



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:57 AM UTC

PDB ID : 3ID8 / pdb_00003id8
Title : Ternary complex of human pancreatic glucokinase crystallized with activator, glucose and AMP-PNP
Authors : Petit, P.; Gluais, L.; Lagarde, A.; Boutin, J.A.; Ferry, G.; Vuillard, L.
Deposited on : 2009-07-20
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

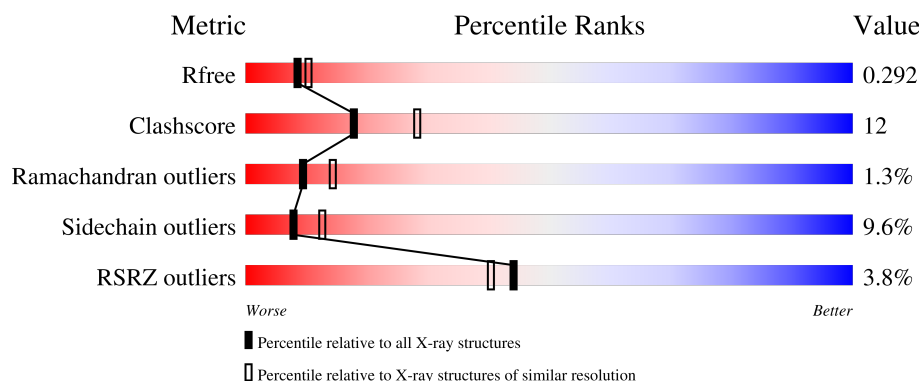
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	470	4% 74% 18% . .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3750 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 Glucokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	450	3557	2215	620	690	32	0	3	0

There are 16 discrepancies between the modelled and reference sequences:

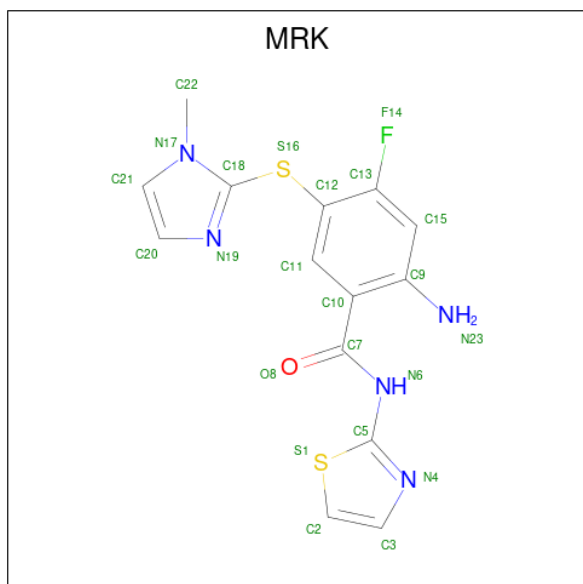
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	expression tag	UNP P35557
A	-3	GLY	-	expression tag	UNP P35557
A	-2	HIS	-	expression tag	UNP P35557
A	-1	HIS	-	expression tag	UNP P35557
A	0	HIS	-	expression tag	UNP P35557
A	1	HIS	-	expression tag	UNP P35557
A	2	HIS	-	expression tag	UNP P35557
A	3	HIS	-	expression tag	UNP P35557
A	4	GLU	-	expression tag	UNP P35557
A	5	ASN	-	expression tag	UNP P35557
A	6	LEU	-	expression tag	UNP P35557
A	7	TYR	-	expression tag	UNP P35557
A	8	PHE	-	expression tag	UNP P35557
A	9	GLN	-	expression tag	UNP P35557
A	10	GLY	-	expression tag	UNP P35557
A	11	MET	-	expression tag	UNP P35557

- Molecule 2 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



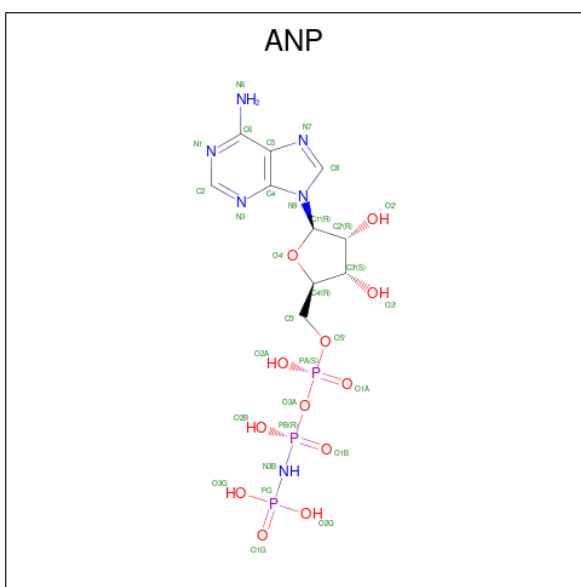
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is 2-AMINO-4-FLUORO-5-[(1-METHYL-1H-IMIDAZOL-2-YL)SULFANYL]-N-(1,3-THIAZOL-2-YL)BENZAMIDE (CCD ID: MRK) (formula: $C_{14}H_{12}FN_5OS_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			23	14	1	5	1	2		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0

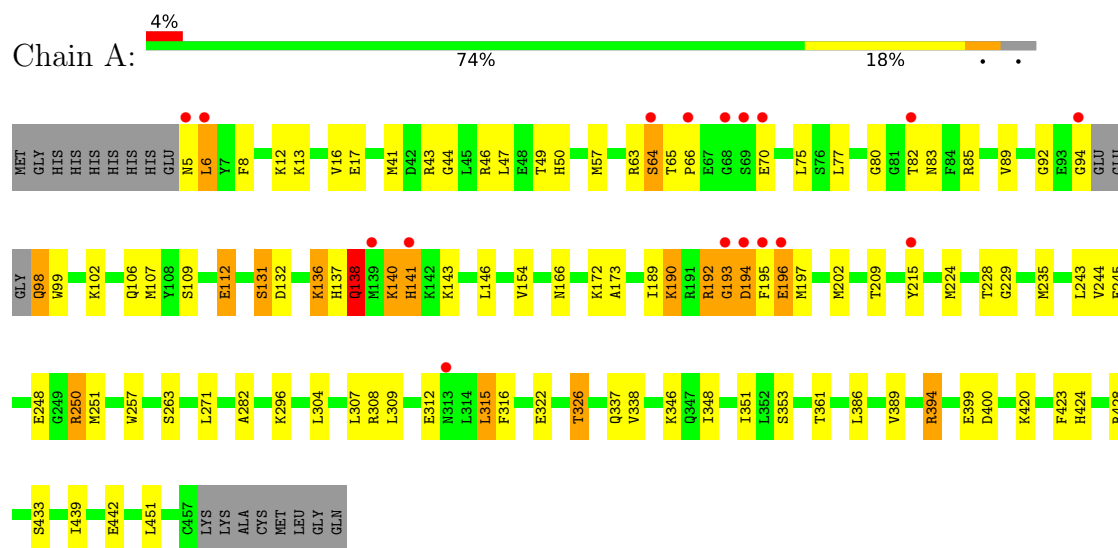
- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total K 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	125	Total O 125 125	0	0

- Molecule 1: Glucokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.00Å 82.60Å 86.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.40 19.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.94-2.40) 99.3 (19.94-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.17 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.279 0.213 , 0.292	Depositor DCC
R_{free} test set	966 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3750	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	1/3620 (0.0%)	0.97	3/4861 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	LYS	C-O	-5.69	1.17	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	LEU	N-CA-C	-9.62	100.97	112.89
1	A	193	GLY	CA-C-N	5.60	132.23	121.54
1	A	193	GLY	C-N-CA	5.60	132.23	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	ARG	Sidechain
1	A	394	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3557	0	3505	87	0
2	A	12	0	12	0	0
3	A	23	0	12	1	0
4	A	31	0	13	2	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	125	0	0	1	0
All	All	3750	0	3542	88	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 12.

All (88) 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)
1:A:194:ASP:HB3	1:A:195:PHE:CA	1.64	1.23
1:A:194:ASP:CB	1:A:195:PHE:HA	1.66	1.21
1:A:195:PHE:CD1	1:A:196:GLU:HB2	1.79	1.16
1:A:106:GLN:HE22	1:A:136:LYS:HE2	1.12	1.14
1:A:394:ARG:HH11	1:A:433:SER:HB3	1.09	1.10
1:A:196:GLU:HA	1:A:196:GLU:OE2	1.55	1.05
1:A:195:PHE:CD1	1:A:196:GLU:N	2.29	1.01
1:A:195:PHE:CD1	1:A:196:GLU:CB	2.49	0.94
1:A:195:PHE:HD1	1:A:196:GLU:HB2	1.15	0.89
1:A:106:GLN:NE2	1:A:136:LYS:HE2	1.88	0.88
1:A:112:GLU:H	1:A:112:GLU:CD	1.82	0.87
1:A:228:THR:H	4:A:600:ANP:HNB1	1.22	0.86
1:A:394:ARG:NH1	1:A:433:SER:HB3	1.90	0.86
1:A:195:PHE:CE1	1:A:196:GLU:CB	2.60	0.84
1:A:194:ASP:HB3	1:A:195:PHE:HA	0.87	0.84
1:A:394:ARG:HH11	1:A:433:SER:CB	1.90	0.84
1:A:195:PHE:HE1	1:A:196:GLU:CG	1.94	0.80
1:A:195:PHE:CD1	1:A:196:GLU:CA	2.64	0.80
1:A:41:MET:HE1	1:A:389:VAL:HG22	1.64	0.78
1:A:85:ARG:NH1	1:A:107:MET:HE3	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:PHE:CG	1:A:196:GLU:N	2.52	0.76
1:A:195:PHE:CE1	1:A:196:GLU:HB2	2.19	0.71
1:A:195:PHE:CE1	1:A:196:GLU:CG	2.74	0.71
1:A:195:PHE:CE1	1:A:196:GLU:OE2	2.46	0.68
1:A:194:ASP:HB3	1:A:195:PHE:CB	2.23	0.67
1:A:228:THR:HG22	1:A:296:LYS:HB2	1.80	0.64
1:A:394:ARG:NH1	1:A:433:SER:CB	2.56	0.64
1:A:224:MET:HE1	1:A:423:PHE:CZ	2.32	0.64
1:A:13:LYS:O	1:A:17:GLU:HG2	1.98	0.63
1:A:195:PHE:CE1	1:A:196:GLU:CD	2.76	0.63
1:A:394:ARG:NH1	1:A:400:ASP:O	2.32	0.62
1:A:194:ASP:N	1:A:195:PHE:HB2	2.14	0.62
3:A:501:MRK:O8	3:A:501:MRK:S1	2.58	0.61
1:A:195:PHE:CE1	1:A:196:GLU:CA	2.85	0.60
1:A:195:PHE:HE1	1:A:196:GLU:CD	2.10	0.60
1:A:193:GLY:C	1:A:195:PHE:HB2	2.26	0.59
1:A:43:ARG:HD2	7:A:580:HOH:O	2.03	0.59
1:A:195:PHE:CD1	1:A:195:PHE:C	2.83	0.56
1:A:5:ASN:OD1	1:A:8:PHE:CE1	2.58	0.56
1:A:194:ASP:CG	1:A:195:PHE:HA	2.34	0.53
1:A:12:LYS:O	1:A:16:VAL:HG23	2.10	0.51
1:A:64:SER:HB3	1:A:250:ARG:HB2	1.92	0.51
1:A:229:GLY:N	4:A:600:ANP:O1G	2.34	0.51
1:A:85:ARG:HH11	1:A:107:MET:HE3	1.75	0.50
1:A:194:ASP:CA	1:A:195:PHE:HB2	2.41	0.50
1:A:228:THR:CG2	1:A:296:LYS:HB2	2.41	0.50
1:A:194:ASP:CB	1:A:195:PHE:CA	2.40	0.50
1:A:195:PHE:HE1	1:A:196:GLU:HG2	1.73	0.50
1:A:75:LEU:O	1:A:146:LEU:HD12	2.11	0.49
1:A:5:ASN:OD1	1:A:8:PHE:CD1	2.66	0.49
1:A:94:GLY:O	1:A:98:GLN:HB3	2.13	0.49
1:A:224:MET:HE1	1:A:423:PHE:CE1	2.49	0.48
1:A:85:ARG:NH1	1:A:107:MET:CE	2.76	0.48
1:A:322:GLU:O	1:A:326:THR:HG22	2.13	0.47
1:A:322:GLU:O	1:A:326:THR:CG2	2.63	0.47
1:A:75:LEU:HD23	1:A:146:LEU:HD13	1.96	0.47
1:A:337:GLN:HE21	1:A:351:ILE:HD11	1.80	0.47
1:A:64:SER:HA	1:A:235:MET:HE2	1.96	0.47
1:A:190:LYS:HA	1:A:195:PHE:CE2	2.49	0.47
1:A:83:ASN:HD22	1:A:109:SER:HA	1.80	0.47
1:A:112:GLU:CD	1:A:112:GLU:N	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:PHE:CE1	1:A:196:GLU:HA	2.50	0.46
1:A:46[A]:ARG:HB2	1:A:49:THR:OG1	2.15	0.46
1:A:424:HIS:O	1:A:428:ARG:HG3	2.15	0.46
1:A:44:GLY:O	1:A:50:HIS:HD2	2.00	0.45
1:A:420:LYS:HG2	1:A:424:HIS:CE1	2.51	0.45
1:A:189:ILE:HG22	1:A:195:PHE:CD2	2.51	0.45
1:A:63:ARG:O	1:A:64:SER:O	2.35	0.45
1:A:338:VAL:HG13	1:A:348:ILE:HG12	1.98	0.45
1:A:154:VAL:HG11	1:A:202:MET:HE3	1.99	0.44
1:A:308:ARG:O	1:A:312:GLU:HG2	2.18	0.43
1:A:41:MET:HE2	1:A:57:MET:HE1	2.00	0.43
1:A:172:LYS:HE3	1:A:282:ALA:HB1	1.99	0.43
1:A:137:HIS:O	1:A:138:GLN:C	2.61	0.43
1:A:190:LYS:HA	1:A:195:PHE:HE2	1.84	0.43
1:A:215:TYR:CE1	1:A:451:LEU:HD13	2.54	0.42
1:A:315:LEU:HD13	1:A:316:PHE:CE2	2.54	0.42
1:A:244:VAL:HG11	1:A:251:MET:HE1	2.02	0.42
1:A:172:LYS:O	1:A:173:ALA:C	2.62	0.41
1:A:194:ASP:CA	1:A:195:PHE:CB	2.99	0.41
1:A:64:SER:HB3	1:A:250:ARG:CB	2.51	0.41
1:A:77:LEU:HD21	1:A:146:LEU:HD11	2.03	0.41
1:A:195:PHE:CZ	1:A:196:GLU:OE2	2.74	0.41
1:A:75:LEU:HD23	1:A:146:LEU:CD1	2.51	0.41
1:A:131:SER:OG	1:A:140:LYS:HE3	2.21	0.41
1:A:257:TRP:CD1	1:A:257:TRP:C	2.99	0.40
1:A:65:THR:HA	1:A:66:PRO:HD3	1.90	0.40
1:A:92:GLY:HA3	1:A:99:TRP:CZ2	2.56	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	A	449/470 (96%)	433 (96%)	10 (2%)	6 (1%)	9	14

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	SER
1	A	194	ASP
1	A	138	GLN
1	A	141	HIS
1	A	136	LYS
1	A	80	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	A	390/403 (97%)	353 (90%)	37 (10%)	8	13

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	47	LEU
1	A	70	GLU
1	A	82	THR
1	A	89	VAL
1	A	98	GLN
1	A	102	LYS
1	A	112	GLU
1	A	131	SER
1	A	132	ASP
1	A	138	GLN
1	A	140	LYS
1	A	141	HIS
1	A	143	LYS
1	A	166	ASN

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Mol	Chain	Res	Type
1	A	192	ARG
1	A	196	GLU
1	A	197	MET
1	A	209	THR
1	A	243	LEU
1	A	245	GLU
1	A	248	GLU
1	A	250	ARG
1	A	263	SER
1	A	271	LEU
1	A	304	LEU
1	A	307	LEU
1	A	309	LEU
1	A	315	LEU
1	A	326	THR
1	A	346	LYS
1	A	353	SER
1	A	361	THR
1	A	386	LEU
1	A	399	GLU
1	A	439	ILE
1	A	442	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	50	HIS
1	A	83	ASN
1	A	106	GLN
1	A	141	HIS
1	A	180	ASN
1	A	313	ASN
1	A	323	GLN
1	A	337	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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$
4	ANP	A	600	5	33,33,33	1.42	4 (12%)	45,52,52	2.20	14 (31%)
3	MRK	A	501	-	25,25,25	4.48	8 (32%)	33,35,35	3.29	9 (27%)
2	GLC	A	500	-	12,12,12	0.59	0	17,17,17	0.65	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
4	ANP	A	600	5	-	6/18/38/38	0/3/3/3
3	MRK	A	501	-	-	2/12/12/12	0/3/3/3
2	GLC	A	500	-	-	0/2/22/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	MRK	C21-C20	14.39	1.67	1.35
3	A	501	MRK	C20-N19	13.03	1.62	1.38
3	A	501	MRK	C12-S16	-6.85	1.70	1.77
3	A	501	MRK	C18-S16	-5.60	1.66	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	ANP	PB-O1B	4.48	1.53	1.46
3	A	501	MRK	C21-N17	-4.33	1.29	1.37
3	A	501	MRK	C5-N4	2.38	1.35	1.31
3	A	501	MRK	C3-C2	2.29	1.39	1.34
4	A	600	ANP	C8-N7	2.27	1.36	1.31
4	A	600	ANP	PG-O1G	2.25	1.49	1.46
3	A	501	MRK	C18-N17	-2.14	1.34	1.36
4	A	600	ANP	PG-O2G	-2.12	1.51	1.56

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	MRK	C21-C20-N19	-15.63	90.28	110.74
4	A	600	ANP	C5-C4-N3	-5.43	119.24	126.72
4	A	600	ANP	N3-C2-N1	-5.20	120.71	128.58
3	A	501	MRK	S16-C18-N19	-5.18	122.38	124.96
4	A	600	ANP	O1G-PG-N3B	-4.95	104.48	111.77
4	A	600	ANP	O2B-PB-O1B	4.29	119.06	109.87
3	A	501	MRK	C9-C10-C7	4.23	123.24	120.14
4	A	600	ANP	O1B-PB-N3B	-4.19	105.60	111.77
4	A	600	ANP	C2-N3-C4	3.96	121.50	111.83
3	A	501	MRK	C21-N17-C18	3.75	112.61	106.81
4	A	600	ANP	N9-C8-N7	-3.58	108.86	113.94
4	A	600	ANP	C4-C5-N7	-3.56	106.51	110.58
3	A	501	MRK	C22-N17-C21	-3.33	119.57	125.11
4	A	600	ANP	C5-N7-C8	3.02	108.20	103.45
4	A	600	ANP	N3-C4-N9	2.98	132.23	127.17
3	A	501	MRK	C15-C13-C12	-2.62	119.30	122.98
3	A	501	MRK	C20-C21-N17	2.59	108.81	106.46
4	A	600	ANP	C5-C4-N9	2.49	108.53	105.81
3	A	501	MRK	F14-C13-C12	2.46	122.11	118.40
4	A	600	ANP	O4'-C1'-N9	2.23	112.38	108.09
4	A	600	ANP	C3'-C2'-C1'	2.17	105.58	101.46
3	A	501	MRK	C2-S1-C5	-2.13	87.64	90.07
4	A	600	ANP	C4-N9-C8	2.06	107.90	105.74

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	MRK	C11-C12-S16-C18
3	A	501	MRK	C13-C12-S16-C18

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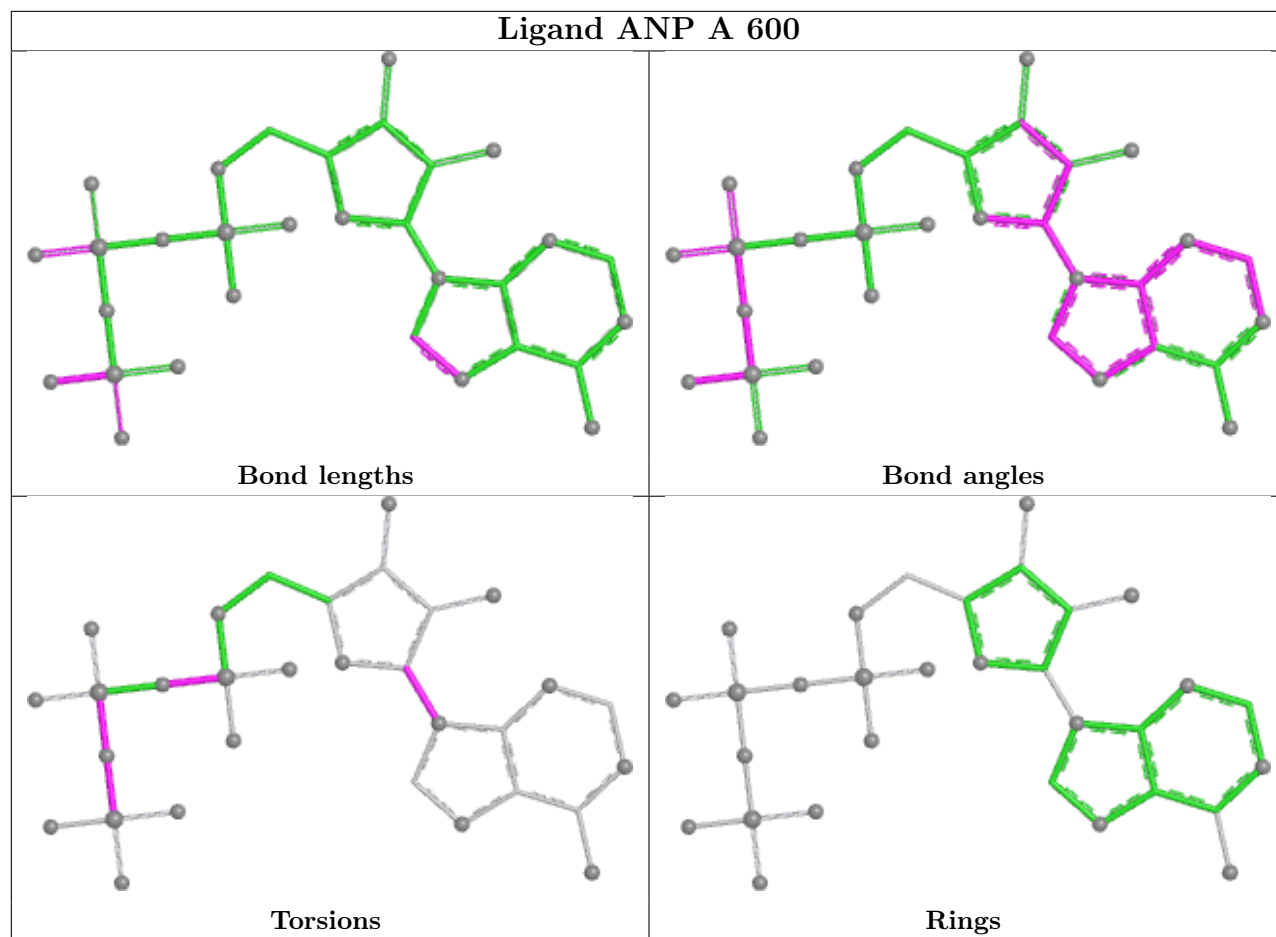
Mol	Chain	Res	Type	Atoms
4	A	600	ANP	PB-N3B-PG-O1G
4	A	600	ANP	PG-N3B-PB-O1B
4	A	600	ANP	PG-N3B-PB-O3A
4	A	600	ANP	C2'-C1'-N9-C8
4	A	600	ANP	O4'-C1'-N9-C8
4	A	600	ANP	PB-O3A-PA-O1A

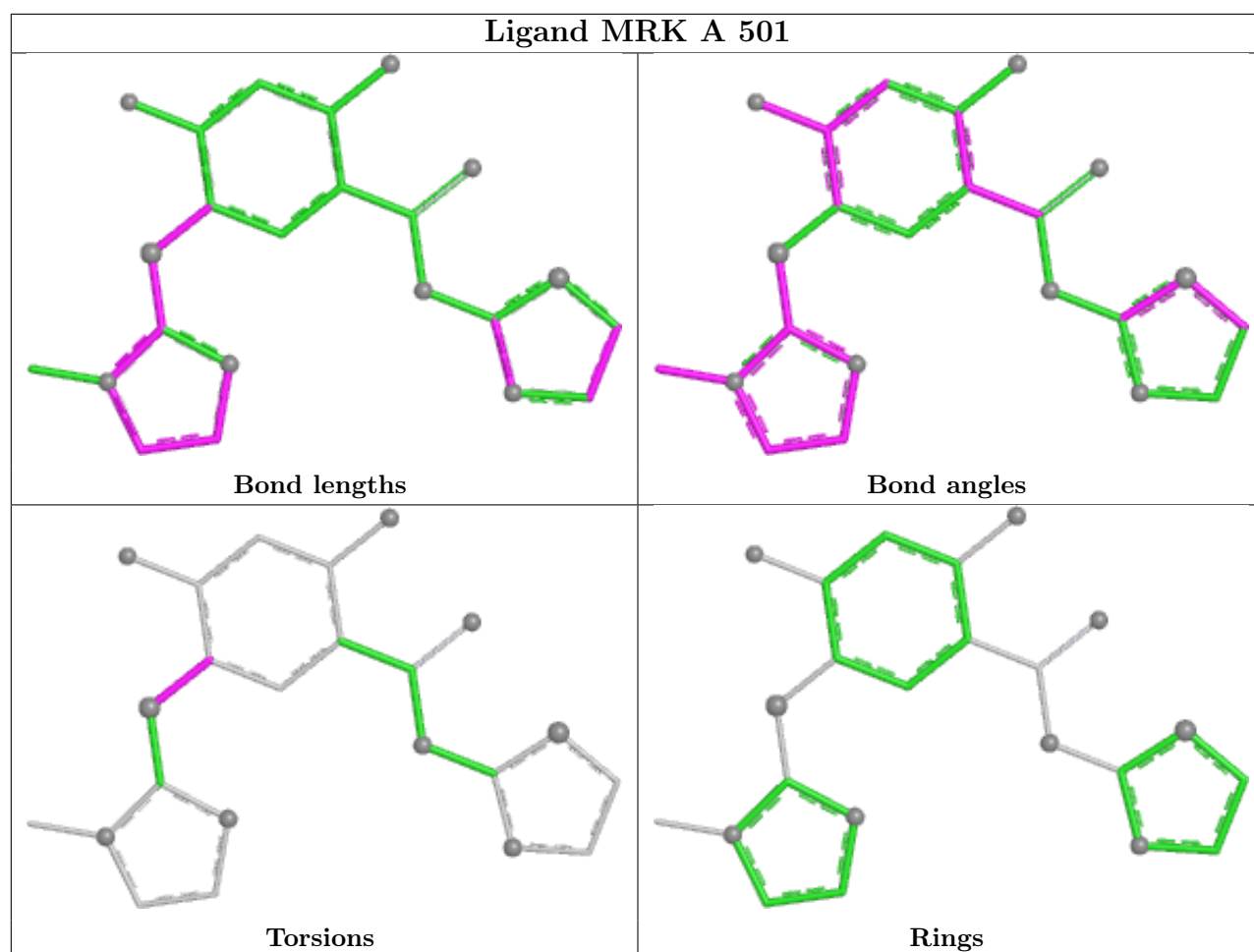
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	ANP	2	0
3	A	501	MRK	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 [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	A	450/470 (95%)	0.03	17 (3%)	44 40	15, 31, 52, 65	3 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	ASP	3.2
1	A	139	MET	3.0
1	A	68	GLY	3.0
1	A	195	PHE	3.0
1	A	6	LEU	2.9
1	A	94	GLY	2.8
1	A	64	SER	2.5
1	A	193	GLY	2.5
1	A	66	PRO	2.4
1	A	70	GLU	2.4
1	A	82	THR	2.3
1	A	141	HIS	2.3
1	A	69	SER	2.2
1	A	215	TYR	2.2
1	A	196	GLU	2.2
1	A	5	ASN	2.1
1	A	313	ASN	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](#)

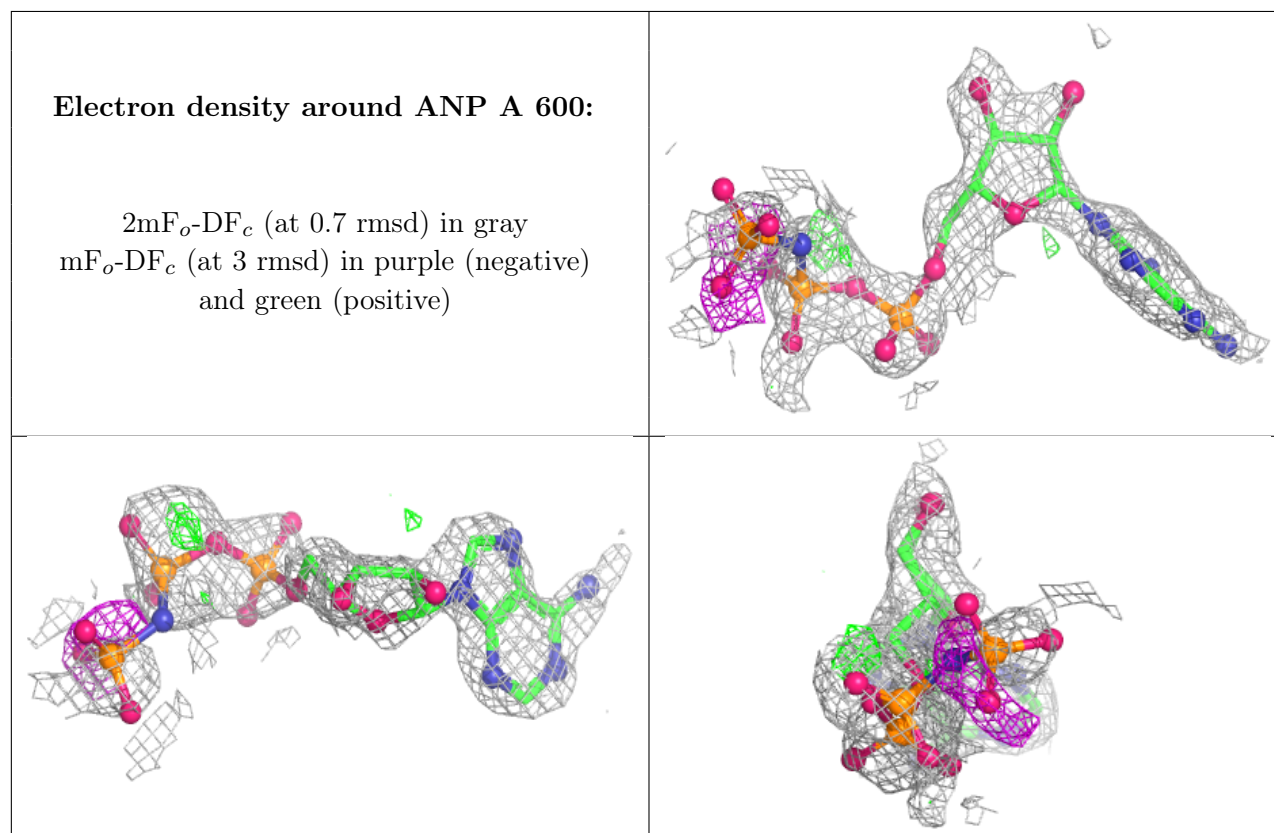
There are no oligosaccharides in this entry.

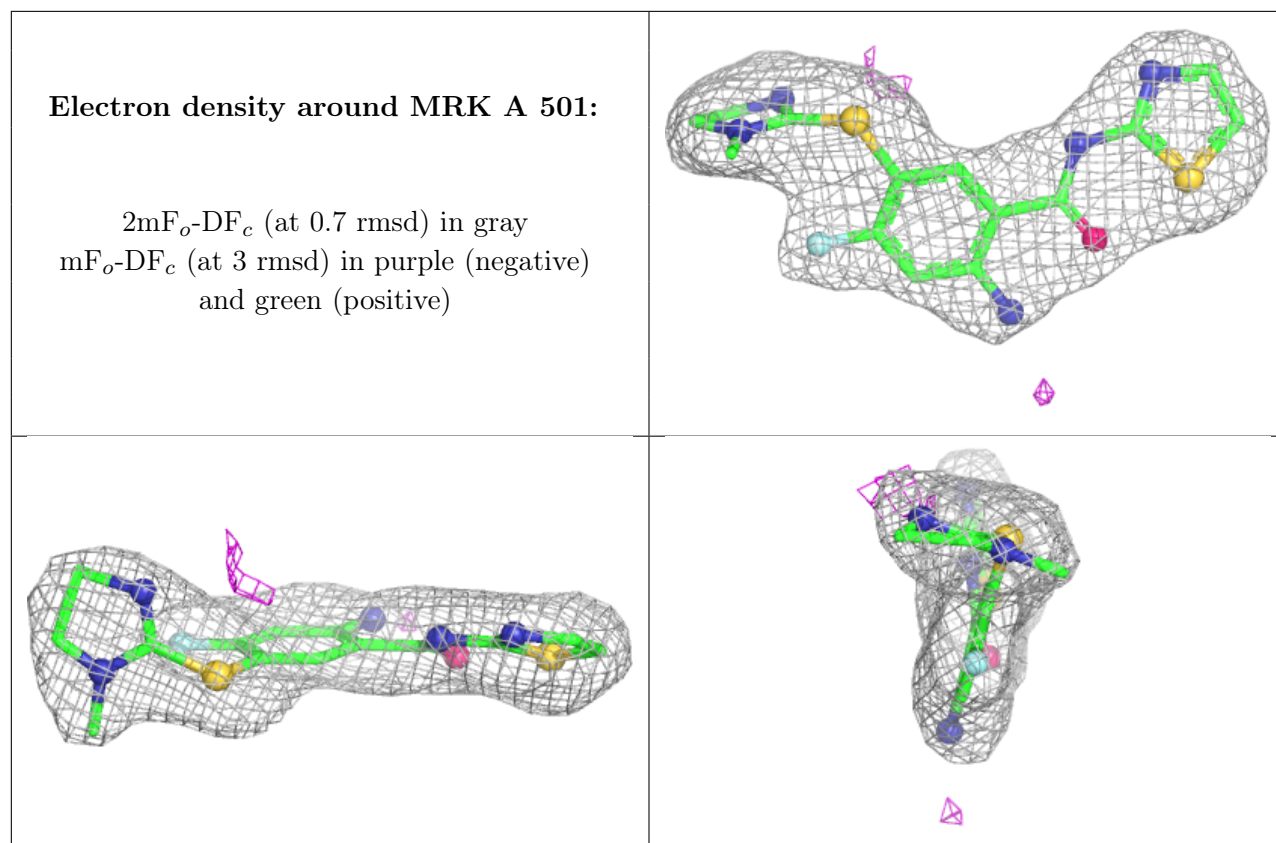
6.4 Ligands ⓘ

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, 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
4	ANP	A	600	31/31	0.75	0.19	19,28,35,35	31
5	MG	A	700	1/1	0.88	0.10	42,42,42,42	0
3	MRK	A	501	23/23	0.94	0.08	32,35,38,39	0
2	GLC	A	500	12/12	0.96	0.07	16,20,21,24	0
6	K	A	800	1/1	0.99	0.03	27,27,27,27	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.