



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 12:14 PM BST

PDB ID : 3PUW
Title : Crystal Structure of an outward-facing MBP-Maltose transporter complex bound to ADP-AIF4
Authors : Oldham, M.L.; Chen, J.
Deposited on : 2010-12-06
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

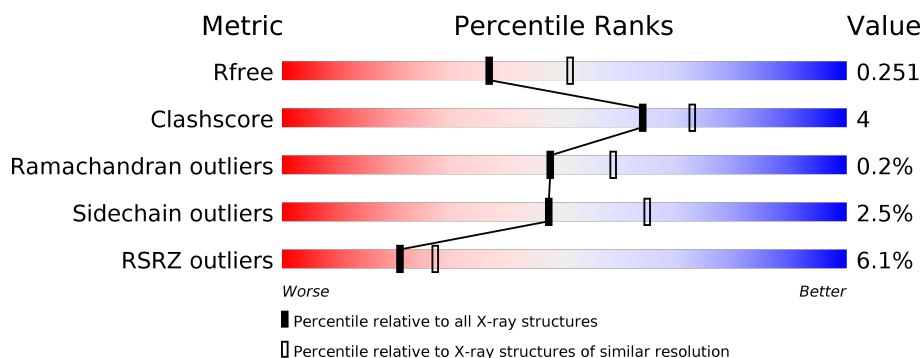
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	378	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>7%</div> <div>•</div> </div> </div>
2	F	514	<div> <div>8%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>• 5%</div> </div> </div>
3	G	296	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>•</div> </div> </div>
4	A	381	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>• •</div> </div> </div>
4	B	381	<div> <div>8%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>• 6%</div> </div> </div>
5	C	2	<div> <div></div> <div> <div></div> <div>100%</div> </div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15229 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	3	0
			2915	1877	474	558	6			

There are 8 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

- 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	2	0
			3831	2517	610	687	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	288	Total	C	N	O	S	0	1	0
			2227	1491	355	373	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	4	0
			2909	1838	521	536	14			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	358	Total	C	N	O	S	0	0	0
			2787	1765	497	512	13			

There are 20 discrepancies between the modelled and reference sequences:

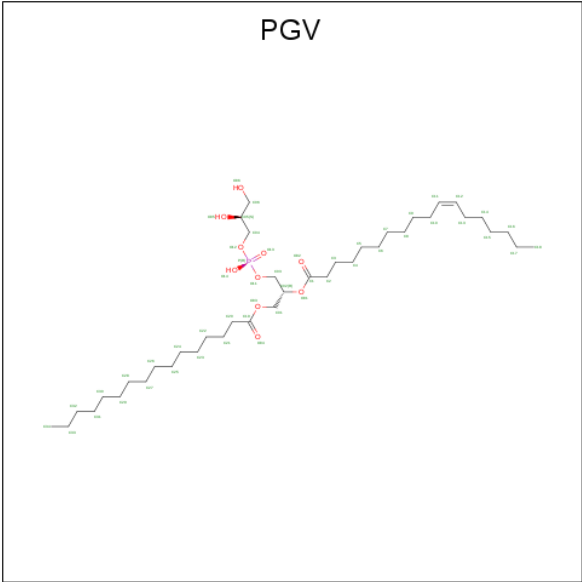
Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	-	expression tag	UNP P68187
A	373	SER	-	expression tag	UNP P68187
A	374	ALA	-	expression tag	UNP P68187
A	375	SER	-	expression tag	UNP P68187
A	376	HIS	-	expression tag	UNP P68187
A	377	HIS	-	expression tag	UNP P68187
A	378	HIS	-	expression tag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



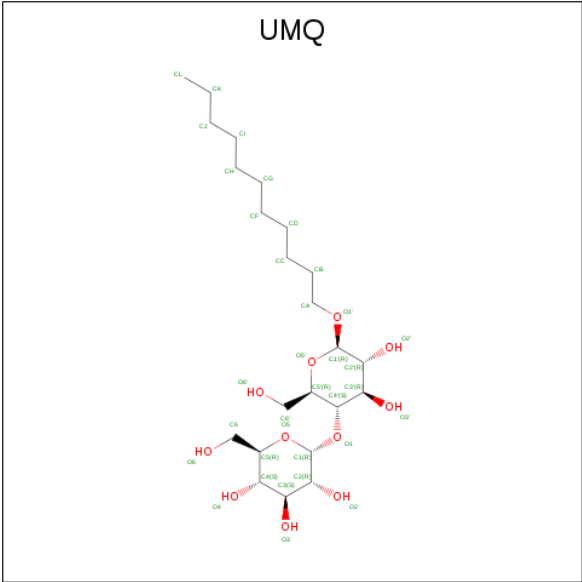
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	C	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 6 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	F	1	Total 51	C 40	O 10	P 1	0	0	
6	F	1	Total 9	C 9				0	0
6	F	1	Total 8	C 8				0	0
6	F	1	Total 17	C 17				0	0
6	G	1	Total 14	C 14				0	0
6	G	1	Total 12	C 12				0	0
6	G	1	Total 12	C 12				0	0
6	G	1	Total 15	C 15				0	0
6	G	1	Total 12	C 12				0	0
6	G	1	Total 14	C 14				0	0

- Molecule 7 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: C₂₃H₄₄O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			34	23	11		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

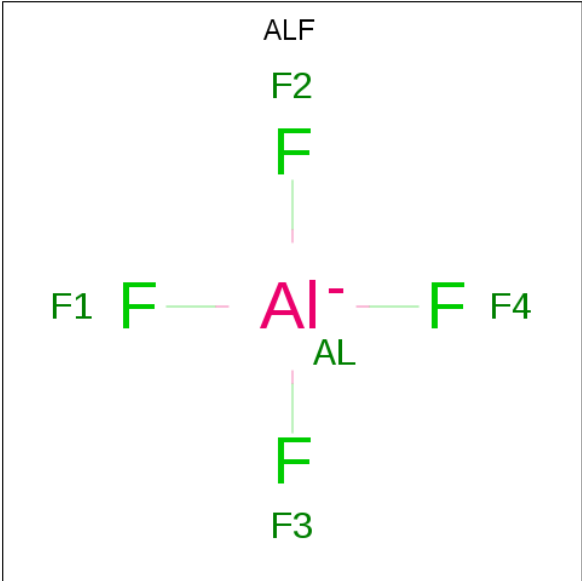
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Mg	0	0
			1	1		
8	A	1	Total	Mg	0	0
			1	1		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 10 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	Al	F	0	0
			5	1	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Al	F	0	0
			5	1	4		

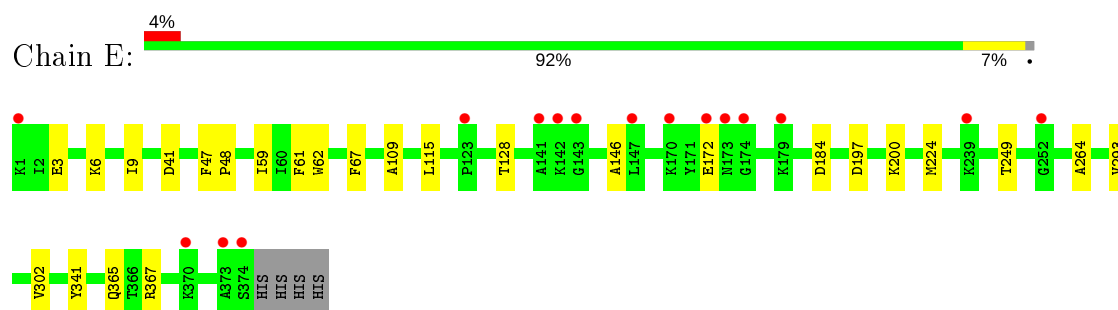
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	E	68	Total	O	0	0
			68	68		
11	F	57	Total	O	0	0
			57	57		
11	G	47	Total	O	0	0
			47	47		
11	A	47	Total	O	0	0
			47	47		
11	B	54	Total	O	0	0
			54	54		

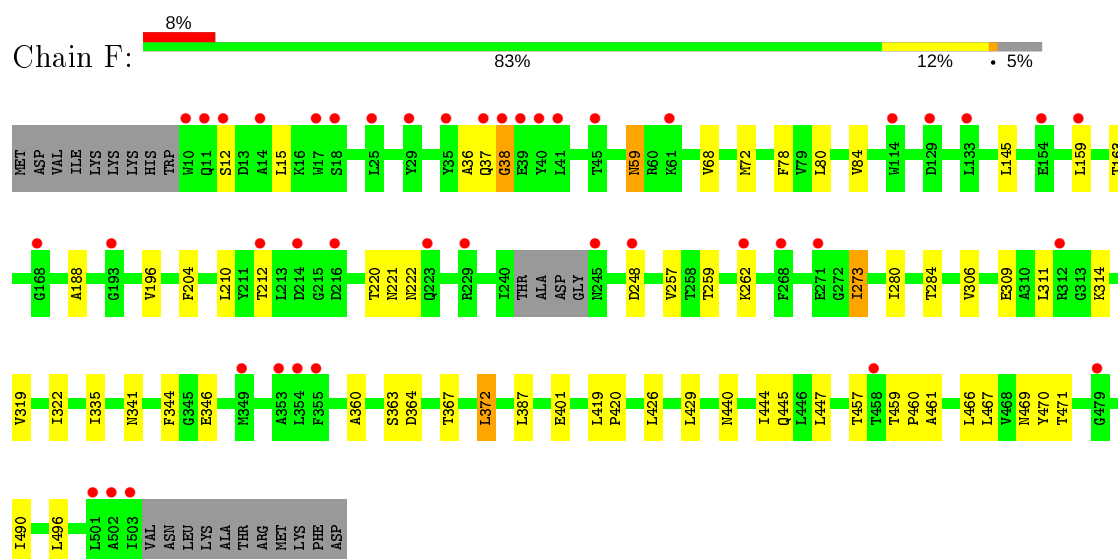
3 Residue-property plots

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

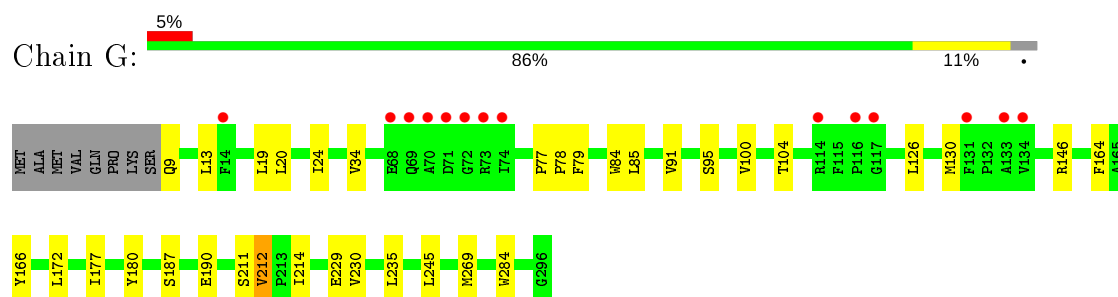
- Molecule 1: Maltose-binding periplasmic protein



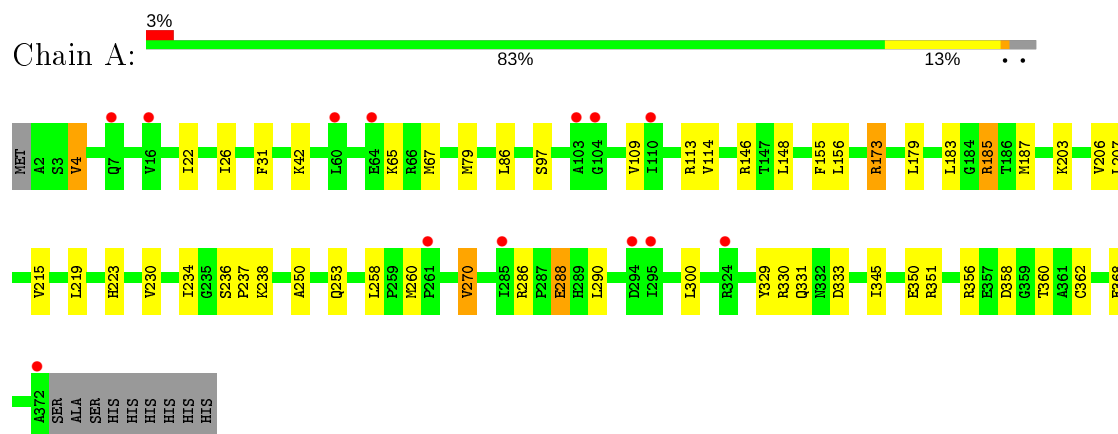
- Molecule 2: Maltose transport system permease protein malF



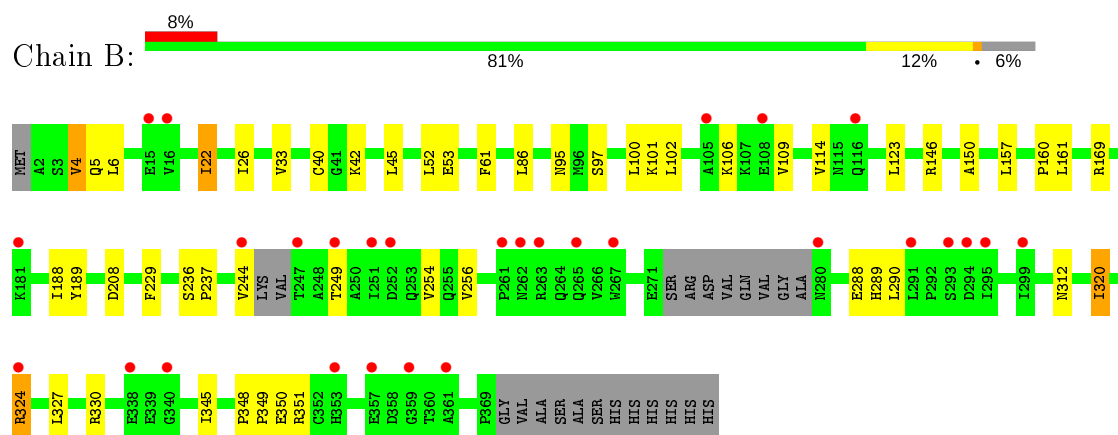
- Molecule 3: Maltose transport system permease protein malG



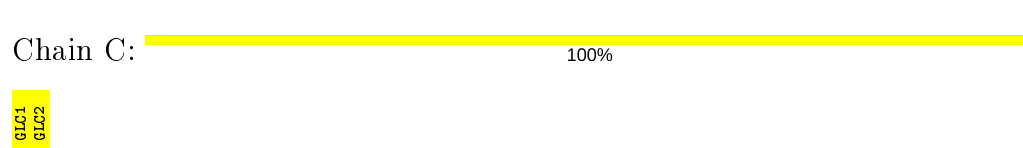
- Molecule 4: Maltose/maltodextrin import ATP-binding protein MalK



- 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	81.88Å 97.34Å 112.34Å 85.76° 79.42° 72.45°	Depositor
Resolution (Å)	19.99 – 2.30 19.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	66.5 (19.99-2.30) 66.5 (19.99-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.220 , 0.255 0.219 , 0.251	Depositor DCC
R_{free} test set	4819 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15229	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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, UMQ, ADP, ALF, GLC, PGV

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	0.34	0/2990	0.47	0/4059
2	F	0.36	0/3932	0.50	0/5352
3	G	0.37	0/2291	0.50	1/3131 (0.0%)
4	A	0.34	0/2962	0.53	0/4016
4	B	0.33	0/2835	0.51	0/3842
All	All	0.35	0/15010	0.50	1/20400 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	235	LEU	CA-CB-CG	5.70	128.42	115.30

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	2915	0	2891	15	0
2	F	3831	0	3861	41	0
3	G	2227	0	2314	21	0
4	A	2909	0	2971	34	0
4	B	2787	0	2845	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	23	0	21	0	0
6	F	85	0	133	1	0
6	G	79	0	122	0	0
7	F	34	0	44	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	27	0	12	0	0
9	B	27	0	12	0	0
10	A	5	0	0	0	0
10	B	5	0	0	0	0
11	A	47	0	0	0	0
11	B	54	0	0	1	0
11	E	68	0	0	1	0
11	F	57	0	0	0	0
11	G	47	0	0	0	0
All	All	15229	0	15226	128	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 (128) 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)
4:A:173[A]:ARG:NH1	4:A:173[A]:ARG:HB2	1.62	1.12
4:A:173[A]:ARG:HH11	4:A:173[A]:ARG:CG	1.73	1.01
4:A:173[A]:ARG:NH1	4:A:173[A]:ARG:CB	2.30	0.94
4:A:173[A]:ARG:CB	4:A:173[A]:ARG:HH11	1.82	0.92
4:A:173[A]:ARG:HH11	4:A:173[A]:ARG:HG3	1.35	0.87
4:B:6:LEU:HD22	4:B:22:ILE:HD11	1.59	0.84
1:E:115:LEU:HD21	1:E:224:MET:HE3	1.59	0.84
4:A:173[A]:ARG:HH11	4:A:173[A]:ARG:HB2	1.36	0.81
4:A:79:MET:HG3	4:A:156:LEU:HB2	1.64	0.78
4:A:223:HIS:CE1	4:A:368:GLU:HG2	2.18	0.78
3:G:91:VAL:O	3:G:95:SER:HB2	1.89	0.72
2:F:471:THR:HG21	2:F:490:ILE:HG21	1.72	0.71
2:F:444:ILE:HG13	2:F:466:LEU:HG	1.73	0.70
1:E:367:ARG:HD2	2:F:460:PRO:HG3	1.75	0.69
4:A:356:ARG:HH11	4:A:360:THR:HG23	1.58	0.68
2:F:335:ILE:HD12	3:G:34:VAL:HG22	1.75	0.67
2:F:284:THR:HG22	2:F:466:LEU:HA	1.76	0.66
4:A:86:LEU:HA	4:A:146:ARG:NH2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:4:VAL:HG13	4:B:26:ILE:HB	1.79	0.65
3:G:104:THR:HG22	3:G:177:ILE:HD13	1.80	0.63
3:G:187:SER:HA	3:G:190:GLU:HB2	1.82	0.61
2:F:471:THR:CG2	2:F:490:ILE:HG21	2.31	0.61
2:F:309:GLU:HA	2:F:314:LYS:NZ	2.16	0.60
4:B:290:LEU:HD22	4:B:345:ILE:HD13	1.84	0.59
2:F:372:LEU:HD13	2:F:447:LEU:HD23	1.85	0.58
2:F:280:ILE:O	2:F:284:THR:HG23	2.04	0.58
2:F:159:LEU:HD11	2:F:188:ALA:HB1	1.84	0.58
2:F:471:THR:HG23	2:F:490:ILE:HD13	1.85	0.58
4:B:106:LYS:HB2	4:B:109:VAL:HB	1.87	0.57
4:A:260[A]:MET:HE2	4:A:300:LEU:HD22	1.86	0.56
2:F:196:VAL:CG1	2:F:204:PHE:HB3	2.36	0.55
2:F:341:ASN:O	2:F:344:PHE:O	2.25	0.54
4:A:173[A]:ARG:CB	4:A:173[A]:ARG:CZ	2.84	0.54
2:F:59:ASN:H	2:F:59:ASN:HD22	1.56	0.54
4:A:4:VAL:HG13	4:A:26:ILE:HB	1.89	0.54
2:F:360:ALA:HB1	2:F:363:SER:HB2	1.89	0.54
4:B:157:LEU:HB3	4:B:160:PRO:HG3	1.91	0.53
2:F:471:THR:HG21	2:F:490:ILE:CG2	2.37	0.52
1:E:146:ALA:O	1:E:224:MET:HG2	2.10	0.52
4:B:288:GLU:HG3	4:B:330:ARG:HD3	1.92	0.52
4:B:249:THR:HG22	4:B:254:VAL:HG13	1.91	0.51
2:F:273:ILE:HA	2:F:470:TYR:OH	2.10	0.51
3:G:126:LEU:O	3:G:130:MET:HG2	2.09	0.51
3:G:100:VAL:O	3:G:104:THR:HG23	2.09	0.51
2:F:36:ALA:O	2:F:38:GLY:N	2.44	0.51
2:F:429:LEU:HD23	3:G:172:LEU:HD22	1.93	0.51
4:A:358:ASP:OD1	4:A:360:THR:HG22	2.11	0.50
4:A:288:GLU:HG2	4:B:312:ASN:HB2	1.92	0.50
4:B:320:ILE:HD11	4:B:327:LEU:HB2	1.94	0.50
1:E:41[B]:ASP:OD2	11:E:407:HOH:O	2.20	0.50
1:E:3:GLU:HB3	1:E:6:LYS:HE2	1.93	0.50
2:F:319:VAL:O	2:F:322:ILE:HG13	2.13	0.49
2:F:335:ILE:HD12	3:G:34:VAL:CG2	2.43	0.49
4:B:324:ARG:H	4:B:324:ARG:HD3	1.77	0.48
4:A:183:LEU:HB3	4:A:185:ARG:HG3	1.95	0.48
4:B:236:SER:HA	4:B:237:PRO:C	2.33	0.48
2:F:68:VAL:HG12	2:F:72:MET:HG3	1.96	0.48
4:B:40:CYS:SG	4:B:42:LYS:HG3	2.54	0.48
4:B:161:LEU:HB3	4:B:169:ARG:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:33:VAL:HG12	4:B:189:TYR:HB3	1.96	0.47
4:A:42:LYS:HG2	4:A:207:LEU:HD12	1.97	0.47
1:E:109:ALA:HA	1:E:302:VAL:HA	1.97	0.47
3:G:20:LEU:O	3:G:24:ILE:HG12	2.14	0.47
4:A:206:VAL:HG21	4:A:234:ILE:HD11	1.98	0.46
4:A:236:SER:HA	4:A:237:PRO:C	2.35	0.46
4:A:329:TYR:CE2	4:A:331:GLN:HG2	2.51	0.46
4:B:86:LEU:HA	4:B:146:ARG:NH2	2.31	0.46
2:F:387:LEU:HD13	2:F:429:LEU:HD13	1.97	0.46
2:F:259:THR:HB	2:F:262:LYS:HD2	1.97	0.46
2:F:419:LEU:HB3	2:F:420:PRO:HD3	1.98	0.46
2:F:309:GLU:HA	2:F:314:LYS:HZ2	1.81	0.45
4:A:250:ALA:HB3	4:A:253:GLN:HG2	1.98	0.45
4:B:100:LEU:HD13	4:B:150:ALA:HA	1.98	0.45
4:A:148:LEU:HD22	4:A:179:LEU:HD22	1.99	0.45
4:A:97:SER:HB3	4:A:114:VAL:HG21	1.98	0.45
2:F:309:GLU:HA	2:F:314:LYS:HZ3	1.81	0.45
3:G:166:TYR:OH	3:G:229[A]:GLU:HG2	2.17	0.45
4:A:351:ARG:NE	4:A:368:GLU:OE2	2.40	0.45
4:B:244:VAL:HB	4:B:256:VAL:HB	1.99	0.45
4:A:65:LYS:O	4:A:67:MET:HG2	2.17	0.45
1:E:9:ILE:HG12	1:E:59:ILE:HB	1.98	0.45
3:G:79:PHE:HB3	3:G:84:TRP:CH2	2.52	0.45
1:E:61:PHE:CE2	1:E:264:ALA:HB2	2.52	0.44
2:F:457:THR:HG21	2:F:461:ALA:HB3	1.99	0.44
4:B:208:ASP:HB2	4:B:229:PHE:CE2	2.52	0.44
4:B:97:SER:HB3	4:B:114:VAL:HG21	1.98	0.44
4:A:203:LYS:HD3	4:A:215:VAL:CG1	2.48	0.44
4:A:270:VAL:HG13	4:A:362:CYS:HB3	2.00	0.44
3:G:180:TYR:CE2	3:G:211:SER:HA	2.52	0.44
4:A:230:VAL:HG13	4:A:234:ILE:HD13	2.00	0.44
1:E:184:ASP:HB2	1:E:365:GLN:CD	2.38	0.44
2:F:12:SER:HB2	2:F:15:LEU:HB2	1.99	0.44
2:F:212:THR:HG23	2:F:222:ASN:HD21	1.83	0.44
3:G:212:VAL:HG22	3:G:284:TRP:CE3	2.53	0.43
4:A:173[A]:ARG:NH1	4:A:173[A]:ARG:HG3	2.15	0.43
6:F:4001:PGV:H82	3:G:19:LEU:HD13	2.00	0.43
1:E:197:ASP:HA	1:E:200:LYS:HB2	2.01	0.43
1:E:62:TRP:HB3	1:E:67:PHE:CE1	2.53	0.43
4:A:290:LEU:HD22	4:A:345:ILE:HD13	2.00	0.43
4:A:286:ARG:HB3	4:A:288:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:341:TYR:CE2	2:F:460:PRO:HB3	2.54	0.42
1:E:47:PHE:HB3	1:E:48:PRO:HD3	2.00	0.42
2:F:78:PHE:HZ	3:G:164:PHE:CD2	2.37	0.42
3:G:9:GLN:O	3:G:9:GLN:HG3	2.19	0.42
2:F:401:GLU:HG2	4:B:52:LEU:HD22	2.02	0.42
3:G:85:LEU:HD22	3:G:269:MET:HE3	2.00	0.42
2:F:80:LEU:O	2:F:84:VAL:HG23	2.20	0.42
2:F:364:ASP:HB3	2:F:367:THR:OG1	2.20	0.42
3:G:214:ILE:HA	3:G:214:ILE:HD12	1.93	0.42
4:A:109:VAL:O	4:A:113:ARG:HG2	2.20	0.42
2:F:273:ILE:HG22	2:F:459:THR:HG21	2.01	0.42
4:B:146:ARG:HD2	11:B:404:HOH:O	2.21	0.41
2:F:284:THR:HG21	2:F:467:LEU:H	1.85	0.41
2:F:78:PHE:HZ	3:G:164:PHE:CE2	2.37	0.41
4:B:348:PRO:HA	4:B:349:PRO:HD3	1.87	0.41
4:B:289:HIS:CG	4:B:351:ARG:HD2	2.55	0.41
4:A:288:GLU:HG3	4:A:330:ARG:HD3	2.03	0.41
4:B:4:VAL:HG11	4:B:188:ILE:HD11	2.03	0.41
1:E:62:TRP:HB3	1:E:67:PHE:HE1	1.85	0.41
1:E:128:THR:HG22	1:E:249:THR:OG1	2.20	0.41
2:F:346:GLU:H	2:F:346:GLU:CD	2.24	0.41
4:B:5:GLN:HG2	4:B:61:PHE:HB2	2.03	0.40
4:A:155:PHE:HB2	4:A:187:MET:HG2	2.02	0.40
3:G:84:TRP:HB3	3:G:245:LEU:HA	2.03	0.40
2:F:445:GLN:HG2	2:F:469:ASN:ND2	2.36	0.40
3:G:77:PRO:HA	3:G:78:PRO:HD3	1.97	0.40
4:B:95:ASN:O	4:B:146:ARG:HG3	2.20	0.40
2:F:210:LEU:HG	2:F:221:ASN:OD1	2.21	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	375/378 (99%)	362 (96%)	12 (3%)	1 (0%)	41	50
2	F	488/514 (95%)	472 (97%)	14 (3%)	2 (0%)	34	42
3	G	287/296 (97%)	281 (98%)	5 (2%)	1 (0%)	41	50
4	A	373/381 (98%)	362 (97%)	11 (3%)	0	100	100
4	B	352/381 (92%)	338 (96%)	14 (4%)	0	100	100
All	All	1875/1950 (96%)	1815 (97%)	56 (3%)	4 (0%)	47	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	37	GLN
2	F	38	GLY
1	E	172	GLU
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	300/303 (99%)	298 (99%)	2 (1%)	84	92
2	F	404/424 (95%)	391 (97%)	13 (3%)	39	54
3	G	231/237 (98%)	228 (99%)	3 (1%)	69	82
4	A	318/323 (98%)	305 (96%)	13 (4%)	30	43
4	B	305/323 (94%)	295 (97%)	10 (3%)	38	53
All	All	1558/1610 (97%)	1517 (97%)	41 (3%)	47	63

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	293[A]	VAL
1	E	293[B]	VAL
2	F	59	ASN
2	F	145	LEU

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Mol	Chain	Res	Type
2	F	163	THR
2	F	220	THR
2	F	248	ASP
2	F	257	VAL
2	F	273	ILE
2	F	306	VAL
2	F	311	LEU
2	F	372	LEU
2	F	426	LEU
2	F	440	ASN
2	F	496	LEU
3	G	13	LEU
3	G	146	ARG
3	G	212	VAL
4	A	4	VAL
4	A	22	ILE
4	A	31	PHE
4	A	173[A]	ARG
4	A	173[B]	ARG
4	A	185	ARG
4	A	219	LEU
4	A	238	LYS
4	A	258	LEU
4	A	270	VAL
4	A	288	GLU
4	A	333	ASP
4	A	350	GLU
4	B	4	VAL
4	B	22	ILE
4	B	45	LEU
4	B	53	GLU
4	B	101	LYS
4	B	102	LEU
4	B	123	LEU
4	B	320	ILE
4	B	324	ARG
4	B	350	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	253	GLN

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Mol	Chain	Res	Type
2	F	59	ASN
2	F	98	ASN
2	F	437	ASN
2	F	440	ASN
4	A	5	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 ⓘ

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	0.47	0	17,17,17	0.94	2 (11%)
5	GLC	C	2	5	11,11,12	0.33	0	15,15,17	0.82	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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	GLC	C1-O5-C5	2.24	117.88	113.66
5	C	2	GLC	C1-O5-C5	2.22	115.20	112.19
5	C	1	GLC	O5-C5-C4	2.11	113.53	109.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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
6	PGV	F	4008	-	7,7,50	0.31	0	6,6,56	0.40	0
9	ADP	B	2502	8	24,29,29	0.76	0	29,45,45	1.39	2 (6%)
6	PGV	G	4005	-	11,11,50	1.01	1 (9%)	10,10,56	1.03	1 (10%)
7	UMQ	F	5004	-	35,35,35	0.45	0	46,46,46	0.61	0
6	PGV	G	4009	-	13,13,50	1.09	1 (7%)	12,12,56	0.78	0
9	ADP	A	2501	8	24,29,29	0.80	0	29,45,45	1.36	2 (6%)
10	ALF	B	3002	-	0,4,4	0.00	-	-	-	-
6	PGV	G	4004	-	11,11,50	1.01	1 (9%)	10,10,56	1.04	1 (10%)
6	PGV	G	4003	-	13,13,50	1.08	1 (7%)	12,12,56	0.79	0
6	PGV	F	4001	-	50,50,50	1.09	3 (6%)	53,56,56	1.05	3 (5%)
6	PGV	G	4007	-	11,11,50	1.00	1 (9%)	10,10,56	1.10	1 (10%)
6	PGV	F	4002	-	8,8,50	0.32	0	7,7,56	0.42	0
6	PGV	G	4006	-	14,14,50	1.05	1 (7%)	13,13,56	0.78	0
10	ALF	A	3001	-	0,4,4	0.00	-	-	-	-
6	PGV	F	4010	-	16,16,50	0.97	1 (6%)	15,15,56	0.75	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
6	PGV	F	4008	-	-	2/5/5/55	-
9	ADP	B	2502	8	-	3/12/32/32	0/3/3/3
6	PGV	G	4005	-	-	4/9/9/55	-
7	UMQ	F	5004	-	-	6/20/60/60	0/2/2/2
6	PGV	G	4009	-	-	4/11/11/55	-
9	ADP	A	2501	8	-	2/12/32/32	0/3/3/3
6	PGV	G	4004	-	-	5/9/9/55	-
6	PGV	G	4003	-	-	7/11/11/55	-
6	PGV	F	4001	-	-	30/55/55/55	-
6	PGV	G	4007	-	-	4/9/9/55	-
6	PGV	F	4002	-	-	3/6/6/55	-
6	PGV	G	4006	-	-	5/12/12/55	-
6	PGV	F	4010	-	-	8/14/14/55	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	4001	PGV	O01-C1	4.39	1.46	1.34
6	F	4001	PGV	O03-C19	4.24	1.45	1.33
6	G	4009	PGV	C12-C11	3.75	1.53	1.31
6	G	4006	PGV	C12-C11	3.72	1.53	1.31
6	G	4003	PGV	C12-C11	3.71	1.53	1.31
6	F	4010	PGV	C12-C11	3.69	1.53	1.31
6	F	4001	PGV	C12-C11	3.67	1.53	1.31
6	G	4007	PGV	C11-C12	3.13	1.53	1.29
6	G	4004	PGV	C11-C12	3.13	1.53	1.29
6	G	4005	PGV	C11-C12	3.13	1.53	1.29

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	2502	ADP	N3-C2-N1	-5.12	120.68	128.68
9	A	2501	ADP	N3-C2-N1	-5.11	120.70	128.68
6	F	4001	PGV	O01-C1-C2	4.17	120.48	111.50
6	F	4001	PGV	O03-C19-C20	2.92	121.08	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	4007	PGV	C10-C11-C12	-2.56	110.70	131.07
6	G	4005	PGV	C10-C11-C12	-2.40	111.98	131.07
6	G	4004	PGV	C10-C11-C12	-2.39	112.08	131.07
6	F	4001	PGV	O03-C19-O04	-2.34	117.68	123.59
9	B	2502	ADP	PA-O3A-PB	-2.32	124.86	132.83
9	A	2501	ADP	PA-O3A-PB	-2.03	125.86	132.83

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	2502	ADP	PA-O3A-PB-O2B
6	G	4005	PGV	C10-C11-C12-C13
9	A	2501	ADP	PA-O3A-PB-O2B
6	G	4003	PGV	C12-C13-C14-C15
6	F	4001	PGV	C03-O11-P-O14
6	F	4001	PGV	C04-O12-P-O11
6	F	4001	PGV	C04-O12-P-O13
6	F	4001	PGV	C04-O12-P-O14
6	F	4001	PGV	C04-C05-C06-O06
6	F	4001	PGV	C2-C1-O01-C02
6	F	4001	PGV	O04-C19-O03-C01
6	F	4001	PGV	C20-C19-O03-C01
6	F	4001	PGV	O02-C1-O01-C02
6	G	4009	PGV	C10-C11-C12-C13
6	F	4001	PGV	C10-C11-C12-C13
6	F	4010	PGV	C10-C11-C12-C13
6	F	4001	PGV	C03-O11-P-O12
6	G	4003	PGV	C3-C4-C5-C6
6	F	4001	PGV	C30-C31-C32-C33
6	F	4001	PGV	O12-C04-C05-O05
6	F	4001	PGV	C24-C25-C26-C27
6	F	4008	PGV	C4-C5-C6-C7
6	G	4003	PGV	C11-C10-C9-C8
6	F	4001	PGV	C11-C10-C9-C8
6	G	4005	PGV	C7-C8-C9-C10
6	F	4001	PGV	C28-C29-C30-C31
6	F	4010	PGV	C6-C7-C8-C9
7	F	5004	UMQ	CD-CF-CG-CH
6	F	4001	PGV	C29-C30-C31-C32
6	F	4002	PGV	C6-C7-C8-C9
7	F	5004	UMQ	CC-CD-CF-CG

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Mol	Chain	Res	Type	Atoms
6	F	4001	PGV	C22-C23-C24-C25
6	F	4001	PGV	C27-C28-C29-C30
6	F	4001	PGV	C20-C21-C22-C23
6	F	4010	PGV	C4-C5-C6-C7
6	G	4003	PGV	C6-C7-C8-C9
6	F	4001	PGV	O05-C05-C06-O06
6	G	4009	PGV	C7-C8-C9-C10
6	F	4001	PGV	C2-C3-C4-C5
6	F	4001	PGV	C19-C20-C21-C22
6	G	4005	PGV	C6-C7-C8-C9
6	G	4004	PGV	C4-C5-C6-C7
6	F	4001	PGV	C6-C7-C8-C9
6	F	4001	PGV	C26-C27-C28-C29
6	F	4002	PGV	C4-C5-C6-C7
7	F	5004	UMQ	CH-CI-CJ-CK
6	G	4006	PGV	C6-C7-C8-C9
6	G	4009	PGV	C5-C6-C7-C8
6	G	4003	PGV	C10-C11-C12-C13
6	F	4010	PGV	C14-C15-C16-C17
6	G	4007	PGV	C2-C3-C4-C5
6	F	4010	PGV	C15-C16-C17-C18
6	F	4001	PGV	C1-C2-C3-C4
6	F	4002	PGV	C2-C3-C4-C5
6	G	4009	PGV	C2-C3-C4-C5
6	G	4006	PGV	C5-C6-C7-C8
6	G	4004	PGV	C5-C6-C7-C8
6	F	4008	PGV	C5-C6-C7-C8
7	F	5004	UMQ	CF-CG-CH-CI
6	F	4001	PGV	C05-C04-O12-P
6	F	4010	PGV	C5-C6-C7-C8
6	F	4010	PGV	C3-C4-C5-C6
6	G	4004	PGV	C3-C4-C5-C6
6	G	4003	PGV	C7-C8-C9-C10
6	G	4007	PGV	C3-C4-C5-C6
6	G	4004	PGV	C6-C7-C8-C9
7	F	5004	UMQ	CI-CJ-CK-CL
6	G	4007	PGV	C5-C6-C7-C8
6	G	4005	PGV	C9-C10-C11-C12
6	G	4003	PGV	C5-C6-C7-C8
6	G	4006	PGV	C11-C10-C9-C8
6	G	4007	PGV	C9-C10-C11-C12
6	G	4006	PGV	C11-C12-C13-C14

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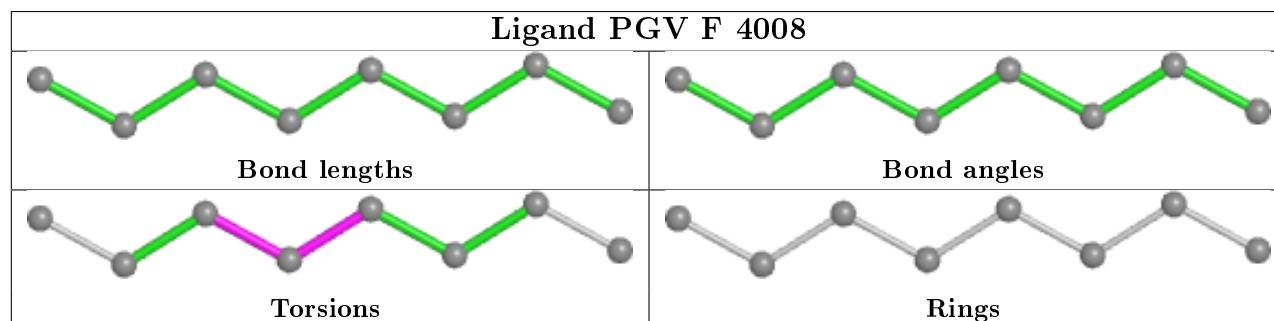
Mol	Chain	Res	Type	Atoms
6	G	4004	PGV	C9-C10-C11-C12
6	F	4001	PGV	C21-C22-C23-C24
6	F	4001	PGV	O03-C01-C02-O01
9	B	2502	ADP	PA-O3A-PB-O1B
9	B	2502	ADP	PA-O3A-PB-O3B
9	A	2501	ADP	PA-O3A-PB-O3B
6	F	4010	PGV	C2-C3-C4-C5
7	F	5004	UMQ	O1'-CA-CB-CC
6	F	4001	PGV	O03-C01-C02-C03
6	G	4006	PGV	C9-C10-C11-C12

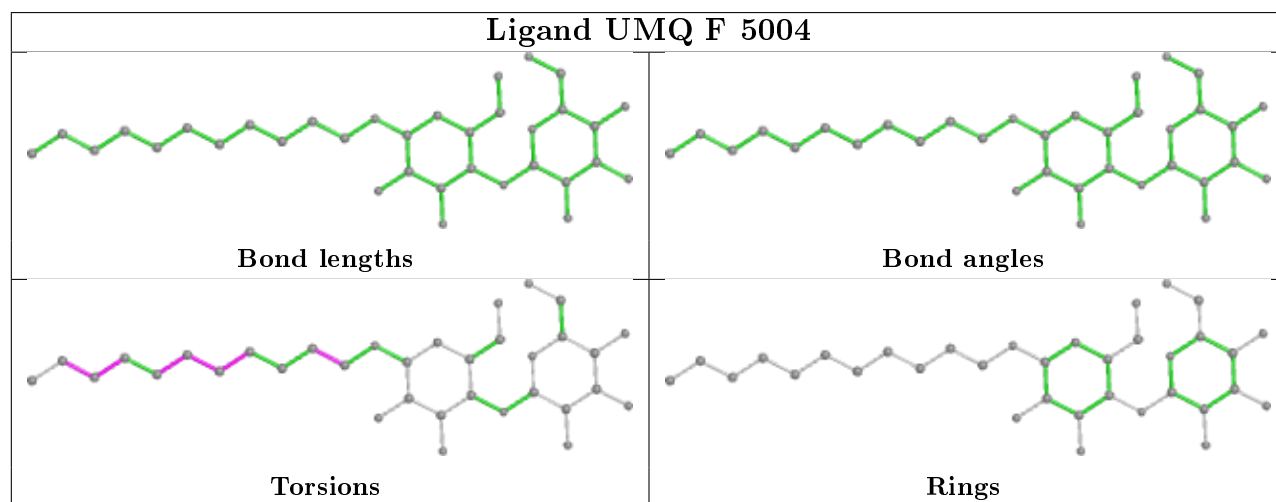
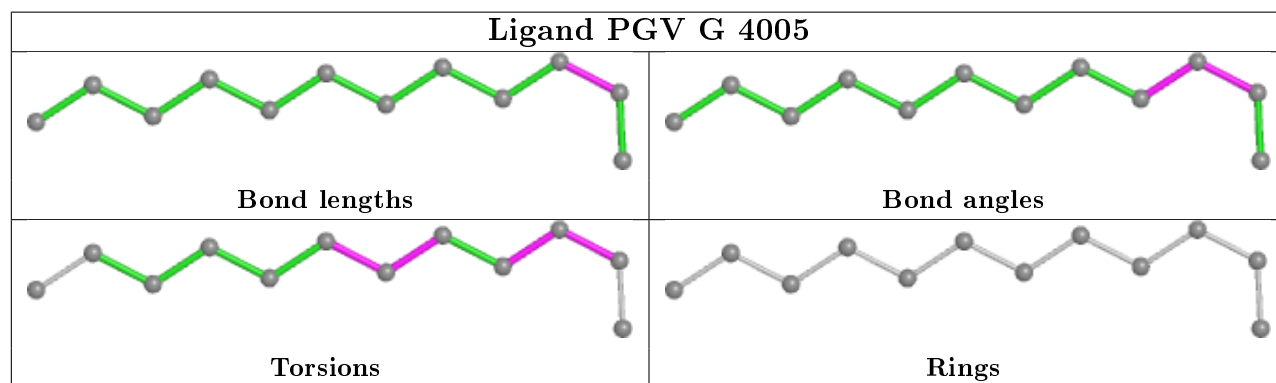
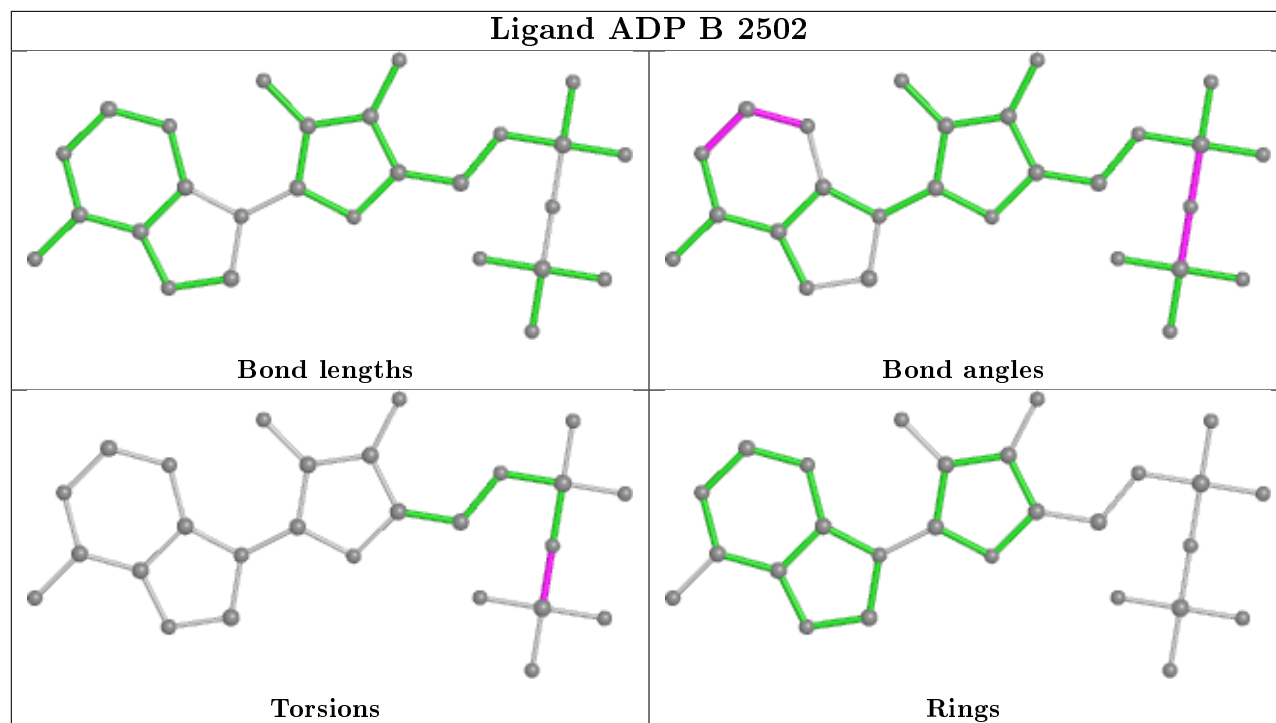
There are no ring outliers.

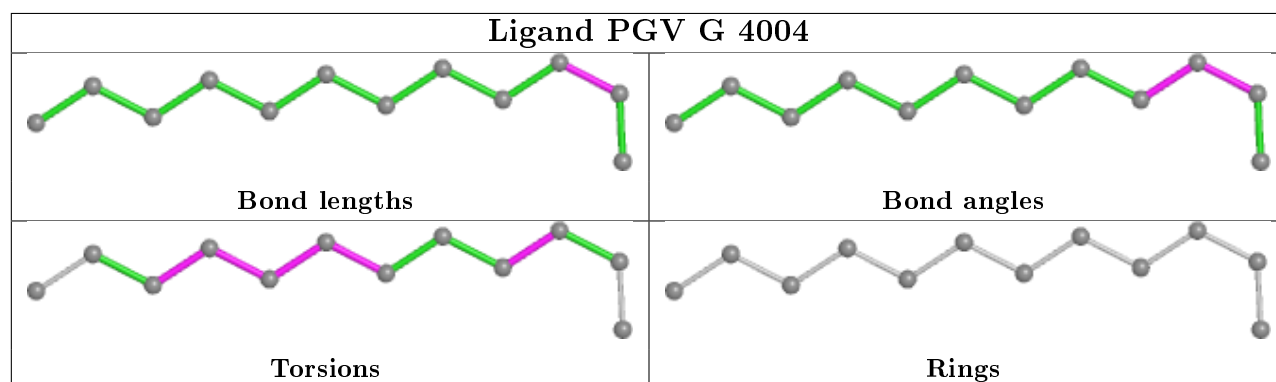
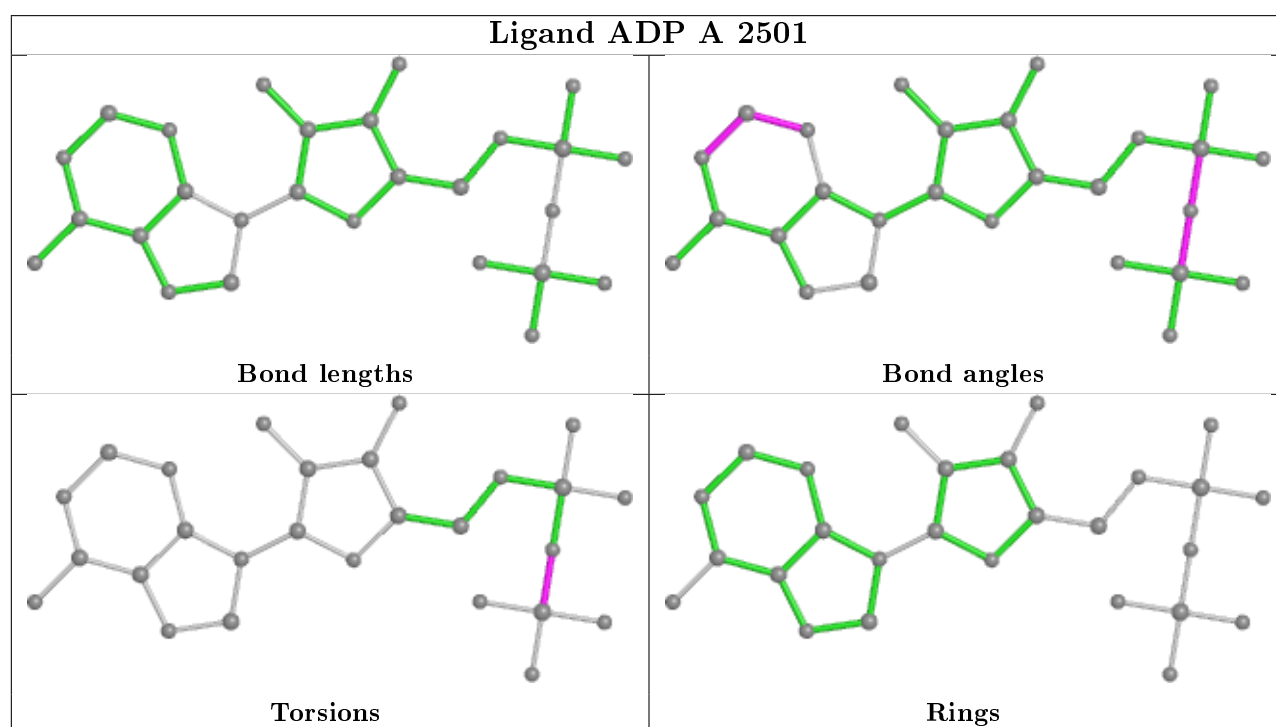
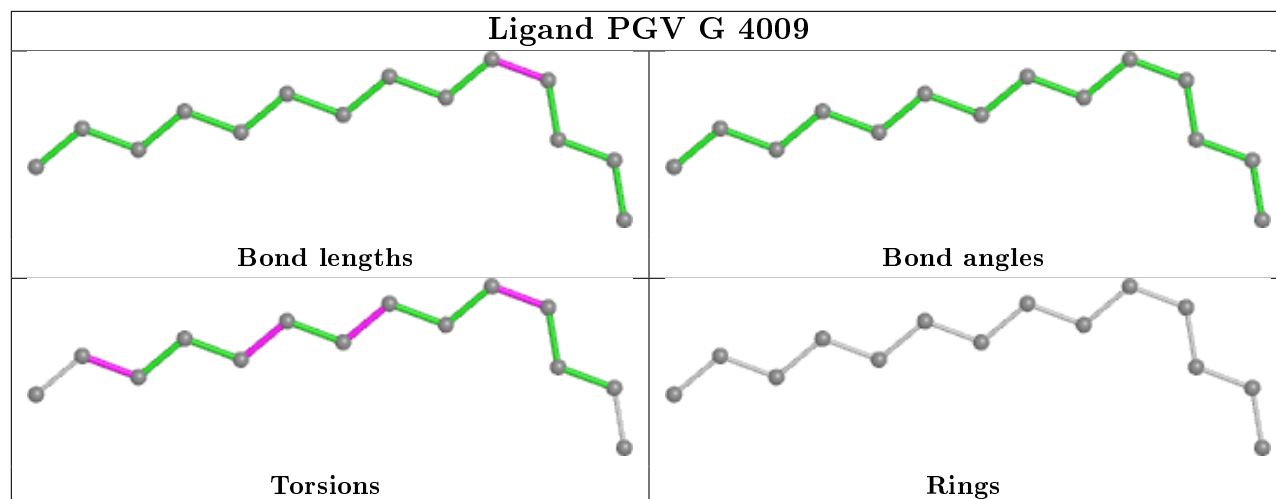
1 monomer is involved in 1 short contact:

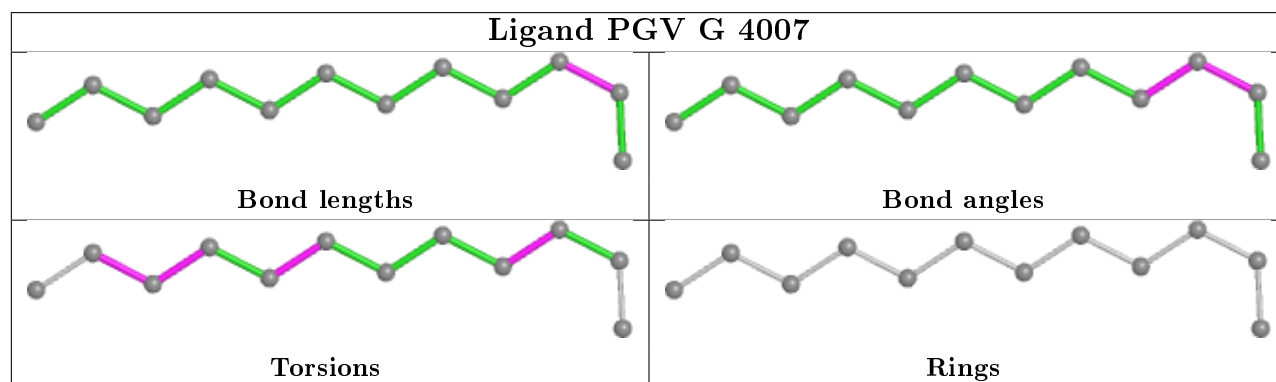
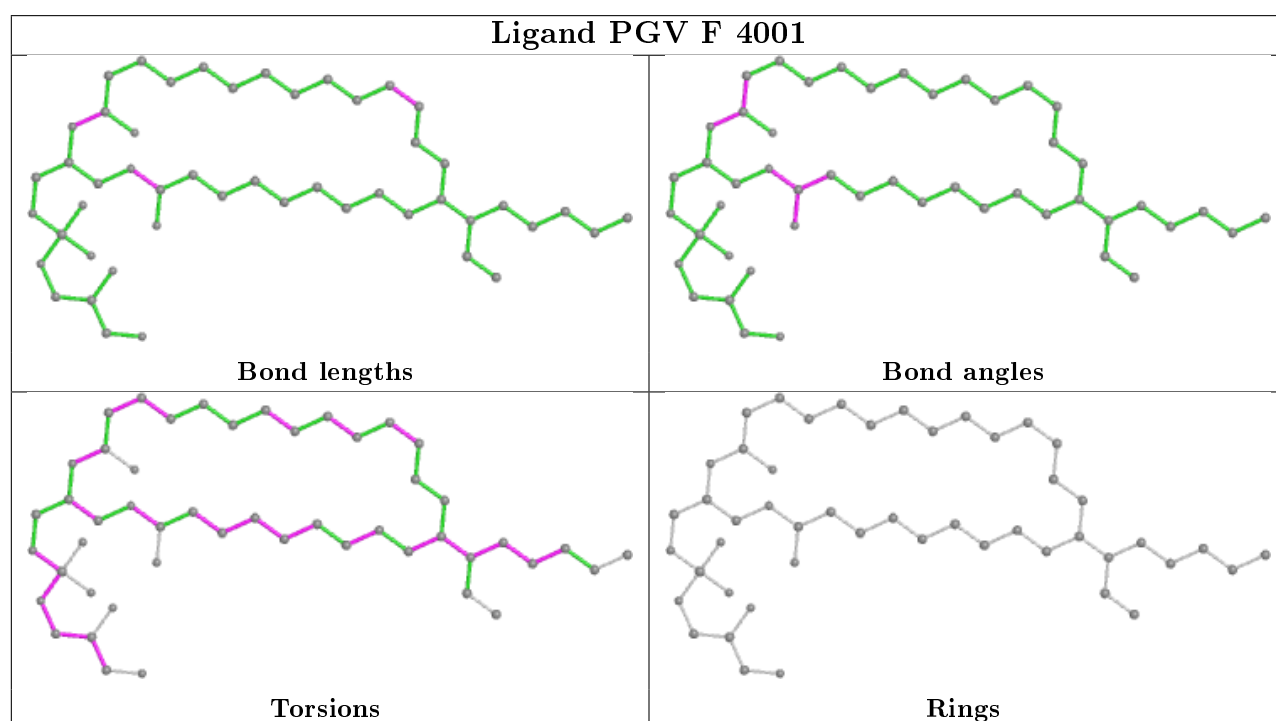
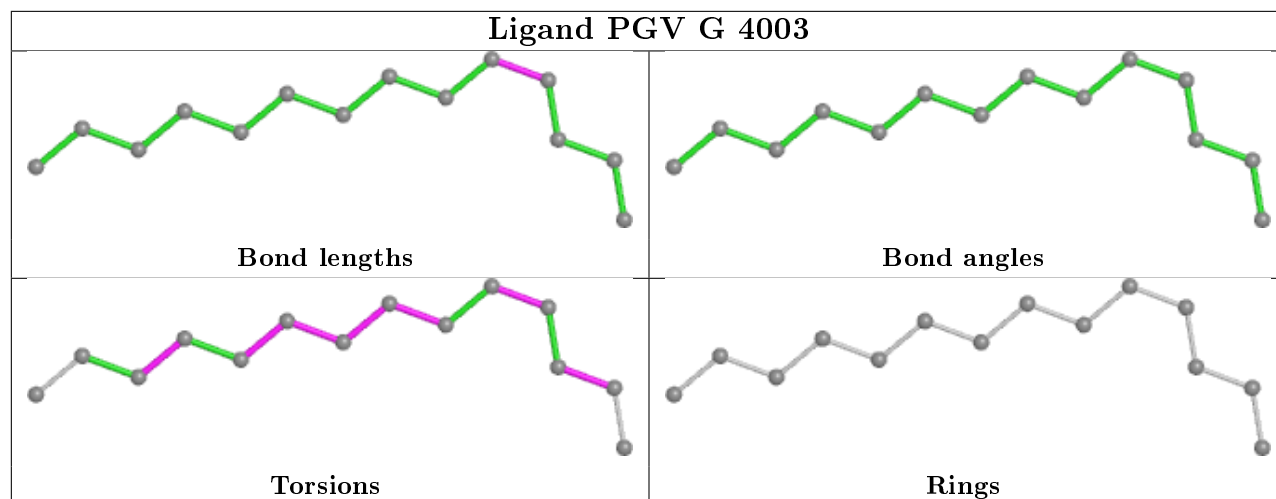
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	4001	PGV	1	0

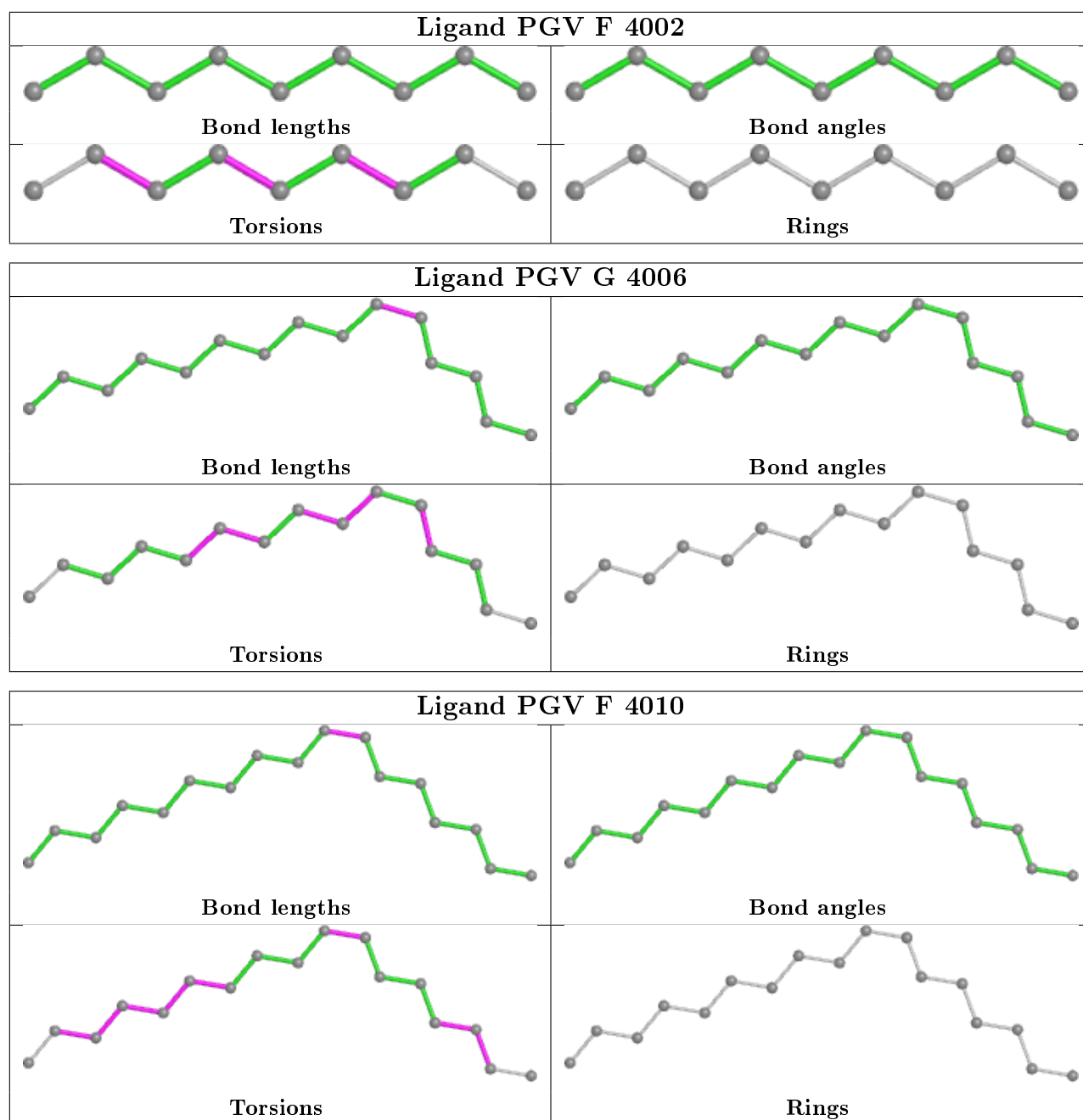
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	E	374/378 (98%)	0.04	16 (4%)	35	42	26, 54, 86, 105	1 (0%)
2	F	490/514 (95%)	0.42	43 (8%)	10	13	27, 56, 112, 162	0
3	G	288/296 (97%)	0.03	14 (4%)	29	36	24, 37, 80, 99	0
4	A	371/381 (97%)	0.11	13 (3%)	44	51	23, 52, 81, 95	1 (0%)
4	B	358/381 (93%)	0.34	29 (8%)	12	16	22, 61, 130, 160	0
All	All	1881/1950 (96%)	0.21	115 (6%)	21	27	22, 53, 101, 162	2 (0%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	37	GLN	8.7
4	B	251	ILE	8.5
2	F	38	GLY	8.1
4	B	16	VAL	7.4
3	G	70	ALA	6.4
4	A	295	ILE	6.0
2	F	40	TYR	6.0
4	B	295	ILE	5.9
4	B	267	TRP	5.9
3	G	133	ALA	5.7
2	F	355	PHE	5.3
3	G	71	ASP	5.0
2	F	29	TYR	5.0
3	G	116	PRO	4.9
2	F	349	MET	4.8
2	F	354	LEU	4.7
1	E	172	GLU	4.4
4	B	105	ALA	4.4
2	F	245	ASN	4.3
3	G	73	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
4	B	357	GLU	4.1
4	B	324	ARG	4.1
3	G	114	ARG	4.1
2	F	503	ILE	4.0
1	E	374	SER	4.0
1	E	179	LYS	4.0
4	A	110	ILE	3.9
3	G	117	GLY	3.8
2	F	11	GLN	3.8
2	F	353	ALA	3.7
2	F	271	GLU	3.7
2	F	248	ASP	3.7
2	F	10	TRP	3.5
4	A	104	GLY	3.5
1	E	143	GLY	3.4
1	E	373	ALA	3.4
4	B	15	GLU	3.3
4	B	249	THR	3.3
1	E	141	ALA	3.2
4	A	103	ALA	3.2
2	F	502	ALA	3.2
2	F	12	SER	3.1
3	G	69	GLN	3.1
4	B	293	SER	3.1
2	F	35	TYR	3.0
2	F	214	ASP	3.0
1	E	1	LYS	3.0
4	B	299	ILE	3.0
4	B	181	LYS	3.0
2	F	312	ARG	2.9
2	F	501	LEU	2.9
2	F	262	LYS	2.9
2	F	229	ARG	2.9
2	F	25	LEU	2.9
2	F	129	ASP	2.7
3	G	72	GLY	2.7
2	F	45	THR	2.7
1	E	142	LYS	2.7
4	B	252	ASP	2.6
4	A	16	VAL	2.6
4	A	324	ARG	2.6
4	A	372	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	193	GLY	2.6
4	B	294	ASP	2.6
1	E	370	LYS	2.6
4	B	261	PRO	2.5
3	G	14	PHE	2.5
2	F	479	GLY	2.5
2	F	18	SER	2.5
3	G	68	GLU	2.5
4	B	265	GLN	2.5
2	F	458	THR	2.5
1	E	252	GLY	2.5
4	B	263	ARG	2.4
2	F	14	ALA	2.4
2	F	168	GLY	2.4
1	E	174	GLY	2.4
4	A	60	LEU	2.4
4	B	108	GLU	2.4
4	B	353	HIS	2.4
2	F	154	GLU	2.3
4	A	64	GLU	2.3
2	F	41	LEU	2.3
2	F	133	LEU	2.3
3	G	134	VAL	2.3
4	B	280	ASN	2.3
1	E	147	LEU	2.2
1	E	170	LYS	2.2
1	E	239	LYS	2.2
4	B	262	ASN	2.2
4	B	359	GLY	2.2
2	F	223	GLN	2.2
1	E	173	ASN	2.2
3	G	74	ILE	2.2
4	B	244	VAL	2.2
4	B	361	ALA	2.2
2	F	17	TRP	2.2
4	A	7	GLN	2.1
4	A	294	ASP	2.1
2	F	159	LEU	2.1
2	F	114	TRP	2.1
2	F	212	THR	2.1
3	G	131	PHE	2.1
4	A	261	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	123	PRO	2.1
4	A	285	ILE	2.1
2	F	61	LYS	2.1
4	B	247	THR	2.1
2	F	268	PHE	2.1
4	B	340	GLY	2.0
2	F	39	GLU	2.0
4	B	338	GLU	2.0
2	F	216	ASP	2.0
4	B	291	LEU	2.0
4	B	116	GLN	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
5	GLC	C	1	12/12	0.96	0.11	39,43,44,45	0
5	GLC	C	2	11/12	0.96	0.08	37,38,38,38	0

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.

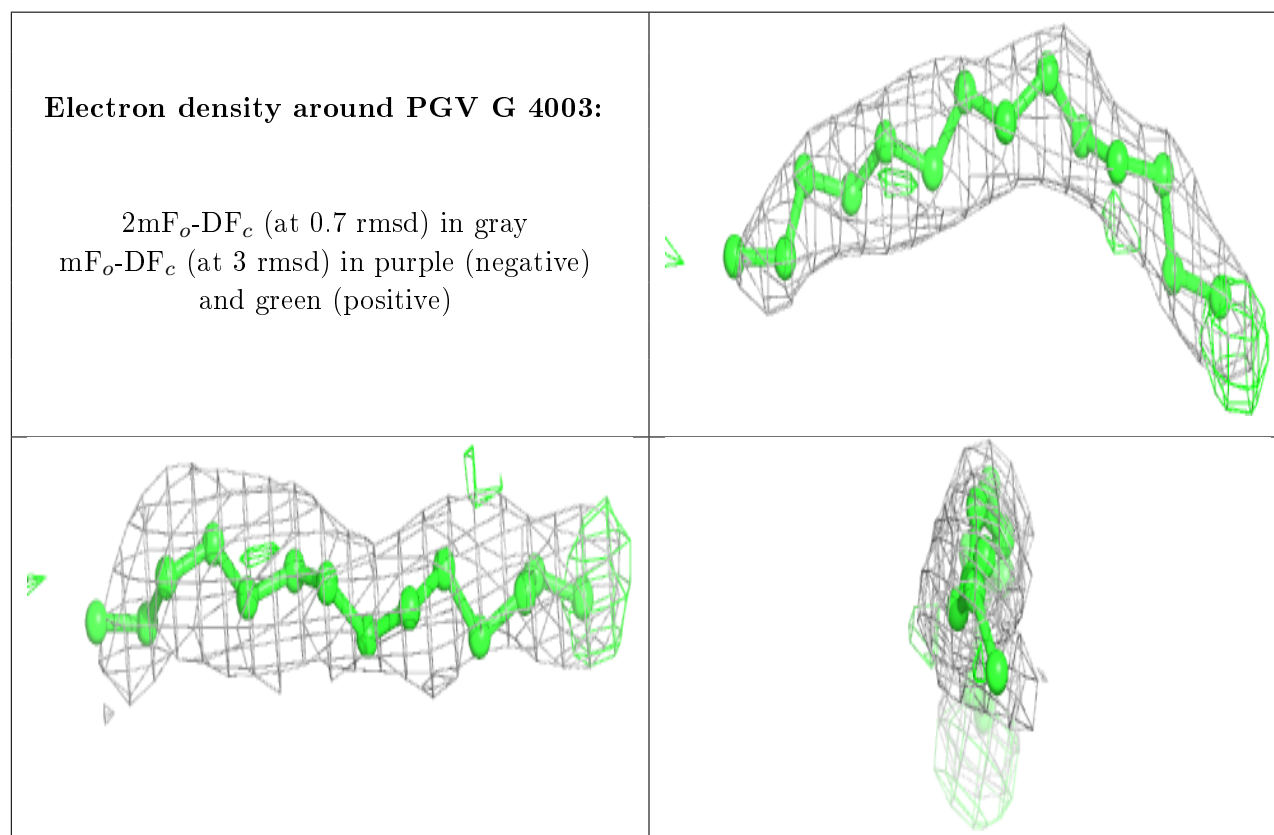
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PGV	G	4003	14/51	0.64	0.29	76,83,85,86	0
6	PGV	G	4005	12/51	0.68	0.15	66,71,73,74	0
6	PGV	F	4010	17/51	0.69	0.24	72,78,80,81	0
6	PGV	G	4006	15/51	0.71	0.16	63,70,78,79	0
6	PGV	G	4009	14/51	0.72	0.21	62,63,66,66	0

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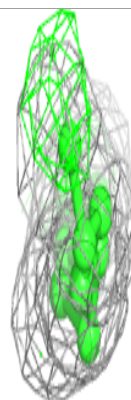
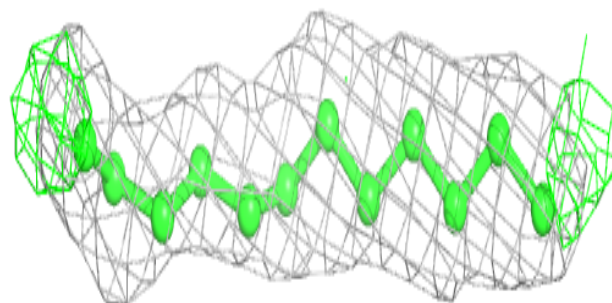
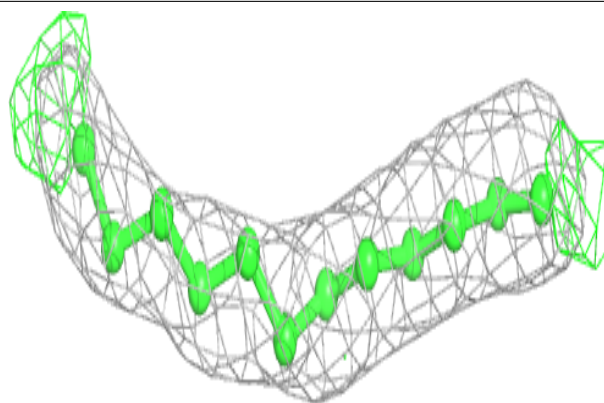
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	PGV	F	4008	8/51	0.79	0.23	60,64,66,67	0
6	PGV	G	4007	12/51	0.81	0.18	86,91,96,97	0
6	PGV	F	4001	51/51	0.83	0.23	61,67,74,76	0
6	PGV	G	4004	12/51	0.85	0.14	50,54,58,59	0
6	PGV	F	4002	9/51	0.86	0.21	38,41,45,47	0
7	UMQ	F	5004	34/34	0.93	0.17	56,66,71,72	0
9	ADP	B	2502	27/27	0.95	0.12	31,43,52,54	0
9	ADP	A	2501	27/27	0.97	0.11	25,37,45,46	0
8	MG	A	1501	1/1	0.99	0.07	26,26,26,26	0
8	MG	B	1502	1/1	0.99	0.11	22,22,22,22	0
10	ALF	A	3001	5/5	0.99	0.09	19,20,21,21	0
10	ALF	B	3002	5/5	0.99	0.10	27,28,28,29	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.

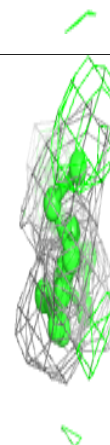
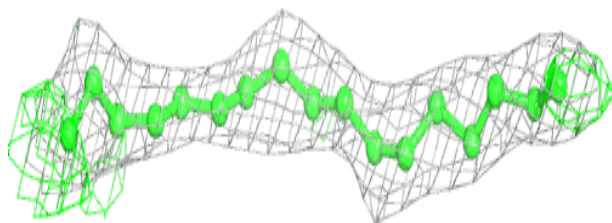
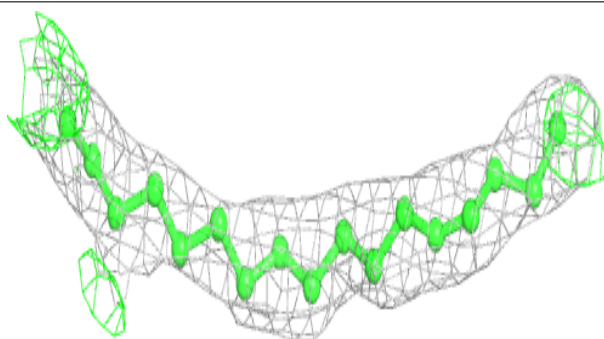


Electron density around PGV G 4005:

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

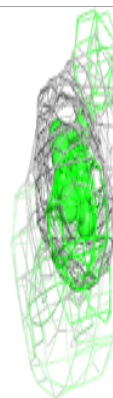
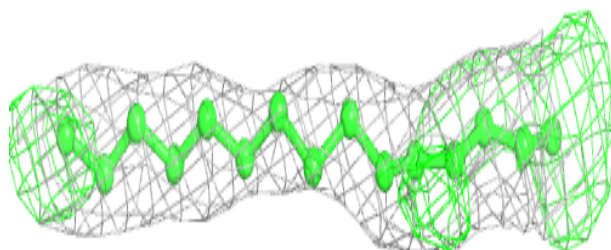
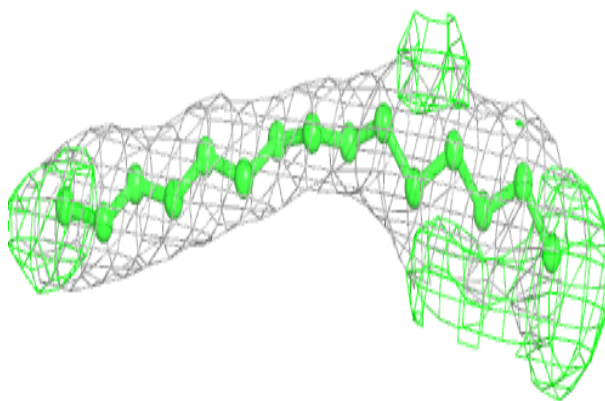
**Electron density around PGV F 4010:**

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

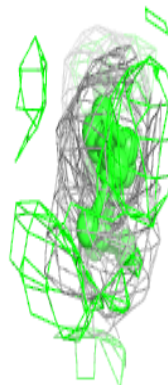
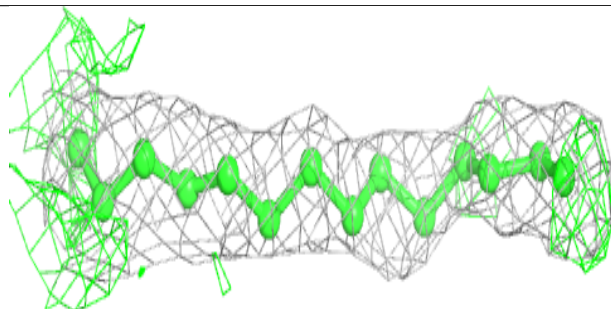
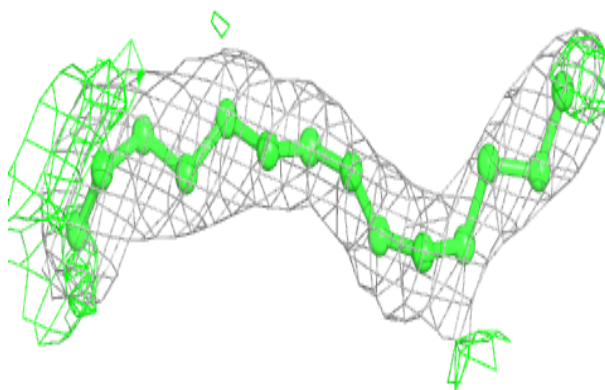


Electron density around PGV G 4006:

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

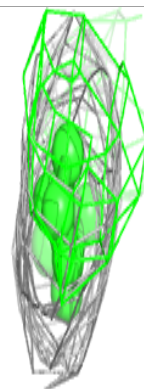
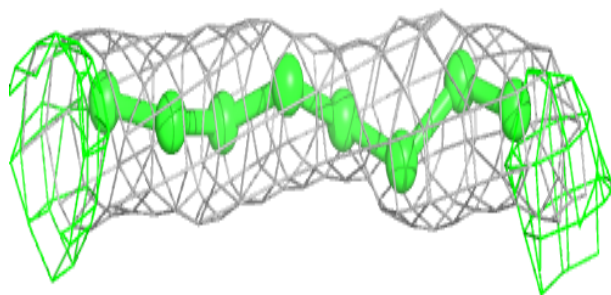
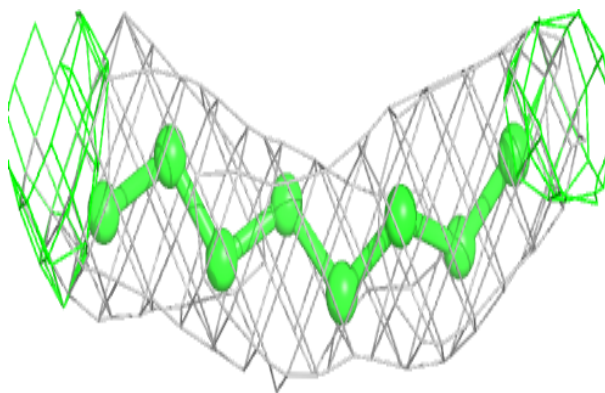
**Electron density around PGV G 4009:**

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

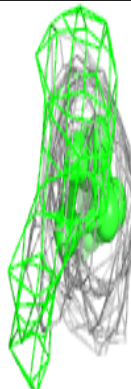
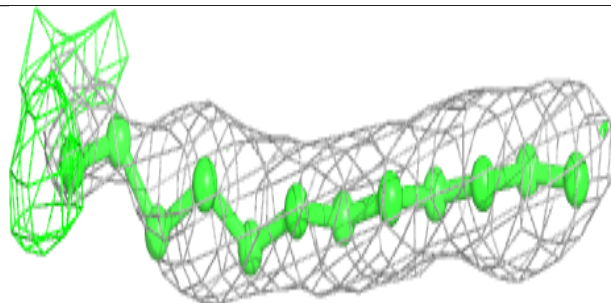
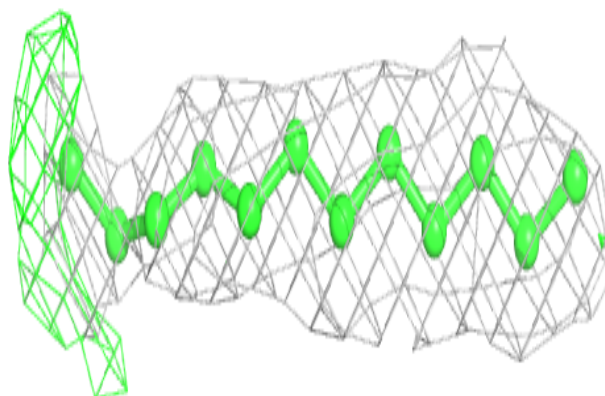


Electron density around PGV F 4008:

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

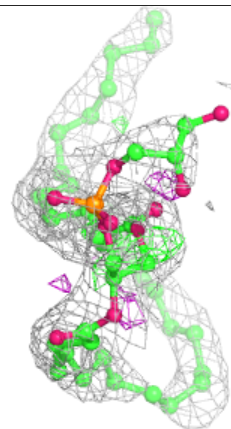
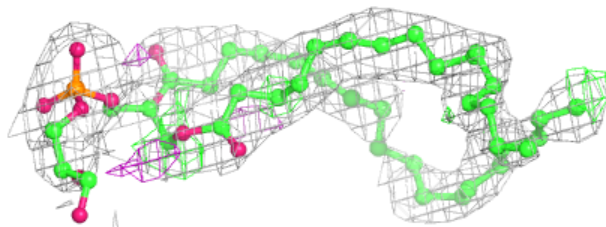
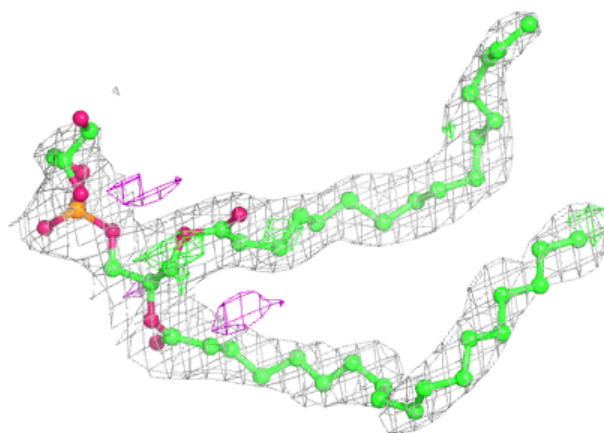
**Electron density around PGV G 4007:**

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

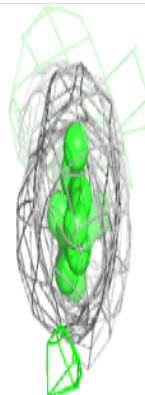
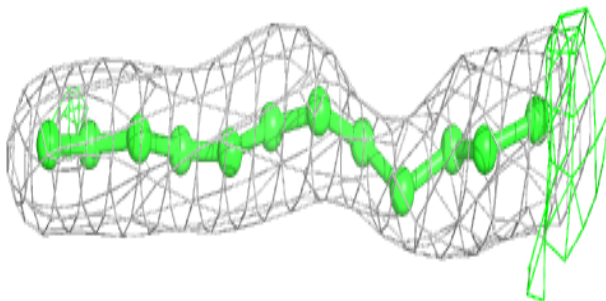
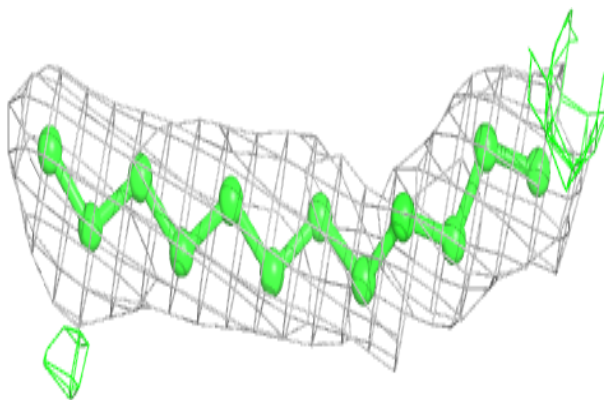


Electron density around PGV F 4001:

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

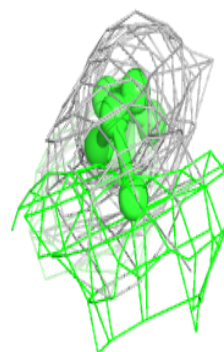
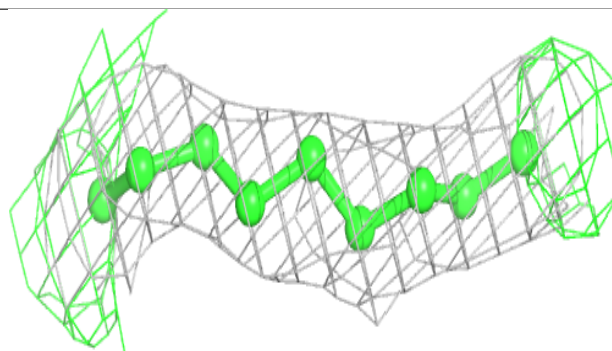
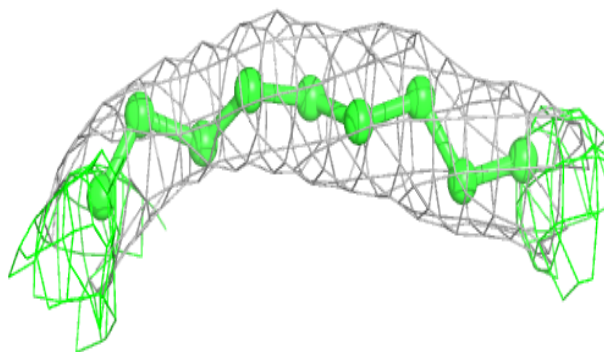
**Electron density around PGV G 4004:**

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

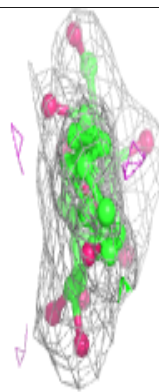
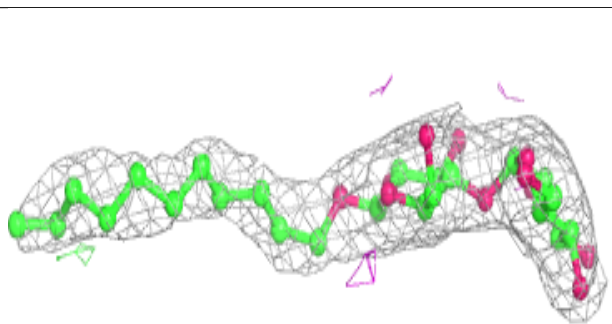
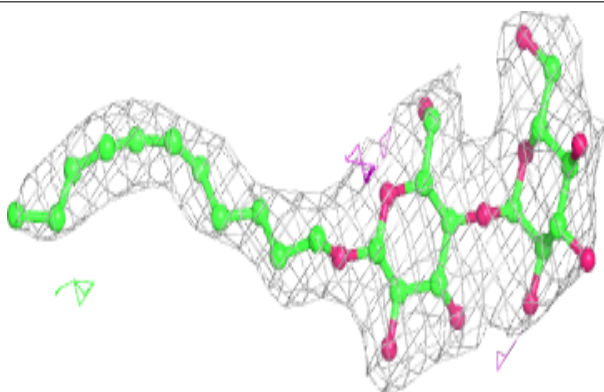


Electron density around PGV F 4002:

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

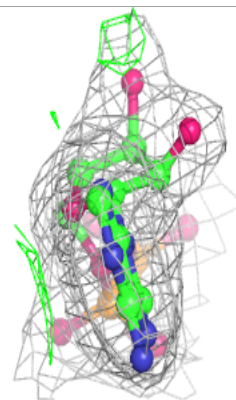
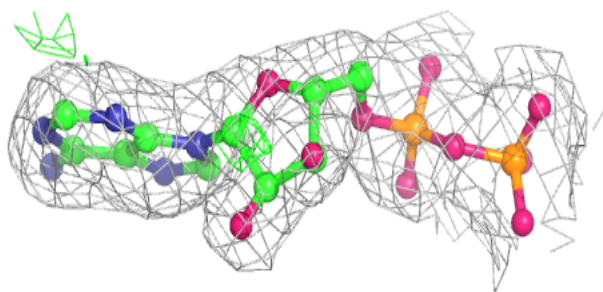
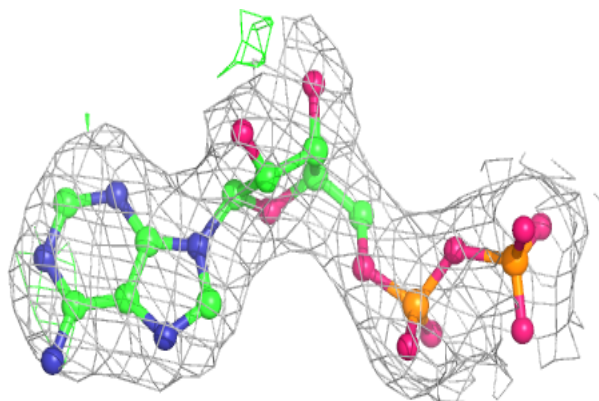
**Electron density around UMQ F 5004:**

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

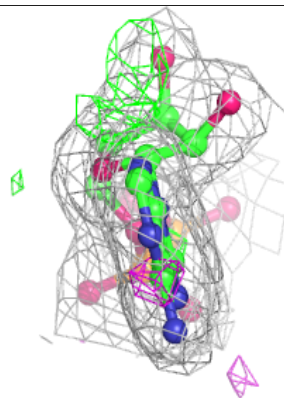
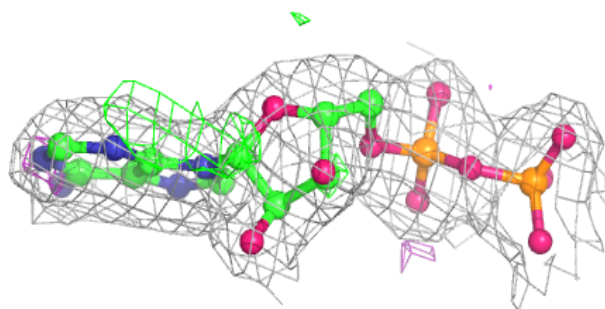
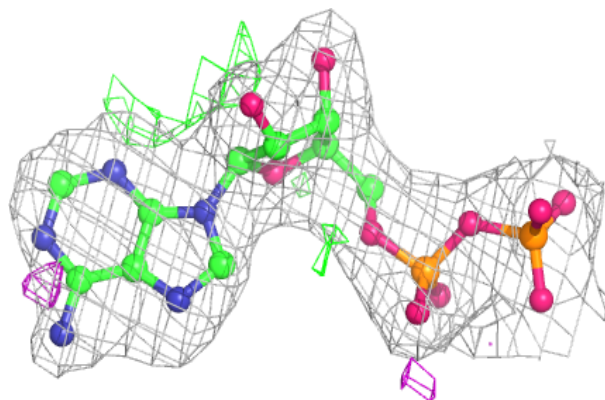


Electron density around ADP B 2502:

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

**Electron density around ADP 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)



6.5 Other polymers

There are no such residues in this entry.