



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:10 PM UTC

PDB ID : 9SQJ / pdb_00009sqj
Title : Crystal Structure of the MurT/GatD Enzyme Complex from *Streptococcus pyogenes* with bound AMPPNP
Authors : Voelpel, S.V.; Stehle, T.
Deposited on : 2025-09-22
Resolution : 1.98 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

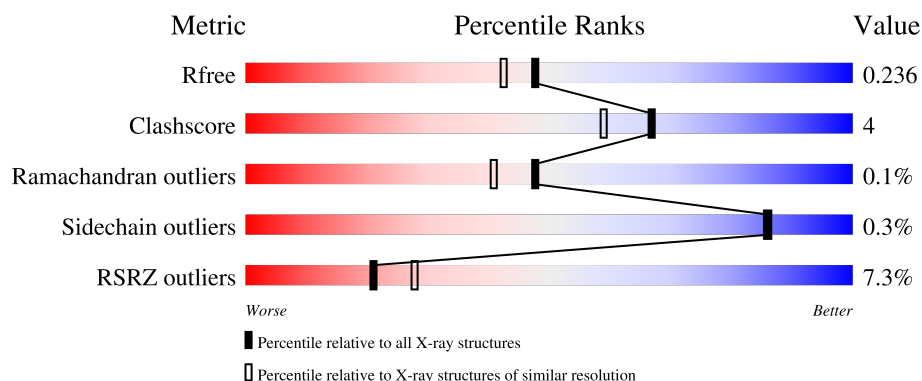
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	AAA	438	
1	BBB	438	
2	CCC	263	
2	DDD	263	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11032 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 Lipid II isoglutaminy synthase (glutamine-hydrolyzing) subunit MurT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	398	Total	C	N	O	S	0	4	0
			3079	1971	505	592	11			
1	BBB	406	Total	C	N	O	S	0	3	0
			3143	2011	514	605	13			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-21	HIS	-	expression tag	UNP A0A8B6J667
AAA	-20	HIS	-	expression tag	UNP A0A8B6J667
AAA	-19	HIS	-	expression tag	UNP A0A8B6J667
AAA	-18	HIS	-	expression tag	UNP A0A8B6J667
AAA	-17	HIS	-	expression tag	UNP A0A8B6J667
AAA	-16	HIS	-	expression tag	UNP A0A8B6J667
AAA	-15	PRO	-	expression tag	UNP A0A8B6J667
AAA	-14	MET	-	expression tag	UNP A0A8B6J667
AAA	-13	SER	-	expression tag	UNP A0A8B6J667
AAA	-12	ASP	-	expression tag	UNP A0A8B6J667
AAA	-11	TYR	-	expression tag	UNP A0A8B6J667
AAA	-10	ASP	-	expression tag	UNP A0A8B6J667
AAA	-9	ILE	-	expression tag	UNP A0A8B6J667
AAA	-8	PRO	-	expression tag	UNP A0A8B6J667
AAA	-7	THR	-	expression tag	UNP A0A8B6J667
AAA	-6	THR	-	expression tag	UNP A0A8B6J667
AAA	-5	GLU	-	expression tag	UNP A0A8B6J667
AAA	-4	ASN	-	expression tag	UNP A0A8B6J667
AAA	-3	LEU	-	expression tag	UNP A0A8B6J667
AAA	-2	TYR	-	expression tag	UNP A0A8B6J667
AAA	-1	PHE	-	expression tag	UNP A0A8B6J667
AAA	0	GLN	-	expression tag	UNP A0A8B6J667
AAA	1	GLY	-	expression tag	UNP A0A8B6J667
AAA	2	ALA	-	expression tag	UNP A0A8B6J667

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	3	MET	-	expression tag	UNP A0A8B6J667
AAA	184	ARG	HIS	conflict	UNP A0A8B6J667
BBB	-21	HIS	-	expression tag	UNP A0A8B6J667
BBB	-20	HIS	-	expression tag	UNP A0A8B6J667
BBB	-19	HIS	-	expression tag	UNP A0A8B6J667
BBB	-18	HIS	-	expression tag	UNP A0A8B6J667
BBB	-17	HIS	-	expression tag	UNP A0A8B6J667
BBB	-16	HIS	-	expression tag	UNP A0A8B6J667
BBB	-15	PRO	-	expression tag	UNP A0A8B6J667
BBB	-14	MET	-	expression tag	UNP A0A8B6J667
BBB	-13	SER	-	expression tag	UNP A0A8B6J667
BBB	-12	ASP	-	expression tag	UNP A0A8B6J667
BBB	-11	TYR	-	expression tag	UNP A0A8B6J667
BBB	-10	ASP	-	expression tag	UNP A0A8B6J667
BBB	-9	ILE	-	expression tag	UNP A0A8B6J667
BBB	-8	PRO	-	expression tag	UNP A0A8B6J667
BBB	-7	THR	-	expression tag	UNP A0A8B6J667
BBB	-6	THR	-	expression tag	UNP A0A8B6J667
BBB	-5	GLU	-	expression tag	UNP A0A8B6J667
BBB	-4	ASN	-	expression tag	UNP A0A8B6J667
BBB	-3	LEU	-	expression tag	UNP A0A8B6J667
BBB	-2	TYR	-	expression tag	UNP A0A8B6J667
BBB	-1	PHE	-	expression tag	UNP A0A8B6J667
BBB	0	GLN	-	expression tag	UNP A0A8B6J667
BBB	1	GLY	-	expression tag	UNP A0A8B6J667
BBB	2	ALA	-	expression tag	UNP A0A8B6J667
BBB	3	MET	-	expression tag	UNP A0A8B6J667
BBB	184	ARG	HIS	conflict	UNP A0A8B6J667

- Molecule 2 is a protein called Lipid II isoglutaminyll synthase (glutamine-hydrolyzing) subunit GatD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	CCC	256	Total	C	N	O	S	0	2	0
			2018	1283	335	396	4			
2	DDD	248	Total	C	N	O	S	0	7	0
			1995	1267	333	390	5			

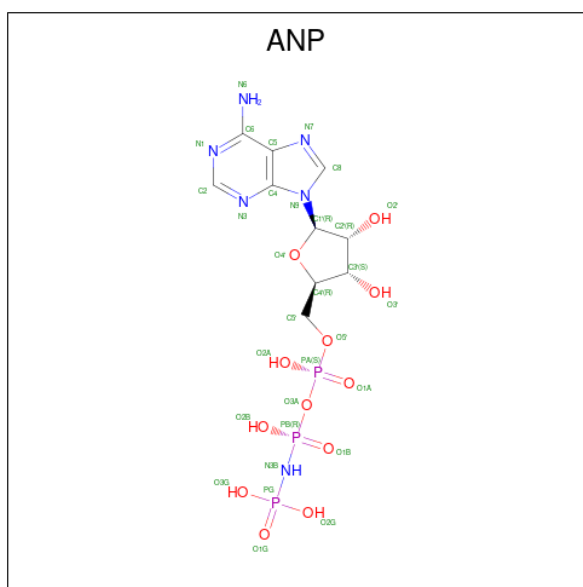
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total	Zn	0	0
			1	1		
3	BBB	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Mg	0	0
			1	1		
4	BBB	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	AAA	1	Total 31	C 10	N 6	O 12	P 3	0	0
5	BBB	1	Total 31	C 10	N 6	O 12	P 3	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AAA	1	Total	C	O	0	0
			6	3	3		
6	BBB	1	Total	C	O	0	0
			6	3	3		

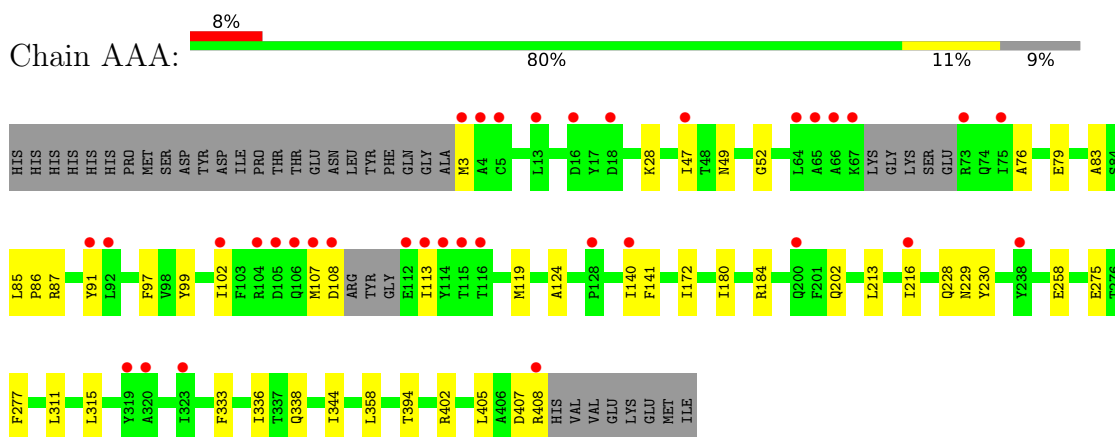
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	193	Total	O	0	0
			193	193		
7	CCC	175	Total	O	0	0
			175	175		
7	BBB	165	Total	O	0	0
			165	165		
7	DDD	186	Total	O	0	0
			186	186		

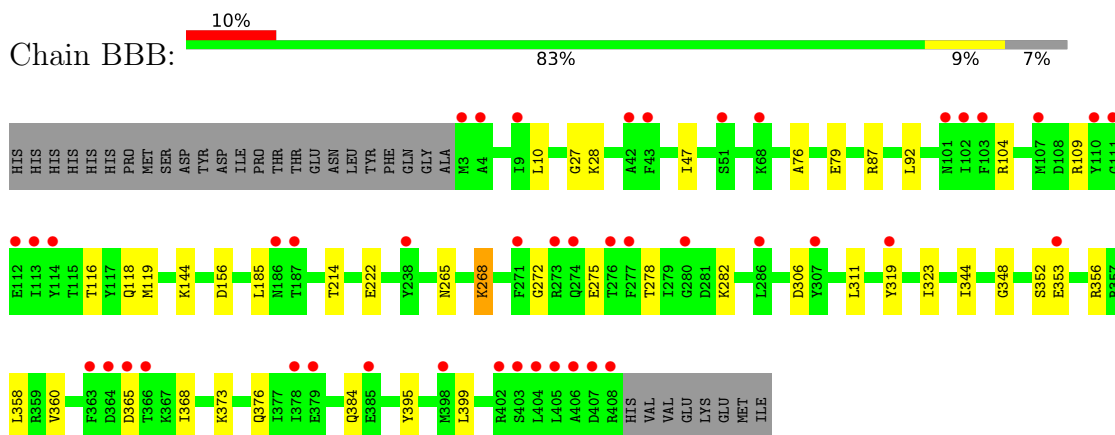
3 Residue-property plots [i](#)

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.

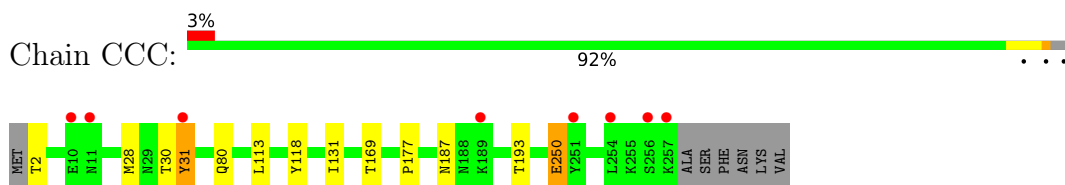
- Molecule 1: Lipid II isoglutaminy synthase (glutamine-hydrolyzing) subunit MurT



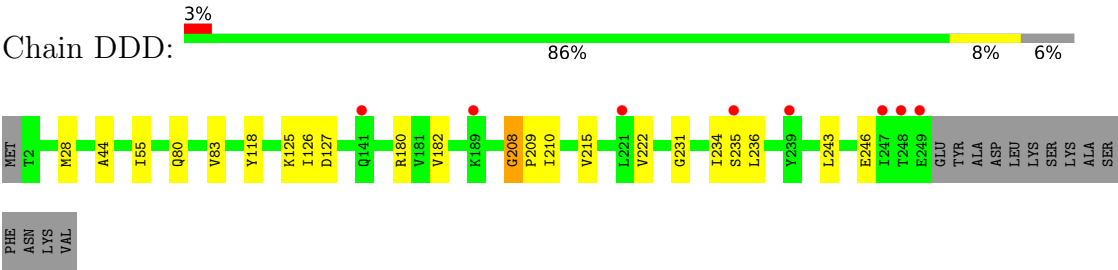
- Molecule 1: Lipid II isoglutaminy synthase (glutamine-hydrolyzing) subunit MurT



- Molecule 2: Lipid II isoglutaminy synthase (glutamine-hydrolyzing) subunit GatD



- Molecule 2: Lipid II isoglutaminy synthase (glutamine-hydrolyzing) subunit GatD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.29Å 101.21Å 177.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.11 – 1.98 49.11 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.11-1.98) 99.6 (49.11-1.98)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0258, PHENIX 1.16_3549	Depositor
R, R_{free}	0.180 , 0.217 0.190 , 0.236	Depositor DCC
R_{free} test set	1547 reflections (1.40%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11032	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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: ZN, MG, ANP, GOL

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	AAA	1.06	0/3134	1.34	2/4263 (0.0%)
1	BBB	1.04	0/3202	1.34	6/4352 (0.1%)
2	CCC	1.07	0/2059	1.28	2/2788 (0.1%)
2	DDD	1.03	1/2035 (0.0%)	1.26	1/2756 (0.0%)
All	All	1.05	1/10430 (0.0%)	1.32	11/14159 (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	BBB	0	1
2	CCC	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	55	ILE	C-O	5.18	1.29	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	250	GLU	CB-CA-C	-6.69	100.41	109.71
1	BBB	348	GLY	CA-C-O	-5.81	117.22	122.57
1	BBB	156	ASP	CA-CB-CG	-5.67	106.93	112.60
2	DDD	182	VAL	N-CA-C	-5.62	106.22	111.45
1	AAA	49	ASN	CA-CB-CG	5.59	118.19	112.60
1	AAA	229	ASN	CB-CA-C	-5.54	100.39	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	272	GLY	CA-C-O	-5.50	118.18	122.52
1	BBB	268	LYS	CB-CA-C	-5.44	101.44	110.68
1	BBB	306	ASP	CA-CB-CG	5.25	117.85	112.60
2	CCC	2	THR	CA-CB-OG1	-5.08	101.98	109.60
1	BBB	10	LEU	CA-C-O	-5.07	115.47	120.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	BBB	352	SER	Mainchain
2	CCC	30	THR	Mainchain
2	CCC	31[A]	TYR	Mainchain

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	AAA	3079	0	3018	31	1
1	BBB	3143	0	3099	23	1
2	CCC	2018	0	1928	7	0
2	DDD	1995	0	1904	15	0
3	AAA	1	0	0	0	0
3	BBB	1	0	0	0	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	0	0
5	AAA	31	0	13	0	0
5	BBB	31	0	13	1	0
6	AAA	6	0	8	0	0
6	BBB	6	0	8	0	0
7	AAA	193	0	0	1	0
7	BBB	165	0	0	2	0
7	CCC	175	0	0	2	0
7	DDD	186	0	0	2	0
All	All	11032	0	9991	75	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 4.

All (75) 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:AAA:213:LEU:HD22	1:AAA:216:ILE:HD11	1.45	0.97
1:AAA:275:GLU:OE1	1:AAA:402:ARG:HD3	1.80	0.81
1:BBB:116:THR:HA	1:BBB:119:MET:HE2	1.66	0.76
1:AAA:83:ALA:HA	1:AAA:119:MET:HE3	1.72	0.70
2:CCC:250:GLU:OE2	7:CCC:301:HOH:O	2.09	0.70
1:AAA:102:ILE:HB	1:AAA:140[B]:ILE:CD1	2.25	0.66
1:AAA:407:ASP:O	1:AAA:408:ARG:HG3	1.97	0.65
1:AAA:83:ALA:CA	1:AAA:119:MET:HE3	2.30	0.62
1:BBB:118:GLN:OE1	1:BBB:144:LYS:NZ	2.32	0.60
2:DDD:215[A]:VAL:HG11	2:DDD:246:GLU:HG2	1.82	0.60
2:DDD:28[A]:MET:SD	2:DDD:80:GLN:HG2	2.41	0.60
1:BBB:265:ASN:HA	1:BBB:268:LYS:HD3	1.83	0.59
2:DDD:28[A]:MET:HE1	2:DDD:80:GLN:HA	1.85	0.59
2:CCC:250:GLU:HG2	7:CCC:345:HOH:O	2.05	0.56
1:AAA:102:ILE:HB	1:AAA:140[B]:ILE:HD11	1.89	0.55
1:AAA:140[B]:ILE:HD11	1:AAA:141:PHE:CE1	2.43	0.54
1:AAA:228:GLN:HG2	1:AAA:230:TYR:CZ	2.43	0.53
1:AAA:338[A]:GLN:OE1	2:DDD:180:ARG:HD2	2.08	0.53
1:AAA:28:LYS:HB3	1:AAA:79:GLU:HG3	1.90	0.53
2:CCC:28:MET:HE1	2:CCC:80:GLN:HG3	1.91	0.52
1:AAA:344:ILE:HG21	1:AAA:358:LEU:HD13	1.93	0.51
1:AAA:184:ARG:HH22	1:AAA:202:GLN:NE2	2.09	0.50
1:AAA:113:ILE:HD12	1:AAA:140[A]:ILE:HD12	1.93	0.50
1:BBB:47:ILE:HD12	1:BBB:47:ILE:N	2.26	0.49
1:BBB:104:ARG:HG2	7:BBB:667:HOH:O	2.12	0.49
2:DDD:234:ILE:HD12	2:DDD:236:LEU:HD21	1.96	0.48
1:AAA:277:PHE:CE2	1:AAA:405:LEU:HD11	2.50	0.47
2:DDD:125:LYS:NZ	2:DDD:127:ASP:OD1	2.47	0.47
1:AAA:102:ILE:HB	1:AAA:140[B]:ILE:HD12	1.97	0.47
1:AAA:87:ARG:HD2	1:AAA:91:TYR:OH	2.15	0.47
1:AAA:113:ILE:HD12	1:AAA:140[A]:ILE:CD1	2.45	0.46
1:BBB:28:LYS:HB3	1:BBB:79:GLU:HG3	1.98	0.46
2:DDD:28[A]:MET:HE2	2:DDD:83:VAL:HG21	1.97	0.46
1:AAA:172:ILE:HD13	1:AAA:180[A]:ILE:HG23	1.98	0.46
2:DDD:208:GLY:N	2:DDD:209:PRO:HA	2.31	0.46
2:DDD:215[B]:VAL:HG11	2:DDD:243:LEU:HD22	1.98	0.46
1:AAA:52:GLY:HA2	7:AAA:607:HOH:O	2.15	0.46
1:AAA:97:PHE:CE2	1:AAA:124:ALA:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:258:GLU:H	1:AAA:258:GLU:CD	2.24	0.45
1:BBB:116:THR:HA	1:BBB:119:MET:CE	2.43	0.45
1:BBB:356:ARG:O	1:BBB:360:VAL:HG13	2.16	0.45
1:BBB:319:TYR:HA	1:BBB:323:ILE:CD1	2.46	0.45
1:BBB:27:GLY:H	5:BBB:503:ANP:H5'1	1.81	0.45
1:AAA:85:LEU:N	1:AAA:86:PRO:CD	2.80	0.44
1:BBB:92:LEU:C	1:BBB:92:LEU:HD12	2.42	0.44
1:BBB:311:LEU:O	1:BBB:344:ILE:HA	2.17	0.44
1:BBB:282:LYS:NZ	1:BBB:384:GLN:O	2.46	0.44
1:AAA:333:PHE:O	1:AAA:336:ILE:HG12	2.18	0.44
2:DDD:28[A]:MET:HE1	2:DDD:80:GLN:HG2	1.99	0.44
1:AAA:83:ALA:N	1:AAA:119:MET:HE3	2.33	0.44
1:BBB:214[A]:THR:OG1	1:BBB:222:GLU:HB2	2.18	0.43
1:BBB:344:ILE:HG21	1:BBB:358:LEU:HD13	2.00	0.43
1:AAA:47:ILE:O	1:AAA:76:ALA:HA	2.18	0.43
2:CCC:177:PRO:HB3	2:CCC:193:THR:HB	2.00	0.43
1:AAA:107:MET:O	1:AAA:108:ASP:C	2.61	0.43
2:CCC:113:LEU:HD21	2:CCC:118:TYR:HE1	1.83	0.43
1:BBB:395:TYR:CE2	1:BBB:399:LEU:HD11	2.54	0.43
2:DDD:235:SER:O	7:DDD:301:HOH:O	2.21	0.43
1:AAA:213:LEU:CD2	1:AAA:216:ILE:HD11	2.33	0.42
1:AAA:315:LEU:HD12	1:AAA:394:THR:HG21	2.01	0.42
1:BBB:278:THR:HA	1:BBB:282:LYS:O	2.20	0.42
2:DDD:44:ALA:HA	2:DDD:222:VAL:HG11	2.01	0.42
2:DDD:231:GLY:O	2:DDD:234:ILE:HG12	2.19	0.42
1:BBB:365:ASP:HA	1:BBB:368:ILE:HD12	2.02	0.42
1:AAA:311:LEU:O	1:AAA:344:ILE:HA	2.19	0.42
2:CCC:169:THR:O	2:CCC:187:ASN:HB3	2.20	0.41
1:BBB:373:LYS:HB2	1:BBB:376:GLN:HE21	1.84	0.41
1:AAA:99:TYR:HB3	1:AAA:141:PHE:CZ	2.55	0.41
1:BBB:109:ARG:HD3	7:BBB:658:HOH:O	2.20	0.41
1:BBB:319:TYR:HA	1:BBB:323:ILE:HD11	2.01	0.41
1:BBB:47:ILE:O	1:BBB:76:ALA:HA	2.21	0.41
2:DDD:210:ILE:HA	7:DDD:404:HOH:O	2.20	0.41
2:DDD:118:TYR:CE1	2:DDD:126:ILE:HB	2.56	0.40
1:BBB:185:LEU:C	1:BBB:185:LEU:HD23	2.46	0.40
2:CCC:131:ILE:O	2:CCC:131:ILE:HG22	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:3:MET:N	1:BBB:275:GLU:OE1[2_555]	2.03	0.17

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	AAA	395/438 (90%)	382 (97%)	13 (3%)	0	100	100
1	BBB	406/438 (93%)	392 (97%)	14 (3%)	0	100	100
2	CCC	254/263 (97%)	246 (97%)	8 (3%)	0	100	100
2	DDD	251/263 (95%)	242 (96%)	8 (3%)	1 (0%)	30	20
All	All	1306/1402 (93%)	1262 (97%)	43 (3%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	DDD	208	GLY

5.3.2 Protein sidechains [i](#)

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	AAA	323/374 (86%)	323 (100%)	0	100	100
1	BBB	333/374 (89%)	330 (99%)	3 (1%)	70	67
2	CCC	212/223 (95%)	211 (100%)	1 (0%)	81	79
2	DDD	210/223 (94%)	210 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1078/1194 (90%)	1074 (100%)	4 (0%)	86	82

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	CCC	31[A]	TYR
1	BBB	87	ARG
1	BBB	353[A]	GLU
1	BBB	353[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
5	ANP	BBB	503	4	33,33,33	1.08	5 (15%)	45,52,52	1.01	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	AAA	504	-	5,5,5	0.15	0	5,5,5	0.39	0
6	GOL	BBB	504	-	5,5,5	0.22	0	5,5,5	0.72	0
5	ANP	AAA	503	4	33,33,33	1.20	6 (18%)	45,52,52	1.21	3 (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	ANP	BBB	503	4	-	12/18/38/38	0/3/3/3
6	GOL	AAA	504	-	-	4/4/4/4	-
6	GOL	BBB	504	-	-	1/4/4/4	-
5	ANP	AAA	503	4	-	3/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AAA	503	ANP	PG-O1G	3.30	1.51	1.46
5	BBB	503	ANP	PG-O1G	3.23	1.51	1.46
5	AAA	503	ANP	PB-O1B	3.01	1.50	1.46
5	BBB	503	ANP	PB-O1B	2.86	1.50	1.46
5	BBB	503	ANP	PB-O2B	-2.43	1.50	1.56
5	AAA	503	ANP	PB-O2B	-2.40	1.50	1.56
5	AAA	503	ANP	PA-O3A	2.23	1.61	1.59
5	BBB	503	ANP	PG-O2G	-2.14	1.51	1.56
5	BBB	503	ANP	PG-O3G	-2.13	1.51	1.56
5	AAA	503	ANP	PG-O3G	-2.09	1.51	1.56
5	AAA	503	ANP	PB-O3A	2.03	1.61	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AAA	503	ANP	O2B-PB-O1B	4.35	119.20	109.87
5	BBB	503	ANP	O2B-PB-O1B	4.28	119.06	109.87
5	AAA	503	ANP	O2G-PG-O1G	-4.25	102.78	113.45
5	AAA	503	ANP	O1B-PB-N3B	-3.93	105.98	111.77
5	BBB	503	ANP	O3G-PG-O1G	-2.05	108.32	113.45

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	AAA	503	ANP	PA-O3A-PB-O2B
5	BBB	503	ANP	PB-N3B-PG-O1G
5	BBB	503	ANP	PG-N3B-PB-O1B
5	BBB	503	ANP	C5'-O5'-PA-O2A
5	BBB	503	ANP	C5'-O5'-PA-O3A
6	AAA	504	GOL	O1-C1-C2-O2
6	AAA	504	GOL	O1-C1-C2-C3
5	BBB	503	ANP	O4'-C4'-C5'-O5'
5	BBB	503	ANP	C3'-C4'-C5'-O5'
6	AAA	504	GOL	C1-C2-C3-O3
6	AAA	504	GOL	O2-C2-C3-O3
5	BBB	503	ANP	C2'-C1'-N9-C8
5	AAA	503	ANP	PG-N3B-PB-O3A
5	BBB	503	ANP	C5'-O5'-PA-O1A
5	BBB	503	ANP	PB-O3A-PA-O2A
6	BBB	504	GOL	O2-C2-C3-O3
5	BBB	503	ANP	O4'-C1'-N9-C8
5	BBB	503	ANP	C2'-C1'-N9-C4
5	AAA	503	ANP	PA-O3A-PB-O1B
5	BBB	503	ANP	PB-O3A-PA-O1A

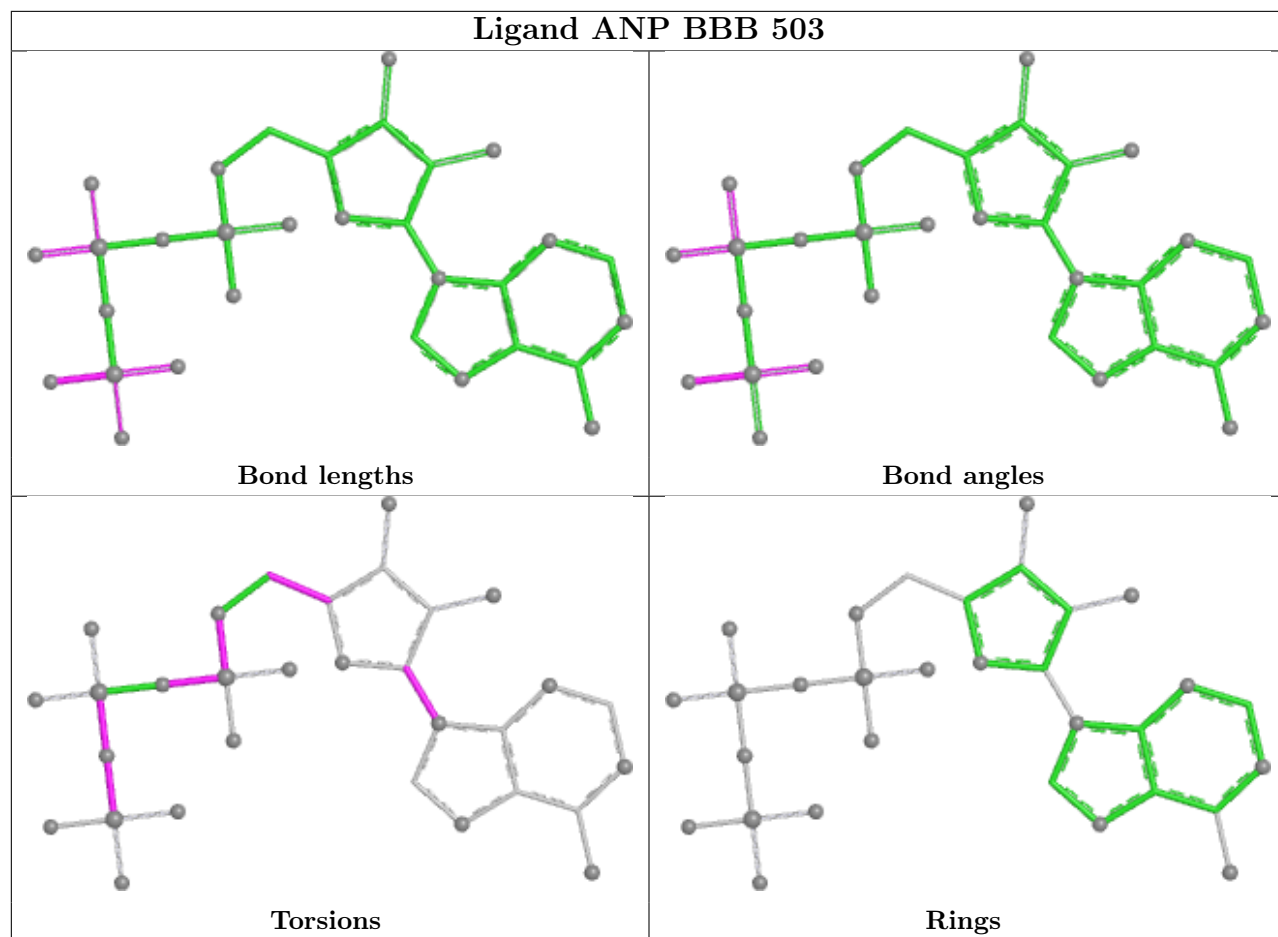
There are no ring outliers.

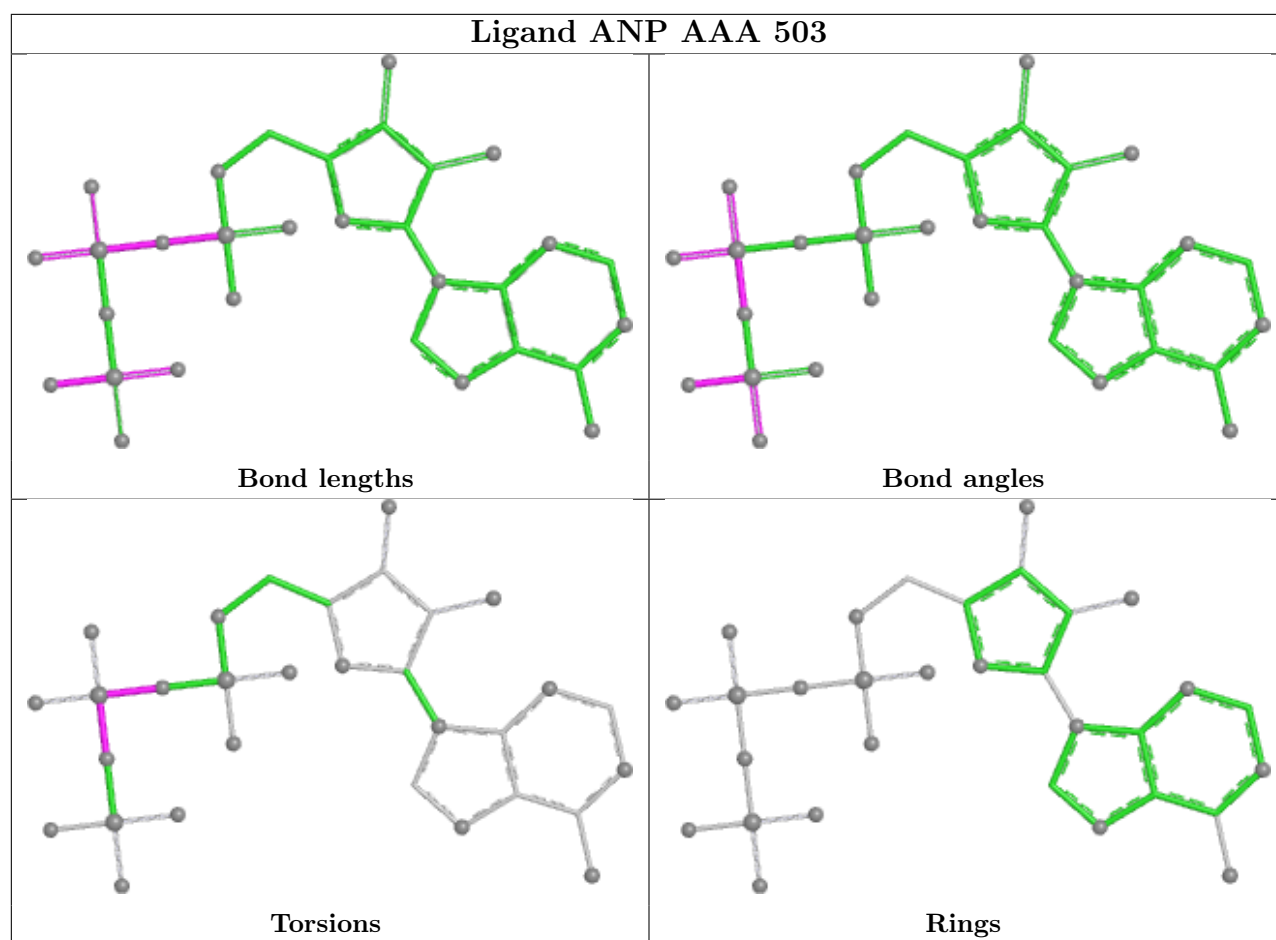
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	BBB	503	ANP	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.

Ligand ANP BBB 503





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	398/438 (90%)	0.75	35 (8%) 15 22	21, 52, 83, 109	3 (0%)
1	BBB	406/438 (92%)	0.80	44 (10%) 11 15	25, 53, 80, 129	2 (0%)
2	CCC	256/263 (97%)	0.28	8 (3%) 51 61	39, 46, 67, 101	1 (0%)
2	DDD	248/263 (94%)	0.35	8 (3%) 50 60	21, 46, 69, 95	5 (2%)
All	All	1308/1402 (93%)	0.60	95 (7%) 21 28	21, 50, 79, 129	11 (0%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	114	TYR	6.5
1	AAA	108	ASP	5.4
1	AAA	92	LEU	5.1
1	BBB	113	ILE	4.8
1	AAA	113	ILE	4.6
2	DDD	247	ILE	4.3
1	AAA	116	THR	4.2
2	CCC	31[A]	TYR	4.1
1	BBB	277	PHE	4.0
1	AAA	107	MET	3.9
1	BBB	114	TYR	3.9
2	DDD	248	THR	3.8
1	BBB	273	ARG	3.7
1	AAA	106	GLN	3.7
1	AAA	216	ILE	3.6
1	AAA	112	GLU	3.6
1	BBB	353[A]	GLU	3.6
1	AAA	64	LEU	3.6
1	BBB	274	GLN	3.5
1	BBB	110	TYR	3.5
1	BBB	112	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	AAA	67	LYS	3.3
1	AAA	4	ALA	3.3
2	CCC	257	LYS	3.2
1	BBB	187	THR	3.1
2	CCC	251	TYR	3.1
1	AAA	73	ARG	3.1
1	BBB	9	ILE	3.1
1	BBB	276	THR	3.1
1	AAA	323	ILE	3.0
1	BBB	364	ASP	3.0
1	AAA	5	CYS	3.0
2	DDD	249	GLU	3.0
2	DDD	239	TYR	2.9
1	BBB	406	ALA	2.9
1	AAA	16	ASP	2.9
2	CCC	256	SER	2.8
2	CCC	254	LEU	2.7
1	AAA	65	ALA	2.7
1	BBB	319	TYR	2.7
1	BBB	102	ILE	2.7
1	BBB	186	ASN	2.7
1	BBB	107	MET	2.6
1	AAA	66	ALA	2.6
1	BBB	404	LEU	2.6
1	AAA	140[A]	ILE	2.6
1	AAA	3	MET	2.5
1	BBB	238	TYR	2.5
1	BBB	307	TYR	2.5
1	AAA	105	ASP	2.5
1	AAA	319	TYR	2.5
2	DDD	221[A]	LEU	2.5
1	AAA	104	ARG	2.4
1	BBB	280	GLY	2.4
1	BBB	271	PHE	2.4
1	BBB	286	LEU	2.4
1	BBB	405	LEU	2.4
1	BBB	3	MET	2.4
1	AAA	320	ALA	2.4
1	BBB	365	ASP	2.4
1	BBB	407	ASP	2.4
1	AAA	408	ARG	2.4
1	AAA	128	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	AAA	47	ILE	2.4
1	BBB	408	ARG	2.4
1	BBB	366	THR	2.3
1	BBB	42	ALA	2.3
2	DDD	235	SER	2.3
1	BBB	402	ARG	2.3
1	AAA	238	TYR	2.3
2	CCC	11	ASN	2.3
1	BBB	4	ALA	2.3
1	AAA	102	ILE	2.3
2	DDD	189	LYS	2.3
1	AAA	18	ASP	2.3
1	BBB	398	MET	2.3
1	AAA	91	TYR	2.3
1	BBB	363	PHE	2.2
2	CCC	189	LYS	2.2
1	AAA	115	THR	2.2
1	BBB	385	GLU	2.2
1	BBB	101	ASN	2.1
1	AAA	75	ILE	2.1
1	BBB	378	ILE	2.1
1	BBB	51	SER	2.1
1	BBB	43	PHE	2.1
1	BBB	111	GLY	2.1
2	CCC	10	GLU	2.1
1	AAA	13	LEU	2.1
1	AAA	200	GLN	2.1
1	BBB	103	PHE	2.1
1	BBB	68	LYS	2.1
1	BBB	379	GLU	2.1
1	BBB	403	SER	2.0
2	DDD	141	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

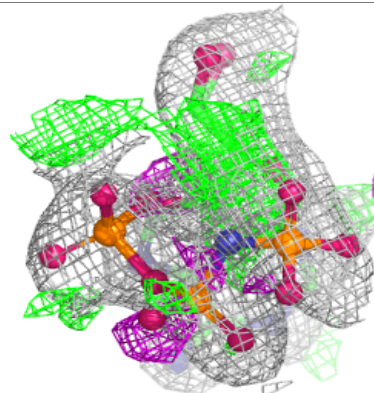
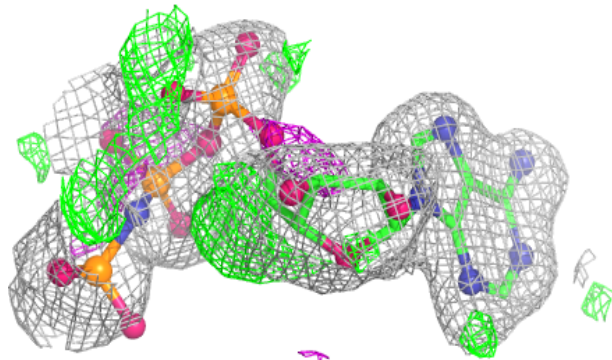
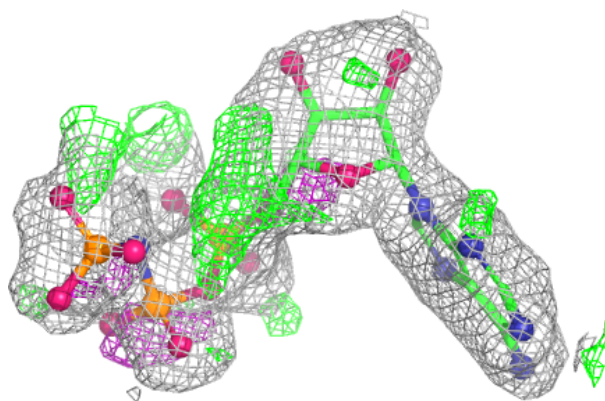
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ANP	BBB	503	31/31	0.81	0.16	49,70,86,97	13
6	GOL	AAA	504	6/6	0.83	0.17	72,79,82,83	0
6	GOL	BBB	504	6/6	0.87	0.17	67,75,79,82	0
4	MG	BBB	502	1/1	0.90	0.10	71,71,71,71	0
5	ANP	AAA	503	31/31	0.96	0.08	40,55,66,75	0
4	MG	AAA	502	1/1	0.99	0.05	64,64,64,64	0
3	ZN	AAA	501	1/1	1.00	0.03	46,46,46,46	0
3	ZN	BBB	501	1/1	1.00	0.02	45,45,45,45	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.

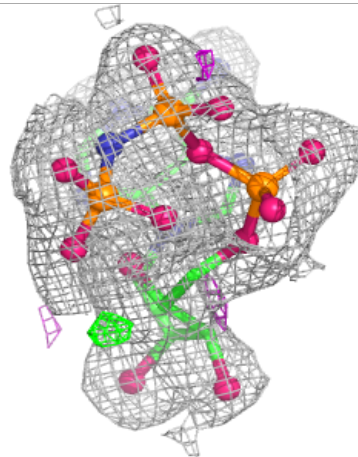
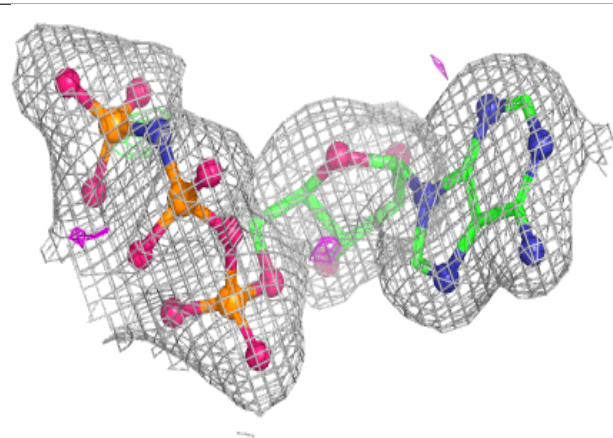
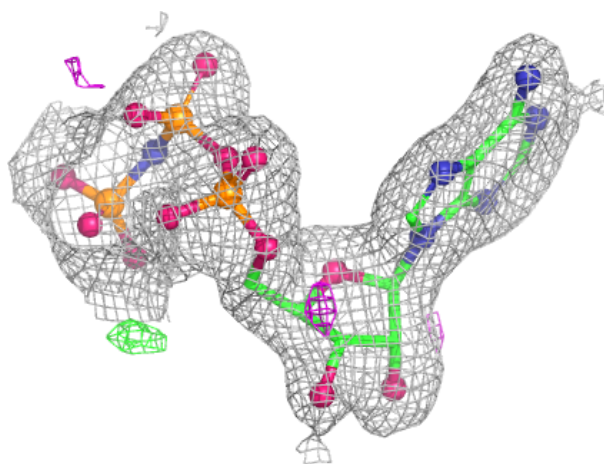
Electron density around ANP BBB 503:

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 AAA 503:

$2mF_o-DF_c$ (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.