



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 05:34 AM BST

PDB ID : 3PUY
Title : Crystal Structure of an outward-facing MBP-Maltose transporter complex bound to AMP-PNP after crystal soaking of the pretranslocation state
Authors : Oldham, M.L.; Chen, J.
Deposited on : 2010-12-06
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

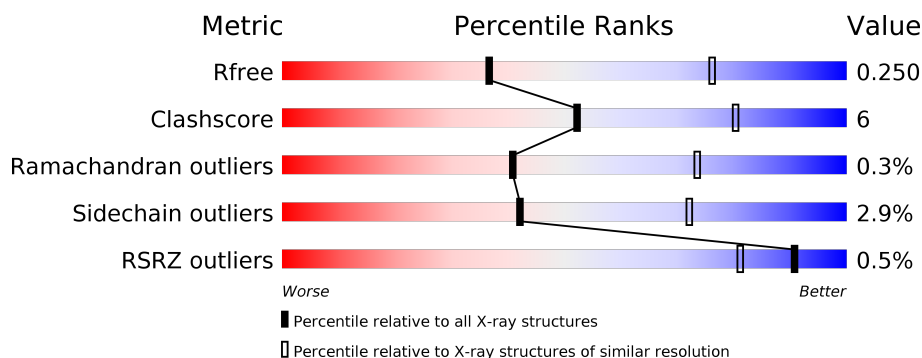
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	378	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 12%, green 87%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 87% 12% • </div> </div>
2	F	514	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 79%, yellow 15%, orange 5%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 79% 15% • 5% </div> </div>
3	G	296	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 84%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 84% 14% •• </div> </div>
4	A	381	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 82%, yellow 14%, orange 4%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 82% 14% •• </div> </div>
4	B	381	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 76%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 76% 18% • 6% </div> </div>
5	C	2	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 50%, orange 50%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 50% 50% </div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14789 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 transporter subunit; periplasmic-binding component of ABC superfamily.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	374	Total	C	N	O	S	0	0	0
			2897	1865	473	553	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	371	ALA	-	expression tag	UNP B1XC33
E	372	SER	-	expression tag	UNP B1XC33
E	373	ALA	-	expression tag	UNP B1XC33
E	374	SER	-	expression tag	UNP B1XC33
E	375	HIS	-	expression tag	UNP B1XC33
E	376	HIS	-	expression tag	UNP B1XC33
E	377	HIS	-	expression tag	UNP B1XC33
E	378	HIS	-	expression tag	UNP B1XC33

- Molecule 2 is a protein called Maltose transporter subunit; membrane component of ABC superfamily.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	490	Total	C	N	O	S	0	0	0
			3821	2511	608	685	17			

- Molecule 3 is a protein called Maltose transporter subunit; membrane component of ABC superfamily.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	293	Total	C	N	O	S	0	0	0
			2257	1510	361	377	9			

- Molecule 4 is a protein called Fused maltose transport subunit, ATP-binding component of ABC superfamily; regulatory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	371	Total	C	N	O	S	0	0	0
			2876	1819	515	529	13			
4	B	358	Total	C	N	O	S	0	0	0
			2789	1767	498	511	13			

There are 20 discrepancies between the modelled and reference sequences:

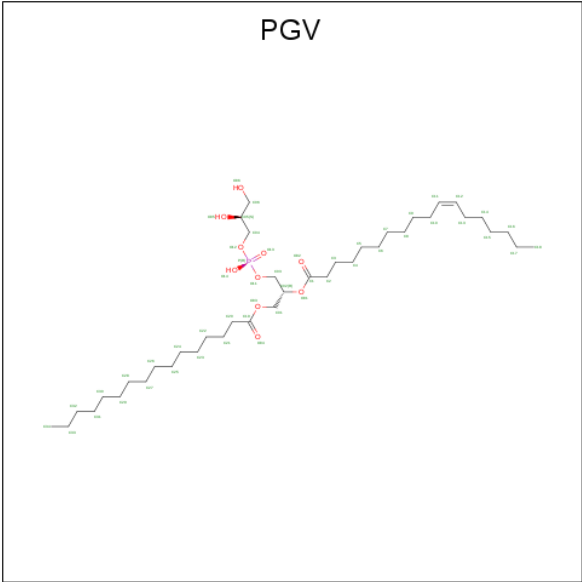
Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	-	expression tag	UNP B1XC34
A	373	SER	-	expression tag	UNP B1XC34
A	374	ALA	-	expression tag	UNP B1XC34
A	375	SER	-	expression tag	UNP B1XC34
A	376	HIS	-	expression tag	UNP B1XC34
A	377	HIS	-	expression tag	UNP B1XC34
A	378	HIS	-	expression tag	UNP B1XC34
A	379	HIS	-	expression tag	UNP B1XC34
A	380	HIS	-	expression tag	UNP B1XC34
A	381	HIS	-	expression tag	UNP B1XC34
B	372	ALA	-	expression tag	UNP B1XC34
B	373	SER	-	expression tag	UNP B1XC34
B	374	ALA	-	expression tag	UNP B1XC34
B	375	SER	-	expression tag	UNP B1XC34
B	376	HIS	-	expression tag	UNP B1XC34
B	377	HIS	-	expression tag	UNP B1XC34
B	378	HIS	-	expression tag	UNP B1XC34
B	379	HIS	-	expression tag	UNP B1XC34
B	380	HIS	-	expression tag	UNP B1XC34
B	381	HIS	-	expression tag	UNP B1XC34

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



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

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

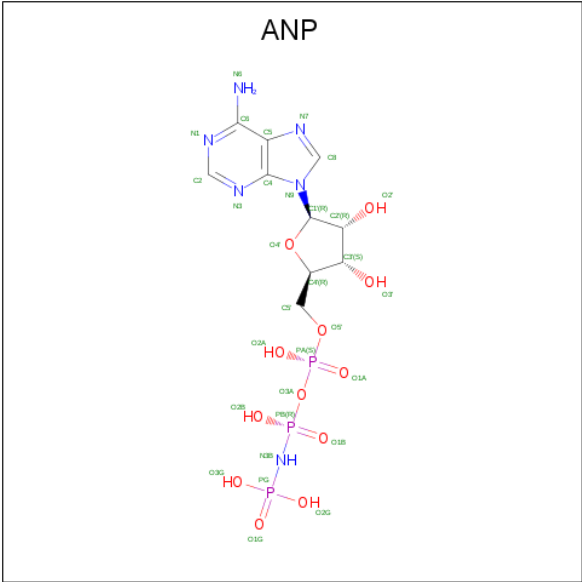


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	F	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 8 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

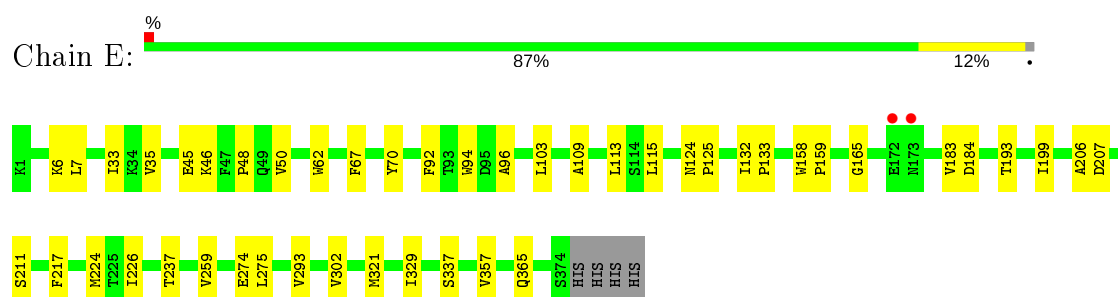
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	2	Total	O	0	0
			2	2		
9	A	6	Total	O	0	0
			6	6		
9	B	3	Total	O	0	0
			3	3		

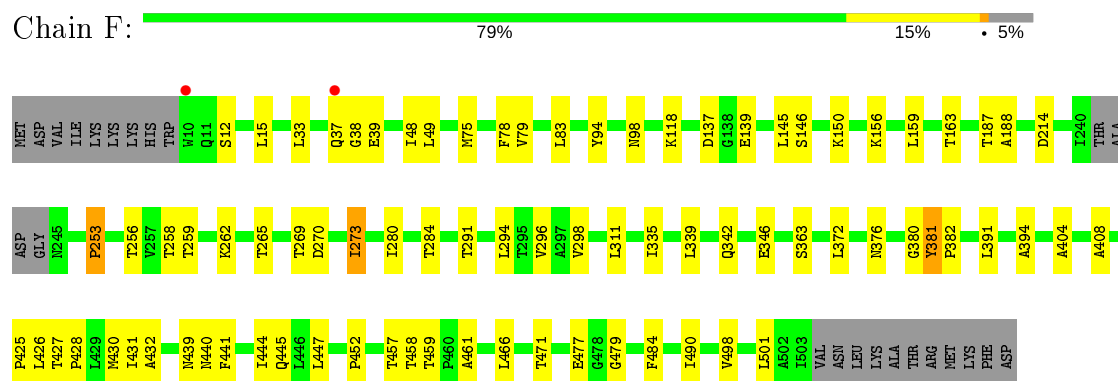
3 Residue-property plots [i](#)

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.

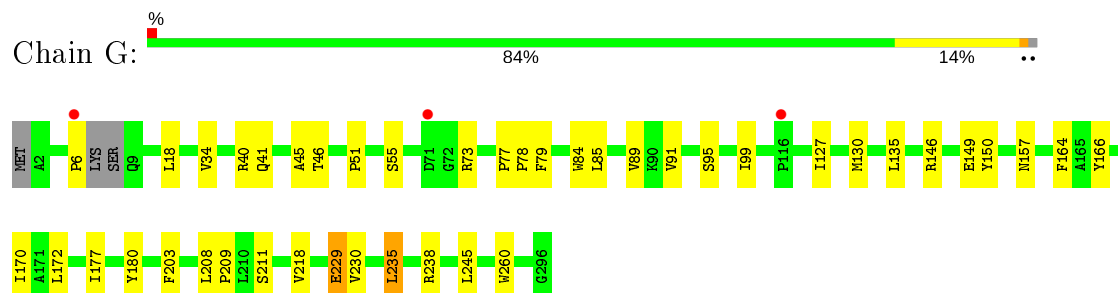
- Molecule 1: Maltose transporter subunit; periplasmic-binding component of ABC superfamily




- Molecule 2: Maltose transporter subunit; membrane component of ABC superfamily

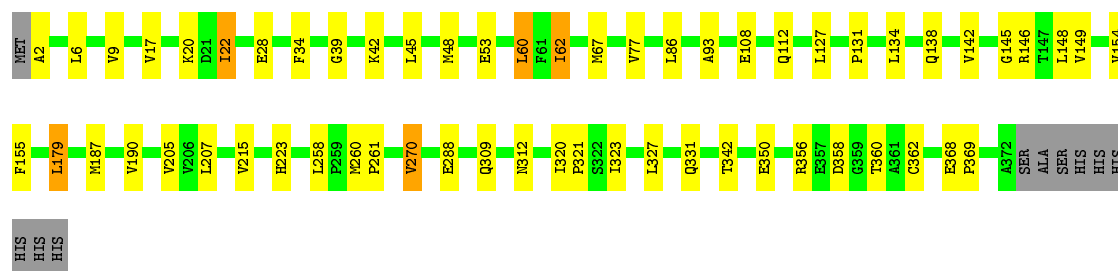


- Molecule 3: Maltose transporter subunit; membrane component of ABC superfamily




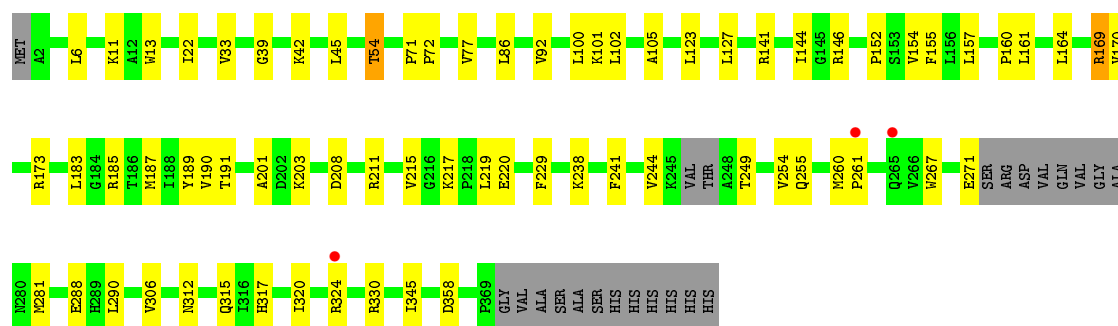
- Molecule 4: Fused maltose transport subunit, ATP-binding component of ABC superfamily; regulatory protein

Chain A:  82% 14% . .



- Molecule 4: Fused maltose transport subunit, ATP-binding component of ABC superfamily; regulatory protein

Chain B:  76% 18% . 6%



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

Chain C:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.55Å 96.28Å 112.28Å 86.91° 80.87° 74.32°	Depositor
Resolution (Å)	20.00 – 3.10 19.91 – 3.10	Depositor EDS
% Data completeness (in resolution range)	82.7 (20.00-3.10) 82.7 (19.91-3.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 3.09Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.214 , 0.254 0.212 , 0.250	Depositor DCC
R_{free} test set	2301 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	65.7	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 27.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14789	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGV, MG, GLC, ANP

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	0.33	0/2966	0.46	0/4026
2	F	0.36	0/3916	0.51	1/5330 (0.0%)
3	G	0.36	0/2318	0.51	1/3167 (0.0%)
4	A	0.34	0/2926	0.53	0/3968
4	B	0.32	0/2837	0.50	0/3843
All	All	0.34	0/14963	0.50	2/20334 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	G	235	LEU	CA-CB-CG	5.98	129.05	115.30
2	F	253	PRO	N-CA-C	5.08	125.31	112.10

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	2897	0	2873	26	0
2	F	3821	0	3849	50	0
3	G	2257	0	2345	31	0
4	A	2876	0	2941	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2789	0	2850	39	0
5	C	23	0	21	1	0
6	F	51	0	76	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	31	0	13	2	0
8	B	31	0	13	2	0
9	A	6	0	0	0	0
9	B	3	0	0	1	0
9	F	2	0	0	0	0
All	All	14789	0	14981	164	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 6.

All (164) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:62:ILE:HG23	4:A:67:MET:HG3	1.40	1.04
2:F:471:THR:HG23	2:F:490:ILE:HD13	1.48	0.96
4:B:39:GLY:H	8:B:2502:ANP:HNB1	1.07	0.94
4:A:39:GLY:N	8:A:2501:ANP:HNB1	1.72	0.87
4:A:39:GLY:H	8:A:2501:ANP:HNB1	0.86	0.80
2:F:335:ILE:HD12	3:G:34:VAL:HG22	1.67	0.76
4:B:39:GLY:N	8:B:2502:ANP:HNB1	1.85	0.73
4:B:260:MET:HB2	4:B:261:PRO:HD2	1.74	0.69
4:A:223:HIS:CE1	4:A:368:GLU:HG2	2.28	0.68
4:A:86:LEU:HA	4:A:146:ARG:HH21	1.59	0.68
2:F:471:THR:HG21	2:F:490:ILE:HG21	1.76	0.67
3:G:41:GLN:HB3	3:G:55:SER:HB2	1.75	0.67
2:F:391:LEU:HD13	2:F:426:LEU:HD12	1.79	0.65
3:G:127:ILE:O	3:G:130:MET:HG2	1.97	0.64
2:F:12:SER:HB2	2:F:15:LEU:HB2	1.80	0.63
2:F:471:THR:CG2	2:F:490:ILE:HG21	2.29	0.62
4:A:288:GLU:HG2	4:B:312:ASN:HB2	1.82	0.61
3:G:180:TYR:CE2	3:G:211:SER:HA	2.37	0.60
4:A:6:LEU:HD22	4:A:22:ILE:HD11	1.83	0.59
4:A:260:MET:CE	4:A:323:ILE:HD11	2.33	0.59
2:F:137:ASP:OD2	2:F:139:GLU:HG2	2.03	0.59
4:A:358:ASP:OD1	4:A:360:THR:HG22	2.02	0.58
1:E:113:LEU:HD22	1:E:226:ILE:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:85:LEU:O	3:G:89:VAL:HG23	2.04	0.58
1:E:62:TRP:HB3	1:E:67:PHE:HE1	1.69	0.57
4:A:312:ASN:HB2	4:B:288:GLU:HG2	1.86	0.57
4:B:6:LEU:HD22	4:B:22:ILE:HD11	1.85	0.57
4:B:244:VAL:HG23	4:B:281:MET:HB2	1.87	0.57
2:F:335:ILE:CD1	3:G:34:VAL:HG22	2.34	0.57
2:F:273:ILE:HG22	2:F:459:THR:HG21	1.89	0.55
4:A:260:MET:HE3	4:A:323:ILE:HD11	1.87	0.55
4:A:356:ARG:HH11	4:A:360:THR:HG23	1.72	0.54
3:G:6:PRO:HA	4:B:71:PRO:HD3	1.88	0.54
2:F:394:ALA:HB2	3:G:180:TYR:CE1	2.41	0.54
4:A:155:PHE:HB2	4:A:187:MET:HG2	1.89	0.54
1:E:48:PRO:HG3	1:E:70:TYR:CE1	2.43	0.53
1:E:6:LYS:HA	1:E:33:ILE:HG23	1.89	0.53
4:A:368:GLU:HG3	4:A:369:PRO:HD2	1.90	0.53
1:E:158:TRP:HH2	1:E:183:VAL:HG12	1.72	0.53
1:E:115:LEU:HD21	1:E:224:MET:HE3	1.91	0.53
2:F:146:SER:HB3	2:F:159:LEU:HD23	1.90	0.53
2:F:294:LEU:O	2:F:298:VAL:HG23	2.08	0.53
2:F:78:PHE:HZ	3:G:164:PHE:CD2	2.27	0.53
4:A:138:GLN:O	4:A:142:VAL:HG23	2.09	0.53
4:A:77:VAL:HG22	4:A:154:VAL:HB	1.91	0.53
3:G:45:ALA:HB2	3:G:260:TRP:CE2	2.44	0.53
4:B:170:VAL:HG22	4:B:173:ARG:HH21	1.74	0.52
4:B:77:VAL:HG12	4:B:154:VAL:HB	1.91	0.52
4:B:86:LEU:HA	4:B:146:ARG:HH21	1.75	0.52
1:E:337:SER:HB2	2:F:479:GLY:H	1.75	0.52
3:G:146:ARG:O	3:G:149:GLU:HG2	2.10	0.51
2:F:441:PHE:CZ	2:F:445:GLN:HG3	2.46	0.51
2:F:291:THR:HG21	2:F:376:ASN:ND2	2.25	0.51
4:A:205:VAL:HG22	4:A:215:VAL:HG13	1.93	0.51
4:A:260:MET:HB3	4:A:261:PRO:HD2	1.92	0.51
3:G:166:TYR:CZ	3:G:229:GLU:HG2	2.46	0.51
1:E:33:ILE:HG13	1:E:275:LEU:HD22	1.93	0.51
1:E:193:THR:HA	1:E:357:VAL:HG21	1.93	0.50
2:F:363:SER:O	2:F:452:PRO:HG3	2.11	0.50
4:B:189:TYR:CE2	4:B:191:THR:HB	2.46	0.50
2:F:284:THR:HG22	2:F:466:LEU:HA	1.92	0.50
4:B:92:VAL:HB	4:B:127:LEU:HA	1.93	0.50
1:E:211:SER:OG	3:G:45:ALA:HB3	2.12	0.50
3:G:41:GLN:CB	3:G:55:SER:HB2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:145:GLY:O	4:A:149:VAL:HG23	2.12	0.50
4:A:86:LEU:HA	4:A:146:ARG:NH2	2.25	0.49
1:E:45:GLU:O	1:E:48:PRO:HD2	2.12	0.49
4:A:34:PHE:HB2	4:A:190:VAL:HG22	1.94	0.49
4:A:6:LEU:HD23	4:A:9:VAL:HG21	1.94	0.49
4:B:141:ARG:HD2	4:B:164:LEU:HD21	1.94	0.49
2:F:408:ALA:HB2	4:B:102:LEU:HD21	1.94	0.49
4:A:2:ALA:HB3	4:A:28:GLU:HG2	1.95	0.49
3:G:203:PHE:O	3:G:208:LEU:HG	2.13	0.49
4:B:155:PHE:HB2	4:B:187:MET:HG2	1.94	0.49
2:F:380:GLY:HA3	5:C:2:GLC:H61	1.93	0.49
4:B:144:ILE:HD11	4:B:160:PRO:O	2.13	0.48
4:B:217:LYS:HB2	4:B:220:GLU:HB2	1.94	0.48
4:B:141:ARG:HD2	4:B:164:LEU:CD2	2.43	0.48
3:G:40:ARG:HG3	3:G:51:PRO:HB3	1.94	0.48
1:E:46:LYS:O	1:E:50:VAL:HG22	2.14	0.48
2:F:78:PHE:HZ	3:G:164:PHE:CE2	2.32	0.47
4:A:6:LEU:HG	4:A:60:LEU:HD23	1.94	0.47
2:F:372:LEU:HD13	2:F:447:LEU:HD23	1.95	0.47
2:F:471:THR:HG21	2:F:490:ILE:CG2	2.45	0.47
3:G:91:VAL:O	3:G:95:SER:HB2	2.14	0.47
2:F:432:ALA:CB	3:G:172:LEU:HD21	2.44	0.47
4:B:101:LYS:HA	4:B:105:ALA:HB2	1.96	0.47
4:B:13:TRP:HZ2	9:B:384:HOH:O	1.97	0.47
4:B:315:GLN:HG2	4:B:330:ARG:HG2	1.96	0.47
2:F:259:THR:HB	2:F:262:LYS:HD2	1.96	0.46
2:F:98:ASN:O	2:F:256:THR:HG22	2.16	0.46
4:B:33:VAL:HG22	4:B:201:ALA:HB2	1.98	0.46
2:F:484:PHE:HB3	3:G:135:LEU:HD11	1.99	0.45
3:G:166:TYR:OH	3:G:229:GLU:HG2	2.17	0.45
4:A:93:ALA:HB2	4:A:127:LEU:HG	1.99	0.45
4:B:33:VAL:HG12	4:B:189:TYR:HB3	1.97	0.45
3:G:99:ILE:HG23	3:G:170:ILE:HG22	1.97	0.45
2:F:156:LYS:HG3	2:F:187:THR:HB	1.99	0.45
2:F:457:THR:HG21	2:F:461:ALA:HB3	1.98	0.45
1:E:158:TRP:N	1:E:159:PRO:HD2	2.32	0.45
2:F:75:MET:O	2:F:79:VAL:HB	2.16	0.45
2:F:498:VAL:HA	2:F:501:LEU:HB2	1.97	0.45
1:E:184:ASP:HB2	1:E:365:GLN:CD	2.38	0.44
2:F:265:THR:O	2:F:269:THR:N	2.50	0.44
2:F:270:ASP:HB3	2:F:273:ILE:HG12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:425:PRO:O	2:F:428:PRO:HD2	2.17	0.44
3:G:208:LEU:HB2	3:G:209:PRO:HD3	1.99	0.44
4:A:108:GLU:O	4:A:112:GLN:HB2	2.17	0.44
4:B:255:GLN:HB2	4:B:267:TRP:CE3	2.53	0.44
4:B:11:LYS:HD3	4:B:54:THR:O	2.17	0.44
1:E:7:LEU:HB2	1:E:35:VAL:HG22	2.00	0.44
4:B:157:LEU:HB3	4:B:160:PRO:HG3	2.00	0.43
4:B:306:VAL:H	4:B:317:HIS:HB2	1.83	0.43
4:B:152:PRO:HD2	4:B:155:PHE:CZ	2.53	0.43
4:B:249:THR:HG22	4:B:254:VAL:HG13	2.01	0.43
4:B:189:TYR:HE2	4:B:191:THR:HB	1.83	0.43
3:G:177:ILE:HD11	3:G:218:VAL:HG21	2.01	0.43
3:G:180:TYR:HE2	3:G:211:SER:HA	1.83	0.43
4:A:270:VAL:HG13	4:A:362:CYS:HB2	1.99	0.43
2:F:346:GLU:H	2:F:346:GLU:CD	2.22	0.43
2:F:432:ALA:HB2	3:G:172:LEU:HD21	2.01	0.43
2:F:94:TYR:HD2	2:F:484:PHE:HB2	1.84	0.43
4:A:223:HIS:ND1	4:A:368:GLU:HG2	2.33	0.42
1:E:94:TRP:HE3	1:E:103:LEU:HD22	1.83	0.42
1:E:207:ASP:OD2	2:F:342:GLN:HB2	2.19	0.42
4:A:45:LEU:HD23	4:A:48:MET:HE3	2.02	0.42
2:F:439:ASN:O	2:F:441:PHE:N	2.52	0.42
4:A:42:LYS:HG2	4:A:207:LEU:HD12	2.00	0.42
2:F:404:ALA:HB1	4:B:72:PRO:HB2	2.01	0.42
4:B:208:ASP:HB2	4:B:229:PHE:CE2	2.55	0.42
1:E:259:VAL:HB	1:E:329:ILE:HD13	2.01	0.42
2:F:159:LEU:HD11	2:F:188:ALA:HB1	2.01	0.42
4:B:290:LEU:HD22	4:B:345:ILE:HD13	2.00	0.42
2:F:372:LEU:HD21	2:F:444:ILE:HD12	2.02	0.42
2:F:296:VAL:HG21	2:F:430:MET:HG2	2.02	0.42
3:G:84:TRP:HB3	3:G:245:LEU:HA	2.02	0.42
4:A:320:ILE:HD12	4:A:327:LEU:HD13	2.01	0.42
3:G:157:ASN:ND2	3:G:238:ARG:HB3	2.35	0.41
4:A:320:ILE:HA	4:A:321:PRO:HD2	1.81	0.41
2:F:335:ILE:O	2:F:339:LEU:HG	2.20	0.41
2:F:381:TYR:N	2:F:382:PRO:CD	2.82	0.41
2:F:48:ILE:HG13	2:F:49:LEU:N	2.35	0.41
4:B:238:LYS:HE2	4:B:241:PHE:HE2	1.86	0.41
1:E:124:ASN:HA	1:E:125:PRO:HD2	1.97	0.41
1:E:92:PHE:HZ	1:E:321:MET:HE1	1.84	0.41
4:A:148:LEU:HD22	4:A:179:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:ILE:HB	1:E:133:PRO:HD3	2.03	0.41
4:B:42:LYS:HD2	4:B:190:VAL:HG13	2.02	0.41
1:E:199:ILE:HG21	1:E:206:ALA:HB2	2.02	0.41
1:E:337:SER:HB3	2:F:477:GLU:HA	2.02	0.41
4:A:62:ILE:HD13	4:A:154:VAL:HG21	2.03	0.41
2:F:428:PRO:HA	2:F:431:ILE:HD12	2.03	0.41
4:B:183:LEU:HB3	4:B:185:ARG:HG3	2.02	0.41
4:A:258:LEU:HB3	4:A:260:MET:SD	2.60	0.41
2:F:39:GLU:HG3	3:G:150:TYR:OH	2.19	0.41
1:E:217:PHE:HE1	1:E:224:MET:HA	1.86	0.41
2:F:280:ILE:O	2:F:284:THR:HG23	2.21	0.41
3:G:79:PHE:HB3	3:G:84:TRP:CH2	2.55	0.41
4:A:309:GLN:HB3	4:B:219:LEU:HD21	2.03	0.40
1:E:109:ALA:HA	1:E:302:VAL:HA	2.03	0.40
4:A:131:PRO:HA	4:A:134:LEU:HD12	2.03	0.40
4:B:161:LEU:HB3	4:B:169:ARG:HG2	2.03	0.40
1:E:96:ALA:HB2	1:E:329:ILE:HD12	2.04	0.40
3:G:77:PRO:HA	3:G:78:PRO:HD3	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	372/378 (98%)	355 (95%)	16 (4%)	1 (0%)	41	73
2	F	486/514 (95%)	461 (95%)	22 (4%)	3 (1%)	25	59
3	G	289/296 (98%)	277 (96%)	11 (4%)	1 (0%)	41	73
4	A	369/381 (97%)	347 (94%)	22 (6%)	0	100	100
4	B	352/381 (92%)	328 (93%)	24 (7%)	0	100	100
All	All	1868/1950 (96%)	1768 (95%)	95 (5%)	5 (0%)	41	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	37	GLN
1	E	165	GLY
2	F	253	PRO
3	G	230	VAL
2	F	38	GLY

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	297/303 (98%)	294 (99%)	3 (1%)	76	90
2	F	402/424 (95%)	388 (96%)	14 (4%)	36	68
3	G	234/237 (99%)	229 (98%)	5 (2%)	53	79
4	A	314/323 (97%)	303 (96%)	11 (4%)	36	68
4	B	305/323 (94%)	293 (96%)	12 (4%)	32	65
All	All	1552/1610 (96%)	1507 (97%)	45 (3%)	42	72

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	237	THR
1	E	274	GLU
1	E	293	VAL
2	F	33	LEU
2	F	83	LEU
2	F	118	LYS
2	F	145	LEU
2	F	150	LYS
2	F	163	THR
2	F	214	ASP
2	F	258	THR
2	F	273	ILE
2	F	311	LEU

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Mol	Chain	Res	Type
2	F	381	TYR
2	F	427	THR
2	F	440	ASN
2	F	458	THR
3	G	18	LEU
3	G	46	THR
3	G	73	ARG
3	G	229	GLU
3	G	235	LEU
4	A	17	VAL
4	A	20	LYS
4	A	22	ILE
4	A	53	GLU
4	A	60	LEU
4	A	62	ILE
4	A	179	LEU
4	A	270	VAL
4	A	331	GLN
4	A	342	THR
4	A	350	GLU
4	B	45	LEU
4	B	54	THR
4	B	100	LEU
4	B	123	LEU
4	B	169	ARG
4	B	203	LYS
4	B	211	ARG
4	B	215	VAL
4	B	271	GLU
4	B	320	ILE
4	B	324	ARG
4	B	358	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	437	ASN
2	F	440	ASN
3	G	41	GLN
3	G	53	GLN
3	G	282	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	GLC	C	1	5	12,12,12	0.55	0	17,17,17	0.74	0
5	GLC	C	2	5	11,11,12	0.28	0	15,15,17	0.81	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GLC	C	1	5	-	2/2/22/22	0/1/1/1
5	GLC	C	2	5	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2	GLC	C1-O5-C5	2.07	115.00	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1	GLC	O5-C5-C6-O6
5	C	1	GLC	C4-C5-C6-O6
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 [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	PGV	F	4001	-	50,50,50	1.10	3 (6%)	53,56,56	1.02	2 (3%)
8	ANP	B	2502	7	29,33,33	1.83	7 (24%)	31,52,52	1.79	9 (29%)
8	ANP	A	2501	7	29,33,33	1.79	8 (27%)	31,52,52	1.79	9 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PGV	F	4001	-	-	31/55/55/55	-
8	ANP	B	2502	7	-	3/14/38/38	0/3/3/3
8	ANP	A	2501	7	-	1/14/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	4001	PGV	O01-C1	4.50	1.47	1.34
8	B	2502	ANP	PB-N3B	4.43	1.74	1.63
8	B	2502	ANP	PG-N3B	4.36	1.74	1.63
8	A	2501	ANP	PB-N3B	4.35	1.74	1.63
6	F	4001	PGV	O03-C19	4.30	1.45	1.33
8	A	2501	ANP	PG-N3B	4.29	1.74	1.63
6	F	4001	PGV	C12-C11	3.66	1.53	1.31
8	B	2502	ANP	PB-O1B	3.22	1.51	1.46
8	B	2502	ANP	PG-O1G	3.19	1.51	1.46
8	A	2501	ANP	PB-O1B	3.03	1.51	1.46
8	A	2501	ANP	PG-O1G	3.00	1.50	1.46
8	A	2501	ANP	C5-C4	2.77	1.48	1.40
8	B	2502	ANP	C5-C4	2.63	1.47	1.40
8	B	2502	ANP	PG-O2G	-2.36	1.50	1.56
8	A	2501	ANP	PG-O2G	-2.36	1.50	1.56
8	A	2501	ANP	PG-O3G	-2.15	1.51	1.56
8	B	2502	ANP	PG-O3G	-2.11	1.51	1.56
8	A	2501	ANP	PB-O2B	-2.05	1.51	1.56

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2501	ANP	O2B-PB-O1B	4.35	119.03	109.92
8	B	2502	ANP	O2B-PB-O1B	4.33	119.00	109.92
6	F	4001	PGV	O01-C1-C2	4.19	120.54	111.50
8	B	2502	ANP	N3-C2-N1	-3.55	123.12	128.68
8	B	2502	ANP	O1B-PB-N3B	-3.49	106.63	111.77
8	A	2501	ANP	N3-C2-N1	-3.41	123.35	128.68
8	B	2502	ANP	PA-O3A-PB	-3.33	120.88	132.62
8	B	2502	ANP	O1G-PG-N3B	-3.26	106.98	111.77
8	A	2501	ANP	PA-O3A-PB	-3.26	121.15	132.62
8	A	2501	ANP	C3'-C2'-C1'	3.20	105.80	100.98
8	A	2501	ANP	O1G-PG-N3B	-3.14	107.14	111.77
8	A	2501	ANP	O1B-PB-N3B	-3.00	107.35	111.77
8	B	2502	ANP	C3'-C2'-C1'	2.85	105.27	100.98
6	F	4001	PGV	O03-C19-C20	2.80	120.69	111.91
8	B	2502	ANP	C4-C5-N7	-2.24	107.07	109.40
8	B	2502	ANP	O3G-PG-O2G	2.19	113.48	107.64
8	A	2501	ANP	C2-N1-C6	2.16	122.45	118.75
8	A	2501	ANP	C4-C5-N7	-2.07	107.24	109.40
8	A	2501	ANP	O3G-PG-O2G	2.07	113.14	107.64
8	B	2502	ANP	C2-N1-C6	2.00	122.18	118.75

There are no chirality outliers.

All (35) torsion outliers are listed below:

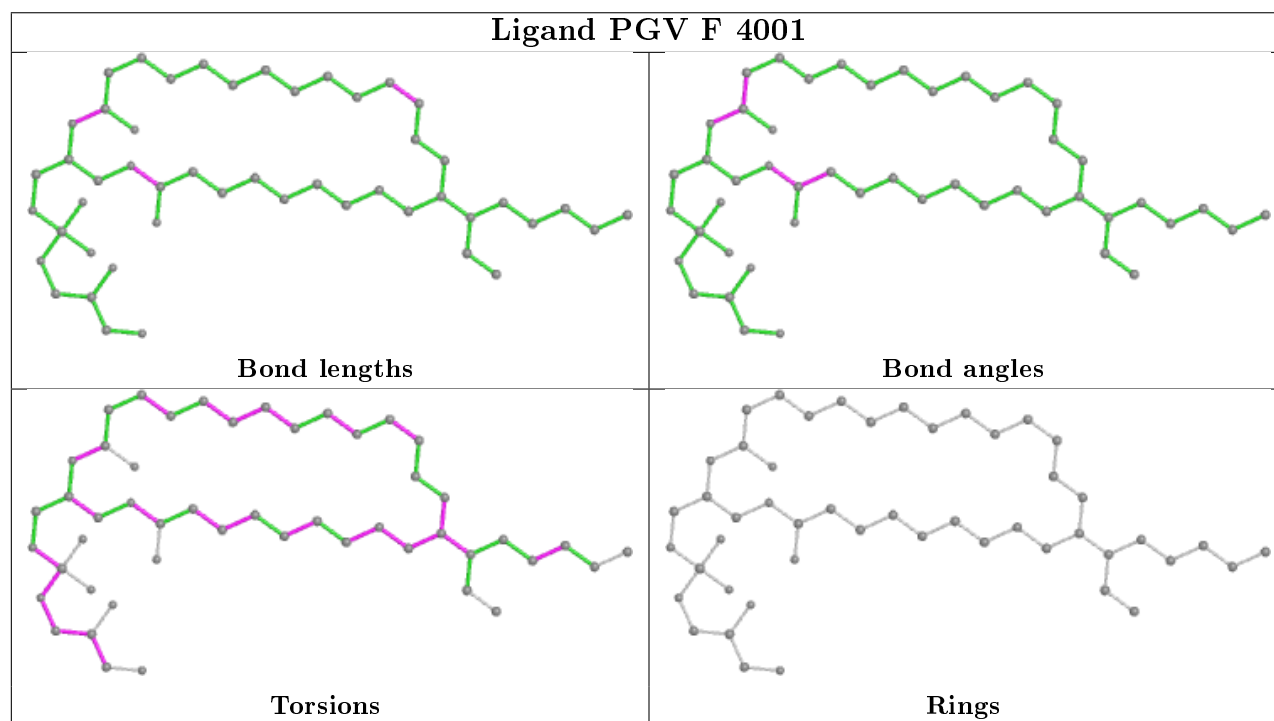
Mol	Chain	Res	Type	Atoms
6	F	4001	PGV	C03-O11-P-O12
6	F	4001	PGV	C03-O11-P-O13
6	F	4001	PGV	C03-O11-P-O14
6	F	4001	PGV	C04-O12-P-O11
6	F	4001	PGV	O12-C04-C05-C06
6	F	4001	PGV	O12-C04-C05-O05
6	F	4001	PGV	C2-C1-O01-C02
8	B	2502	ANP	PG-N3B-PB-O1B
8	B	2502	ANP	C5'-O5'-PA-O3A
8	A	2501	ANP	PG-N3B-PB-O1B
6	F	4001	PGV	O02-C1-O01-C02
6	F	4001	PGV	C10-C11-C12-C13
6	F	4001	PGV	C19-C20-C21-C22
6	F	4001	PGV	C20-C19-O03-C01
6	F	4001	PGV	C04-C05-C06-O06
6	F	4001	PGV	C26-C27-C28-C29
6	F	4001	PGV	C2-C3-C4-C5
6	F	4001	PGV	C24-C25-C26-C27
6	F	4001	PGV	C6-C7-C8-C9
6	F	4001	PGV	C27-C28-C29-C30
6	F	4001	PGV	C25-C26-C27-C28
6	F	4001	PGV	O05-C05-C06-O06
6	F	4001	PGV	C22-C23-C24-C25
6	F	4001	PGV	O04-C19-O03-C01
6	F	4001	PGV	C13-C14-C15-C16
6	F	4001	PGV	C20-C21-C22-C23
6	F	4001	PGV	C11-C10-C9-C8
6	F	4001	PGV	C4-C5-C6-C7
6	F	4001	PGV	C05-C04-O12-P
6	F	4001	PGV	C04-O12-P-O14
6	F	4001	PGV	O03-C01-C02-O01
6	F	4001	PGV	C30-C31-C32-C33
6	F	4001	PGV	C5-C6-C7-C8
6	F	4001	PGV	O03-C01-C02-C03
8	B	2502	ANP	C5'-O5'-PA-O1A

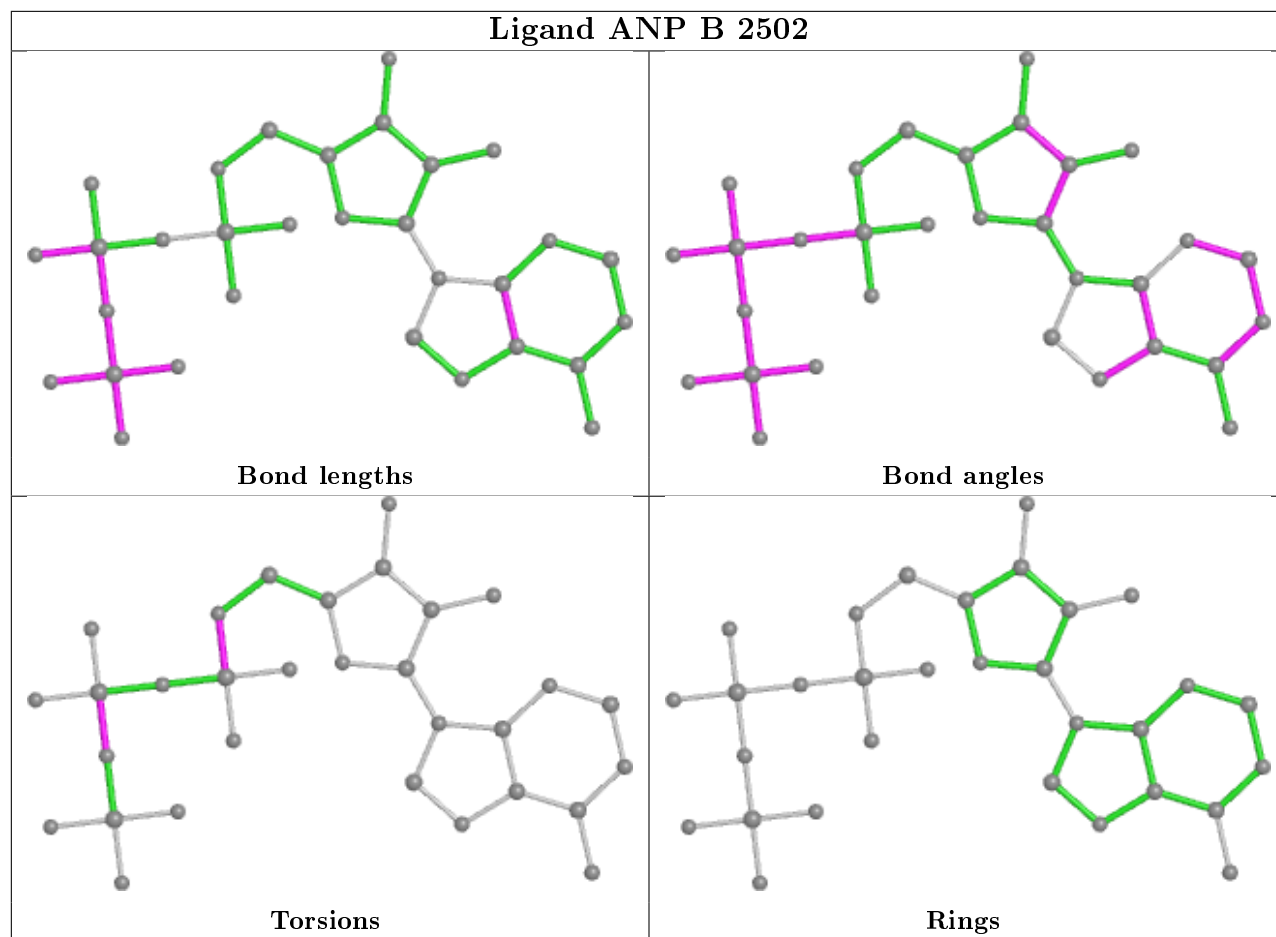
There are no ring outliers.

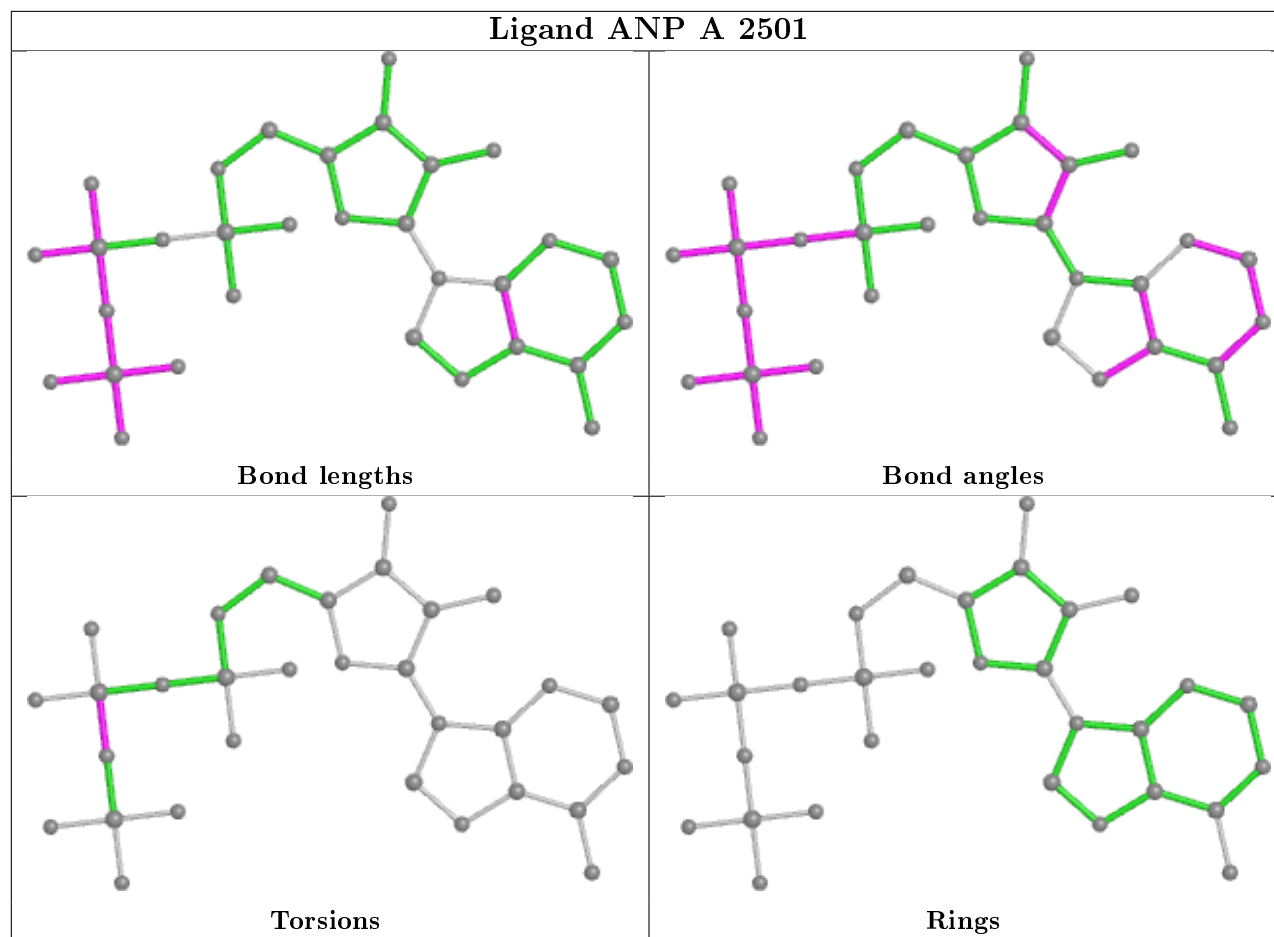
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	2502	ANP	2	0
8	A	2501	ANP	2	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	374/378 (98%)	-0.49	2 (0%) 91 81	41, 78, 122, 140	0
2	F	490/514 (95%)	-0.40	2 (0%) 92 84	34, 82, 136, 183	0
3	G	293/296 (98%)	-0.57	3 (1%) 82 67	32, 58, 104, 162	0
4	A	371/381 (97%)	-0.56	0 100 100	43, 74, 101, 112	0
4	B	358/381 (93%)	-0.37	3 (0%) 86 72	44, 91, 188, 261	0
All	All	1886/1950 (96%)	-0.47	10 (0%) 91 81	32, 78, 133, 261	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	6	PRO	5.8
2	F	37	GLN	3.4
1	E	172	GLU	3.4
1	E	173	ASN	3.3
3	G	71	ASP	2.7
2	F	10	TRP	2.5
4	B	261	PRO	2.4
3	G	116	PRO	2.3
4	B	324	ARG	2.2
4	B	265	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GLC	C	1	12/12	0.93	0.15	80,81,82,83	0
5	GLC	C	2	11/12	0.96	0.14	80,81,82,82	0

6.4 Ligands [i](#)

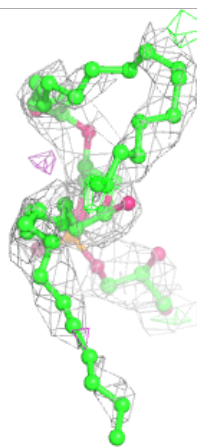
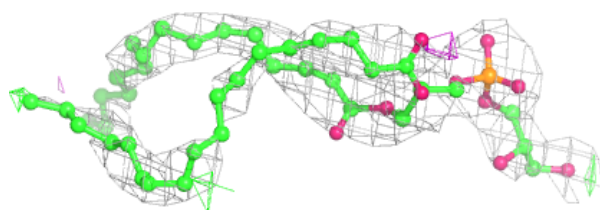
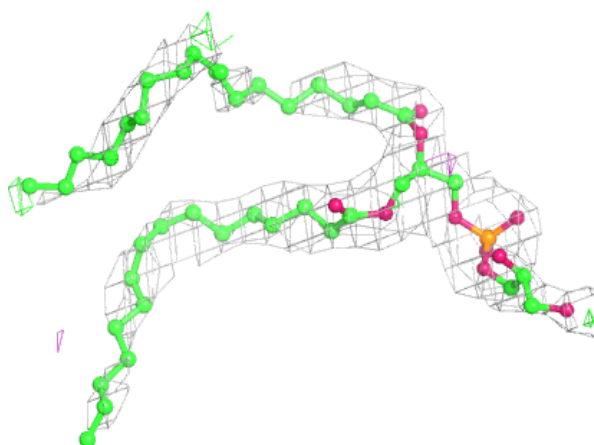
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PGV	F	4001	51/51	0.81	0.32	106,110,114,115	0
8	ANP	B	2502	31/31	0.96	0.15	59,74,82,84	0
8	ANP	A	2501	31/31	0.97	0.15	52,64,73,75	0
7	MG	A	1501	1/1	0.98	0.11	53,53,53,53	0
7	MG	B	1502	1/1	0.99	0.13	54,54,54,54	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.

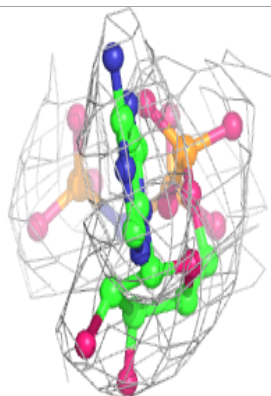
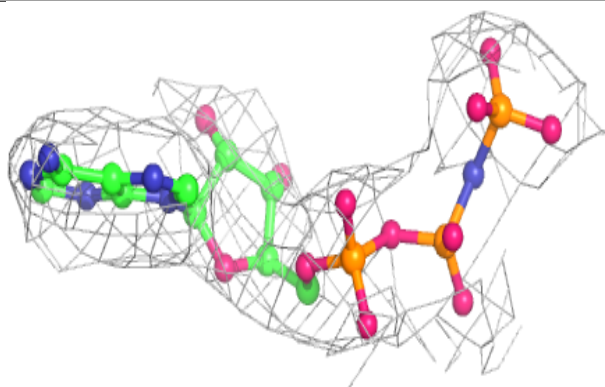
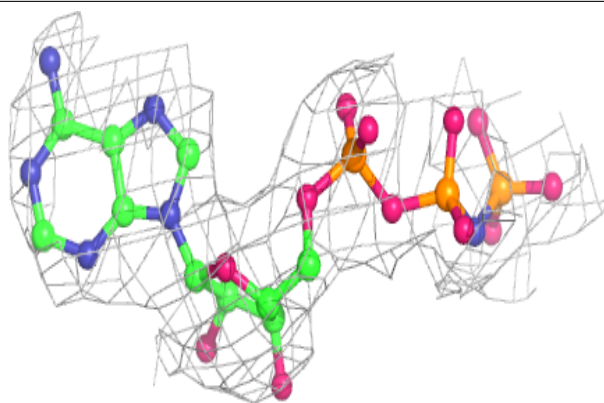
Electron density around PGV F 4001:

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

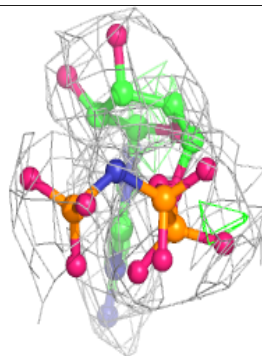
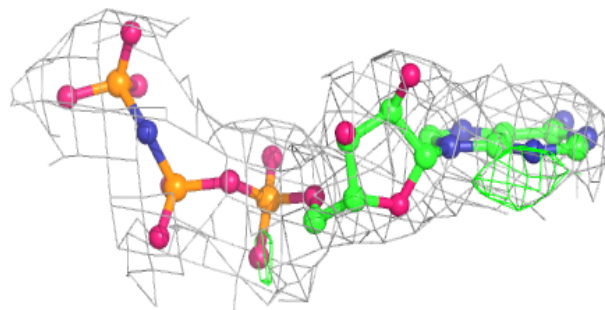
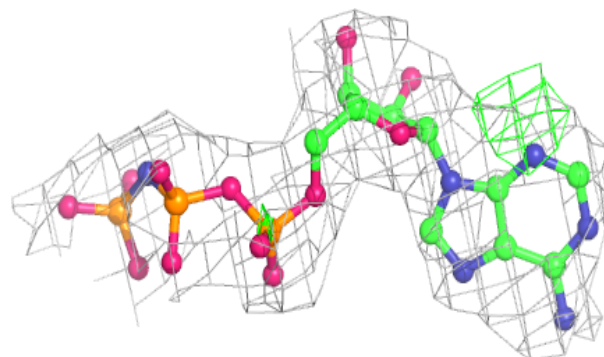


Electron density around ANP B 2502:

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

**Electron density around ANP A 2501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.