



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 04:39 AM BST

PDB ID : 3PUX  
Title : Crystal Structure of an outward-facing MBP-Maltose transporter complex bound to ADP-BeF<sub>3</sub>  
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](mailto: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.

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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

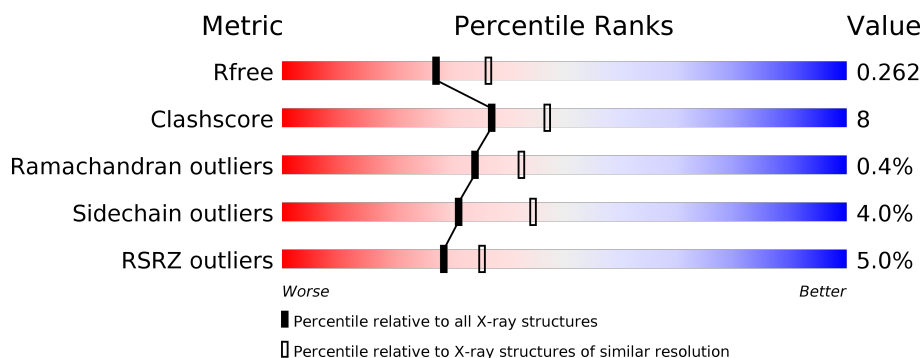
# 1 Overall quality at a glance

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  $\geq 3$ , 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>85%</div> <div>13%</div> <div>..</div> </div> </div>
2	F	514	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>5%</div> </div> </div>
3	G	296	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>..</div> </div> </div>
4	A	381	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>..</div> </div> </div>
4	B	381	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>19%</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 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:

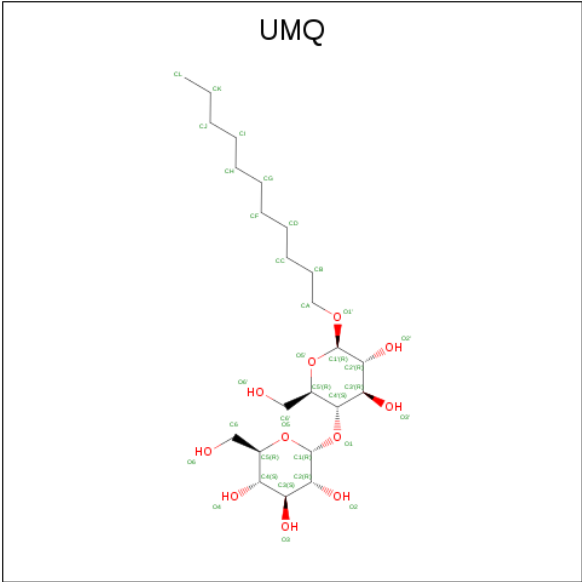
Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	-	expression tag	UNP P68187
A	373	SER	-	expression tag	UNP P68187
A	374	ALA	-	expression tag	UNP P68187
A	375	SER	-	expression tag	UNP P68187
A	376	HIS	-	expression tag	UNP P68187
A	377	HIS	-	expression tag	UNP P68187
A	378	HIS	-	expression tag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



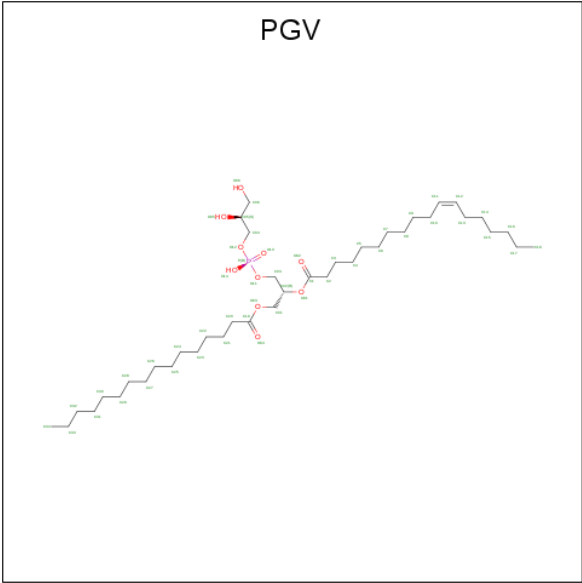
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	C	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 6 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: C<sub>23</sub>H<sub>44</sub>O<sub>11</sub>).



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 (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	F	1	Total	C	O	P	0	0
			51	40	10	1		
7	F	1	Total		C			
			9		9			

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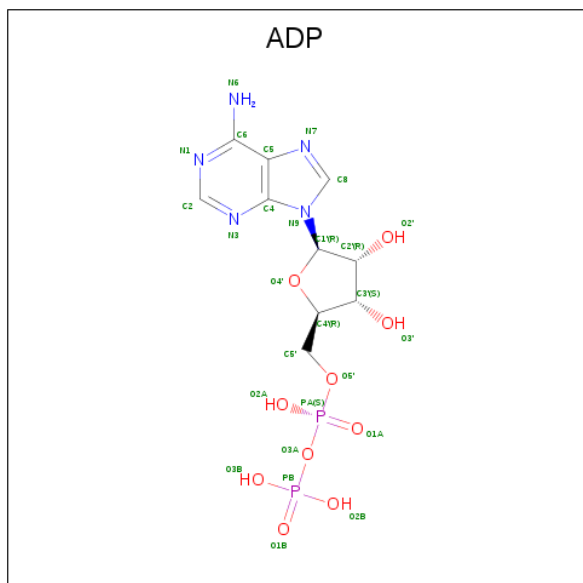
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total C 8 8	0	0
7	F	1	Total C 13 13	0	0
7	G	1	Total C 8 8	0	0
7	G	1	Total C 12 12	0	0
7	G	1	Total C 10 10	0	0
7	G	1	Total C 7 7	0	0
7	G	1	Total C 9 9	0	0
7	G	1	Total C 12 12	0	0

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

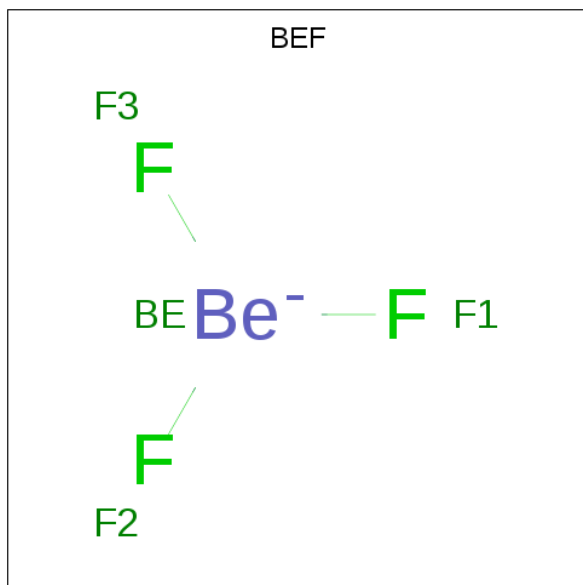
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Mg 1 1	0	0
8	A	1	Total Mg 1 1	0	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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 (three-letter code: BEF) (formula: BeF<sub>3</sub>).



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		

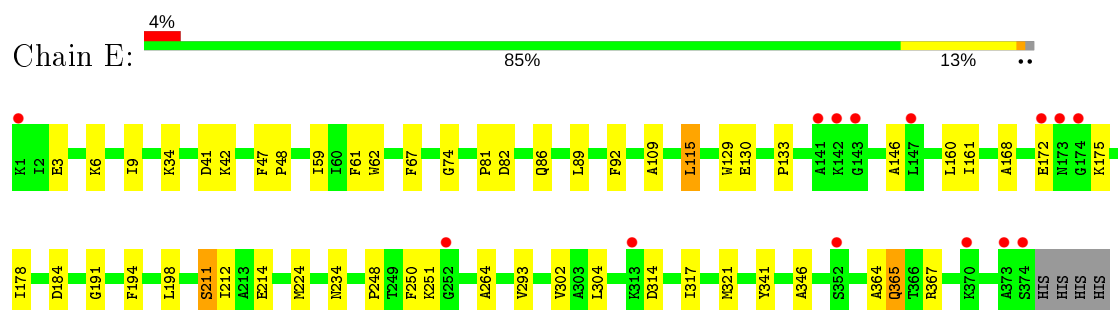
- Molecule 11 is water.

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		

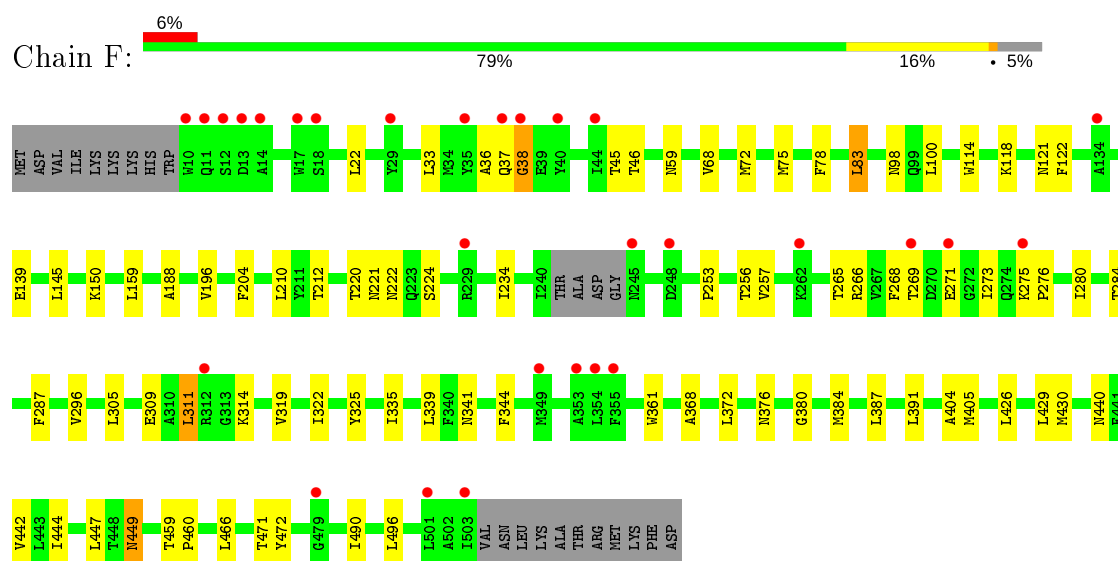
### 3 Residue-property plots [i](#)

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.

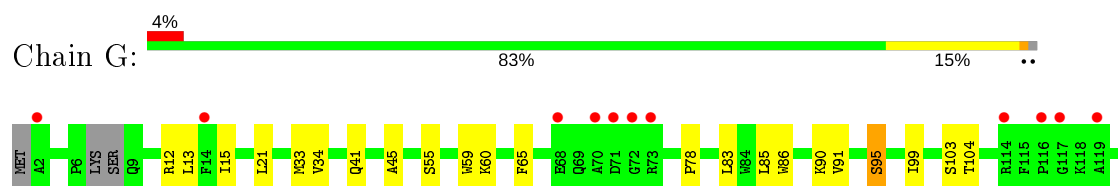
- Molecule 1: Maltose-binding periplasmic protein



- Molecule 2: Maltose transport system permease protein malF



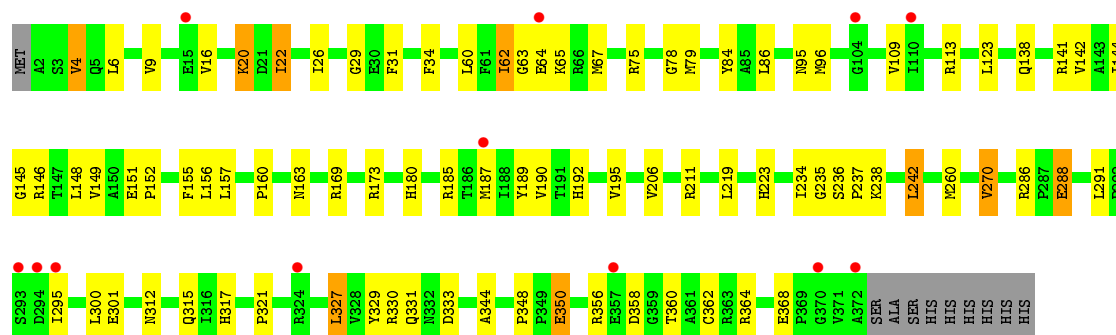
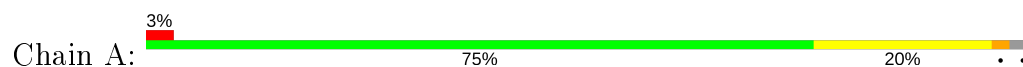
- Molecule 3: Maltose transport system permease protein malG



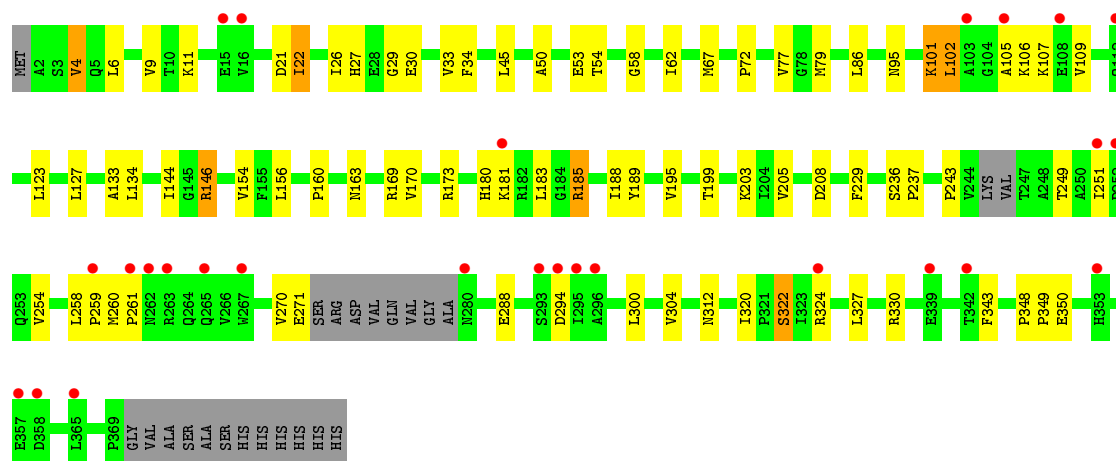
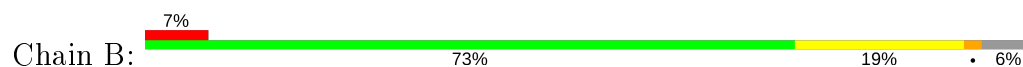




- Molecule 4: Maltose/maltodextrin import ATP-binding protein MalK



- 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, $\alpha$ , $\beta$ , $\gamma$	82.13Å 97.34Å 112.84Å 85.58° 78.98° 72.25°	Depositor
Resolution (Å)	19.81 – 2.30 19.81 – 2.20	Depositor EDS
% Data completeness (in resolution range)	64.8 (19.81-2.30) 57.8 (19.81-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	36.1	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, GLC, BEF, 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	0.57	2/2990 (0.1%)	0.60	0/4059
2	F	0.51	0/3932	0.62	1/5351 (0.0%)
3	G	0.58	0/2334	0.61	1/3188 (0.0%)
4	A	0.54	0/2991	0.68	1/4055 (0.0%)
4	B	0.50	0/2870	0.63	1/3889 (0.0%)
All	All	0.54	2/15117 (0.0%)	0.63	4/20542 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	251	LYS	CD-CE	7.38	1.69	1.51
1	E	250	PHE	CG-CD1	5.08	1.46	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	235	LEU	CA-CB-CG	6.78	130.89	115.30
4	B	146	ARG	NE-CZ-NH2	-6.14	117.23	120.30
2	F	33	LEU	CA-CB-CG	5.52	128.00	115.30
4	A	242	LEU	CA-CB-CG	5.43	127.78	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	2898	32	0
2	F	3831	0	3869	59	0
3	G	2270	0	2364	32	0
4	A	2929	0	3011	75	0
4	B	2816	0	2881	47	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	3	0
All	All	15273	0	15316	237	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 (237) 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: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
1:E:115:LEU:HD21	1:E:224:MET:HE3	1.50	0.91
2:F:471:THR:HG21	2:F:490:ILE:CG2	2.00	0.91
4:A:187[B]:MET:CE	4:A:187[B]:MET:C	2.43	0.87
4:A:286:ARG:HB3	4:A:288:GLU:OE1	1.76	0.84
2:F:405[B]:MET:HA	2:F:405[B]:MET:HE3	1.59	0.83
2:F:339:LEU:HD21	3:G:33[B]:MET:SD	2.19	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:187[B]:MET:HE3	4:A:187[B]:MET:O	1.79	0.82
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
4:A:31:PHE:CE1	4:A:187[B]:MET:HE1	2.16	0.81
3:G:91:VAL:O	3:G:95:SER:HB2	1.79	0.81
4:A:187[B]:MET:HE3	4:A:187[B]:MET:C	2.00	0.81
4:A:235:GLY:HA2	11:A:431:HOH:O	1.81	0.79
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: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
4:A:187[B]:MET:CE	4:A:187[B]:MET:O	2.37	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
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
4:A:67:MET:HE1	4:A:75:ARG:HA	1.73	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
2:F:405[A]:MET:HE1	4:B:77[A]:VAL:HG12	1.78	0.66
4:B:133:ALA:O	11:B:400:HOH:O	2.13	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
4:A:301:GLU:HG3	4:A:344:ALA:HB2	1.79	0.64
1:E:211:SER:HB2	11:E:390:HOH:O	1.98	0.64
1:E:367:ARG:HD2	2:F:460:PRO:HG3	1.82	0.61
4:B:188[B]:ILE:HD12	4:B:188[B]:ILE:C	2.21	0.60
4:A:86:LEU:HA	4:A:146:ARG:NH2	2.17	0.60
4:A:65:LYS:O	4:A:67:MET:HG2	2.02	0.58
2:F:405[B]:MET:HA	2:F:405[B]:MET:HE2	1.84	0.58
4:A:270:VAL:HG13	4:A:362:CYS:HB3	1.86	0.58
1:E:146:ALA:O	1:E:224:MET:HG2	2.03	0.58
4:A:260[B]:MET:SD	4:A:321:PRO:HG2	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:86:TRP:CE2	3:G:90:LYS:HD2	2.39	0.57
4:B:34:PHE:CD1	4:B:188[B]:ILE:HD11	2.40	0.57
4:A:206:VAL:HG21	4:A:234:ILE:HD11	1.87	0.56
2:F:372:LEU:HD21	2:F:444:ILE:HD12	1.87	0.56
4:A:187[B]:MET:HE1	4:A:189:TYR:HB2	1.86	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
4:A:187[B]:MET:SD	4:A:187[B]:MET:C	2.85	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
4:A:60[B]:LEU:HD11	4:A:62[B]:ILE:HG13	1.90	0.54
4:B:183:LEU:HB3	4:B:185:ARG:HG3	1.89	0.54
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
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
4:A:187[B]:MET:CE	4:A:189:TYR:HB2	2.39	0.53
3:G:104:THR:HG21	3:G:208:LEU:HD21	1.91	0.53
2:F:449:ASN:ND2	11:F:547:HOH:O	2.35	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
4:A:60[B]:LEU:CD1	4:A:62[B]:ILE:HG13	2.40	0.52
2:F:391:LEU:HD13	2:F:426:LEU:HD12	1.91	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
2:F:118:LYS:HE3	2:F:139:GLU:CD	2.30	0.51
4:A:260[A]:MET:HE2	4:A:300:LEU:HD22	1.92	0.51
4:A:291:LEU:HD11	4:A:348:PRO:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:170:VAL:HG22	4:B:173:ARG:HH21	1.75	0.51
4:B:27:HIS:O	4:B:30:GLU:HB2	2.11	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:A:151:GLU:O	4:A:185:ARG:NH2	2.42	0.50
4:A:173[B]:ARG:NH1	4:A:195:VAL:CG1	2.74	0.50
4:A:6:LEU:HB3	4:A:9:VAL:HG21	1.94	0.50
3:G:230:VAL:HG22	3:G:246:ALA:HB1	1.93	0.49
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
4:A:173[B]:ARG:NH1	4:A:195:VAL:HG11	2.28	0.49
2:F:471:THR:HG22	2:F:472:TYR:CD1	2.48	0.49
4:A:157:LEU:HD12	4:A:187[B]:MET:SD	2.52	0.49
1:E:184:ASP:HB2	1:E:365:GLN:CD	2.34	0.48
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
3:G:166:TYR:OH	3:G:229:GLU:CG	2.60	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:85:LEU:HD22	3:G:269:MET:HE3	1.96	0.48
3:G:129:GLN:HB3	3:G:130:MET:CE	2.43	0.48
4:A:236:SER:HA	4:A:237:PRO:C	2.34	0.48
4:A:260[A]:MET:N	4:A:260[A]:MET:SD	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
4:A:350:GLU:H	4:A:350:GLU:HG3	1.53	0.47
2:F:325:TYR:O	11:F:525:HOH:O	2.20	0.47
1:E:41:ASP:HB2	11:G:305:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:245:LEU:HG	3:G:249:MET:HE2	1.96	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
1:E:92:PHE:HZ	1:E:321:MET:HE1	1.79	0.46
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
2:F:75:MET:HE1	11:G:330:HOH:O	2.15	0.46
3:G:214:ILE:HA	3:G:214:ILE:HD12	1.77	0.46
4:A:145:GLY:O	4:A:149:VAL:HG23	2.16	0.46
4:A:144:ILE:HD11	4:A:160:PRO:O	2.16	0.46
3:G:60:LYS:HB3	3:G:65:PHE:HB2	1.97	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
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
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
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
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:305:LEU:O	2:F:311:LEU:HD12	2.17	0.44
2:F:68:VAL:HG12	2:F:72:MET:HG3	1.98	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
4:B:34:PHE:HD2	4:B:205:VAL:HB	1.83	0.44
4:A:96:MET:HE3	4:A:145:GLY:HA3	1.99	0.44
2:F:83:LEU:C	2:F:83:LEU:HD23	2.38	0.44
4:B:50:ALA:HB2	4:B:79:MET:HE3	2.00	0.43
1:E:341:TYR:CE2	2:F:460:PRO:HB2	2.53	0.43
2:F:309:GLU:HA	2:F:314:LYS:HZ3	1.83	0.43
2:F:391:LEU:HD13	2:F:426:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2501:ADP:H1'	11:B:384:HOH:O	2.17	0.43
4:B:259:PRO:HD2	4:B:260:MET:HE2	2.00	0.43
4:A:173[B]:ARG:NH2	11:A:428:HOH:O	2.51	0.43
4:A:260[A]:MET:CE	4:A:300:LEU:HD22	2.48	0.43
2:F:405[B]:MET:CE	4:B:77[B]:VAL:HG23	2.48	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: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
4:A:29:GLY:O	4:A:180:HIS:NE2	2.51	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
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
2:F:380:GLY:HA3	5:C:2:GLC:H61	2.01	0.43
1:E:129:TRP:CD2	1:E:160:LEU:HD13	2.52	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
4:A:20:LYS:HB2	4:A:211:ARG:HD2	2.00	0.42
1:E:3:GLU:HB3	1:E:6:LYS:HE2	2.00	0.42
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
4:A:95:ASN:O	4:A:146:ARG:HG3	2.20	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
4:B:146:ARG:HD2	11:B:396:HOH:O	2.19	0.42
4:A:187[B]:MET:O	4:A:187[B]:MET:HE2	2.20	0.42
4:B:62:ILE:HB	4:B:67:MET:HG3	2.02	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
4:B:102:LEU:HA	4:B:102:LEU:HD12	1.91	0.42
4:B:236:SER:HA	4:B:237:PRO:C	2.41	0.42
4:A:317:HIS:HA	4:A:327:LEU:O	2.20	0.41
3:G:180:TYR:CE2	3:G:211:SER:HA	2.54	0.41
4:A:34:PHE:HB2	4:A:190:VAL:HG22	2.02	0.41
2:F:404:ALA:HB1	4:B:72:PRO:HB2	2.01	0.41
1:E:314:ASP:HB3	1:E:317:ILE:HD12	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
4:B:106:LYS:HB2	4:B:109:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:391:LEU:CD1	2:F:426:LEU:HD12	2.50	0.41
1:E:82:ASP:O	1:E:86:GLN:HG3	2.21	0.41
4:A:315:GLN:HG2	4:A:330:ARG:HG2	2.01	0.41
4:A:173[B]:ARG:NH1	4:A:195:VAL:HG12	2.36	0.41
1:E:61:PHE:CE2	1:E:264:ALA:HB2	2.55	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:214:GLU:OE1	1:E:234:ASN:ND2	2.50	0.41
4:A:187[B]:MET:HE2	4:A:187[B]:MET:HB3	1.38	0.40
4:B:29:GLY:O	4:B:180:HIS:CE1	2.74	0.40
1:E:9:ILE:HG12	1:E:59:ILE:HB	2.02	0.40
4:B:86:LEU:HA	4:B:146:ARG:NH2	2.36	0.40
1:E:129:TRP:CE2	1:E:160:LEU:HD13	2.56	0.40
1:E:81:PRO:HA	11:E:418:HOH:O	2.20	0.40
4:A:6:LEU:HB3	4:A:9:VAL:HG23	2.03	0.40
6:E:5004:UMQ:C6	11:F:535:HOH:O	2.70	0.40
1:E:89:LEU:HD22	1:E:304:LEU:HA	2.03	0.40
3:G:99:ILE:O	3:G:103:SER:OG	2.34	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%)	29	35
2	F	488/514 (95%)	468 (96%)	18 (4%)	2 (0%)	34	42
3	G	291/296 (98%)	286 (98%)	4 (1%)	1 (0%)	41	50
4	A	377/381 (99%)	360 (96%)	16 (4%)	1 (0%)	41	50
4	B	356/381 (93%)	335 (94%)	19 (5%)	2 (1%)	25	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1887/1950 (97%)	1812 (96%)	67 (4%)	8 (0%)	34	42

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%)	292 (97%)	8 (3%)	44	61
2	F	404/424 (95%)	385 (95%)	19 (5%)	26	37
3	G	236/237 (100%)	232 (98%)	4 (2%)	60	76
4	A	322/323 (100%)	308 (96%)	14 (4%)	29	40
4	B	309/323 (96%)	290 (94%)	19 (6%)	18	25
All	All	1571/1610 (98%)	1507 (96%)	64 (4%)	31	43

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	115	LEU
1	E	175	LYS
1	E	178	ILE
1	E	211	SER
1	E	212	ILE
1	E	293[A]	VAL

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Mol	Chain	Res	Type
1	E	293[B]	VAL
1	E	365	GLN
2	F	22	LEU
2	F	45	THR
2	F	46	THR
2	F	59	ASN
2	F	83	LEU
2	F	145	LEU
2	F	150	LYS
2	F	196	VAL
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	440	ASN
2	F	449	ASN
2	F	496	LEU
3	G	13	LEU
3	G	21	LEU
3	G	95	SER
3	G	212	VAL
4	A	4	VAL
4	A	20	LYS
4	A	22	ILE
4	A	62[A]	ILE
4	A	62[B]	ILE
4	A	84	TYR
4	A	219	LEU
4	A	242	LEU
4	A	270	VAL
4	A	288	GLU
4	A	295	ILE
4	A	327	LEU
4	A	333	ASP
4	A	350	GLU
4	B	4	VAL
4	B	21	ASP
4	B	22	ILE

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Mol	Chain	Res	Type
4	B	45	LEU
4	B	53	GLU
4	B	101	LYS
4	B	102	LEU
4	B	123	LEU
4	B	127	LEU
4	B	181	LYS
4	B	185	ARG
4	B	203	LYS
4	B	251	ILE
4	B	271	GLU
4	B	294	ASP
4	B	300	LEU
4	B	322	SER
4	B	324	ARG
4	B	350	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	282	ASN
2	F	59	ASN
2	F	437	ASN
2	F	440	ASN
4	A	5	GLN
4	A	317	HIS
4	B	180	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	GLC	C	1	5	12,12,12	0.58	0	17,17,17	1.75	3 (17%)
5	GLC	C	2	5	11,11,12	0.40	0	15,15,17	0.55	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
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	4.05	121.31	113.66
5	C	1	GLC	C6-C5-C4	-3.51	104.79	113.00
5	C	1	GLC	O5-C5-C4	2.79	114.76	109.69

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

## 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
7	PGV	F	4010	-	12,12,50	1.15	1 (8%)	10,11,56	0.68	0
7	PGV	G	4005	-	9,9,50	1.18	1 (11%)	8,8,56	1.09	1 (12%)
7	PGV	F	4002	-	8,8,50	0.29	0	7,7,56	0.68	0
7	PGV	G	4009	-	11,11,50	1.31	1 (9%)	10,10,56	0.72	0
9	ADP	B	2502	8,10	24,29,29	0.86	0	29,45,45	1.53	4 (13%)
7	PGV	G	4006	-	6,6,50	1.41	1 (16%)	5,5,56	1.38	1 (20%)
7	PGV	F	4001	-	50,50,50	1.15	3 (6%)	53,56,56	1.11	3 (5%)
7	PGV	G	4003	-	7,7,50	0.37	0	6,6,56	0.64	0
7	PGV	G	4007	-	8,8,50	1.15	1 (12%)	7,7,56	1.29	2 (28%)
10	BEF	A	3001	9	0,3,3	0.00	-	-	-	-
6	UMQ	E	5004	-	35,35,35	0.60	0	46,46,46	1.25	5 (10%)
9	ADP	A	2501	8,10	24,29,29	0.85	0	29,45,45	1.55	3 (10%)
7	PGV	G	4004	-	11,11,50	1.06	1 (9%)	10,10,56	0.94	1 (10%)
10	BEF	B	3002	9	0,3,3	0.00	-	-	-	-
7	PGV	F	4008	-	7,7,50	0.42	0	6,6,56	0.45	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
7	PGV	F	4010	-	-	6/10/10/55	-
7	PGV	G	4005	-	-	3/7/7/55	-
7	PGV	F	4002	-	-	2/6/6/55	-
7	PGV	G	4009	-	-	4/9/9/55	-
9	ADP	B	2502	8,10	-	3/12/32/32	0/3/3/3
7	PGV	G	4006	-	-	1/4/4/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PGV	F	4001	-	-	29/55/55/55	-
7	PGV	G	4003	-	-	0/5/5/55	-
7	PGV	G	4007	-	-	3/6/6/55	-
6	UMQ	E	5004	-	-	8/20/60/60	0/2/2/2
9	ADP	A	2501	8,10	-	0/12/32/32	0/3/3/3
7	PGV	G	4004	-	-	4/9/9/55	-
7	PGV	F	4008	-	-	2/5/5/55	-

All (9) 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	4.01	1.55	1.31
7	F	4001	PGV	C12-C11	3.77	1.53	1.31
7	F	4010	PGV	C12-C11	3.74	1.53	1.31
7	G	4005	PGV	C11-C12	3.22	1.53	1.29
7	G	4006	PGV	C12-C11	3.19	1.53	1.29
7	G	4004	PGV	C11-C12	3.17	1.53	1.29
7	G	4007	PGV	C11-C12	3.04	1.52	1.29

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2501	ADP	N3-C2-N1	-5.89	119.47	128.68
9	B	2502	ADP	N3-C2-N1	-5.30	120.39	128.68
7	F	4001	PGV	O01-C1-C2	4.63	121.49	111.50
7	F	4001	PGV	O03-C19-C20	3.50	122.90	111.91
9	B	2502	ADP	O4'-C1'-C2'	-3.18	102.28	106.93
9	B	2502	ADP	O3B-PB-O2B	3.01	119.15	107.64
6	E	5004	UMQ	C1-O5-C5	2.97	119.51	113.69
6	E	5004	UMQ	CA-O1'-C1'	2.83	118.54	113.84
7	G	4006	PGV	C13-C12-C11	-2.69	109.65	131.07
9	A	2501	ADP	PA-O3A-PB	-2.60	123.92	132.83
7	G	4005	PGV	C10-C11-C12	-2.50	111.19	131.07
7	G	4007	PGV	C10-C11-C12	-2.47	111.41	131.07
9	A	2501	ADP	C3'-C2'-C1'	2.40	104.59	100.98
6	E	5004	UMQ	C1'-O5'-C5'	-2.34	109.09	113.69
6	E	5004	UMQ	O2'-C2'-C1'	2.33	115.70	110.05
7	G	4004	PGV	C10-C11-C12	-2.30	112.79	131.07
7	F	4001	PGV	O03-C19-O04	-2.20	118.04	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	5004	UMQ	O1'-C1'-C2'	2.17	111.69	108.30
7	G	4007	PGV	C13-C12-C11	-2.14	108.66	126.37
9	B	2502	ADP	PA-O3A-PB	-2.05	125.79	132.83

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	4010	PGV	C10-C11-C12-C13
7	G	4005	PGV	C10-C11-C12-C13
9	B	2502	ADP	PA-O3A-PB-O2B
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	4007	PGV	C10-C11-C12-C13
7	G	4004	PGV	C10-C11-C12-C13
7	F	4001	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	G	4009	PGV	C5-C6-C7-C8
7	F	4002	PGV	C6-C7-C8-C9
7	G	4007	PGV	C6-C7-C8-C9
6	E	5004	UMQ	CC-CD-CF-CG
7	F	4010	PGV	C3-C4-C5-C6
7	F	4001	PGV	C11-C10-C9-C8
7	F	4001	PGV	C30-C31-C32-C33
7	F	4010	PGV	C11-C10-C9-C8
7	G	4009	PGV	C11-C10-C9-C8
7	G	4004	PGV	C6-C7-C8-C9
7	F	4001	PGV	C05-C04-O12-P
7	F	4001	PGV	C25-C26-C27-C28
7	F	4001	PGV	C20-C19-O03-C01
7	G	4004	PGV	C4-C5-C6-C7
7	F	4001	PGV	O03-C01-C02-C03

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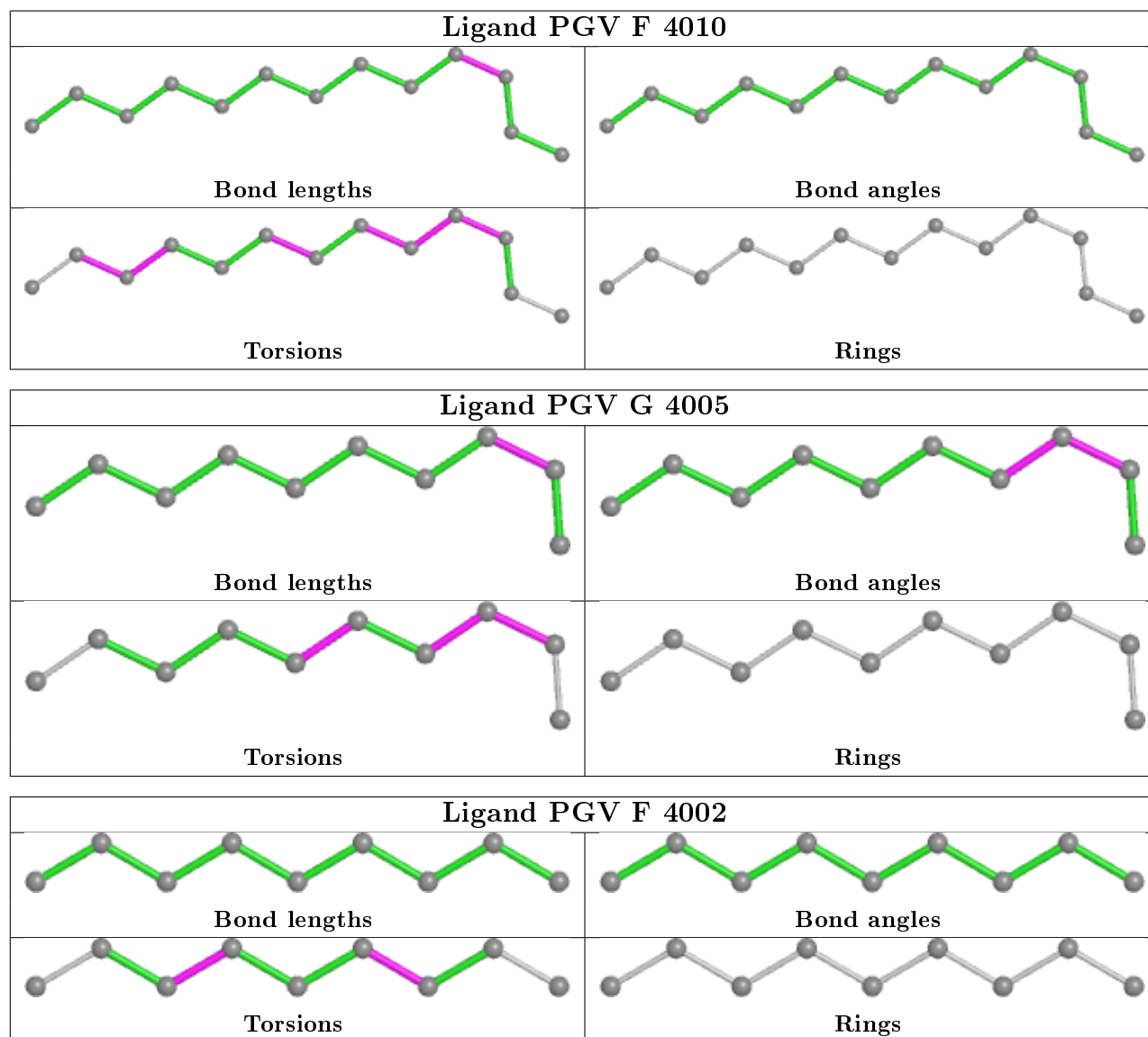
Mol	Chain	Res	Type	Atoms
7	F	4001	PGV	C24-C25-C26-C27
7	G	4004	PGV	C2-C3-C4-C5
7	G	4009	PGV	C4-C5-C6-C7
7	F	4001	PGV	O03-C01-C02-O01
6	E	5004	UMQ	O5'-C1'-O1'-CA
7	G	4007	PGV	C5-C6-C7-C8
7	F	4002	PGV	C3-C4-C5-C6
7	F	4001	PGV	O04-C19-O03-C01
7	F	4001	PGV	C23-C24-C25-C26
9	B	2502	ADP	PA-O3A-PB-O3B
6	E	5004	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	F	4001	PGV	C03-O11-P-O12
6	E	5004	UMQ	C2'-C1'-O1'-CA
6	E	5004	UMQ	CF-CG-CH-CI
7	G	4006	PGV	C11-C12-C13-C14
7	F	4001	PGV	C6-C7-C8-C9
6	E	5004	UMQ	CG-CH-CI-CJ
7	F	4001	PGV	C22-C23-C24-C25
7	F	4001	PGV	C21-C22-C23-C24
7	G	4005	PGV	C9-C10-C11-C12
7	F	4010	PGV	C6-C7-C8-C9
7	F	4001	PGV	O05-C05-C06-O06
7	F	4010	PGV	C9-C10-C11-C12
9	B	2502	ADP	PA-O3A-PB-O1B
7	F	4001	PGV	O03-C19-C20-C21
7	F	4001	PGV	O04-C19-C20-C21

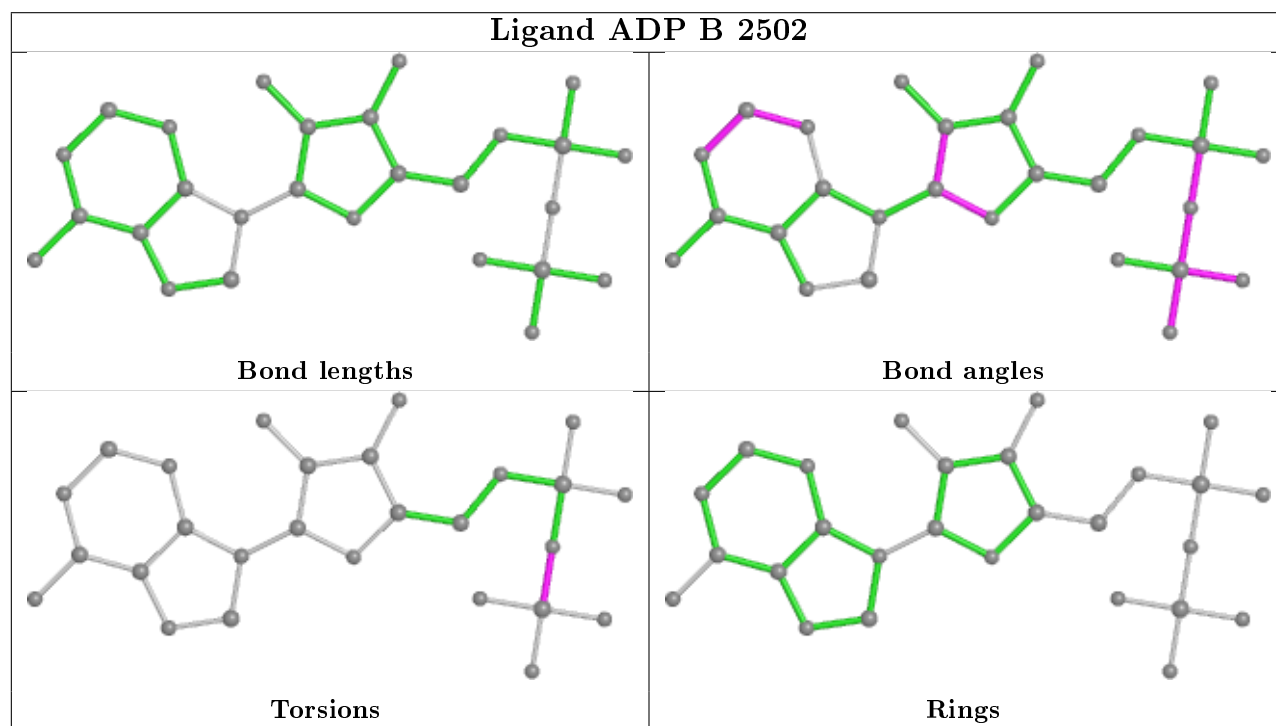
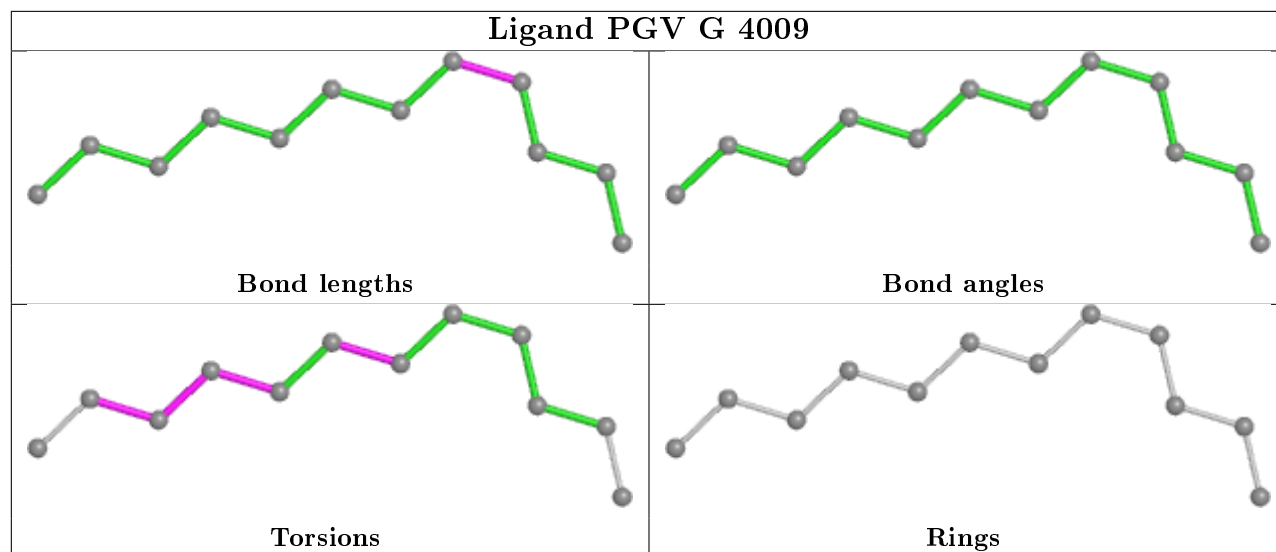
There are no ring outliers.

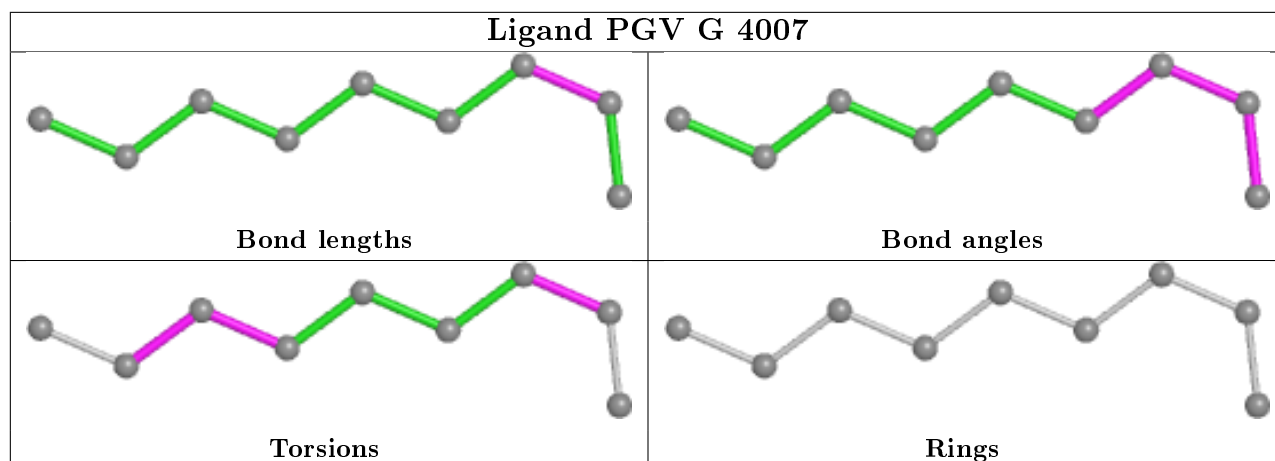
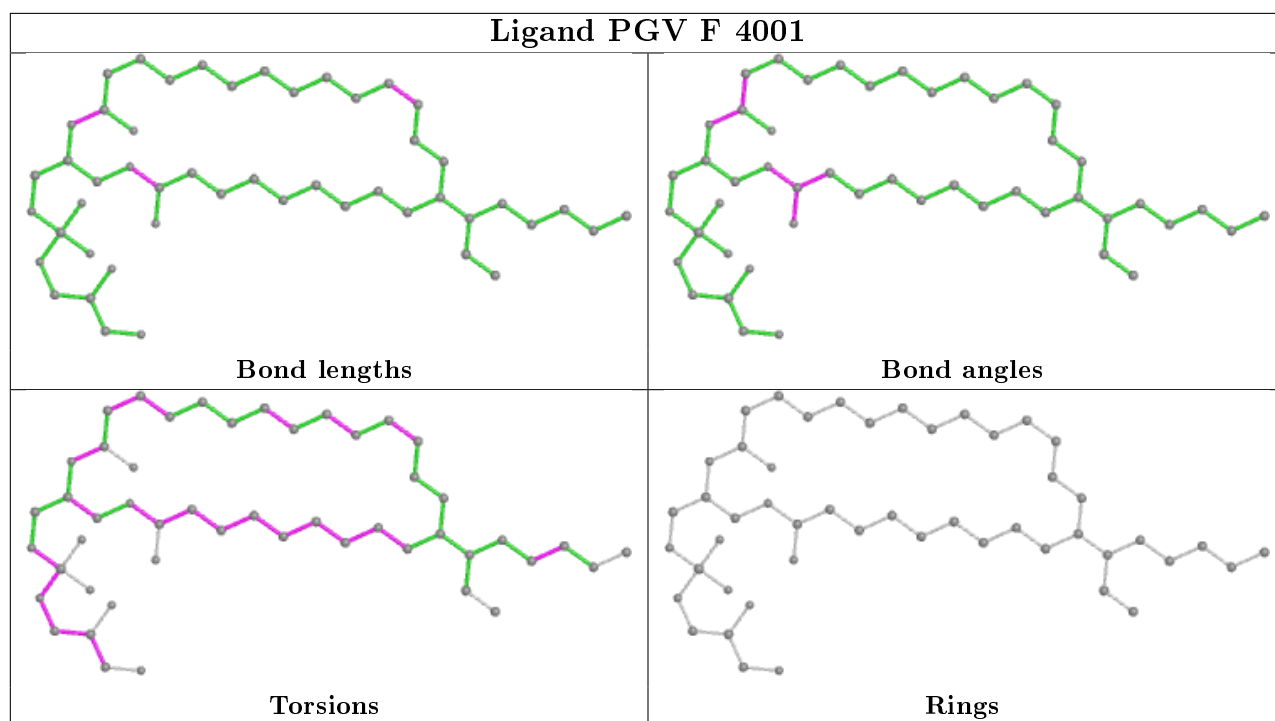
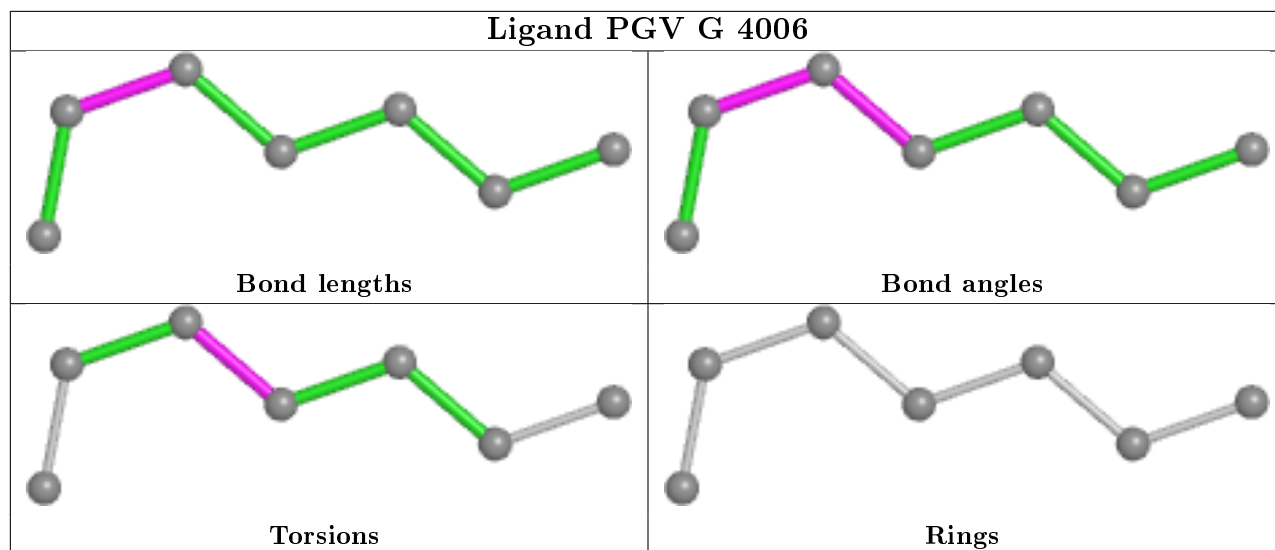
5 monomers are involved in 7 short contacts:

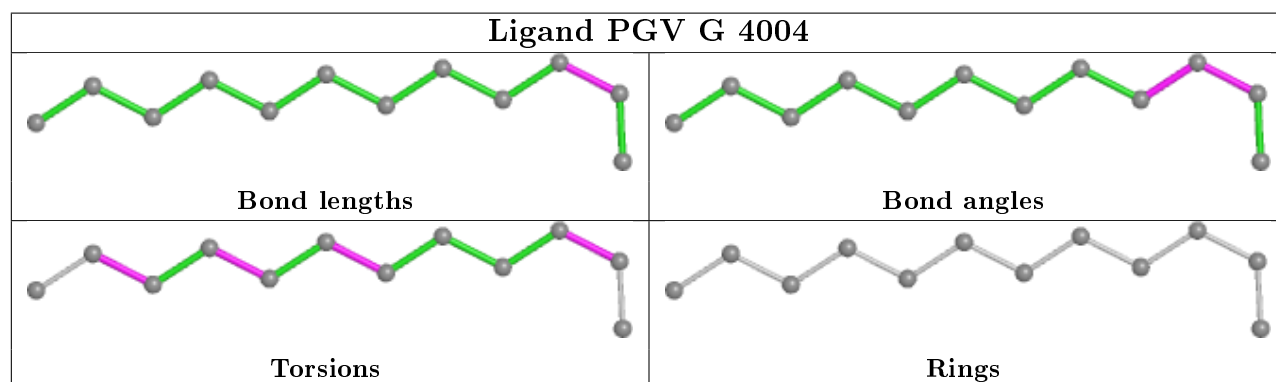
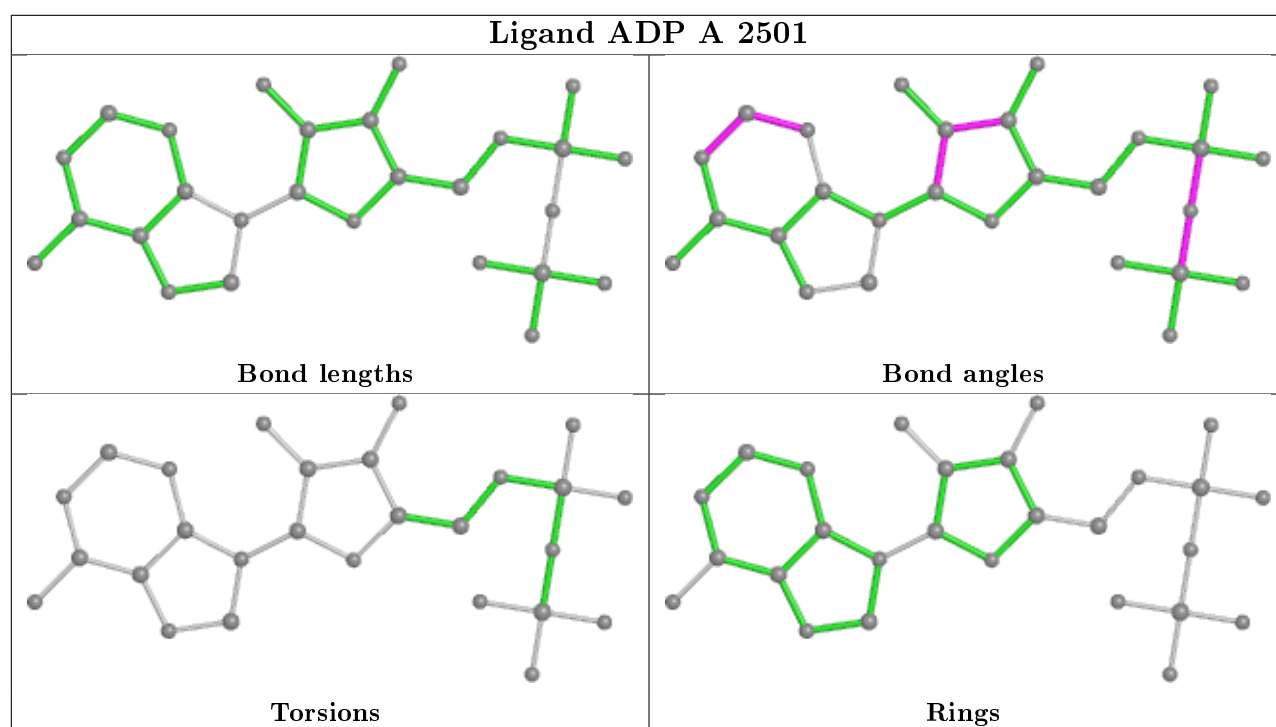
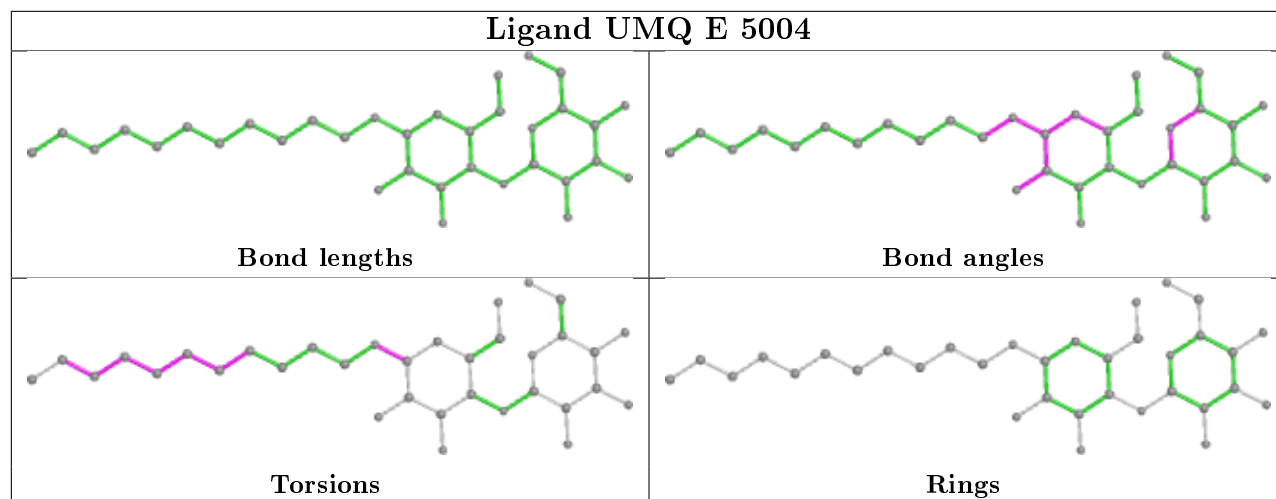
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	4006	PGV	1	0
7	G	4003	PGV	2	0
6	E	5004	UMQ	2	0
9	A	2501	ADP	2	0
7	G	4004	PGV	1	0

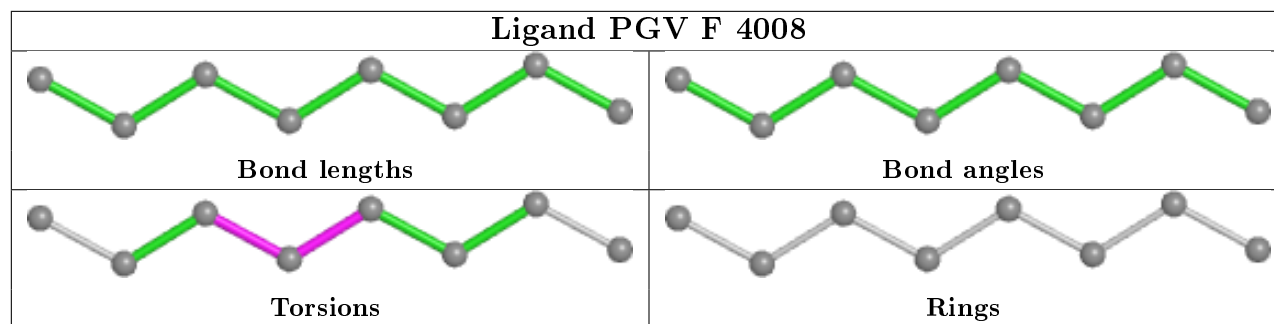
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	E	374/378 (98%)	0.05	14 (3%) 41 48	21, 50, 82, 94	1 (0%)
2	F	490/514 (95%)	0.24	29 (5%) 22 28	21, 52, 98, 119	0
3	G	293/296 (98%)	-0.11	13 (4%) 34 41	15, 33, 74, 94	0
4	A	371/381 (97%)	0.01	12 (3%) 47 54	17, 44, 69, 80	1 (0%)
4	B	358/381 (93%)	0.22	27 (7%) 14 19	16, 55, 105, 122	0
All	All	1886/1950 (96%)	0.10	95 (5%) 28 35	15, 47, 88, 122	2 (0%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	267	TRP	10.8
2	F	37	GLN	8.1
4	B	16	VAL	7.6
2	F	38	GLY	6.8
3	G	70	ALA	6.4
4	B	295	ILE	6.0
4	A	295	ILE	5.5
4	B	251	ILE	5.5
4	A	104	GLY	5.4
2	F	354	LEU	5.2
2	F	245	ASN	5.2
4	A	372	ALA	5.1
2	F	355	PHE	4.8
2	F	29	TYR	4.5
4	B	259	PRO	4.5
3	G	71	ASP	4.4
4	B	15	GLU	4.3
1	E	172	GLU	4.2
2	F	18	SER	4.2
2	F	271	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
4	B	261	PRO	4.0
1	E	374	SER	4.0
3	G	114	ARG	3.9
3	G	116	PRO	3.8
4	B	357	GLU	3.8
4	A	324	ARG	3.6
2	F	10	TRP	3.6
4	B	294	ASP	3.6
2	F	349	MET	3.5
2	F	503	ILE	3.4
4	A	110	ILE	3.4
2	F	479	GLY	3.3
3	G	133	ALA	3.3
4	B	105	ALA	3.3
2	F	312	ARG	3.2
4	B	324	ARG	3.1
3	G	2	ALA	3.1
4	B	262	ASN	3.0
2	F	17	TRP	3.0
3	G	117	GLY	3.0
1	E	252	GLY	3.0
1	E	142	LYS	2.9
4	B	296	ALA	2.9
4	B	339	GLU	2.9
1	E	370	LYS	2.8
2	F	275	LYS	2.8
3	G	134	VAL	2.8
3	G	14	PHE	2.7
4	B	265	GLN	2.7
4	B	181	LYS	2.7
2	F	262	LYS	2.7
4	A	294	ASP	2.7
1	E	174	GLY	2.7
3	G	72	GLY	2.7
2	F	12	SER	2.7
1	E	147	LEU	2.7
2	F	269	THR	2.6
2	F	40	TYR	2.6
2	F	13	ASP	2.6
4	B	342	THR	2.6
1	E	1	LYS	2.6
4	A	64	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	44	ILE	2.6
4	B	280	ASN	2.5
4	B	252	ASP	2.5
4	B	353	HIS	2.5
1	E	173	ASN	2.5
2	F	501	LEU	2.5
4	A	187[A]	MET	2.5
4	B	263	ARG	2.5
4	B	103	ALA	2.4
4	A	357	GLU	2.4
1	E	352	SER	2.4
2	F	229	ARG	2.3
3	G	73	ARG	2.3
2	F	353	ALA	2.3
4	A	293	SER	2.3
1	E	373	ALA	2.3
4	B	293	SER	2.3
4	B	108	GLU	2.2
1	E	141	ALA	2.2
4	B	358	ASP	2.2
4	A	370	GLY	2.2
4	A	15	GLU	2.1
2	F	134	ALA	2.1
1	E	313	LYS	2.1
2	F	35	TYR	2.1
2	F	248	ASP	2.1
1	E	143	GLY	2.1
3	G	68	GLU	2.1
4	B	112	GLN	2.0
4	B	365	LEU	2.0
2	F	14	ALA	2.0
3	G	119	ALA	2.0
2	F	11	GLN	2.0

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

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

## 6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	GLC	C	1	12/12	0.95	0.11	30,33,35,35	0
5	GLC	C	2	11/12	0.97	0.08	30,31,32,32	0

## 6.4 Ligands

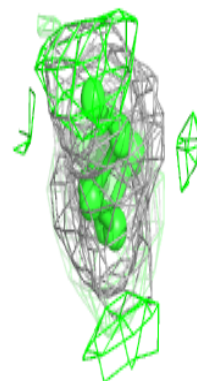
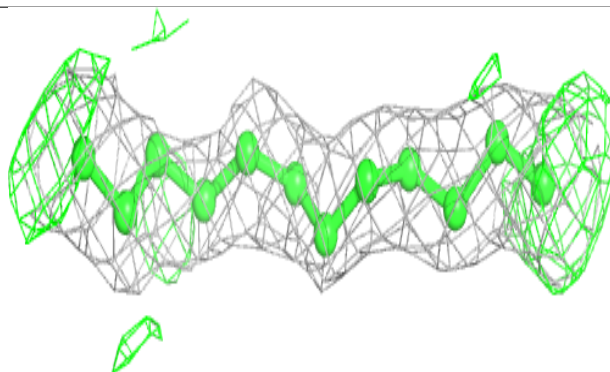
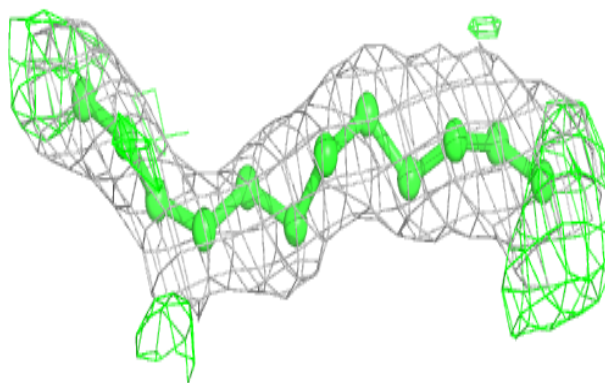
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	PGV	G	4009	12/51	0.69	0.20	48,49,51,52	0
7	PGV	G	4003	8/51	0.73	0.25	50,54,56,58	0
7	PGV	F	4008	8/51	0.83	0.16	47,49,50,50	0
7	PGV	G	4004	12/51	0.84	0.16	43,48,58,60	0
7	PGV	F	4001	51/51	0.84	0.20	50,57,69,71	0
7	PGV	F	4010	13/51	0.85	0.24	66,68,70,70	0
7	PGV	G	4007	9/51	0.87	0.23	46,50,55,56	0
7	PGV	G	4005	10/51	0.88	0.16	52,56,57,57	0
7	PGV	G	4006	7/51	0.90	0.11	43,45,49,51	0
7	PGV	F	4002	9/51	0.90	0.13	31,33,36,39	0
6	UMQ	E	5004	34/34	0.93	0.18	23,28,33,34	0
10	BEF	A	3001	4/4	0.97	0.08	17,18,19,20	0
9	ADP	B	2502	27/27	0.97	0.11	24,40,53,54	0
8	MG	A	1501	1/1	0.98	0.09	18,18,18,18	0
9	ADP	A	2501	27/27	0.98	0.09	17,27,38,39	0
10	BEF	B	3002	4/4	0.99	0.09	21,21,22,26	0
8	MG	B	1502	1/1	1.00	0.09	15,15,15,15	0

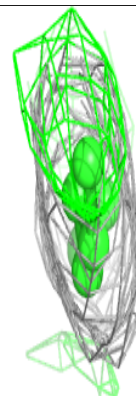
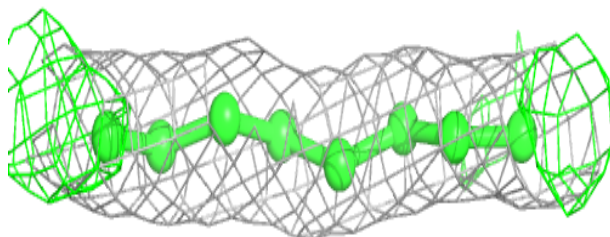
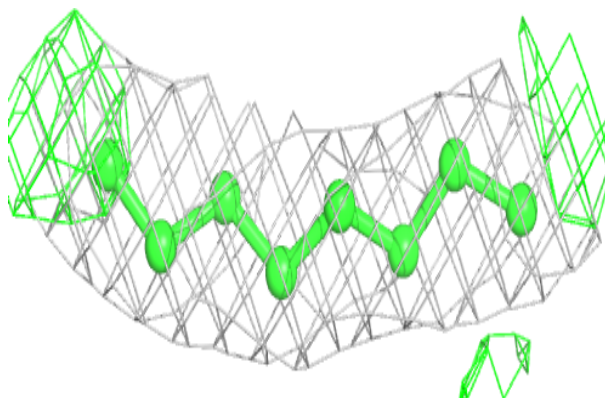
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

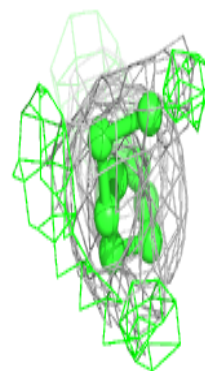
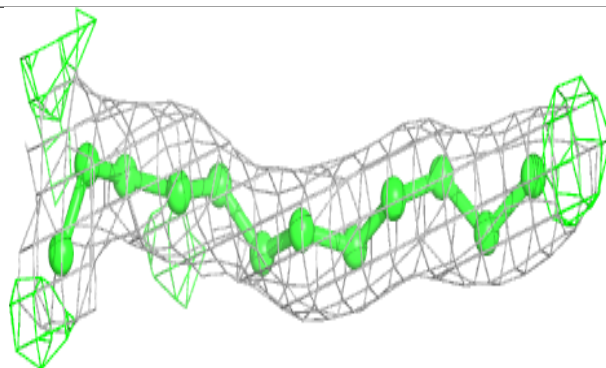
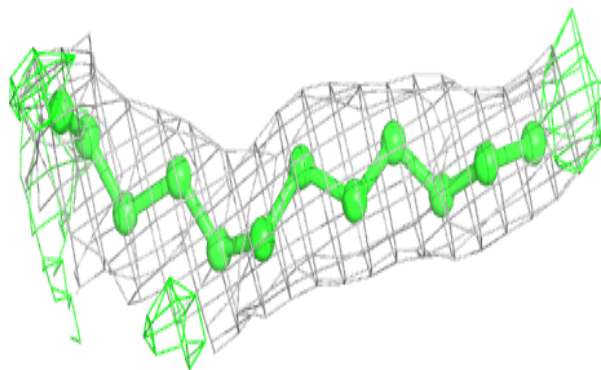
**Electron density around PGV F 4008:**

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



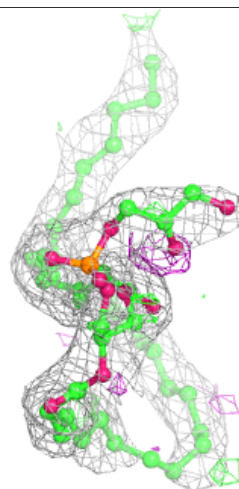
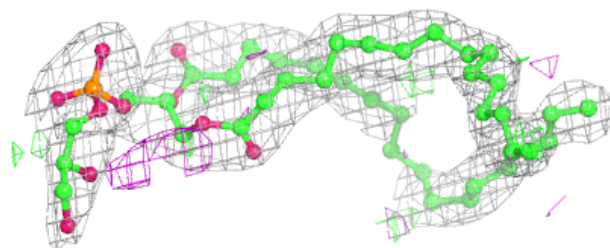
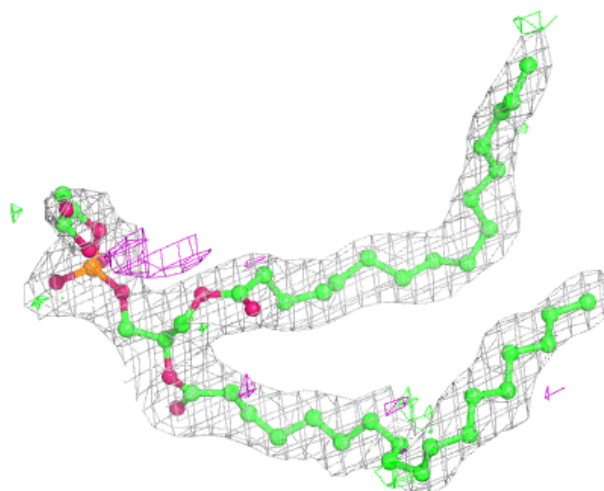
**Electron density around PGV G 4004:**

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



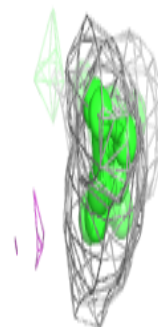
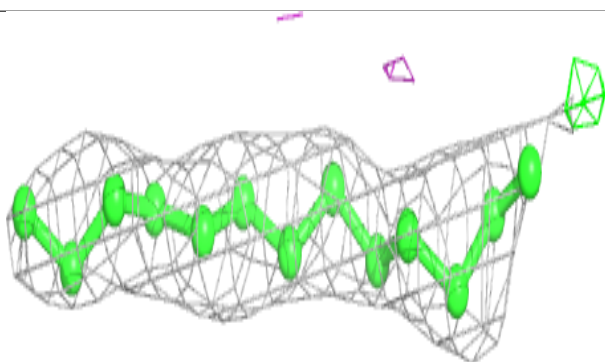
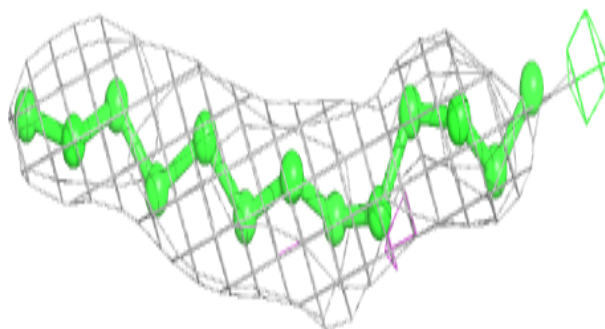
**Electron density around PGV F 4001:**

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

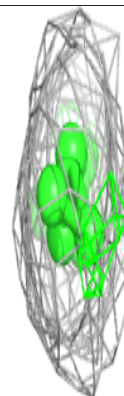
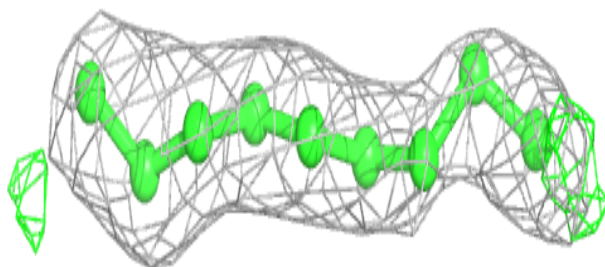
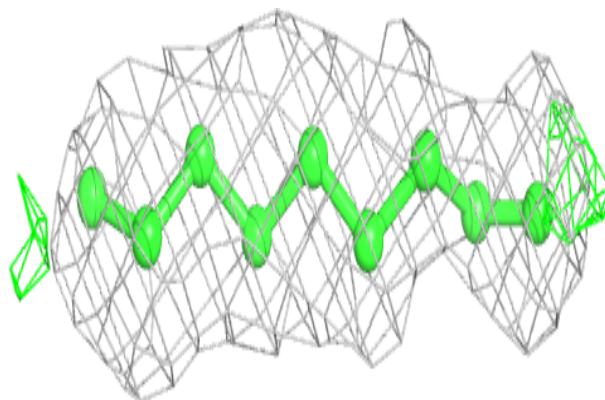


**Electron density around PGV F 4010:**

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

**Electron density around PGV G 4007:**

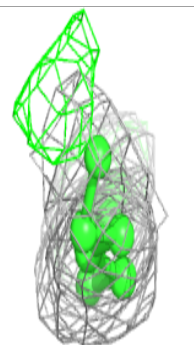
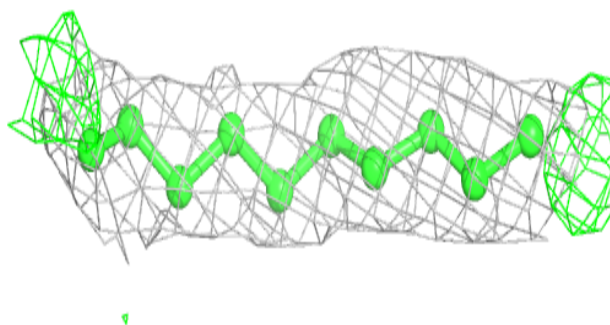
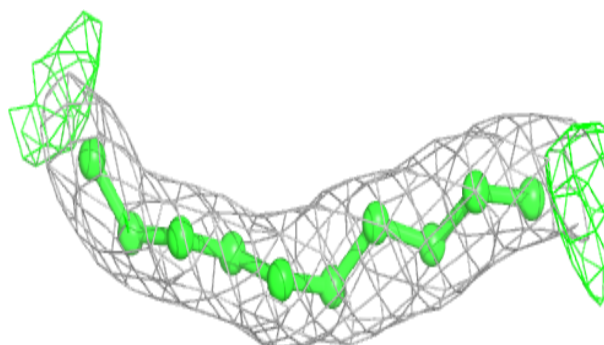
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



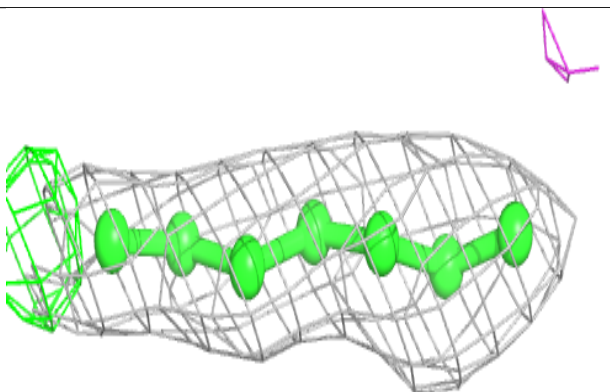
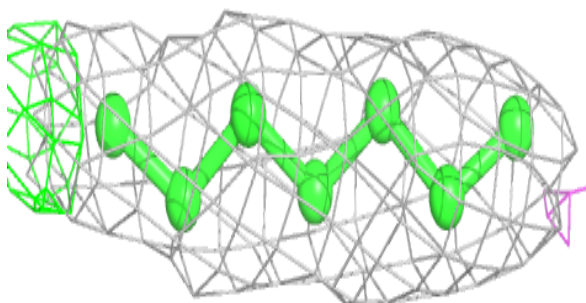


**Electron density around PGV G 4005:**

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

**Electron density around PGV G 4006:**

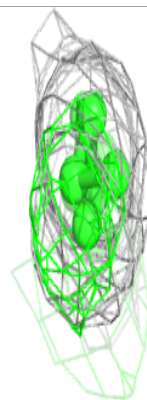
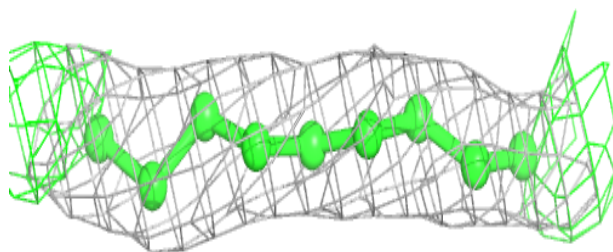
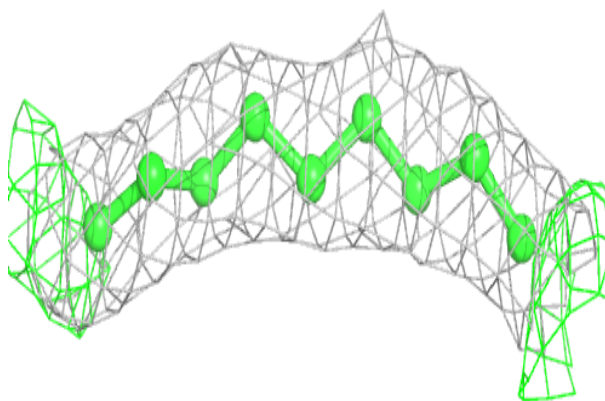
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



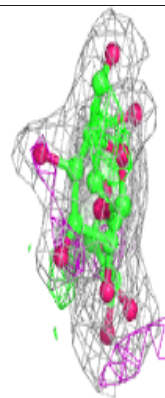
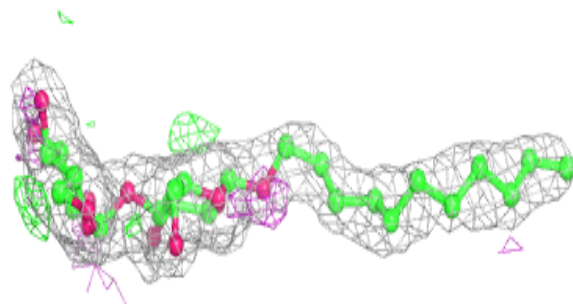
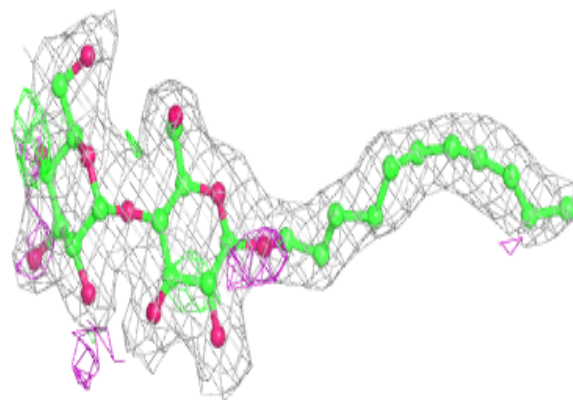


**Electron density around PGV F 4002:**

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

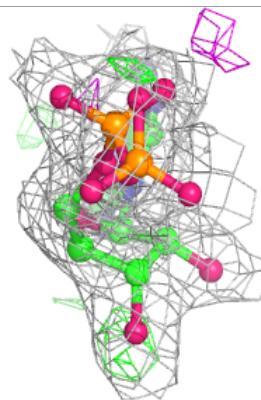
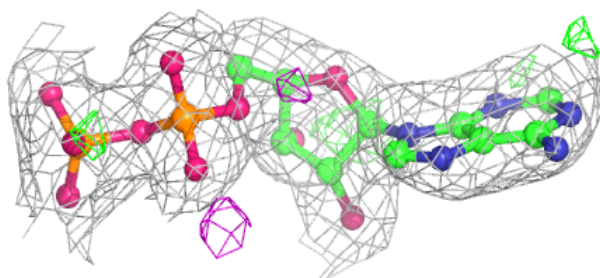
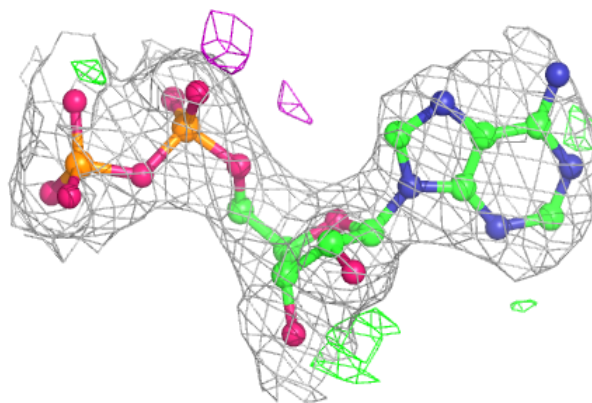
**Electron density around UMQ E 5004:**

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

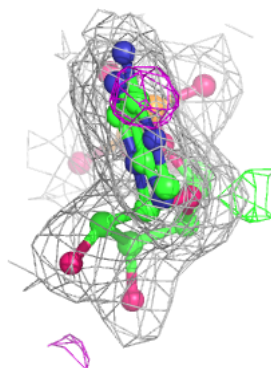
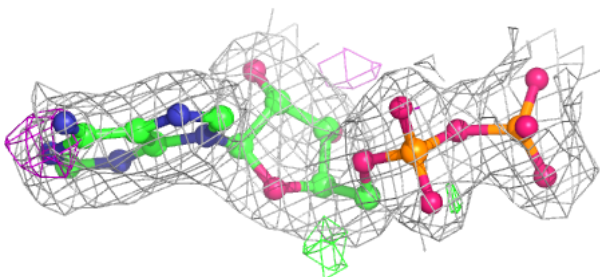
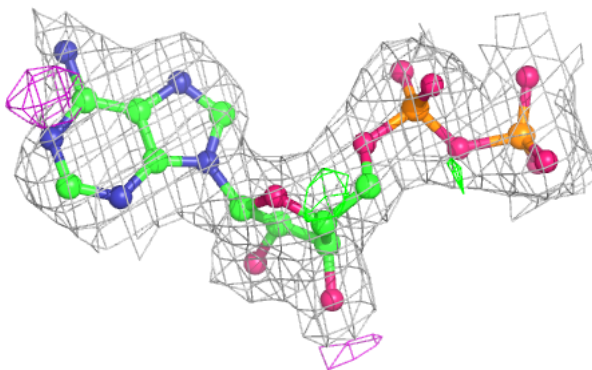


**Electron density around ADP B 2502:**

$2mF_o-DF_c$  (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 [i](#)

There are no such residues in this entry.