



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 03:14 PM UTC

PDB ID : 3PUX / pdb_00003pux
Title : Crystal Structure of an outward-facing MBP-Maltose transporter complex bound to ADP-BeF3
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 types of validation reports are described at

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

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

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

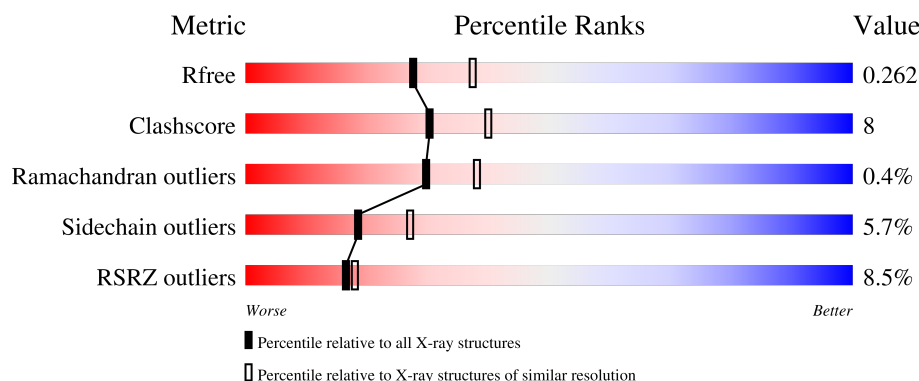
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

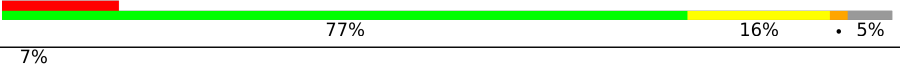
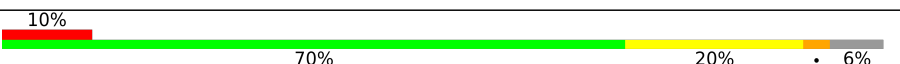
The reported resolution of this entry is 2.30 Å.

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	378	
2	F	514	
3	G	296	
4	A	381	
4	B	381	

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Mol	Chain	Length	Quality of chain
5	C	2	 100%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15273 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	1879	474	556	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	2520	608	685	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	293	Total	C	N	O	S	0	2	0
			2270	1520	362	378	10			

- 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	8	0
			2929	1856	522	536	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	358	Total	C	N	O	S	0	4	0
			2816	1785	502	516	13			

There are 20 discrepancies between the modelled and reference sequences:

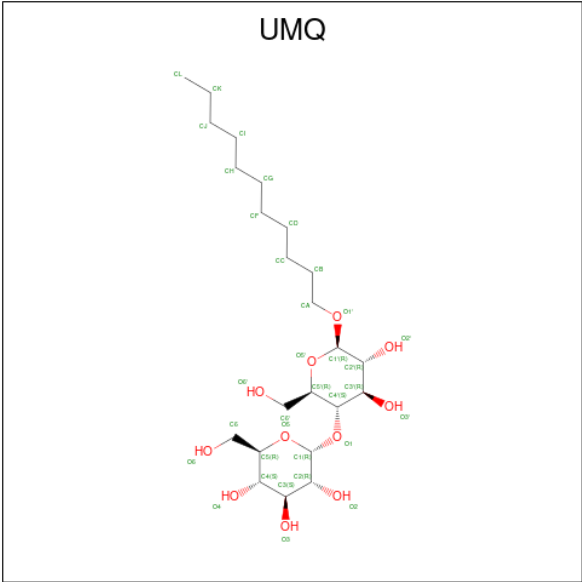
Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	-	expression tag	UNP P68187
A	373	SER	-	expression tag	UNP P68187
A	374	ALA	-	expression tag	UNP P68187
A	375	SER	-	expression tag	UNP P68187
A	376	HIS	-	expression tag	UNP P68187
A	377	HIS	-	expression tag	UNP P68187
A	378	HIS	-	expression tag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



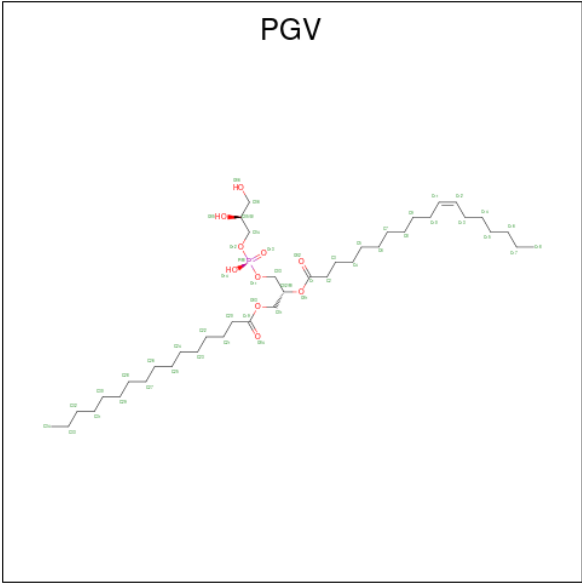
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	C	2	Total	C	O	0	0	0
			23	12	11			

- 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	0
			9		9			

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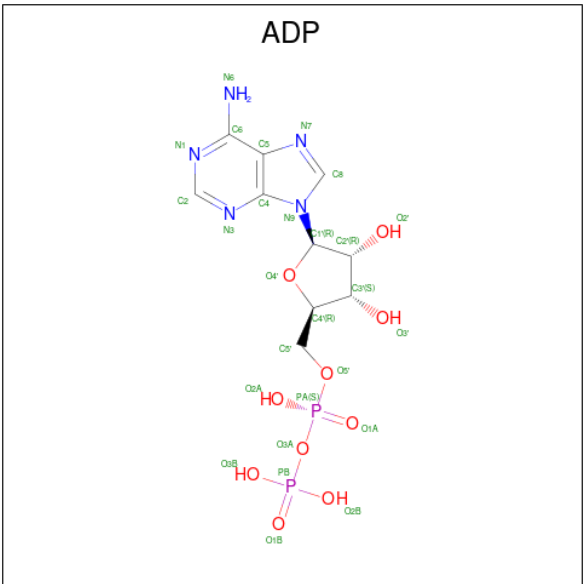
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total C 8 8	0	0
7	F	1	Total C 13 13	0	0
7	G	1	Total C 8 8	0	0
7	G	1	Total C 12 12	0	0
7	G	1	Total C 10 10	0	0
7	G	1	Total C 7 7	0	0
7	G	1	Total C 9 9	0	0
7	G	1	Total C 12 12	0	0

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

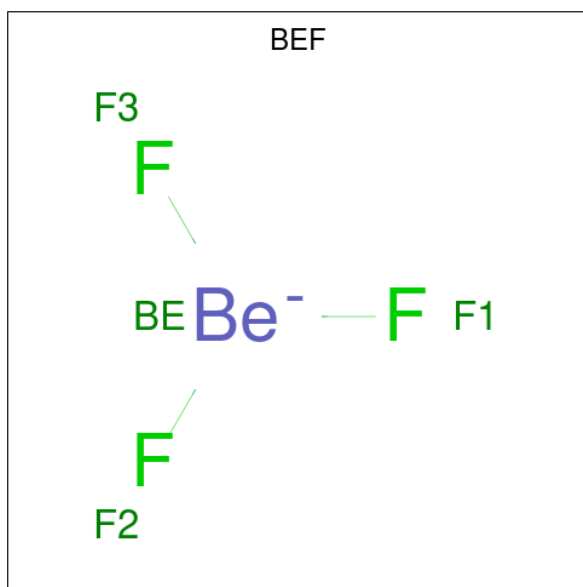
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Mg 1 1	0	0
8	B	1	Total Mg 1 1	0	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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 BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	Be	F	0	0
			4	1	3		
10	B	1	Total	Be	F	0	0
			4	1	3		

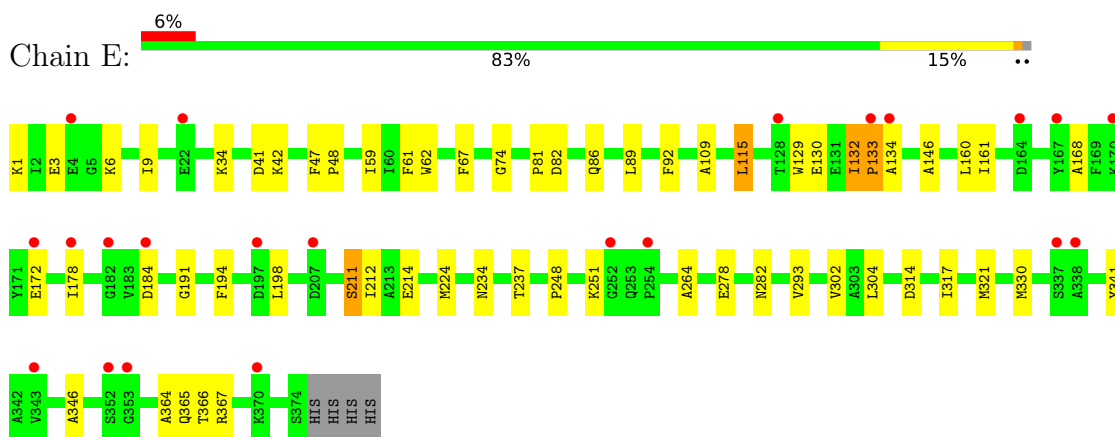
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	E	56	Total	O	0	0
			56	56		
11	F	44	Total	O	0	0
			44	44		
11	G	51	Total	O	0	0
			51	51		
11	A	61	Total	O	0	0
			61	61		
11	B	40	Total	O	0	0
			40	40		

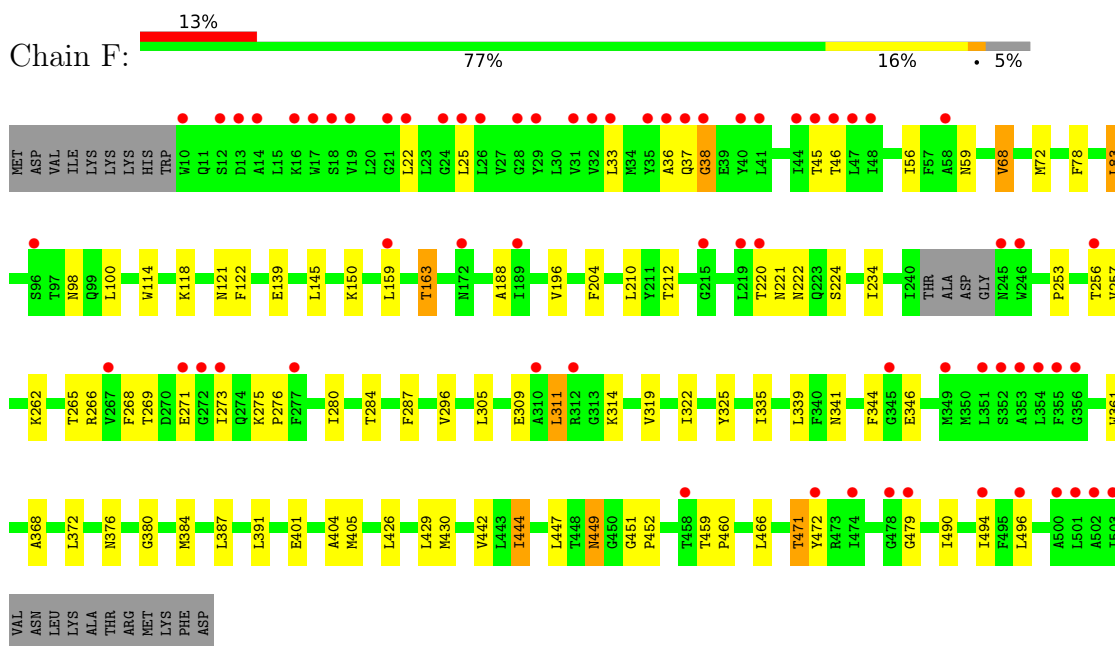
3 Residue-property plots [i](#)

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.

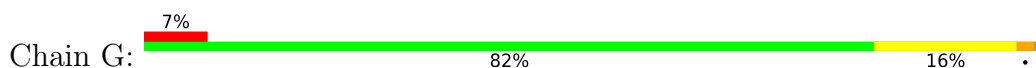
- Molecule 1: Maltose-binding periplasmic protein

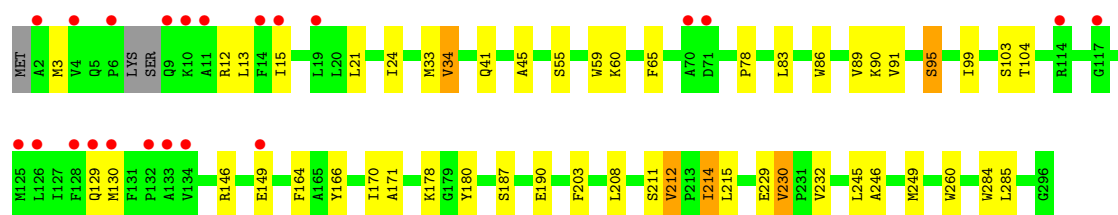


- Molecule 2: Maltose transport system permease protein malF

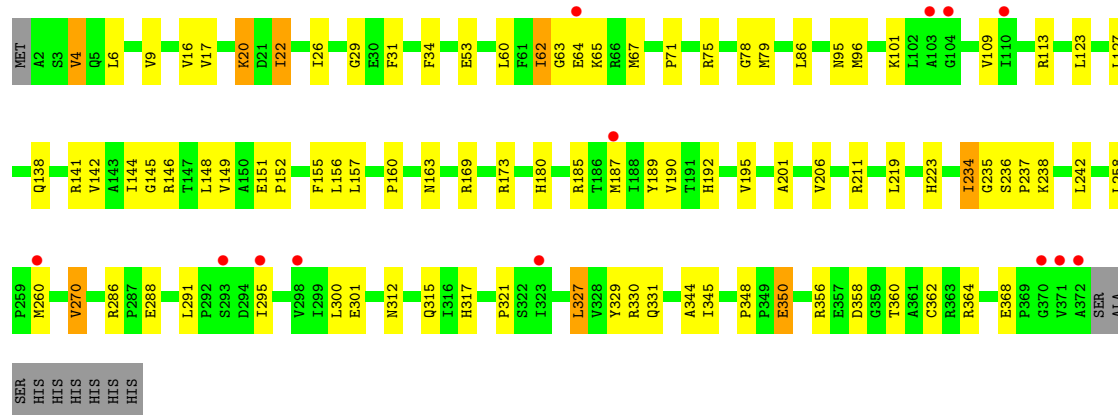
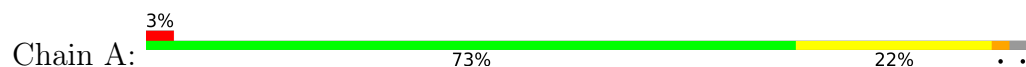


- Molecule 3: Maltose transport system permease protein malG

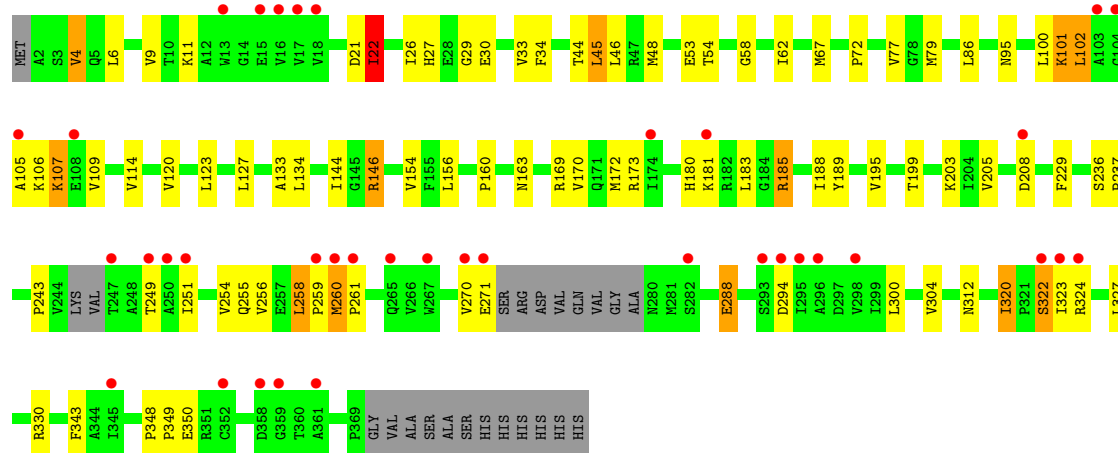




• Molecule 4: Maltose/maltodextrin import ATP-binding protein MalK



• 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	82.13Å 97.34Å 112.84Å 85.58° 78.98° 72.25°	Depositor
Resolution (Å)	19.81 – 2.30 19.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	64.8 (19.81-2.30) 64.6 (19.81-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.228 , 0.265 0.226 , 0.262	Depositor DCC
R_{free} test set	4829 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15273	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, BEF, MG, UMQ, ADP, 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	0.68	4/2990 (0.1%)	0.89	1/4059 (0.0%)
2	F	0.63	0/3932	0.91	3/5351 (0.1%)
3	G	0.75	2/2334 (0.1%)	0.91	1/3188 (0.0%)
4	A	0.69	1/2991 (0.0%)	0.94	3/4055 (0.1%)
4	B	0.63	1/2870 (0.0%)	0.90	2/3889 (0.1%)
All	All	0.67	8/15117 (0.1%)	0.91	10/20542 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	132	ILE	CA-CB	7.67	1.58	1.54
1	E	134	ALA	N-CA	7.66	1.55	1.46
1	E	133	PRO	CA-C	6.46	1.62	1.52
4	A	71	PRO	CA-C	6.40	1.55	1.51
4	B	22	ILE	CA-CB	5.87	1.61	1.54
1	E	251	LYS	CD-CE	5.75	1.69	1.52
3	G	89	VAL	CA-CB	5.25	1.60	1.54
3	G	232	VAL	CA-CB	5.01	1.60	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	71	PRO	CA-C-N	5.70	125.82	119.32
4	A	71	PRO	C-N-CA	5.70	125.82	119.32
2	F	163	THR	N-CA-C	-5.50	107.22	114.31
2	F	262	LYS	N-CA-C	5.21	118.42	111.75
4	A	201	ALA	N-CA-C	5.14	117.89	110.28
1	E	132	ILE	CB-CA-C	-5.13	107.28	114.00
4	B	260	MET	CA-C-N	5.03	124.75	119.82
4	B	260	MET	C-N-CA	5.03	124.75	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	479	GLY	N-CA-C	5.01	122.24	115.32
3	G	34	VAL	N-CA-C	-5.01	105.82	110.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2915	0	2898	37	0
2	F	3831	0	3869	61	0
3	G	2270	0	2364	35	0
4	A	2929	0	3011	76	0
4	B	2816	0	2881	54	0
5	C	23	0	21	1	0
6	E	34	0	44	2	0
7	F	81	0	122	0	0
7	G	58	0	82	3	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	27	0	12	2	0
9	B	27	0	12	0	0
10	A	4	0	0	0	0
10	B	4	0	0	0	0
11	A	61	0	0	10	0
11	B	40	0	0	5	0
11	E	56	0	0	4	0
11	F	44	0	0	8	0
11	G	51	0	0	2	0
All	All	15273	0	15316	254	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 8.

All (254) 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	1.18	1.16
4:A:187[B]:MET:HE3	4:A:187[B]:MET:C	1.70	1.14
4:A:187[B]:MET:HE3	4:A:187[B]:MET:O	1.50	1.12
2:F:405[B]:MET:HE3	2:F:405[B]:MET:HA	1.13	1.07
4:B:6:LEU:HD22	4:B:22:ILE:HD11	1.36	1.06
2:F:471:THR:CG2	2:F:490:ILE:HG21	1.87	1.04
4:A:62[A]:ILE:HG23	4:A:67:MET:HG3	1.38	1.02
2:F:405[B]:MET:HA	2:F:405[B]:MET:CE	1.92	0.99
4:B:134:LEU:HD23	11:B:400:HOH:O	1.66	0.93
2:F:471:THR:HG21	2:F:490:ILE:CG2	2.00	0.91
4:A:187[B]:MET:C	4:A:187[B]:MET:CE	2.43	0.90
2:F:405[B]:MET:HE2	4:B:77[B]:VAL:HG23	1.57	0.87
4:A:286:ARG:HB3	4:A:288:GLU:OE1	1.76	0.84
2:F:339:LEU:HD21	3:G:33[B]:MET:SD	2.19	0.82
4:A:31:PHE:CE1	4:A:187[B]:MET:HE2	2.14	0.81
2:F:471:THR:HG23	2:F:490:ILE:HD13	1.60	0.81
4:A:356:ARG:HH11	4:A:360:THR:HG23	1.46	0.81
3:G:91:VAL:O	3:G:95:SER:HB2	1.79	0.81
4:A:235:GLY:HA2	11:A:431:HOH:O	1.81	0.79
1:E:115:LEU:HD21	1:E:224:MET:HE3	1.66	0.78
4:A:223:HIS:CE1	4:A:368:GLU:HG2	2.19	0.78
4:A:163:ASN:OD1	11:A:425:HOH:O	2.01	0.77
4:B:188[B]:ILE:HD12	4:B:189:TYR:N	1.98	0.77
4:A:96:MET:HE3	4:A:145:GLY:HA3	1.67	0.76
4:B:320:ILE:HD11	4:B:327:LEU:HB2	1.70	0.73
4:A:79:MET:HG3	4:A:156:LEU:HB2	1.71	0.73
3:G:166:TYR:OH	3:G:229:GLU:HG2	1.90	0.72
2:F:284:THR:HG22	2:F:466:LEU:HA	1.72	0.72
2:F:159:LEU:HD11	2:F:188:ALA:HB1	1.72	0.71
3:G:129:GLN:HB3	3:G:130:MET:HE2	1.72	0.71
11:A:425:HOH:O	4:B:163:ASN:OD1	2.07	0.71
4:B:169:ARG:HD3	11:B:404:HOH:O	1.91	0.70
4:A:288:GLU:HG2	4:B:312:ASN:HB2	1.72	0.70
1:E:62:TRP:HB3	1:E:67:PHE:HE1	1.56	0.70
2:F:372:LEU:HD12	2:F:447:LEU:HD23	1.74	0.69
4:A:329:TYR:CE2	4:A:331:GLN:HG2	2.28	0.69
2:F:280:ILE:O	2:F:284:THR:HG23	1.93	0.68
1:E:34:LYS:HD3	11:E:407:HOH:O	1.95	0.67
2:F:78:PHE:HZ	3:G:164:PHE:CE2	2.13	0.67
4:A:60[B]:LEU:HD12	4:A:67:MET:HB2	1.75	0.67
4:A:187[B]:MET:O	4:A:187[B]:MET:CE	2.37	0.66
4:B:133:ALA:O	11:B:400:HOH:O	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:188[B]:ILE:HD12	4:B:188[B]:ILE:C	2.21	0.65
4:A:157:LEU:CD1	4:A:187[B]:MET:SD	2.84	0.65
3:G:78:PRO:HD2	11:G:344:HOH:O	1.95	0.65
1:E:115:LEU:HD11	1:E:224:MET:HE3	1.78	0.65
4:B:45:LEU:HA	4:B:48:MET:HE3	1.78	0.65
4:A:301:GLU:HG3	4:A:344:ALA:HB2	1.79	0.64
4:A:260[A]:MET:HE2	4:A:300:LEU:HD22	1.77	0.64
1:E:211:SER:HB2	11:E:390:HOH:O	1.98	0.64
2:F:405[B]:MET:HE3	2:F:405[B]:MET:CA	2.08	0.63
1:E:367:ARG:HD2	2:F:460:PRO:HG3	1.82	0.61
4:A:86:LEU:HA	4:A:146:ARG:NH2	2.17	0.60
4:A:187[B]:MET:C	4:A:187[B]:MET:SD	2.85	0.59
4:B:44:THR:HG22	4:B:48:MET:HE2	1.85	0.59
4:A:65:LYS:O	4:A:67:MET:HG2	2.02	0.58
4:A:270:VAL:HG13	4:A:362:CYS:HB3	1.86	0.58
4:A:67:MET:HE1	4:A:75:ARG:HA	1.84	0.58
1:E:146:ALA:O	1:E:224:MET:HG2	2.03	0.58
3:G:86:TRP:CE2	3:G:90:LYS:HD2	2.39	0.57
4:A:260[B]:MET:SD	4:A:321:PRO:HG2	2.44	0.57
4:B:34:PHE:CD1	4:B:188[B]:ILE:HD11	2.40	0.57
4:A:31:PHE:CD1	4:A:187[B]:MET:HE2	2.40	0.56
4:A:187[B]:MET:HE1	4:A:189:TYR:HB2	1.88	0.56
4:A:206:VAL:HG21	4:A:234:ILE:HD11	1.87	0.56
2:F:118:LYS:HE3	2:F:139:GLU:CD	2.30	0.56
2:F:372:LEU:HD21	2:F:444:ILE:HD12	1.87	0.56
4:A:6:LEU:HB3	4:A:9:VAL:CG2	2.35	0.56
4:B:101:LYS:HE2	4:B:105:ALA:HB1	1.87	0.56
4:B:156:LEU:HD23	4:B:188[B]:ILE:HG23	1.88	0.55
4:B:11:LYS:HD3	4:B:54:THR:O	2.07	0.55
3:G:166:TYR:CZ	3:G:229:GLU:HG2	2.42	0.55
4:B:195:VAL:O	4:B:199:THR:HG23	2.07	0.55
4:B:288:GLU:HG3	4:B:330:ARG:HD3	1.86	0.55
2:F:341:ASN:O	2:F:344:PHE:O	2.25	0.55
1:E:92:PHE:HZ	1:E:321:MET:HE1	1.71	0.54
2:F:442:VAL:HG23	11:F:530:HOH:O	2.06	0.54
4:B:208:ASP:HB2	4:B:229:PHE:CE2	2.41	0.54
1:E:92:PHE:CZ	1:E:321:MET:HE1	2.42	0.54
4:A:60[B]:LEU:HD11	4:A:62[B]:ILE:HG13	1.90	0.54
4:B:46:LEU:HG	4:B:79:MET:HE2	1.90	0.54
4:B:183:LEU:HB3	4:B:185:ARG:HG3	1.89	0.54
4:B:260:MET:HE2	4:B:323:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:LYS:HD2	11:E:393:HOH:O	2.08	0.54
2:F:444:ILE:HG13	2:F:466:LEU:HG	1.89	0.54
4:A:329:TYR:CZ	4:A:331:GLN:HG2	2.43	0.54
4:B:4:VAL:HG13	4:B:26:ILE:HB	1.89	0.54
3:G:99:ILE:HG23	3:G:170:ILE:HG22	1.90	0.53
2:F:405[A]:MET:HE3	2:F:405[A]:MET:HA	1.90	0.53
1:E:184:ASP:HB2	1:E:365:GLN:CD	2.34	0.53
4:A:358:ASP:OD1	4:A:360:THR:HG22	2.08	0.53
4:B:249:THR:HG22	4:B:254:VAL:HG13	1.91	0.53
2:F:121:ASN:HB3	11:F:534:HOH:O	2.08	0.53
3:G:104:THR:HG21	3:G:208:LEU:HD21	1.91	0.53
4:A:187[B]:MET:CE	4:A:189:TYR:HB2	2.39	0.53
2:F:449:ASN:ND2	11:F:547:HOH:O	2.35	0.52
4:A:236:SER:HA	4:A:237:PRO:C	2.34	0.52
2:F:265:THR:O	2:F:268:PHE:N	2.41	0.52
2:F:36:ALA:O	2:F:38:GLY:N	2.40	0.52
2:F:309:GLU:HA	2:F:314:LYS:NZ	2.24	0.52
3:G:83:LEU:HD13	7:G:4003:PGV:H52	1.92	0.52
2:F:391:LEU:HD13	2:F:426:LEU:HD12	1.91	0.52
4:A:60[B]:LEU:CD1	4:A:62[B]:ILE:HG13	2.40	0.52
4:A:109:VAL:O	4:A:113:ARG:HG2	2.11	0.51
4:A:173[B]:ARG:HH12	4:A:195:VAL:HG11	1.76	0.51
4:A:364:ARG:NH2	11:A:421:HOH:O	2.44	0.51
4:A:31:PHE:CZ	4:A:187[B]:MET:HE2	2.45	0.51
1:E:133:PRO:HG3	1:E:198:LEU:HD23	1.93	0.51
2:F:212:THR:HG23	2:F:222:ASN:OD1	2.11	0.51
2:F:387:LEU:HD13	2:F:429:LEU:HD13	1.92	0.51
3:G:212:VAL:HG22	3:G:284:TRP:CE3	2.45	0.51
4:A:291:LEU:HD11	4:A:348:PRO:HB3	1.91	0.51
4:B:27:HIS:O	4:B:30:GLU:HB2	2.11	0.51
4:B:170:VAL:HG22	4:B:173:ARG:HH21	1.75	0.51
3:G:146:ARG:O	3:G:149:GLU:HG2	2.11	0.51
4:B:144:ILE:HD11	4:B:160:PRO:O	2.11	0.50
4:A:16:VAL:HG11	11:A:393:HOH:O	2.11	0.50
4:B:95:ASN:O	4:B:146:ARG:HG3	2.12	0.50
4:B:258:LEU:HB3	4:B:260:MET:HE3	1.93	0.50
4:A:96:MET:HE3	4:A:145:GLY:CA	2.39	0.50
4:A:151:GLU:O	4:A:185:ARG:NH2	2.42	0.50
4:A:6:LEU:HB3	4:A:9:VAL:HG21	1.94	0.50
4:A:173[B]:ARG:NH1	4:A:195:VAL:CG1	2.74	0.50
3:G:230:VAL:HG22	3:G:246:ALA:HB1	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:TRP:HB3	1:E:67:PHE:CE1	2.43	0.49
3:G:208:LEU:HD22	3:G:215:LEU:HD11	1.93	0.49
2:F:83:LEU:C	2:F:83:LEU:HD23	2.38	0.49
2:F:471:THR:HG22	2:F:472:TYR:CD1	2.48	0.49
4:A:173[B]:ARG:NH1	4:A:195:VAL:HG11	2.28	0.49
4:A:157:LEU:HD12	4:A:187[B]:MET:SD	2.52	0.49
4:A:146:ARG:HD2	11:A:391:HOH:O	2.13	0.48
4:A:356:ARG:NH1	4:A:360:THR:HG23	2.23	0.48
1:E:346:ALA:HB2	1:E:364:ALA:HB2	1.96	0.48
3:G:59:TRP:CE2	7:G:4006:PGV:H152	2.49	0.48
4:A:312:ASN:HB2	4:B:288:GLU:HG2	1.94	0.48
2:F:335[A]:ILE:HD12	3:G:34:VAL:HG22	1.94	0.48
3:G:41:GLN:HB3	3:G:55:SER:HB2	1.94	0.48
3:G:166:TYR:OH	3:G:229:GLU:CG	2.60	0.48
2:F:401:GLU:HG2	3:G:3:MET:HE2	1.95	0.48
3:G:129:GLN:HB3	3:G:130:MET:CE	2.43	0.48
4:A:260[A]:MET:SD	4:A:260[A]:MET:N	2.87	0.48
4:A:169:ARG:HD3	11:A:405:HOH:O	2.13	0.47
3:G:212:VAL:HG13	3:G:284:TRP:HB3	1.95	0.47
4:A:78:GLY:HA3	4:A:152:PRO:HG3	1.97	0.47
3:G:187:SER:HA	3:G:190:GLU:HB2	1.96	0.47
1:E:109:ALA:HA	1:E:302:VAL:HA	1.96	0.47
6:E:5004:UMQ:H62	11:F:535:HOH:O	2.14	0.47
2:F:325:TYR:O	11:F:525:HOH:O	2.20	0.47
2:F:405[A]:MET:HE1	4:B:77[A]:VAL:HG12	1.96	0.47
4:A:350:GLU:H	4:A:350:GLU:HG3	1.53	0.47
1:E:41:ASP:HB2	11:G:305:HOH:O	2.15	0.47
3:G:45:ALA:HB2	3:G:260:TRP:CE2	2.50	0.47
2:F:98:ASN:O	2:F:256:THR:HG22	2.15	0.47
4:A:123:LEU:HD11	4:A:141:ARG:HB3	1.97	0.46
4:B:6:LEU:CD2	4:B:22:ILE:HD11	2.25	0.46
1:E:47:PHE:HB3	1:E:48:PRO:HD3	1.97	0.46
3:G:214:ILE:HD12	3:G:214:ILE:HA	1.77	0.46
3:G:60:LYS:HB3	3:G:65:PHE:HB2	1.97	0.46
4:A:144:ILE:HD11	4:A:160:PRO:O	2.16	0.46
4:A:145:GLY:O	4:A:149:VAL:HG23	2.16	0.46
4:B:236:SER:HA	4:B:237:PRO:C	2.41	0.46
4:A:329:TYR:CE2	4:A:331:GLN:CG	2.97	0.46
4:B:77[B]:VAL:HG12	4:B:154:VAL:HB	1.97	0.45
2:F:335[A]:ILE:HD12	3:G:34:VAL:CG2	2.47	0.45
4:B:348:PRO:HA	4:B:349:PRO:HD3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:4003:PGV:H92	7:G:4004:PGV:H71	1.98	0.45
1:E:130:GLU:HA	1:E:194:PHE:CZ	2.52	0.45
2:F:296:VAL:HG21	2:F:430:MET:HG2	1.99	0.45
2:F:471:THR:HG23	2:F:490:ILE:HG21	1.91	0.45
4:A:6:LEU:HD22	4:A:22:ILE:HD11	1.98	0.45
4:B:243:PRO:O	4:B:259:PRO:HG3	2.16	0.45
4:B:261:PRO:HD3	4:B:322:SER:HB2	1.97	0.45
4:B:304:VAL:HG23	4:B:343:PHE:HB2	1.98	0.45
1:E:161:ILE:HA	1:E:191:GLY:HA3	1.99	0.45
2:F:275:LYS:HB2	2:F:276:PRO:HD3	1.99	0.45
2:F:384:MET:CE	11:F:553:HOH:O	2.65	0.45
2:F:114:TRP:HB3	2:F:210:LEU:HD13	1.99	0.45
2:F:384:MET:HE3	11:F:553:HOH:O	2.17	0.45
4:A:63:GLY:O	4:A:64:GLU:HB2	2.15	0.44
2:F:68:VAL:HG12	2:F:72:MET:HG3	1.98	0.44
2:F:305:LEU:O	2:F:311:LEU:HD12	2.17	0.44
4:B:258:LEU:HA	4:B:259:PRO:HD3	1.86	0.44
2:F:100:LEU:O	2:F:256:THR:HG23	2.17	0.44
3:G:170:ILE:O	3:G:171:ALA:C	2.61	0.44
4:B:34:PHE:HD2	4:B:205:VAL:HB	1.83	0.44
1:E:341:TYR:CE2	2:F:460:PRO:HB2	2.53	0.43
2:F:391:LEU:HD13	2:F:426:LEU:CD1	2.48	0.43
9:A:2501:ADP:H1'	11:B:384:HOH:O	2.17	0.43
4:A:173[B]:ARG:NH2	11:A:428:HOH:O	2.51	0.43
1:E:74:GLY:HA3	2:F:253:PRO:HB3	2.01	0.43
2:F:122:PHE:CD1	2:F:204:PHE:HD2	2.36	0.43
4:A:29:GLY:O	4:A:180:HIS:NE2	2.51	0.43
4:A:138:GLN:O	4:A:142:VAL:HG23	2.19	0.43
9:A:2501:ADP:N3	11:A:393:HOH:O	2.36	0.43
1:E:115:LEU:HG	1:E:248:PRO:HD3	2.01	0.43
2:F:287:PHE:CZ	2:F:376:ASN:ND2	2.87	0.43
1:E:129:TRP:CD2	1:E:160:LEU:HD13	2.52	0.43
2:F:380:GLY:HA3	5:C:2:GLC:H61	2.01	0.43
4:A:148:LEU:HD23	4:A:155:PHE:HE2	1.84	0.43
4:B:33:VAL:HA	4:B:189:TYR:O	2.19	0.43
1:E:133:PRO:HG3	1:E:198:LEU:CD2	2.49	0.42
2:F:319:VAL:O	2:F:322:ILE:HG13	2.19	0.42
1:E:3:GLU:HB3	1:E:6:LYS:HE2	2.00	0.42
4:A:20:LYS:HB2	4:A:211:ARG:HD2	2.00	0.42
4:A:260[A]:MET:CE	4:A:300:LEU:HD22	2.48	0.42
4:B:62:ILE:HB	4:B:67:MET:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:192:HIS:HA	11:A:396:HOH:O	2.20	0.42
4:A:223:HIS:ND1	4:A:368:GLU:HG2	2.34	0.42
2:F:221:ASN:ND2	2:F:224:SER:H	2.17	0.42
3:G:12:ARG:O	3:G:15:ILE:HG22	2.19	0.42
3:G:245:LEU:HG	3:G:249:MET:HE2	2.01	0.42
4:A:95:ASN:O	4:A:146:ARG:HG3	2.20	0.42
4:B:146:ARG:HD2	11:B:396:HOH:O	2.19	0.42
4:B:62:ILE:HB	4:B:67:MET:HG3	2.02	0.42
1:E:115:LEU:HD21	1:E:224:MET:CE	2.44	0.42
2:F:451:GLY:HA2	2:F:452:PRO:C	2.45	0.42
1:E:130:GLU:HA	1:E:194:PHE:HZ	1.85	0.42
3:G:104:THR:HG22	3:G:203:PHE:CZ	2.55	0.42
3:G:129:GLN:C	3:G:130:MET:HE2	2.45	0.42
4:B:102:LEU:HD12	4:B:102:LEU:HA	1.91	0.42
3:G:180:TYR:CE2	3:G:211:SER:HA	2.54	0.41
4:A:317:HIS:HA	4:A:327:LEU:O	2.20	0.41
1:E:314:ASP:HB3	1:E:317:ILE:HD12	2.02	0.41
2:F:404:ALA:HB1	4:B:72:PRO:HB2	2.01	0.41
4:A:34:PHE:HB2	4:A:190:VAL:HG22	2.02	0.41
2:F:78:PHE:HZ	3:G:164:PHE:CD2	2.39	0.41
2:F:361:TRP:O	2:F:368:ALA:HA	2.19	0.41
2:F:459:THR:HA	2:F:460:PRO:HD3	1.91	0.41
2:F:391:LEU:CD1	2:F:426:LEU:HD12	2.50	0.41
4:B:106:LYS:HB2	4:B:109:VAL:HB	2.03	0.41
4:B:259:PRO:HD2	4:B:260:MET:HE3	2.03	0.41
1:E:82:ASP:O	1:E:86:GLN:HG3	2.21	0.41
2:F:309:GLU:HA	2:F:314:LYS:HZ3	1.85	0.41
4:A:315:GLN:HG2	4:A:330:ARG:HG2	2.01	0.41
1:E:61:PHE:CE2	1:E:264:ALA:HB2	2.55	0.41
4:A:173[B]:ARG:NH1	4:A:195:VAL:HG12	2.36	0.41
4:B:120:VAL:O	4:B:172:MET:HE1	2.21	0.41
1:E:214:GLU:OE1	1:E:234:ASN:ND2	2.50	0.41
4:A:4:VAL:HG13	4:A:26[A]:ILE:HB	2.02	0.41
4:A:270:VAL:HG13	4:A:362:CYS:CB	2.49	0.41
4:B:9:VAL:HA	4:B:58:GLY:HA3	2.01	0.41
1:E:9:ILE:HG12	1:E:59:ILE:HB	2.02	0.40
1:E:330:MET:HE2	1:E:330:MET:HB2	1.95	0.40
4:B:29:GLY:O	4:B:180:HIS:CE1	2.74	0.40
1:E:81:PRO:HA	11:E:418:HOH:O	2.20	0.40
1:E:129:TRP:CE2	1:E:160:LEU:HD13	2.56	0.40
1:E:278:GLU:CD	1:E:282:ASN:HD22	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:86:LEU:HA	4:B:146:ARG:NH2	2.36	0.40
1:E:89:LEU:HD22	1:E:304:LEU:HA	2.03	0.40
6:E:5004:UMQ:C6	11:F:535:HOH:O	2.70	0.40
3:G:99:ILE:O	3:G:103:SER:OG	2.34	0.40
4:A:6:LEU:HB3	4:A:9:VAL:HG23	2.03	0.40
4:B:106:LYS:O	4:B:107:LYS:C	2.63	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%)	363 (97%)	10 (3%)	2 (0%)	24	31
2	F	488/514 (95%)	468 (96%)	18 (4%)	2 (0%)	30	38
3	G	291/296 (98%)	286 (98%)	4 (1%)	1 (0%)	36	46
4	A	377/381 (99%)	360 (96%)	16 (4%)	1 (0%)	36	46
4	B	356/381 (93%)	335 (94%)	19 (5%)	2 (1%)	21	27
All	All	1887/1950 (97%)	1812 (96%)	67 (4%)	8 (0%)	30	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	37	GLN
4	B	107	LYS
1	E	172	GLU
1	E	168	ALA
3	G	230	VAL
4	A	238	LYS
2	F	38	GLY
4	B	270	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%)	290 (97%)	10 (3%)	33	50
2	F	404/424 (95%)	377 (93%)	27 (7%)	15	21
3	G	236/237 (100%)	228 (97%)	8 (3%)	32	49
4	A	322/323 (100%)	304 (94%)	18 (6%)	19	28
4	B	309/323 (96%)	282 (91%)	27 (9%)	9	12
All	All	1571/1610 (98%)	1481 (94%)	90 (6%)	18	27

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1	LYS
1	E	115	LEU
1	E	132	ILE
1	E	178	ILE
1	E	211	SER
1	E	212	ILE
1	E	237	THR
1	E	293[A]	VAL
1	E	293[B]	VAL
1	E	366	THR
2	F	22	LEU
2	F	25	LEU
2	F	33	LEU
2	F	45	THR
2	F	46	THR
2	F	56	ILE
2	F	59	ASN
2	F	68	VAL
2	F	83	LEU
2	F	145	LEU
2	F	150	LYS
2	F	163	THR
2	F	196	VAL

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Mol	Chain	Res	Type
2	F	220	THR
2	F	234	ILE
2	F	257	VAL
2	F	266	ARG
2	F	269	THR
2	F	271	GLU
2	F	273	ILE
2	F	311	LEU
2	F	346	GLU
2	F	444	ILE
2	F	449	ASN
2	F	471	THR
2	F	494	ILE
2	F	496	LEU
3	G	13	LEU
3	G	21	LEU
3	G	24	ILE
3	G	95	SER
3	G	178	LYS
3	G	212	VAL
3	G	214	ILE
3	G	285	LEU
4	A	4	VAL
4	A	17	VAL
4	A	20	LYS
4	A	22	ILE
4	A	53	GLU
4	A	62[A]	ILE
4	A	62[B]	ILE
4	A	101	LYS
4	A	127	LEU
4	A	219	LEU
4	A	234	ILE
4	A	242	LEU
4	A	258	LEU
4	A	270	VAL
4	A	295	ILE
4	A	327	LEU
4	A	345	ILE
4	A	350	GLU
4	B	4	VAL
4	B	21	ASP

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Mol	Chain	Res	Type
4	B	22	ILE
4	B	45	LEU
4	B	53	GLU
4	B	100	LEU
4	B	101	LYS
4	B	102	LEU
4	B	114	VAL
4	B	123	LEU
4	B	127	LEU
4	B	146	ARG
4	B	181	LYS
4	B	185	ARG
4	B	203	LYS
4	B	251	ILE
4	B	255	GLN
4	B	256	VAL
4	B	258	LEU
4	B	271	GLU
4	B	288	GLU
4	B	294	ASP
4	B	300	LEU
4	B	320	ILE
4	B	322	SER
4	B	324	ARG
4	B	350	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	49	GLN
1	E	253	GLN
1	E	282	ASN
2	F	59	ASN
2	F	155	GLN
2	F	165	GLN
2	F	203	GLN
2	F	437	ASN
2	F	440	ASN
2	F	449	ASN
2	F	469	ASN
3	G	5	GLN
3	G	53	GLN

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Mol	Chain	Res	Type
3	G	129	GLN
4	A	5	GLN
4	A	253	GLN
4	A	280	ASN
4	A	305	GLN
4	A	317	HIS
4	B	125	HIS
4	B	180	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	0.59	0	17,17,17	1.71	3 (17%)
5	GLC	C	2	5	11,11,12	0.40	0	15,15,17	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
5	GLC	C	1	5	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GLC	C	2	5	-	1/2/19/22	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	3.96	121.31	113.65
5	C	1	GLC	C6-C5-C4	-3.35	104.79	113.02
5	C	1	GLC	O5-C5-C4	2.81	114.76	109.70

There are no chirality outliers.

All (1) torsion outliers are listed below:

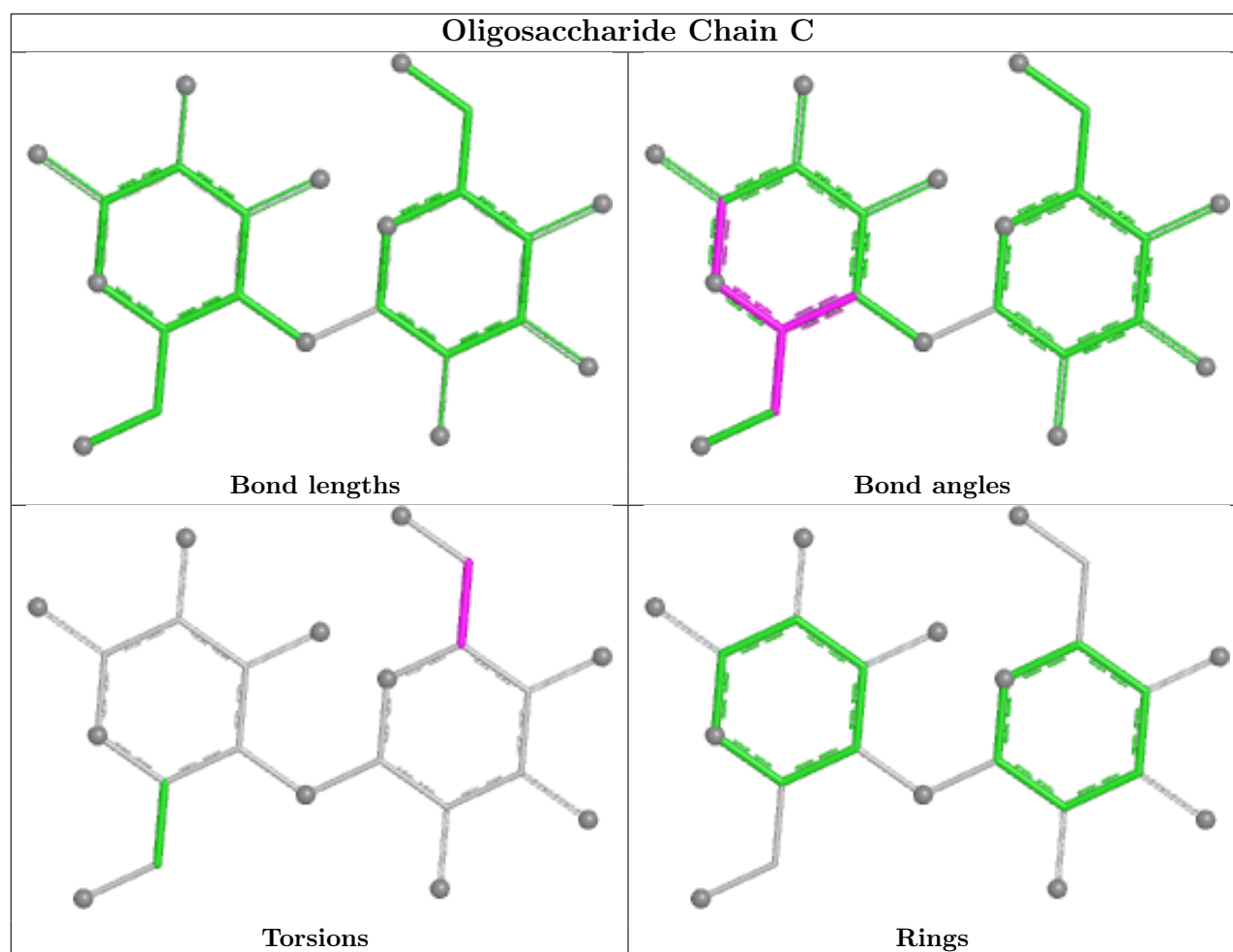
Mol	Chain	Res	Type	Atoms
5	C	2	GLC	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2	GLC	1	0

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



5.6 Ligand geometry [i](#)

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$
9	ADP	A	2501	10,8	28,29,29	1.04	2 (7%)	43,45,45	1.77	5 (11%)
7	PGV	F	4002	-	8,8,50	0.30	0	7,7,56	0.69	0
7	PGV	G	4004	-	11,11,50	1.09	1 (9%)	10,10,56	0.96	1 (10%)
7	PGV	G	4007	-	8,8,50	1.19	1 (12%)	7,7,56	1.33	2 (28%)
7	PGV	G	4003	-	7,7,50	0.39	0	6,6,56	0.66	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	0.60	0	46,46,46	1.27	5 (10%)
10	BEF	A	3001	9	0,3,3	-	-	-		
7	PGV	F	4008	-	7,7,50	0.44	0	6,6,56	0.45	0
7	PGV	G	4006	-	6,6,50	1.44	1 (16%)	5,5,56	1.42	1 (20%)
7	PGV	G	4005	-	9,9,50	1.21	1 (11%)	8,8,56	1.12	1 (12%)
7	PGV	F	4010	-	12,12,50	1.18	1 (8%)	11,11,56	1.02	1 (9%)
7	PGV	G	4009	-	11,11,50	1.34	1 (9%)	10,10,56	0.73	0
9	ADP	B	2502	10,8	28,29,29	1.06	3 (10%)	43,45,45	1.84	7 (16%)
7	PGV	F	4001	-	50,50,50	1.16	3 (6%)	53,56,56	1.13	4 (7%)
10	BEF	B	3002	9	0,3,3	-	-	-		

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	ADP	A	2501	10,8	-	0/16/32/32	0/3/3/3
7	PGV	F	4002	-	-	2/6/6/55	-
7	PGV	G	4004	-	-	4/9/9/55	-
7	PGV	G	4007	-	-	3/6/6/55	-
7	PGV	G	4003	-	-	0/5/5/55	-
6	UMQ	E	5004	-	-	8/20/60/60	0/2/2/2
7	PGV	F	4008	-	-	2/5/5/55	-
7	PGV	G	4006	-	-	1/4/4/55	-
7	PGV	G	4005	-	-	3/7/7/55	-
7	PGV	F	4010	-	-	6/10/10/55	-
7	PGV	G	4009	-	-	4/9/9/55	-
9	ADP	B	2502	10,8	-	3/16/32/32	0/3/3/3
7	PGV	F	4001	-	-	27/55/55/55	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	4001	PGV	O01-C1	4.73	1.47	1.34
7	F	4001	PGV	O03-C19	4.14	1.45	1.33
7	G	4009	PGV	C12-C11	4.10	1.55	1.31
7	F	4001	PGV	C12-C11	3.86	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	4010	PGV	C12-C11	3.83	1.53	1.31
7	G	4005	PGV	C11-C12	3.32	1.53	1.29
7	G	4006	PGV	C12-C11	3.28	1.53	1.29
7	G	4004	PGV	C11-C12	3.27	1.53	1.29
7	G	4007	PGV	C11-C12	3.13	1.52	1.29
9	B	2502	ADP	PA-O3A	2.43	1.62	1.59
9	A	2501	ADP	C8-N7	2.40	1.36	1.31
9	B	2502	ADP	C5-N7	-2.38	1.34	1.39
9	A	2501	ADP	C5-N7	-2.28	1.34	1.39
9	B	2502	ADP	C8-N7	2.14	1.35	1.31

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2501	ADP	N3-C2-N1	-6.02	119.47	128.58
9	B	2502	ADP	C5-C4-N3	-5.58	119.04	126.72
9	B	2502	ADP	N3-C2-N1	-5.41	120.39	128.58
9	A	2501	ADP	C5-C4-N3	-4.95	119.90	126.72
7	F	4001	PGV	O01-C1-C2	4.63	121.49	111.48
9	A	2501	ADP	C2-N3-C4	3.98	121.55	111.83
9	B	2502	ADP	N3-C4-N9	3.82	133.67	127.17
9	B	2502	ADP	C2-N3-C4	3.81	121.13	111.83
7	F	4001	PGV	O03-C19-C20	3.63	122.90	111.83
9	A	2501	ADP	N3-C4-N9	3.18	132.58	127.17
9	B	2502	ADP	O3B-PB-O2B	3.03	119.15	107.80
6	E	5004	UMQ	C1-O5-C5	2.97	119.51	113.72
6	E	5004	UMQ	CA-O1'-C1'	2.85	118.54	113.68
7	G	4006	PGV	C13-C12-C11	-2.75	109.65	130.48
9	A	2501	ADP	N9-C8-N7	-2.73	110.06	113.94
9	B	2502	ADP	N9-C8-N7	-2.66	110.16	113.94
7	F	4010	PGV	C13-C12-C11	-2.58	110.91	126.42
7	G	4005	PGV	C10-C11-C12	-2.55	111.19	130.48
7	G	4007	PGV	C10-C11-C12	-2.52	111.41	130.48
6	E	5004	UMQ	C1'-O5'-C5'	-2.37	109.09	113.72
6	E	5004	UMQ	O2'-C2'-C1'	2.36	115.70	110.08
7	G	4004	PGV	C10-C11-C12	-2.33	112.79	130.48
7	G	4007	PGV	C13-C12-C11	-2.27	108.66	126.43
6	E	5004	UMQ	O1'-C1'-C2'	2.25	111.69	108.27
7	F	4001	PGV	O03-C19-O04	-2.23	118.04	123.63
9	B	2502	ADP	O4'-C1'-C2'	-2.02	102.28	106.62
7	F	4001	PGV	O01-C1-O02	-2.00	119.02	123.70

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	4001	PGV	C04-O12-P-O11
7	F	4001	PGV	C04-O12-P-O13
7	F	4001	PGV	C04-O12-P-O14
7	F	4001	PGV	O12-C04-C05-C06
7	F	4001	PGV	O02-C1-O01-C02
7	F	4001	PGV	C2-C1-O01-C02
7	G	4004	PGV	C10-C11-C12-C13
7	G	4005	PGV	C10-C11-C12-C13
7	G	4007	PGV	C10-C11-C12-C13
9	B	2502	ADP	PA-O3A-PB-O2B
7	F	4001	PGV	C10-C11-C12-C13
7	F	4010	PGV	C10-C11-C12-C13
7	F	4001	PGV	O12-C04-C05-O05
7	F	4001	PGV	C19-C20-C21-C22
7	F	4001	PGV	C1-C2-C3-C4
7	F	4001	PGV	C20-C21-C22-C23
7	G	4005	PGV	C7-C8-C9-C10
7	G	4009	PGV	C6-C7-C8-C9
6	E	5004	UMQ	CD-CF-CG-CH
7	F	4001	PGV	C11-C10-C9-C8
7	F	4002	PGV	C6-C7-C8-C9
7	G	4009	PGV	C5-C6-C7-C8
7	F	4001	PGV	C05-C04-O12-P
6	E	5004	UMQ	CC-CD-CF-CG
7	G	4007	PGV	C6-C7-C8-C9
7	F	4010	PGV	C11-C10-C9-C8
7	F	4010	PGV	C3-C4-C5-C6
7	F	4001	PGV	C30-C31-C32-C33
7	F	4001	PGV	C20-C19-O03-C01
7	G	4009	PGV	C11-C10-C9-C8
7	G	4004	PGV	C6-C7-C8-C9
7	F	4001	PGV	C25-C26-C27-C28
7	F	4001	PGV	O03-C01-C02-C03
7	G	4004	PGV	C4-C5-C6-C7
7	G	4004	PGV	C2-C3-C4-C5
7	F	4001	PGV	O03-C01-C02-O01
7	F	4001	PGV	C24-C25-C26-C27
6	E	5004	UMQ	O5'-C1'-O1'-CA
7	G	4009	PGV	C4-C5-C6-C7
7	F	4001	PGV	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
7	G	4007	PGV	C5-C6-C7-C8
7	F	4002	PGV	C3-C4-C5-C6
9	B	2502	ADP	PA-O3A-PB-O3B
7	F	4001	PGV	C23-C24-C25-C26
6	E	5004	UMQ	CH-CI-CJ-CK
7	F	4008	PGV	C5-C6-C7-C8
7	F	4010	PGV	C2-C3-C4-C5
7	F	4008	PGV	C4-C5-C6-C7
7	F	4001	PGV	C2-C3-C4-C5
6	E	5004	UMQ	CI-CJ-CK-CL
7	G	4006	PGV	C11-C12-C13-C14
6	E	5004	UMQ	CF-CG-CH-CI
7	F	4001	PGV	C6-C7-C8-C9
7	F	4001	PGV	O05-C05-C06-O06
7	F	4001	PGV	C22-C23-C24-C25
6	E	5004	UMQ	CG-CH-CI-CJ
6	E	5004	UMQ	C2'-C1'-O1'-CA
7	G	4005	PGV	C9-C10-C11-C12
7	F	4001	PGV	C21-C22-C23-C24
7	F	4010	PGV	C9-C10-C11-C12
7	F	4010	PGV	C6-C7-C8-C9
9	B	2502	ADP	PA-O3A-PB-O1B
7	F	4001	PGV	O03-C19-C20-C21

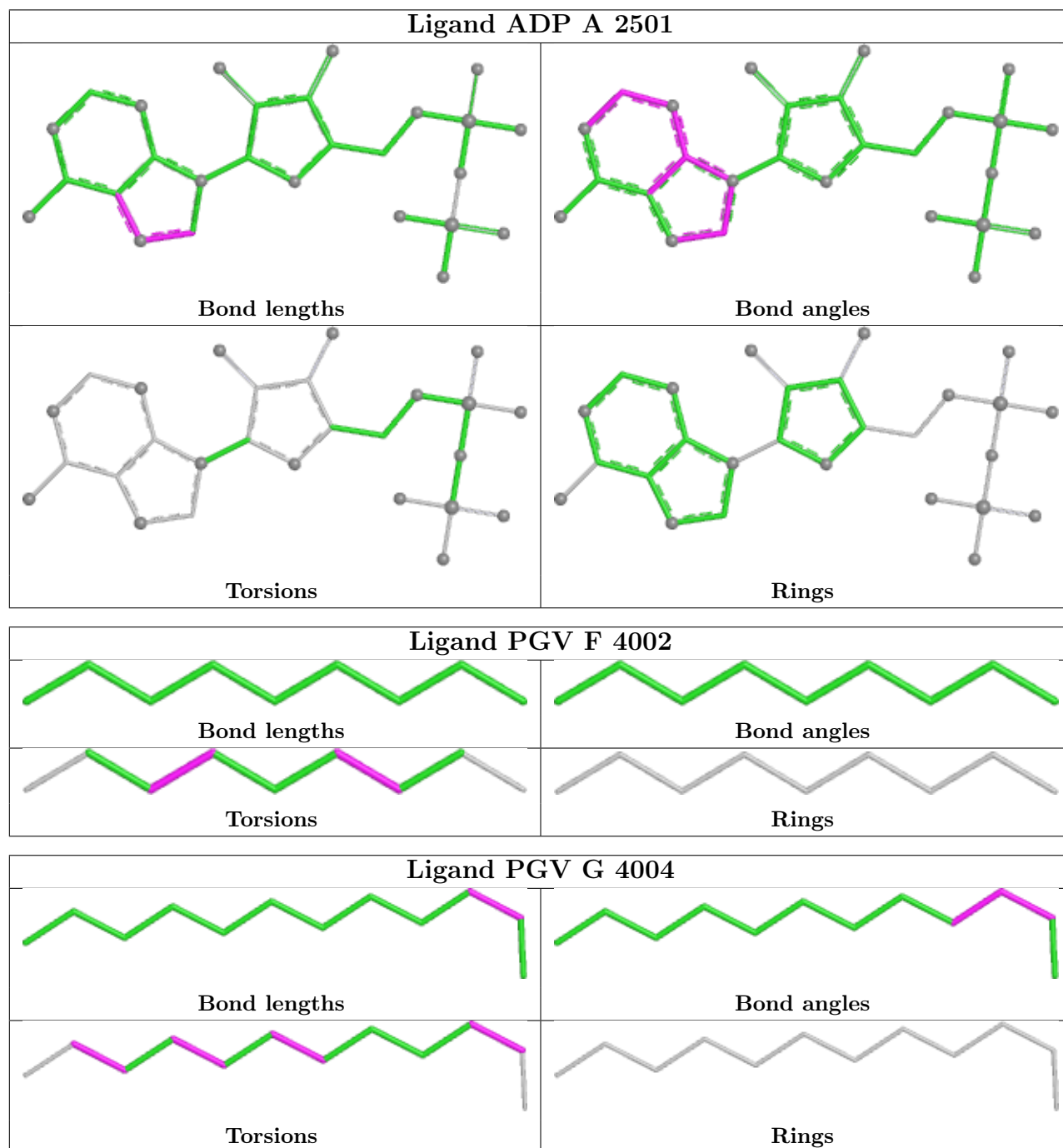
There are no ring outliers.

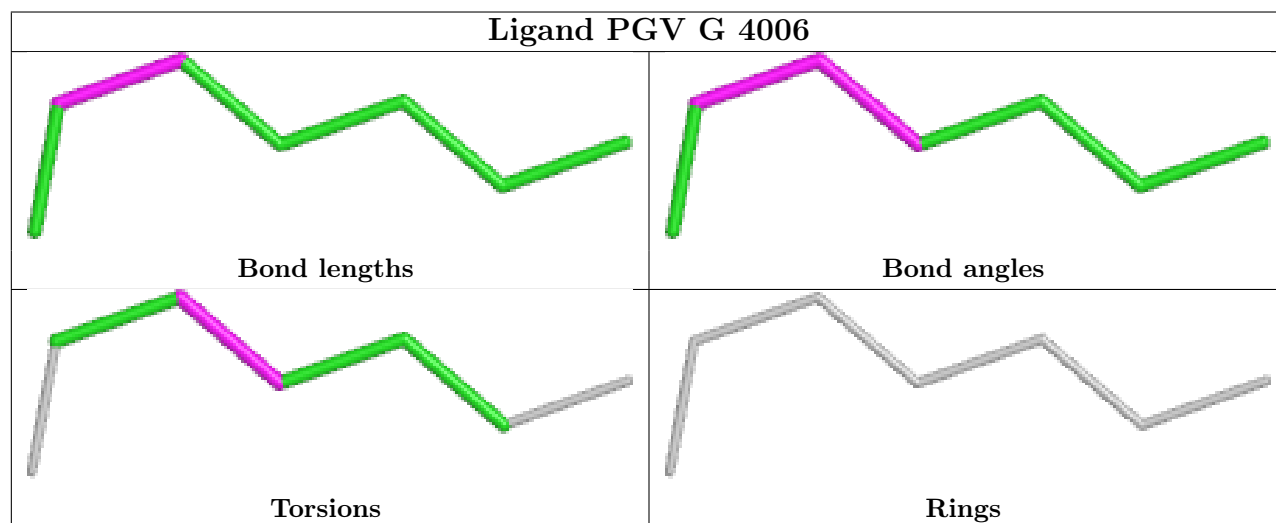
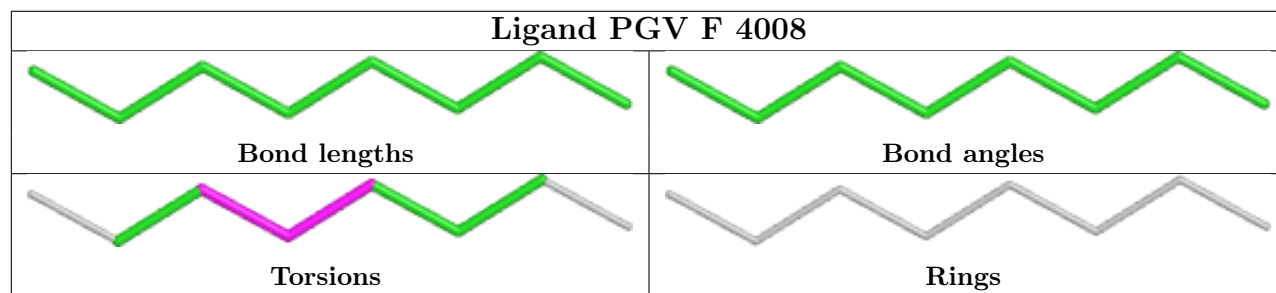
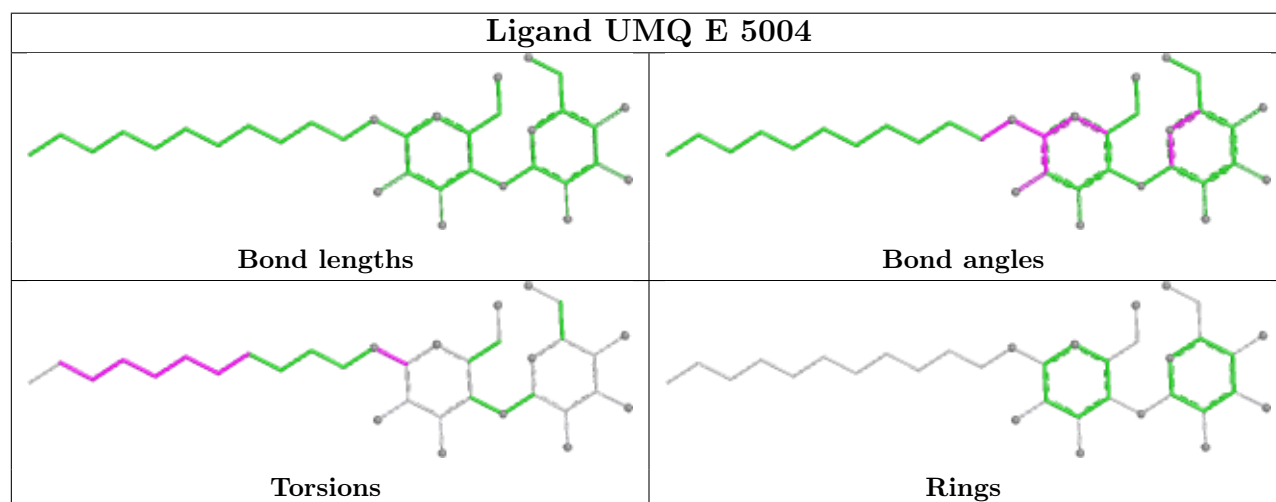
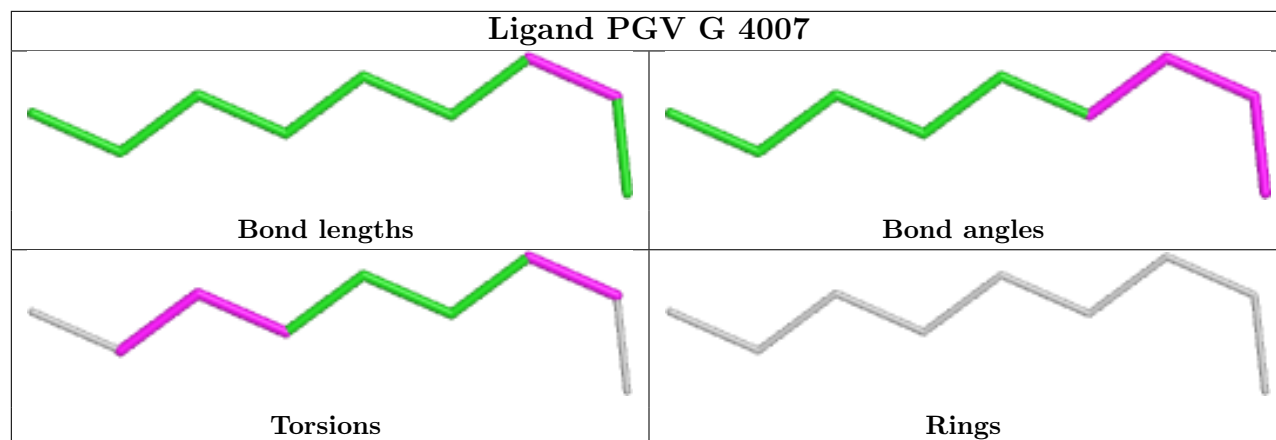
5 monomers are involved in 7 short contacts:

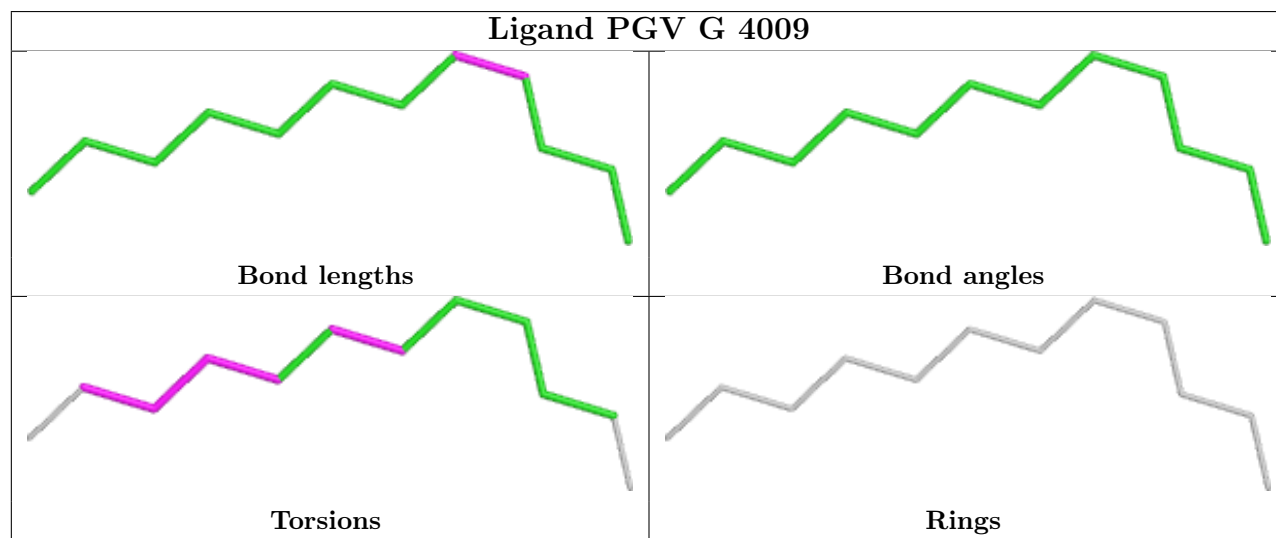
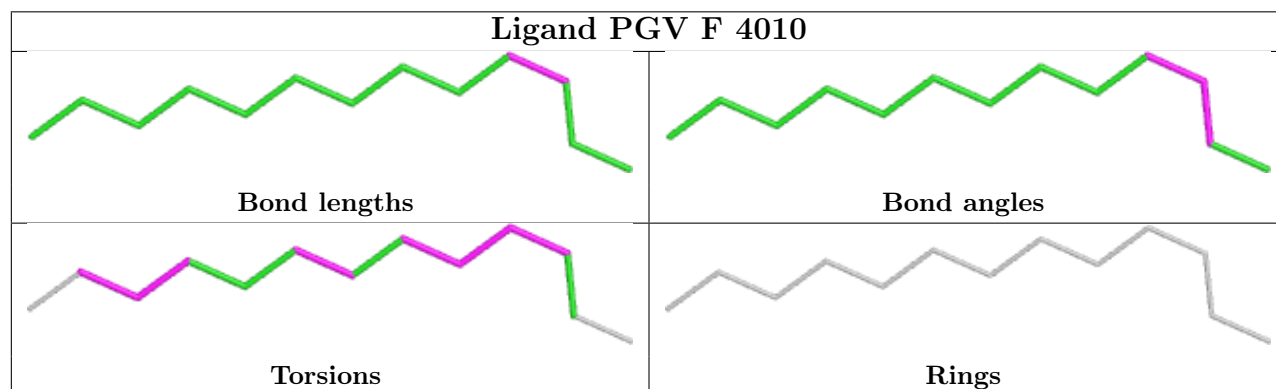
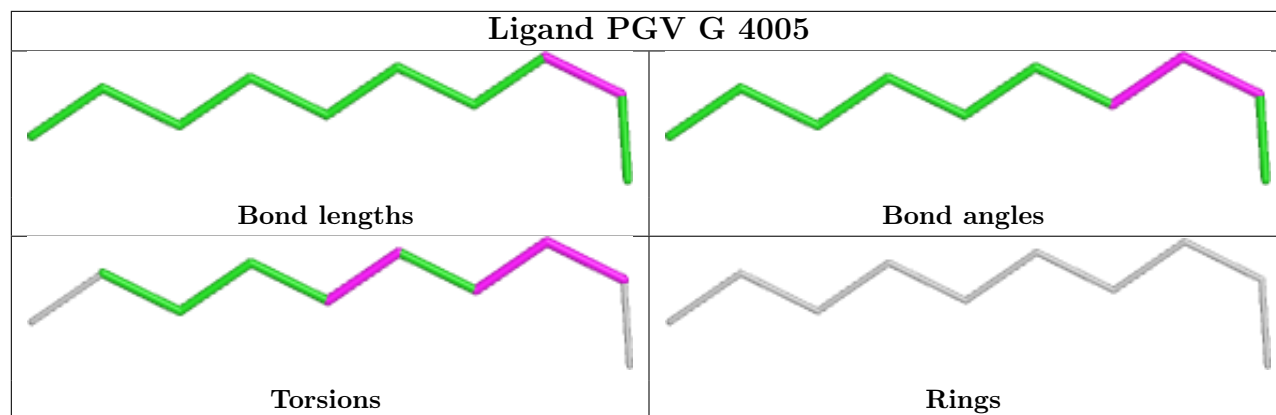
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2501	ADP	2	0
7	G	4004	PGV	1	0
7	G	4003	PGV	2	0
6	E	5004	UMQ	2	0
7	G	4006	PGV	1	0

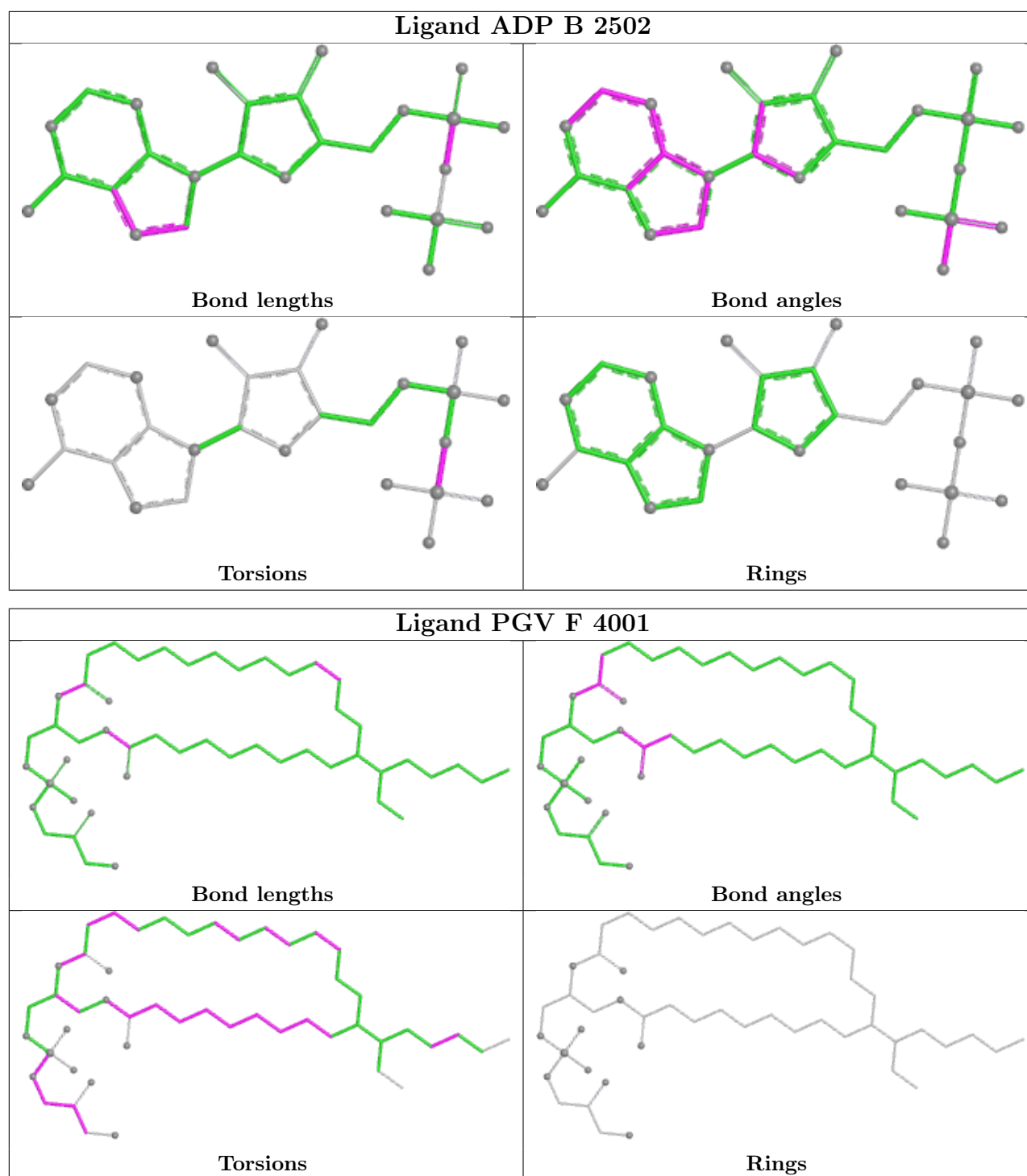
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.51	22 (5%) 28 30	14, 50, 82, 94	4 (1%)
2	F	490/514 (95%)	0.79	66 (13%) 7 8	20, 52, 98, 119	2 (0%)
3	G	293/296 (98%)	0.29	22 (7%) 20 22	13, 32, 74, 94	2 (0%)
4	A	371/381 (97%)	0.45	13 (3%) 47 49	8, 44, 69, 80	9 (2%)
4	B	358/381 (93%)	0.73	37 (10%) 12 13	16, 54, 105, 122	4 (1%)
All	All	1886/1950 (96%)	0.58	160 (8%) 16 18	8, 47, 88, 122	21 (1%)

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	110	ILE	9.0
2	F	10	TRP	8.6
4	B	251	ILE	8.1
4	B	267	TRP	7.1
4	A	104	GLY	6.6
2	F	37	GLN	6.3
4	B	16	VAL	5.9
3	G	133	ALA	5.6
2	F	503	ILE	5.3
4	A	295	ILE	5.2
2	F	18	SER	4.4
4	A	103	ALA	4.3
2	F	479	GLY	4.2
2	F	16	LYS	3.9
2	F	38	GLY	3.9
2	F	356	GLY	3.8
3	G	11	ALA	3.7
1	E	128	THR	3.6
2	F	31	VAL	3.6
2	F	22	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
4	B	295	ILE	3.5
4	B	323	ILE	3.5
2	F	245	ASN	3.4
2	F	17	TRP	3.4
3	G	134	VAL	3.4
4	B	259	PRO	3.3
3	G	126	LEU	3.3
4	B	271	GLU	3.3
2	F	354	LEU	3.3
4	B	261	PRO	3.3
4	B	108	GLU	3.3
2	F	32	VAL	3.3
2	F	352	SER	3.2
2	F	48	ILE	3.2
2	F	14	ALA	3.2
2	F	267	VAL	3.1
4	B	247	THR	3.1
4	B	105	ALA	3.1
3	G	71	ASP	3.0
4	A	371	VAL	3.0
1	E	197	ASP	3.0
3	G	70	ALA	3.0
2	F	472	TYR	3.0
2	F	36	ALA	3.0
4	A	64	GLU	3.0
4	A	372	ALA	2.9
1	E	134	ALA	2.9
2	F	13	ASP	2.9
2	F	35	TYR	2.9
3	G	4	VAL	2.9
2	F	44	ILE	2.9
4	B	324	ARG	2.8
4	B	322	SER	2.8
2	F	501	LEU	2.8
2	F	500	ALA	2.8
4	B	249	THR	2.8
2	F	478	GLY	2.8
1	E	133	PRO	2.8
2	F	25	LEU	2.7
3	G	130	MET	2.7
1	E	370	LYS	2.7
1	E	182	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	29	TYR	2.7
2	F	310	ALA	2.6
4	B	361	ALA	2.6
2	F	355	PHE	2.6
4	B	359	GLY	2.6
2	F	40	TYR	2.6
1	E	254	PRO	2.6
2	F	271	GLU	2.6
4	B	270	VAL	2.6
1	E	184	ASP	2.5
1	E	353	GLY	2.5
4	B	260	MET	2.5
2	F	45	THR	2.5
1	E	337	SER	2.5
4	B	18	VAL	2.5
1	E	4	GLU	2.5
1	E	22	GLU	2.5
4	B	294	ASP	2.5
2	F	33	LEU	2.5
4	B	293	SER	2.4
4	B	298	VAL	2.4
4	B	13	TRP	2.4
1	E	178	ILE	2.4
1	E	338	ALA	2.4
2	F	272	GLY	2.4
3	G	117	GLY	2.4
3	G	10	LYS	2.4
2	F	349	MET	2.4
4	A	187[A]	MET	2.4
3	G	114	ARG	2.4
4	B	104	GLY	2.3
4	B	296	ALA	2.3
4	A	293	SER	2.3
4	B	282	SER	2.3
2	F	19	VAL	2.3
4	B	17	VAL	2.3
2	F	172	ASN	2.3
4	B	181	LYS	2.3
4	B	352	CYS	2.3
4	B	208	ASP	2.3
2	F	28	GLY	2.3
2	F	345	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
4	A	260[A]	MET	2.3
2	F	26	LEU	2.3
2	F	496	LEU	2.3
4	B	358	ASP	2.3
1	E	252	GLY	2.3
4	B	103	ALA	2.3
1	E	352	SER	2.3
2	F	277	PHE	2.2
2	F	215	GLY	2.2
2	F	494	ILE	2.2
2	F	46	THR	2.2
3	G	2	ALA	2.2
4	B	250	ALA	2.2
2	F	96	SER	2.2
2	F	273	ILE	2.2
2	F	351	LEU	2.2
1	E	343	VAL	2.2
3	G	14	PHE	2.2
2	F	21	GLY	2.2
4	A	370	GLY	2.2
2	F	353	ALA	2.2
1	E	167	TYR	2.2
2	F	219	LEU	2.2
2	F	312	ARG	2.2
1	E	207	ASP	2.2
4	B	15	GLU	2.2
2	F	220	THR	2.2
2	F	458	THR	2.2
3	G	128	PHE	2.1
3	G	149	GLU	2.1
2	F	58	ALA	2.1
2	F	24	GLY	2.1
2	F	256	THR	2.1
2	F	502	ALA	2.1
2	F	159	LEU	2.1
1	E	164	ASP	2.1
3	G	15	ILE	2.1
3	G	19	LEU	2.1
4	A	323	ILE	2.1
3	G	129	GLN	2.1
3	G	6	PRO	2.1
2	F	246	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	170	LYS	2.1
2	F	474	ILE	2.1
4	B	174	ILE	2.1
4	B	265	GLN	2.1
3	G	132	PRO	2.1
2	F	12	SER	2.0
1	E	172	GLU	2.0
3	G	9	GLN	2.0
2	F	189	ILE	2.0
4	B	345	ILE	2.0
4	A	298	VAL	2.0
3	G	125	MET	2.0
2	F	41	LEU	2.0
2	F	47	LEU	2.0

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

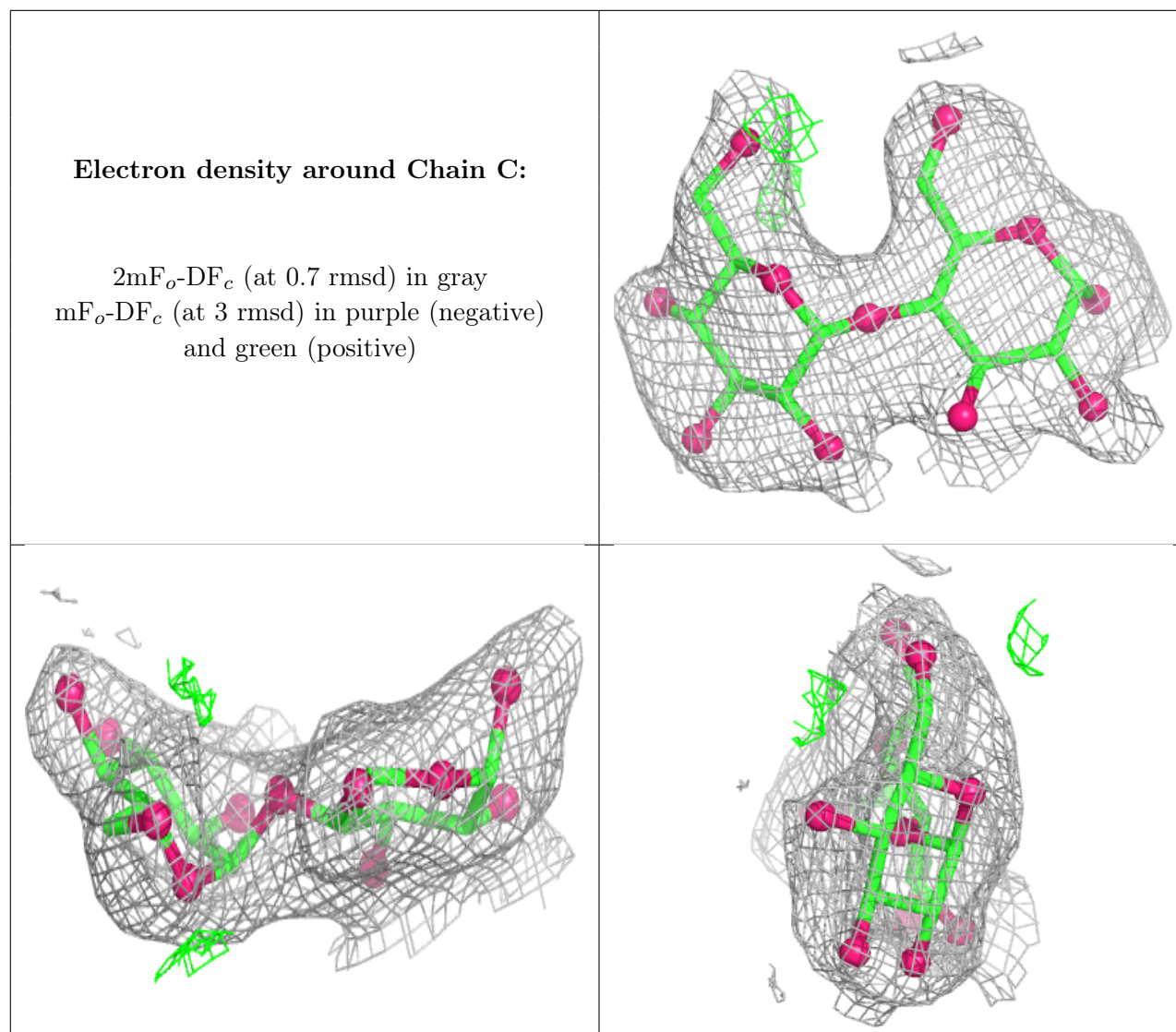
There are no non-standard protein/DNA/RNA residues in this entry.

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	-	-	30,33,35,35	0
5	GLC	C	2	11/12	-	-	30,31,32,32	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(Å ²)	Q<0.9
7	PGV	G	4009	12/51	0.61	0.22	48,49,51,52	0
7	PGV	F	4008	8/51	0.63	0.19	47,49,50,50	0
7	PGV	G	4003	8/51	0.69	0.22	50,54,56,58	0
7	PGV	G	4005	10/51	0.72	0.13	52,56,57,57	0
7	PGV	G	4007	9/51	0.76	0.14	46,50,55,56	0
7	PGV	G	4004	12/51	0.76	0.14	43,48,58,60	0
7	PGV	F	4002	9/51	0.78	0.13	31,33,36,39	0

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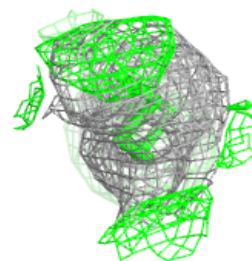
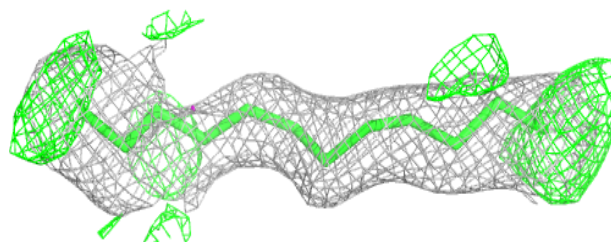
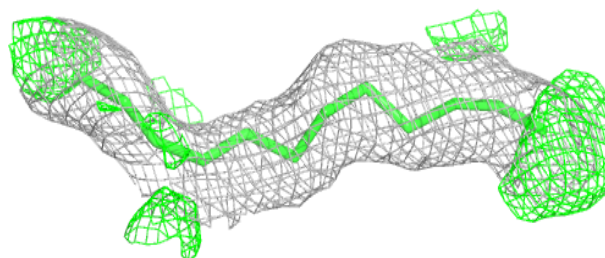
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PGV	G	4006	7/51	0.79	0.15	43,45,49,51	0
7	PGV	F	4010	13/51	0.84	0.16	66,68,70,70	0
7	PGV	F	4001	51/51	0.86	0.14	50,57,69,71	0
6	UMQ	E	5004	34/34	0.90	0.09	23,28,33,34	0
9	ADP	B	2502	27/27	0.96	0.09	24,40,53,54	0
10	BEF	A	3001	4/4	0.96	0.06	17,18,19,20	0
8	MG	A	1501	1/1	0.98	0.03	18,18,18,18	0
9	ADP	A	2501	27/27	0.98	0.06	17,27,38,39	0
10	BEF	B	3002	4/4	0.98	0.05	21,21,22,26	0
8	MG	B	1502	1/1	1.00	0.04	15,15,15,15	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.

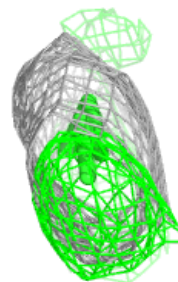
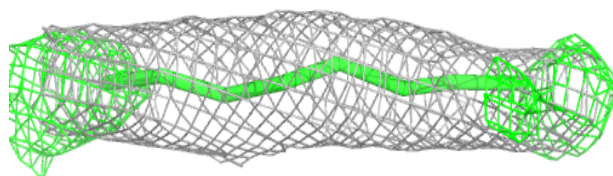
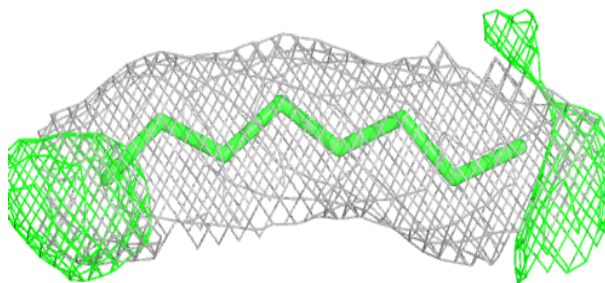
Electron density around PGV G 4009:

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

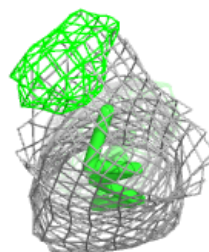
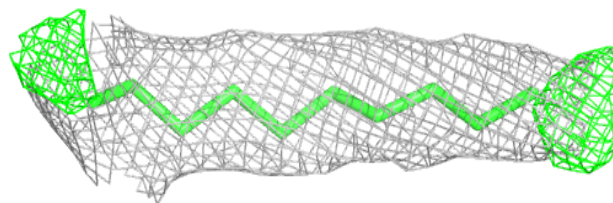
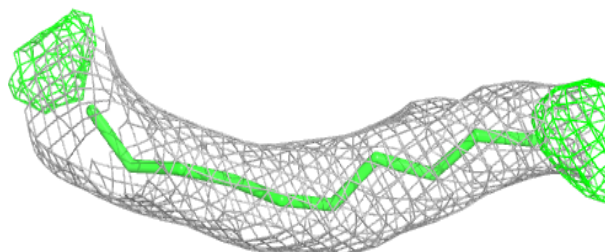


Electron density around PGV F 4008:

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

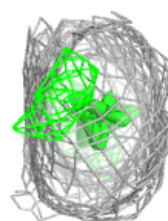
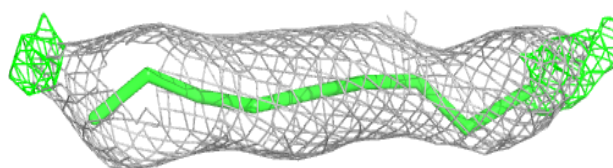
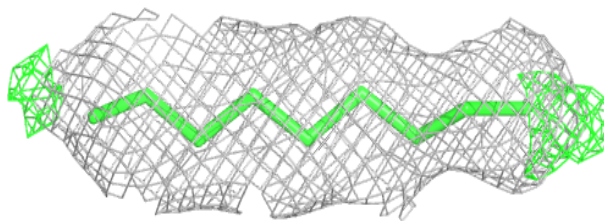
**Electron density around PGV G 4005:**

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

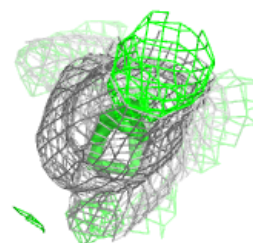
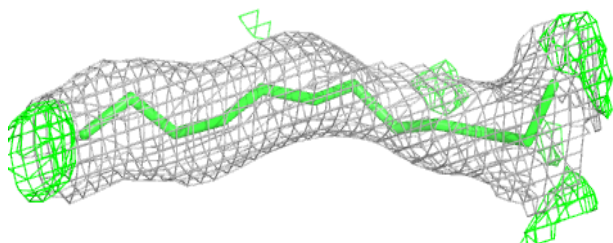
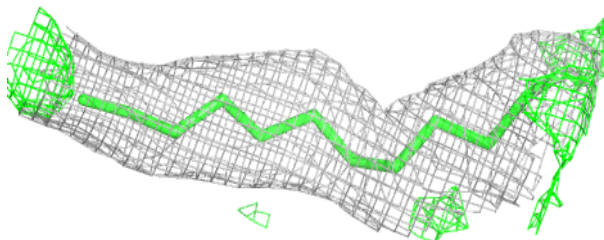


Electron density around PGV G 4007:

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

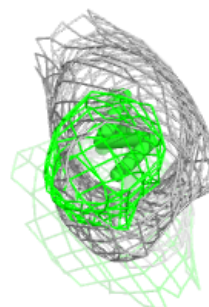
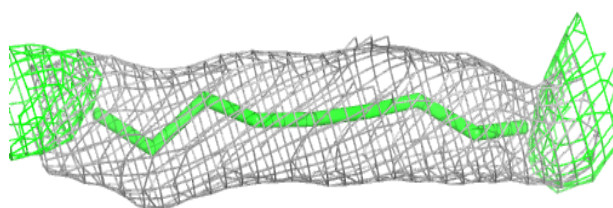
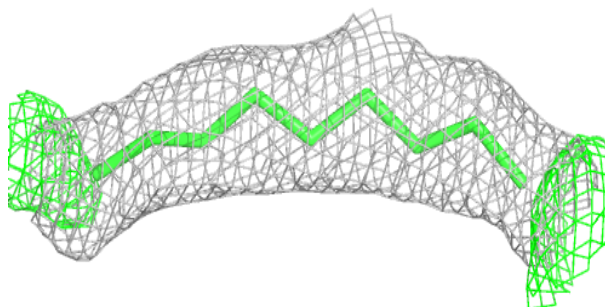
**Electron density around PGV G 4004:**

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

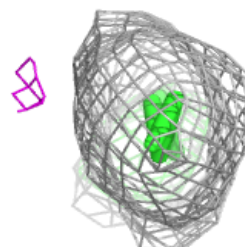
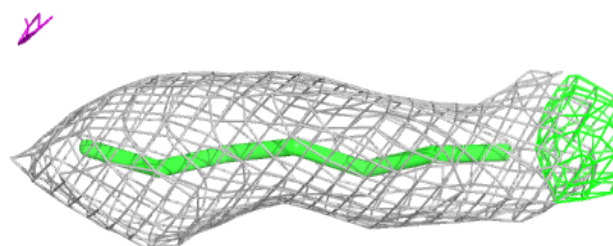
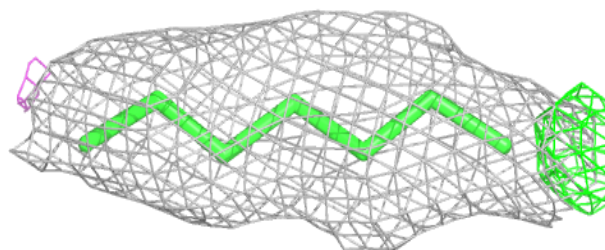


Electron density around PGV F 4002:

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

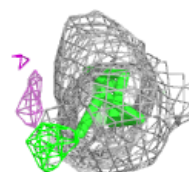
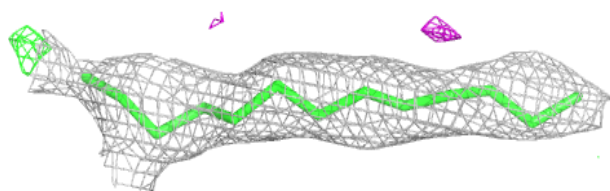
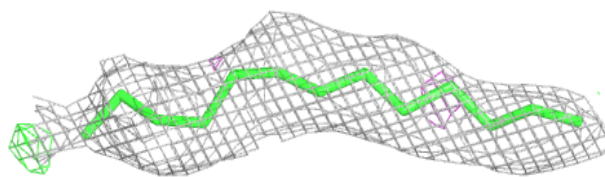
**Electron density around PGV G 4006:**

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



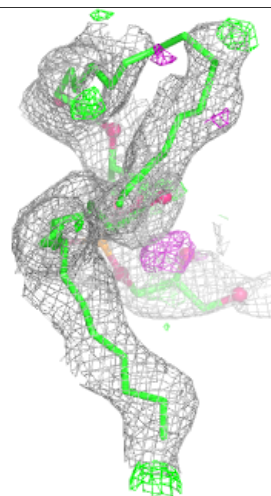
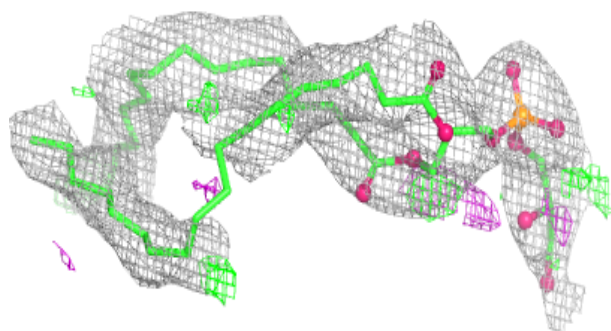
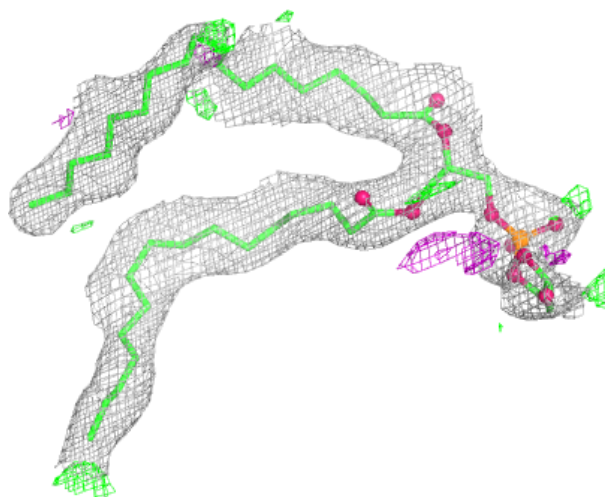
Electron density around PGV F 4010:

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



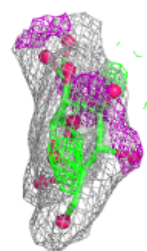
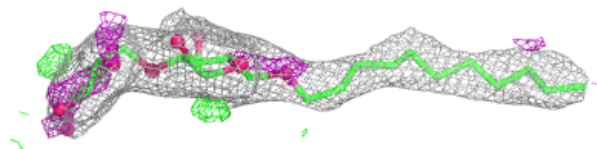
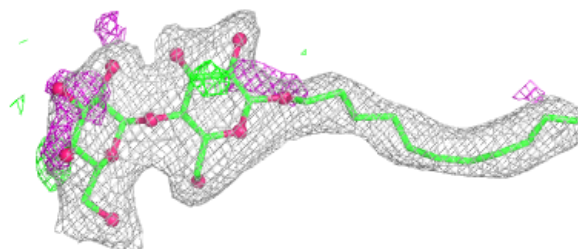
Electron density around PGV F 4001:

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

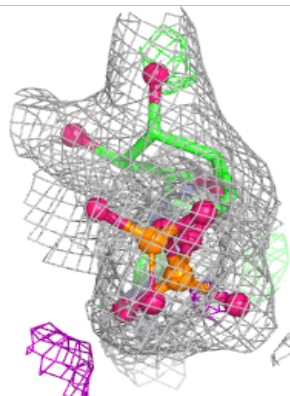
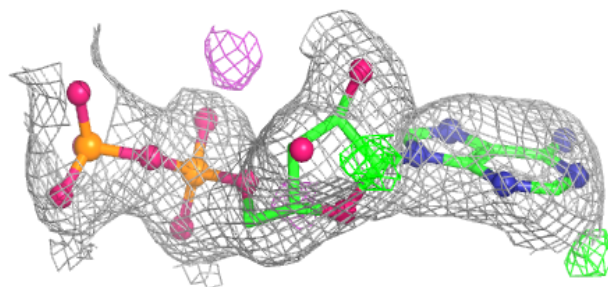
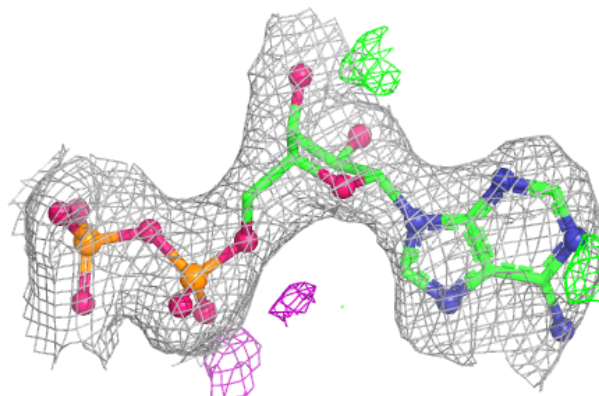


Electron density around UMQ E 5004:

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

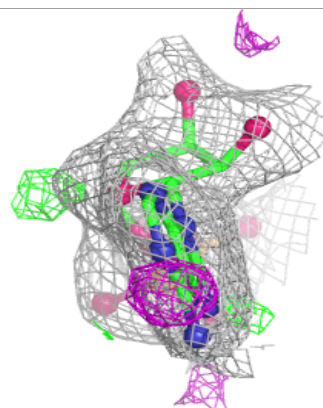
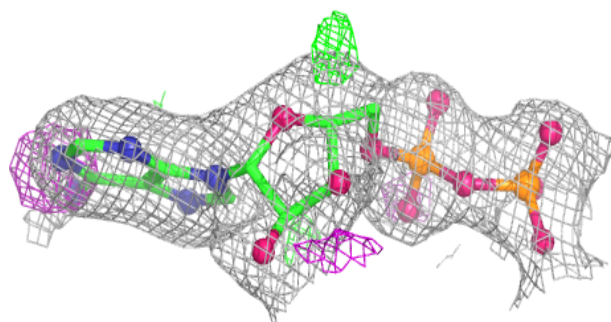
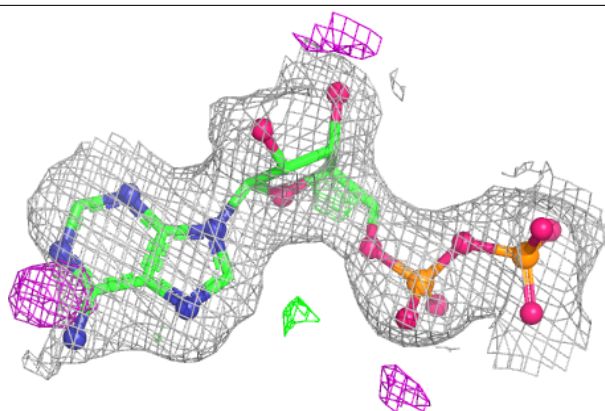
**Electron density around ADP B 2502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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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 [i](#)

There are no such residues in this entry.