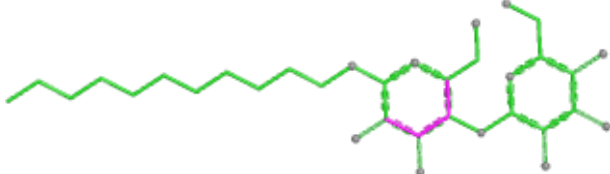
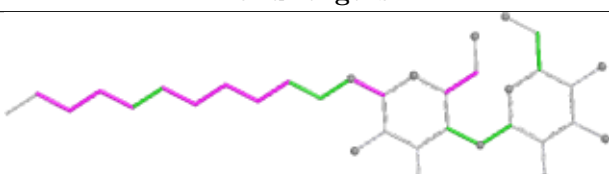
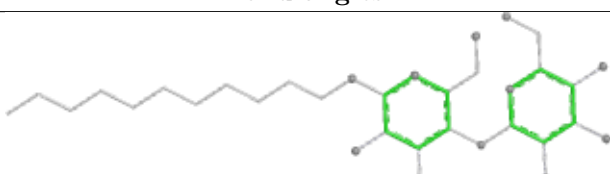
Ligand ANP B 2502

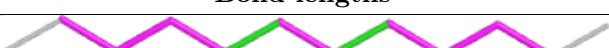


Ligand PGV F 4001



Ligand PGV F 4002	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UMQ E 5004	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV G 4009	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	E	374/380 (98%)	0.90	53 (14%) 6 4	18, 66, 111, 133	3 (0%)
2	F	490/514 (95%)	1.22	111 (22%) 2 1	19, 61, 127, 188	1 (0%)
3	G	286/296 (96%)	0.54	16 (5%) 30 27	19, 44, 81, 108	2 (0%)
4	A	371/381 (97%)	0.42	13 (3%) 47 44	27, 44, 69, 94	0
4	B	371/381 (97%)	0.52	25 (6%) 24 21	23, 46, 84, 112	1 (0%)
All	All	1892/1952 (96%)	0.76	218 (11%) 9 7	18, 51, 104, 188	7 (0%)

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	104	GLY	6.6
4	B	105	ALA	6.6
3	G	133	ALA	6.5
2	F	32	VAL	6.1
2	F	28	GLY	5.8
2	F	38	GLY	5.4
2	F	269	THR	5.3
2	F	217	GLY	5.0
2	F	503	ILE	5.0
1	E	141	ALA	4.8
2	F	10	TRP	4.8
1	E	353	GLY	4.7
2	F	21	GLY	4.6
2	F	277	PHE	4.6
2	F	345	GLY	4.5
2	F	220	THR	4.5
2	F	500	ALA	4.4
2	F	26	LEU	4.2
2	F	280	ILE	4.2
2	F	22	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
4	B	263	ARG	4.2
2	F	25	LEU	4.1
2	F	17	TRP	4.1
2	F	499	GLY	4.1
4	B	260	MET	4.0
2	F	411	PHE	3.9
1	E	253	GLN	3.9
2	F	43	ALA	3.9
1	E	374	SER	3.8
2	F	51	SER	3.8
2	F	265	THR	3.8
2	F	260	GLY	3.8
3	G	70	ALA	3.7
3	G	11	ALA	3.7
2	F	36	ALA	3.6
2	F	24	GLY	3.6
3	G	149	GLU	3.6
1	E	178	ILE	3.5
2	F	14	ALA	3.5
2	F	352	SER	3.5
1	E	191	GLY	3.5
1	E	222	THR	3.4
4	A	64	GLU	3.4
2	F	40	TYR	3.4
2	F	31	VAL	3.4
2	F	62	ALA	3.4
2	F	44	ILE	3.4
2	F	481	GLY	3.3
2	F	485	GLY	3.3
2	F	46	THR	3.2
1	E	186	ALA	3.2
2	F	267	VAL	3.2
2	F	11	GLN	3.2
2	F	48	ILE	3.2
1	E	119	LYS	3.2
1	E	190	ALA	3.2
2	F	278	LEU	3.2
2	F	29	TYR	3.1
2	F	474	ILE	3.1
4	B	322	SER	3.1
3	G	69	GLN	3.0
3	G	71	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	41	LEU	3.0
2	F	37	GLN	3.0
2	F	268	PHE	3.0
2	F	357	VAL	3.0
2	F	50	SER	3.0
4	B	112	GLN	3.0
1	E	145	SER	2.9
1	E	134	ALA	2.9
1	E	370	LYS	2.9
2	F	19	VAL	2.9
2	F	349	MET	2.9
4	A	177	SER	2.9
2	F	456	GLY	2.9
2	F	219	LEU	2.9
3	G	146	ARG	2.8
1	E	170	LYS	2.8
2	F	245	ASN	2.8
1	E	341	TYR	2.8
2	F	274	GLN	2.8
2	F	463	TYR	2.8
2	F	15	LEU	2.8
1	E	177	ASP	2.8
3	G	116	PRO	2.8
2	F	45	THR	2.8
2	F	218	THR	2.8
1	E	143	GLY	2.8
1	E	182	GLY	2.8
1	E	163	ALA	2.8
4	A	295	ILE	2.7
2	F	491	ALA	2.7
4	A	103	ALA	2.7
2	F	214	ASP	2.7
4	B	259	PRO	2.7
1	E	22	GLU	2.7
2	F	33	LEU	2.7
2	F	355	PHE	2.7
1	E	369	THR	2.7
2	F	129	ASP	2.7
4	B	300	LEU	2.7
4	B	15	GLU	2.6
4	B	21	ASP	2.6
3	G	72	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	60	ARG	2.6
1	E	207	ASP	2.6
2	F	215	GLY	2.6
2	F	247	GLY	2.6
2	F	16	LYS	2.6
4	B	245	LYS	2.6
2	F	477	GLU	2.6
1	E	183	VAL	2.6
2	F	47	LEU	2.6
1	E	373	ALA	2.6
1	E	363	ASP	2.6
2	F	72	MET	2.6
4	A	342	THR	2.6
3	G	74	ILE	2.6
1	E	237	THR	2.5
1	E	241	ASN	2.5
2	F	344	PHE	2.5
2	F	35	TYR	2.5
1	E	139	LEU	2.5
2	F	475	ALA	2.5
4	B	279	ALA	2.5
2	F	462	GLY	2.5
1	E	372	SER	2.5
3	G	280	LEU	2.5
4	A	263	ARG	2.4
3	G	131	PHE	2.4
1	E	135	LEU	2.4
2	F	195	LYS	2.4
2	F	445	GLN	2.4
2	F	27	VAL	2.4
2	F	354	LEU	2.4
2	F	501	LEU	2.4
2	F	489	ALA	2.4
2	F	459	THR	2.4
2	F	18	SER	2.4
2	F	56	ILE	2.4
3	G	75	THR	2.4
4	B	360	THR	2.4
4	B	320	ILE	2.4
2	F	467	LEU	2.4
2	F	496	LEU	2.4
2	F	206	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	234	ILE	2.3
2	F	423	ILE	2.3
2	F	49	LEU	2.3
4	A	174	ILE	2.3
1	E	194	PHE	2.3
2	F	257	VAL	2.3
4	B	119	GLU	2.3
1	E	255	SER	2.3
1	E	122	LEU	2.3
2	F	20	LEU	2.3
1	E	205	ASN	2.3
2	F	216	ASP	2.3
1	E	187	GLY	2.3
2	F	53	GLY	2.3
1	E	345	THR	2.3
2	F	498	VAL	2.3
4	B	336	LEU	2.2
4	B	274	ASP	2.2
1	E	101	GLY	2.2
1	E	99	TYR	2.2
1	E	188	ALA	2.2
1	E	179	LYS	2.2
1	E	118	ASN	2.2
2	F	13	ASP	2.2
4	A	294	ASP	2.2
2	F	312	ARG	2.2
1	E	360	ALA	2.2
4	A	323	ILE	2.2
2	F	258	THR	2.2
2	F	284	THR	2.2
2	F	457	THR	2.2
4	B	342	THR	2.2
1	E	124	ASN	2.2
4	B	16	VAL	2.2
1	E	151	LEU	2.1
1	E	78	GLU	2.1
2	F	271	GLU	2.1
4	B	261	PRO	2.1
1	E	350	ALA	2.1
2	F	58	ALA	2.1
4	A	105	ALA	2.1
1	E	132	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
3	G	122	LEU	2.1
3	G	127	ILE	2.1
4	B	323	ILE	2.1
1	E	136	ASP	2.1
2	F	226	VAL	2.1
1	E	327	GLY	2.1
4	A	169	ARG	2.1
2	F	279	ALA	2.1
2	F	502	ALA	2.1
2	F	227	LYS	2.1
2	F	273	ILE	2.1
3	G	148	GLY	2.1
2	F	360	ALA	2.1
4	A	262	ASN	2.1
4	B	171	GLN	2.1
4	B	295	ILE	2.1
1	E	117	TYR	2.1
2	F	338	GLY	2.1
2	F	246	TRP	2.1
2	F	261	TRP	2.1
1	E	274	GLU	2.0
2	F	353	ALA	2.0
4	B	339	GLU	2.0
2	F	248	ASP	2.0
4	B	321	PRO	2.0
2	F	356	GLY	2.0
2	F	262	LYS	2.0
1	E	128	THR	2.0
1	E	359	GLU	2.0
4	B	349	PRO	2.0

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

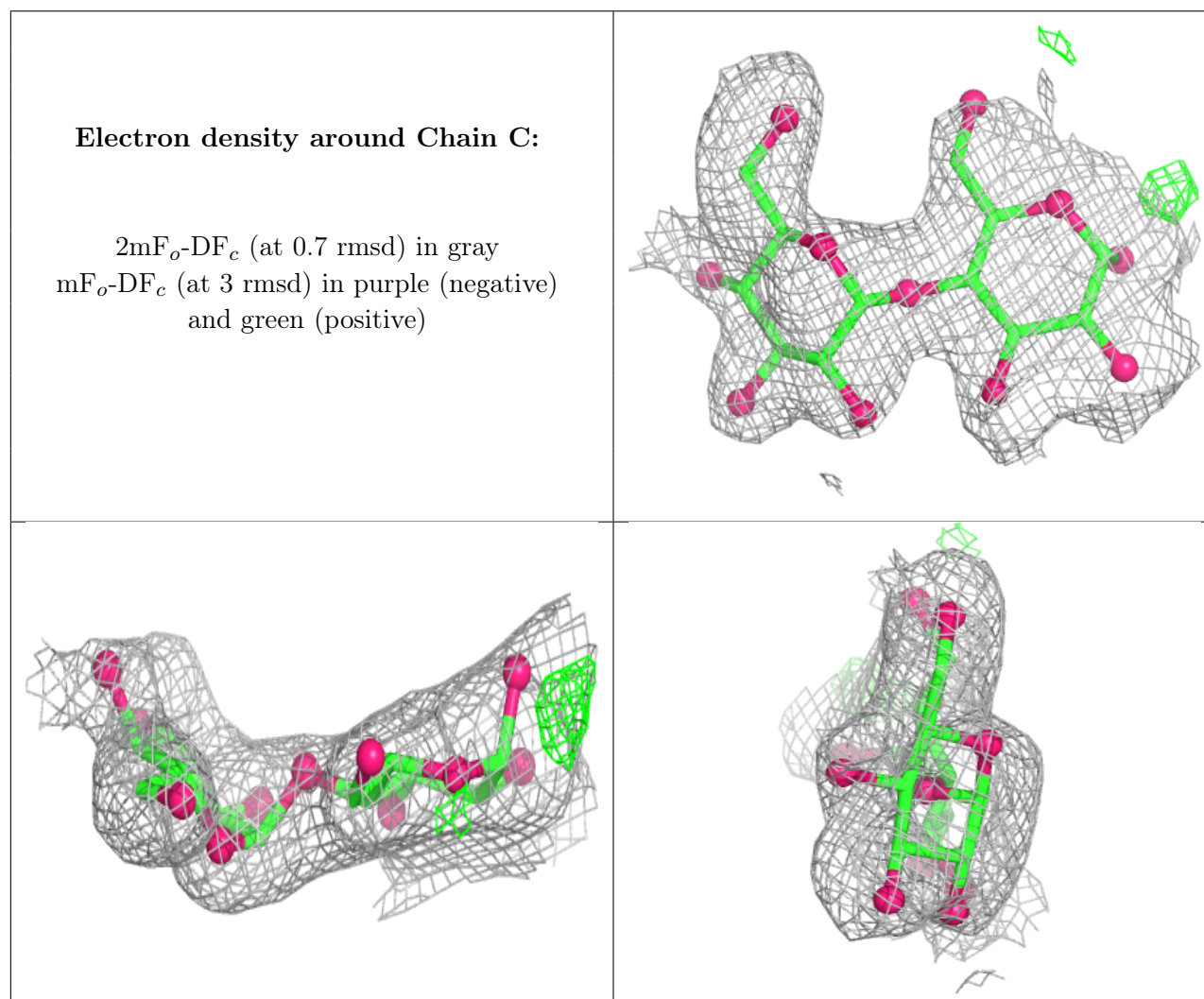
There are no non-standard protein/DNA/RNA residues in this entry.

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
5	GLC	C	1	12/12	-	-	47,49,52,54	0
5	GLC	C	2	11/12	-	-	46,48,50,51	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
7	PGV	G	4006	14/51	0.72	0.19	71,75,82,84	0
7	PGV	F	4002	14/51	0.73	0.13	58,60,65,66	0

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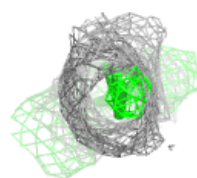
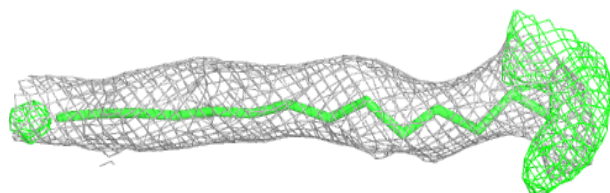
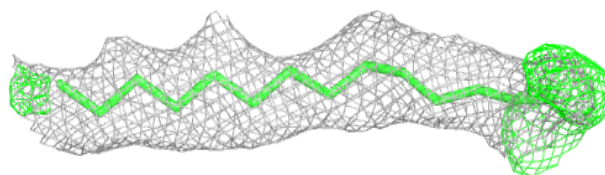
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PGV	G	4009	12/51	0.76	0.20	70,71,74,74	0
6	UMQ	E	5004	34/34	0.79	0.18	74,80,82,83	0
7	PGV	F	4001	51/51	0.83	0.15	75,83,86,91	0
9	ANP	A	2501	31/31	0.98	0.06	25,32,41,41	0
9	ANP	B	2502	31/31	0.98	0.07	28,35,41,42	0
8	MG	A	1501	1/1	0.99	0.03	28,28,28,28	0
8	MG	B	1502	1/1	0.99	0.06	30,30,30,30	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.

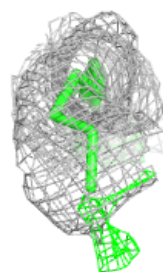
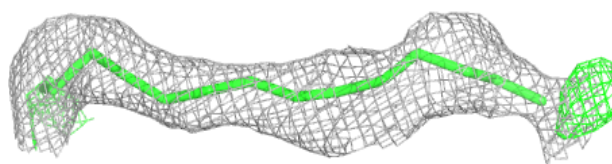
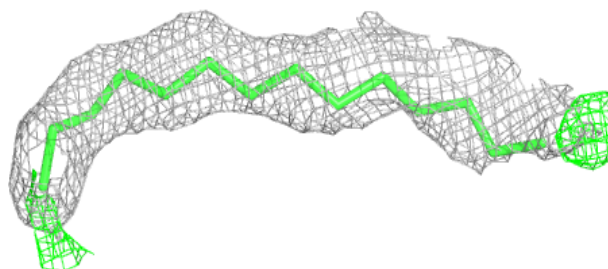
Electron density around PGV G 4006:

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

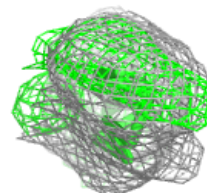
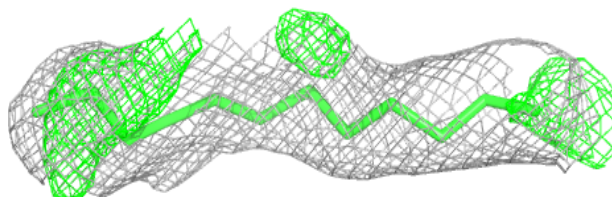
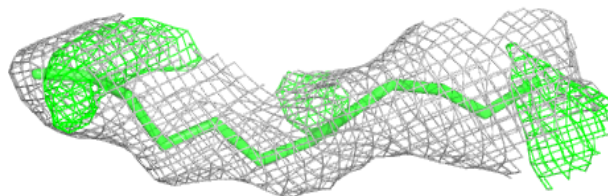


Electron density around PGV F 4002:

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

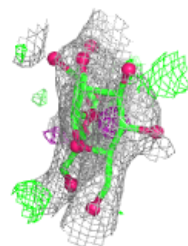
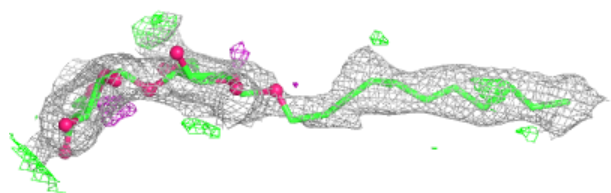
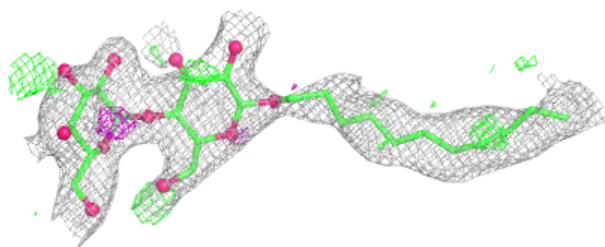
**Electron density around PGV G 4009:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

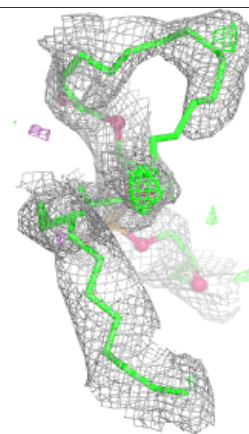
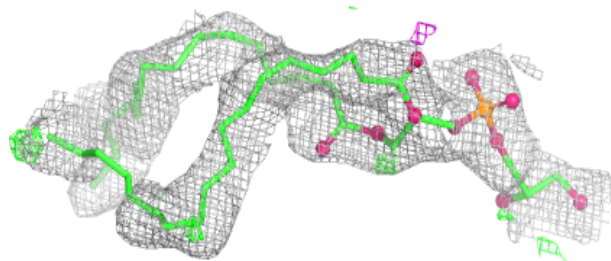
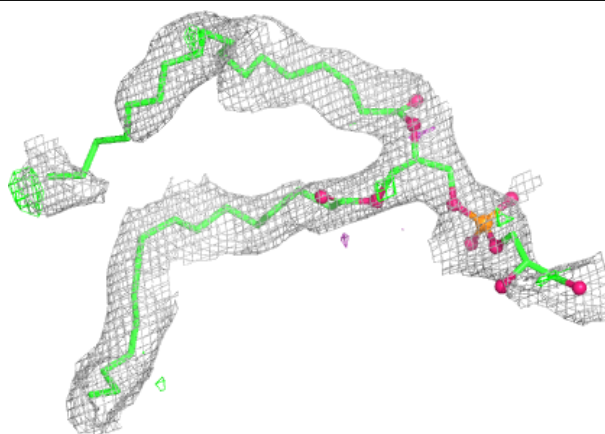


Electron density around UMQ E 5004:

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

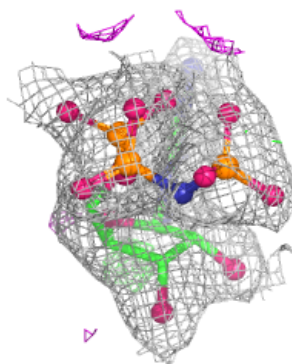
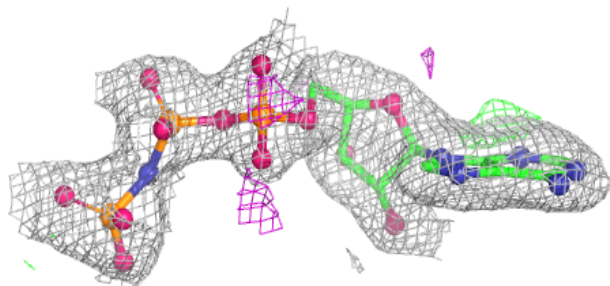
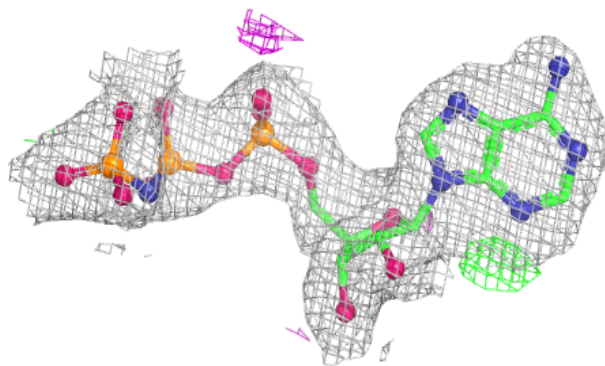
**Electron density around PGV F 4001:**

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

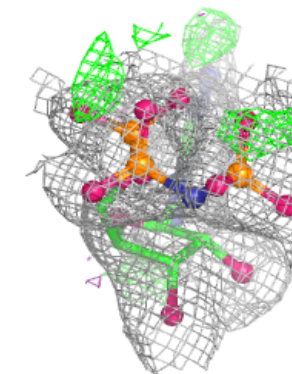
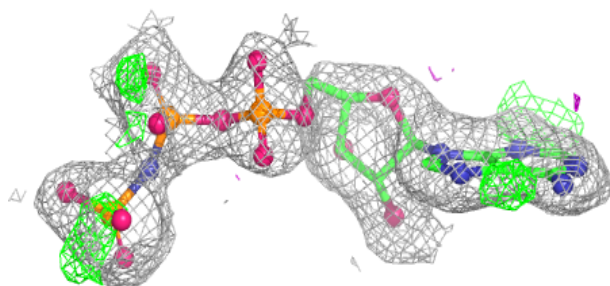
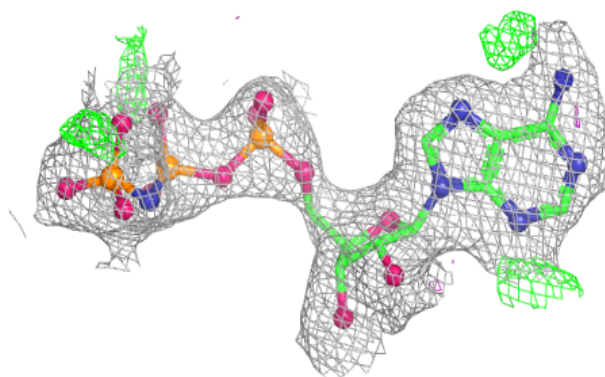


Electron density around ANP A 2501:

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

**Electron density around ANP B 2502:**

$2mF_o-DF_c$ (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.