



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2025 – 01:27 pm BST

PDB ID : 9ERQ / pdb_00009erq
Title : Citramalate lyase - AMPPNP- citramalate complex
Authors : Ermler, U.; Berg, I.A.; Demmer, U.
Deposited on : 2024-03-25
Resolution : 1.20 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

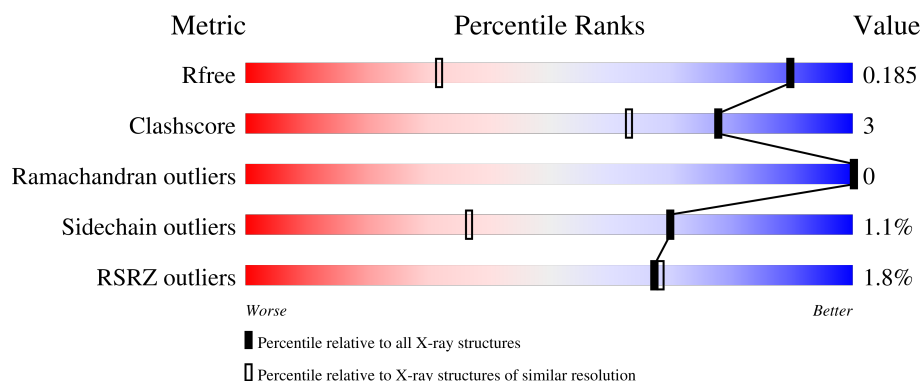
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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}	164625	1079 (1.20-1.20)
Clashscore	180529	1183 (1.20-1.20)
Ramachandran outliers	177936	1146 (1.20-1.20)
Sidechain outliers	177891	1146 (1.20-1.20)
RSRZ outliers	164620	1078 (1.20-1.20)

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	456	<div> <div>2%</div> <div>94%</div> <div>6%</div> </div>
1	C	456	<div> <div>2%</div> <div>94%</div> <div>5%</div> </div>
2	B	105	<div> <div>2%</div> <div>96%</div> <div>..</div> </div>
2	D	105	<div> <div>%</div> <div>94%</div> <div>6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	S2G	B	202	-	X	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 19000 atoms, of which 9007 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.

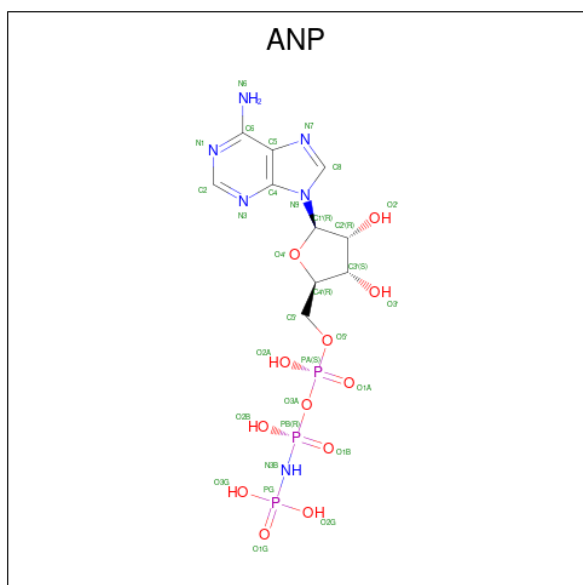
- Molecule 1 is a protein called Acyclic terpene utilization AtuA family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	456	Total	C	H	N	O	S	0	37	0
			7160	2271	3560	614	694	21			
1	C	456	Total	C	H	N	O	S	0	31	0
			7085	2249	3529	605	680	22			

- Molecule 2 is a protein called DUF4387 domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	105	Total	C	H	N	O	S	0	15	0
			1849	584	938	158	165	4			
2	D	105	Total	C	H	N	O	S	0	9	0
			1797	570	908	154	161	4			

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

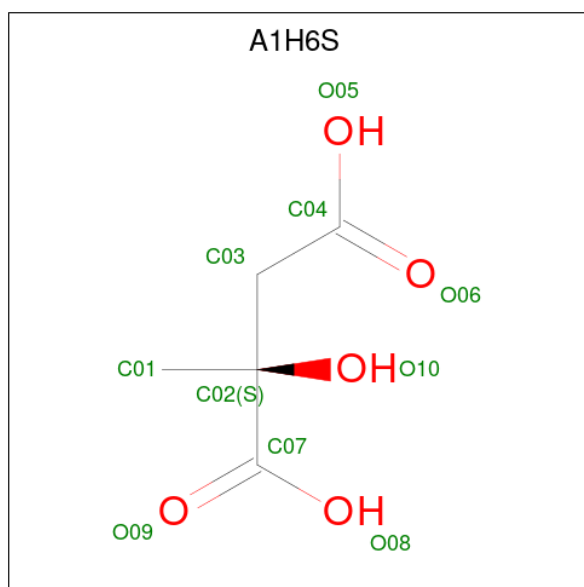


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	
			42	10	11	6	12	3	
3	C	1	Total	C	H	N	O	P	
			42	10	11	6	12	3	

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mg	0	0
			3	3		
4	C	3	Total	Mg	0	0
			3	3		

- Molecule 5 is (2 {S})-2-methyl-2-oxidanyl-butanedioic acid (CCD ID: A1H6S) (formula: C₅H₈O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			16	5	6	5		
5	C	1	Total	C	H	O	0	0
			16	5	6	5		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).

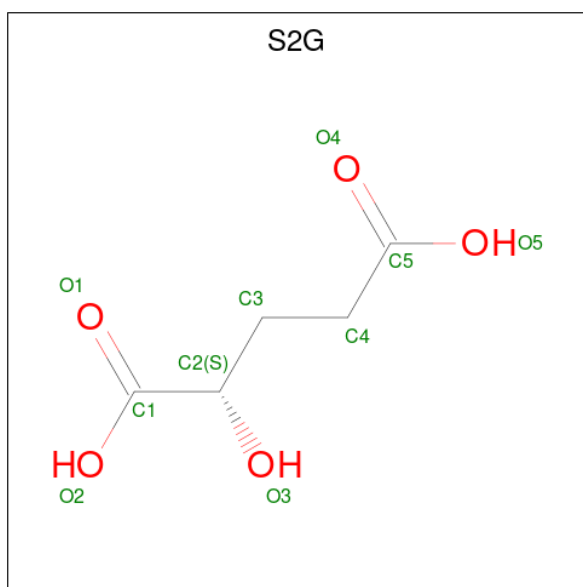


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
6	C	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		

- Molecule 8 is (2S)-2-HYDROXPENTANEDIOIC ACID (CCD ID: S2G) (formula: C₅H₈O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	H	O	0	0
			16	5	6	5		
8	D	1	Total	C	H	O	0	0
			16	5	6	5		

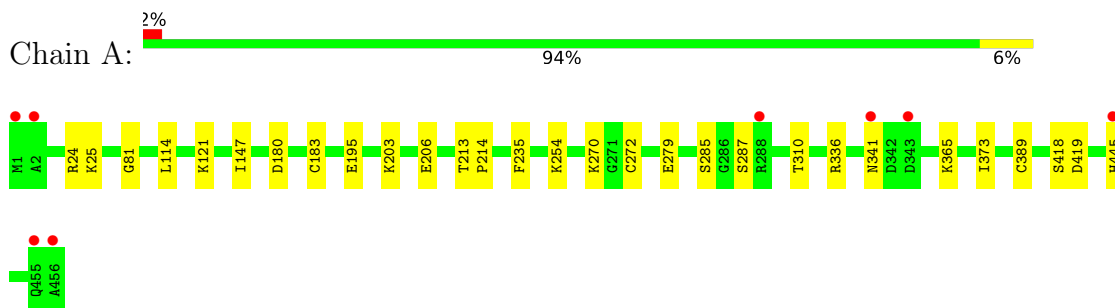
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	345	Total	O	0	5
			350	350		
9	B	75	Total	O	0	1
			76	76		
9	C	385	Total	O	0	3
			388	388		
9	D	89	Total	O	0	1
			90	90		

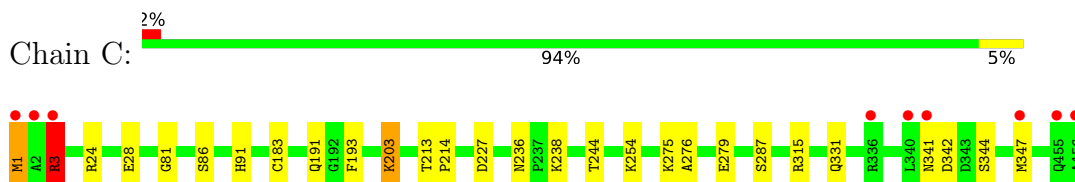
3 Residue-property plots [i](#)

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.

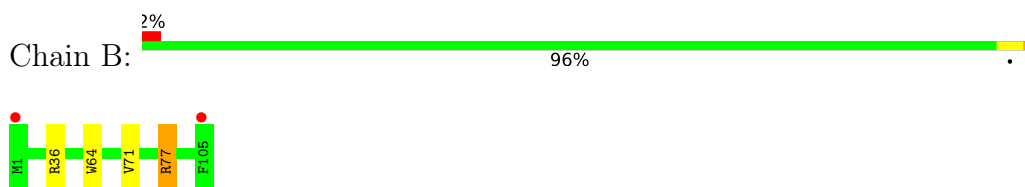
- Molecule 1: Acyclic terpene utilization AtuA family protein



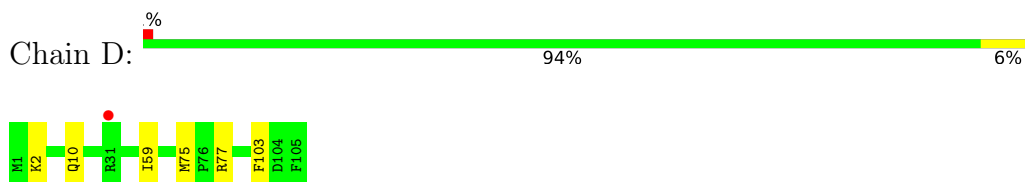
- Molecule 1: Acyclic terpene utilization AtuA family protein



- Molecule 2: DUF4387 domain-containing protein



- Molecule 2: DUF4387 domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.24Å 107.29Å 98.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.73 – 1.20 44.73 – 1.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (44.73-1.20) 99.3 (44.73-1.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 1.20Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.163 , 0.185 0.163 , 0.185	Depositor DCC
R_{free} test set	17532 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	14.0	Xtriage
Anisotropy	0.682	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	19000	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: CL, MES, MG, ANP, S2G, A1H6S

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	0.45	1/3791 (0.0%)	0.60	1/5140 (0.0%)
1	C	0.41	0/3751	0.63	2/5088 (0.0%)
2	B	0.38	0/987	0.60	0/1335
2	D	0.38	0/941	0.58	0/1274
All	All	0.42	1/9470 (0.0%)	0.61	3/12837 (0.0%)

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
2	B	0	1
2	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	ASP	C-N	13.26	1.49	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	ARG	CB-CA-C	6.47	123.29	110.42
1	A	180	ASP	O-C-N	-6.21	114.65	120.55
1	C	315	ARG	CG-CD-NE	-5.39	100.13	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	77	ARG	Sidechain
2	D	77	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	3600	3560	3422	23	0
1	C	3556	3529	3399	17	0
2	B	911	938	869	5	0
2	D	889	908	877	3	0
3	A	31	11	13	0	0
3	C	31	11	13	0	0
4	A	3	0	0	0	0
4	C	3	0	0	0	0
5	A	10	6	0	0	0
5	C	10	6	0	0	0
6	A	12	13	13	0	0
6	C	12	13	13	0	0
7	B	1	0	0	0	0
8	B	10	6	5	1	0
8	D	10	6	5	0	0
9	A	350	0	0	4	0
9	B	76	0	0	2	0
9	C	388	0	0	2	0
9	D	90	0	0	0	0
All	All	9993	9007	8629	48	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 3.

All (48) 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:310[B]:THR:HG23	1:A:389:CYS:SG	2.26	0.75
1:A:310[A]:THR:HG23	1:A:418:SER:O	1.89	0.73
1:C:331:GLN:HG2	1:C:347[B]:MET:HE1	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ARG:NH1	1:C:28:GLU:OE2	2.27	0.67
1:C:1:MET:HG3	1:C:191:GLN:O	1.99	0.62
1:C:1:MET:N	1:C:227:ASP:OD1	2.33	0.61
1:A:195[A]:GLU:HG3	9:A:865:HOH:O	2.02	0.60
1:A:270[B]:LYS:HG2	9:A:604:HOH:O	2.00	0.60
1:A:203[A]:LYS:O	1:A:206[A]:GLU:HG2	2.03	0.59
1:A:24:ARG:HH11	1:A:24:ARG:HG2	1.68	0.57
1:C:81:GLY:HA3	1:C:183[A]:CYS:SG	2.44	0.57
1:C:3:ARG:HA	1:C:3:ARG:HE	1.69	0.57
2:B:36[B]:ARG:HG3	9:B:350:HOH:O	2.04	0.57
1:C:1:MET:HB3	1:C:193:PHE:CZ	2.40	0.56
1:A:341:ASN:ND2	9:A:602:HOH:O	2.35	0.56
1:C:331:GLN:HG2	1:C:347[B]:MET:CE	2.34	0.56
1:C:3:ARG:HA	1:C:3:ARG:NE	2.22	0.54
2:B:77:ARG:HA	8:B:202:S2G:H3	1.90	0.53
1:A:310[B]:THR:HG22	1:A:419:ASP:HA	1.91	0.53
1:C:213:THR:HA	1:C:214:PRO:C	2.35	0.51
1:A:25:LYS:HE3	1:A:235:PHE:O	2.13	0.48
1:A:203[B]:LYS:HE2	1:A:254:LYS:CE	2.43	0.48
1:C:342:ASP:OD2	1:C:344:SER:HB2	2.14	0.48
1:A:81:GLY:HA3	1:A:183[A]:CYS:SG	2.54	0.47
1:A:203[B]:LYS:HD2	1:A:203[B]:LYS:O	2.14	0.47
1:A:213:THR:HA	1:A:214:PRO:C	2.40	0.46
1:C:236:ASN:OD1	1:C:238:LYS:HG2	2.16	0.45
1:C:275:LYS:HD2	1:C:276:ALA:N	2.32	0.45
1:A:114:LEU:HD12	1:A:445:HIS:NE2	2.32	0.45
1:A:310[B]:THR:CG2	1:A:389:CYS:SG	3.02	0.45
2:B:64:TRP:CE3	2:B:71[B]:VAL:HG22	2.52	0.45
1:A:121:LYS:HE2	1:A:147:ILE:O	2.17	0.44
1:A:203[B]:LYS:HE2	1:A:254:LYS:HE3	1.99	0.44
1:C:203[A]:LYS:HD2	1:C:203[A]:LYS:O	2.18	0.43
1:C:244:THR:HG21	2:D:10:GLN:HG2	2.01	0.43
2:D:59:ILE:CD1	2:D:75[B]:MET:CE	2.97	0.43
2:B:64:TRP:CZ3	2:B:71[B]:VAL:HG21	2.54	0.42
1:A:272[B]:CYS:HA	1:A:285[B]:SER:O	2.19	0.42
1:A:24:ARG:HG2	1:A:24:ARG:NH1	2.35	0.42
1:A:270[B]:LYS:CG	9:A:604:HOH:O	2.65	0.42
2:B:36[B]:ARG:CG	9:B:350:HOH:O	2.67	0.42
2:D:2:LYS:HA	2:D:103:PHE:O	2.20	0.41
1:C:254:LYS:NZ	9:C:603:HOH:O	2.37	0.41
1:C:86:SER:HB2	1:C:91:HIS:CE1	2.56	0.41

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	491/456 (108%)	477 (97%)	14 (3%)	0	100	100
1	C	485/456 (106%)	470 (97%)	15 (3%)	0	100	100
2	B	118/105 (112%)	115 (98%)	3 (2%)	0	100	100
2	D	112/105 (107%)	110 (98%)	2 (2%)	0	100	100
All	All	1206/1122 (108%)	1172 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	392/360 (109%)	387 (99%)	5 (1%)	65	29
1	C	387/360 (108%)	380 (98%)	7 (2%)	54	18
2	B	108/93 (116%)	108 (100%)	0	100	100
2	D	102/93 (110%)	102 (100%)	0	100	100
All	All	989/906 (109%)	977 (99%)	12 (1%)	70	32

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	279[A]	GLU
1	A	279[B]	GLU
1	A	287	SER
1	A	336	ARG
1	A	365	LYS
1	C	1	MET
1	C	3	ARG
1	C	203[A]	LYS
1	C	203[C]	LYS
1	C	279	GLU
1	C	287	SER
1	C	341	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
2	B	83	ASN
2	D	83	ASN

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 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 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	A1H6S	C	505	4	8,9,9	1.19	0	9,13,13	1.63	3 (33%)
8	S2G	B	202	-	9,9,9	1.53	1 (11%)	10,11,11	2.91	6 (60%)
5	A1H6S	A	505	4	8,9,9	1.80	3 (37%)	9,13,13	1.24	2 (22%)
8	S2G	D	201	-	9,9,9	1.69	1 (11%)	10,11,11	1.71	2 (20%)
3	ANP	C	501	4	29,33,33	1.28	3 (10%)	31,52,52	1.12	2 (6%)
3	ANP	A	501	4	29,33,33	1.29	4 (13%)	31,52,52	1.10	2 (6%)
6	MES	C	506	-	12,12,12	1.56	1 (8%)	14,16,16	0.84	0
6	MES	A	506	-	12,12,12	1.59	1 (8%)	14,16,16	1.20	1 (7%)

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	A1H6S	C	505	4	-	0/11/11/11	-
8	S2G	B	202	-	-	8/9/9/9	-
5	A1H6S	A	505	4	-	0/11/11/11	-
8	S2G	D	201	-	-	8/9/9/9	-
3	ANP	C	501	4	-	3/14/38/38	0/3/3/3
3	ANP	A	501	4	-	2/14/38/38	0/3/3/3
6	MES	C	506	-	-	0/6/14/14	0/1/1/1
6	MES	A	506	-	-	0/6/14/14	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	506	MES	C8-S	-5.14	1.70	1.77
6	C	506	MES	C8-S	-4.99	1.70	1.77
3	C	501	ANP	PG-O3G	-4.51	1.44	1.56
3	A	501	ANP	PG-O3G	-3.52	1.47	1.56
5	A	505	A1H6S	O06-C04	3.42	1.33	1.22
8	B	202	S2G	O3-C2	-3.35	1.35	1.42
8	D	201	S2G	O3-C2	-3.34	1.35	1.42
3	A	501	ANP	PG-O2G	-3.13	1.48	1.56
3	C	501	ANP	PB-O2B	-2.29	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	505	A1H6S	O09-C07	2.18	1.29	1.22
5	A	505	A1H6S	O10-C02	-2.14	1.39	1.43
3	A	501	ANP	PB-O3A	2.06	1.61	1.59
3	A	501	ANP	C8-N7	-2.04	1.31	1.34
3	C	501	ANP	C8-N7	-2.02	1.31	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	202	S2G	C4-C3-C2	-6.04	106.21	114.46
8	B	202	S2G	O2-C1-C2	3.94	121.37	112.72
8	B	202	S2G	O1-C1-C2	-3.74	115.24	122.54
3	C	501	ANP	O1G-PG-N3B	-3.63	106.42	111.77
3	A	501	ANP	O3G-PG-O1G	-3.30	105.15	113.45
8	D	201	S2G	O5-C5-C4	3.08	123.92	114.03
5	C	505	A1H6S	O08-C07-C02	3.06	118.64	113.18
5	C	505	A1H6S	O09-C07-C02	-2.72	118.53	122.31
6	A	506	MES	O3S-S-C8	2.71	110.15	105.77
5	A	505	A1H6S	O08-C07-C02	2.47	117.58	113.18
8	B	202	S2G	O5-C5-C4	2.39	121.72	114.03
8	B	202	S2G	O4-C5-C4	-2.34	115.56	123.08
8	D	201	S2G	O4-C5-C4	-2.23	115.91	123.08
8	B	202	S2G	O3-C2-C1	-2.22	104.43	110.36
3	A	501	ANP	O1B-PB-N3B	2.16	114.95	111.77
5	A	505	A1H6S	O09-C07-C02	-2.12	119.37	122.31
3	C	501	ANP	O3G-PG-O1G	-2.07	108.25	113.45
5	C	505	A1H6S	C03-C02-C07	-2.03	105.76	110.05

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	ANP	PB-N3B-PG-O1G
3	C	501	ANP	PB-N3B-PG-O1G
8	B	202	S2G	C2-C3-C4-C5
8	B	202	S2G	C1-C2-C3-C4
8	B	202	S2G	O3-C2-C3-C4
8	D	201	S2G	C2-C3-C4-C5
8	D	201	S2G	C1-C2-C3-C4
8	D	201	S2G	O3-C2-C3-C4
8	B	202	S2G	O2-C1-C2-O3
8	B	202	S2G	O1-C1-C2-O3

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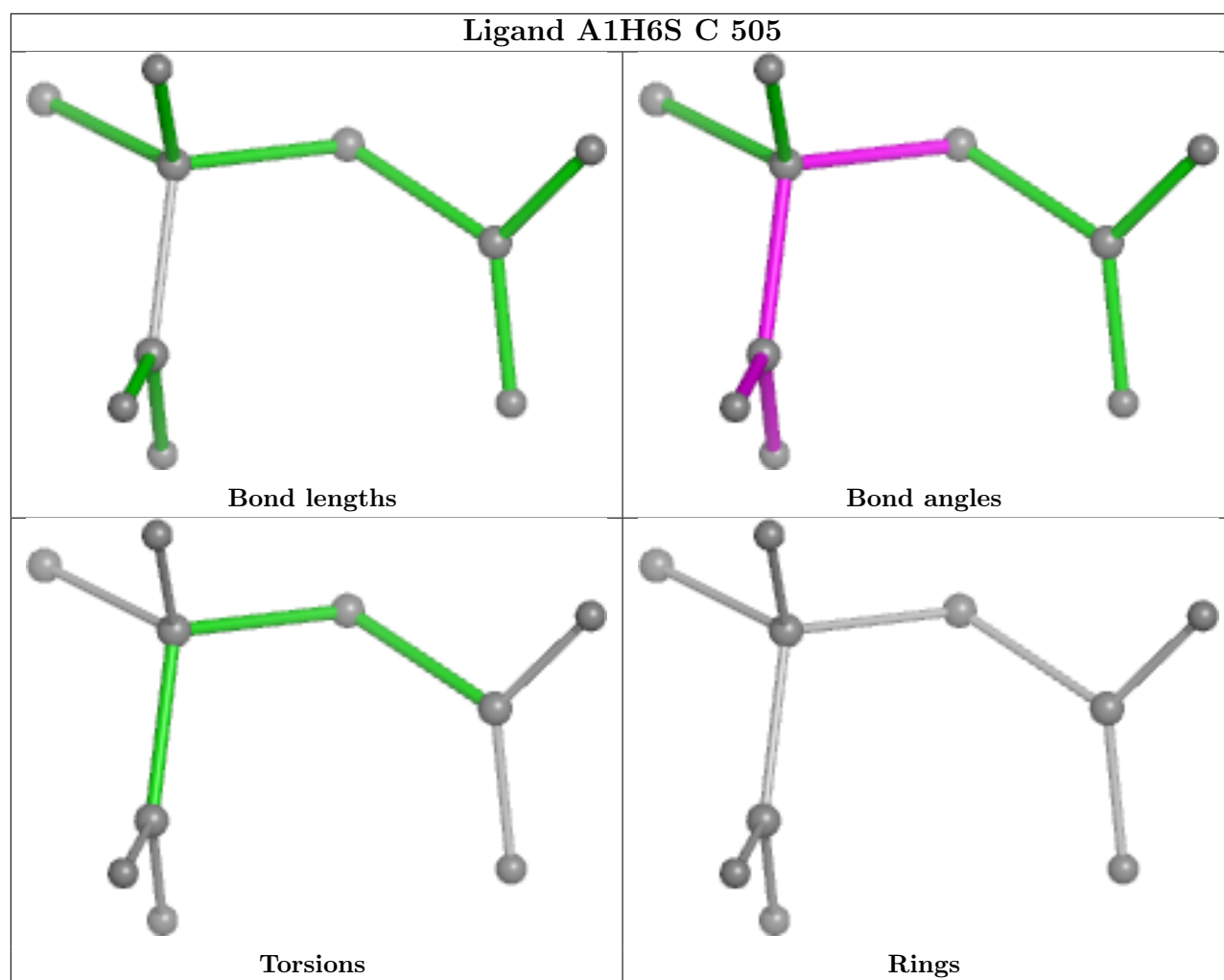
Mol	Chain	Res	Type	Atoms
8	D	201	S2G	O1-C1-C2-O3
8	B	202	S2G	O2-C1-C2-C3
8	B	202	S2G	O1-C1-C2-C3
8	D	201	S2G	O2-C1-C2-O3
8	D	201	S2G	O1-C1-C2-C3
3	C	501	ANP	PG-N3B-PB-O1B
3	C	501	ANP	O4'-C4'-C5'-O5'
3	A	501	ANP	O4'-C4'-C5'-O5'
8	D	201	S2G	C3-C4-C5-O5
8	D	201	S2G	O2-C1-C2-C3
8	B	202	S2G	C3-C4-C5-O5

There are no ring outliers.

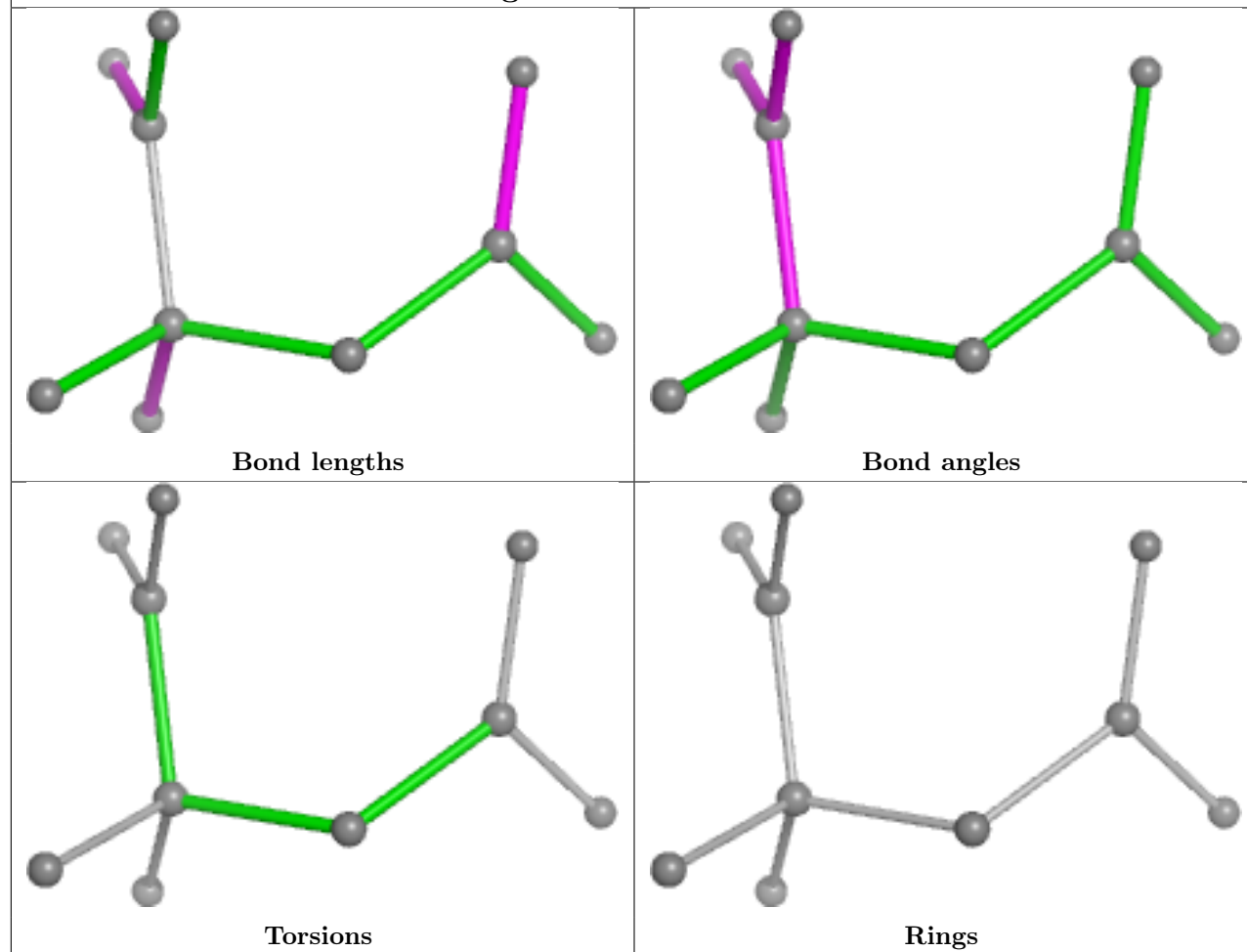
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	202	S2G	1	0

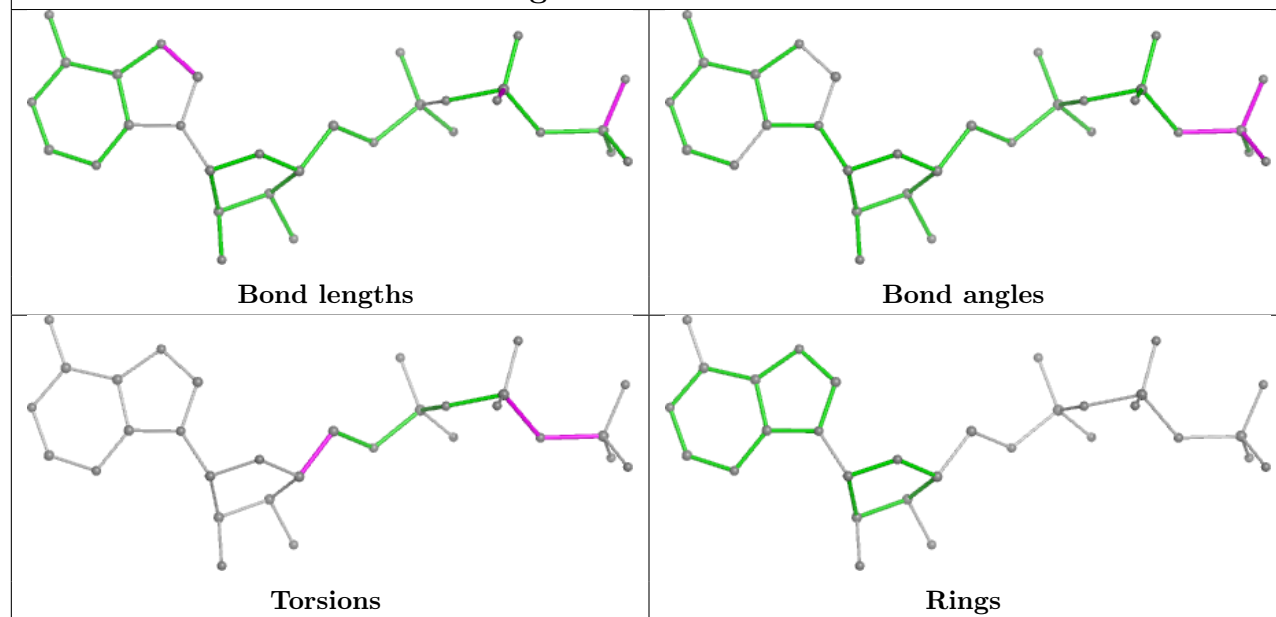
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

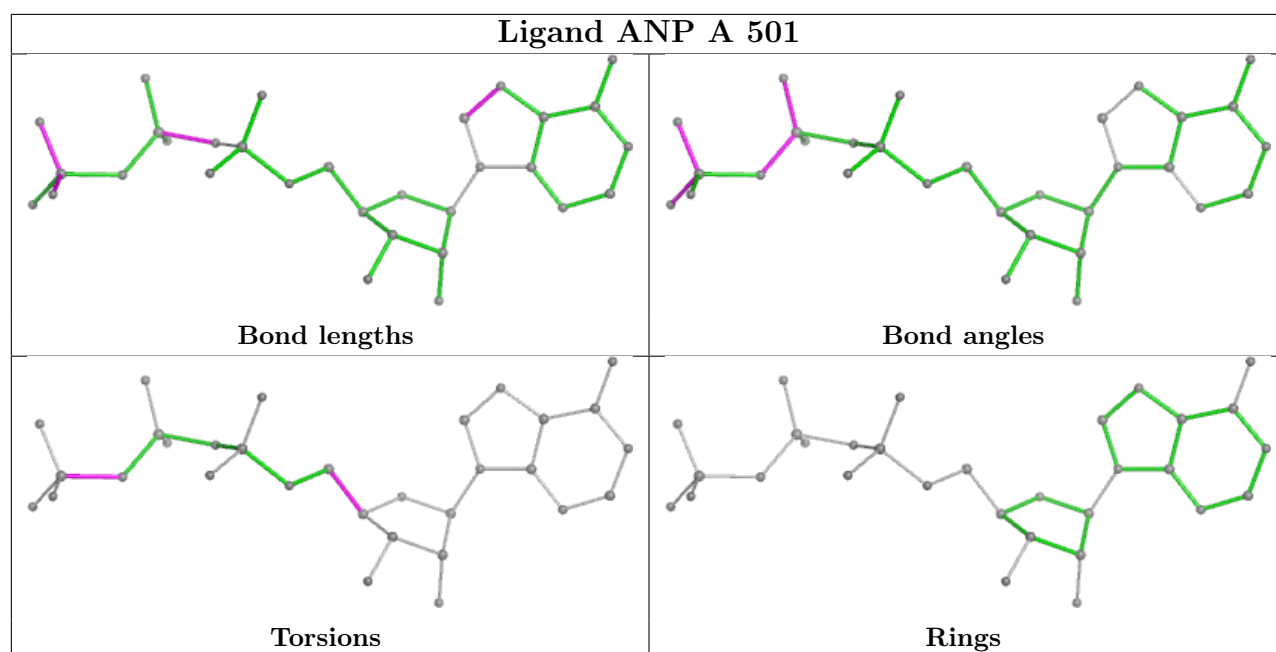


Ligand A1H6S A 505



Ligand ANP C 501





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	A	456/456 (100%)	-0.15	8 (1%) 67 68	9, 20, 34, 69	20 (4%)
1	C	456/456 (100%)	-0.16	9 (1%) 64 65	9, 20, 33, 58	15 (3%)
2	B	105/105 (100%)	-0.12	2 (1%) 66 66	10, 21, 33, 52	8 (7%)
2	D	105/105 (100%)	-0.27	1 (0%) 79 81	10, 20, 31, 41	5 (4%)
All	All	1122/1122 (100%)	-0.16	20 (1%) 67 68	9, 20, 33, 69	48 (4%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	8.2
1	A	456	ALA	6.5
1	A	2	ALA	6.4
1	C	1	MET	5.6
1	C	456	ALA	5.4
1	A	1	MET	4.7
1	A	341	ASN	3.2
2	B	1	MET	3.0
1	C	3	ARG	2.9
2	B	105	PHE	2.8
1	A	343	ASP	2.7
1	A	288[A]	ARG	2.7
1	C	347[A]	MET	2.7
1	C	341	ASN	2.6
1	C	336	ARG	2.6
1	C	340	LEU	2.2
2	D	31[A]	ARG	2.2
1	C	455	GLN	2.2
1	A	455	GLN	2.1
1	A	445	HIS	2.1

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 [i](#)

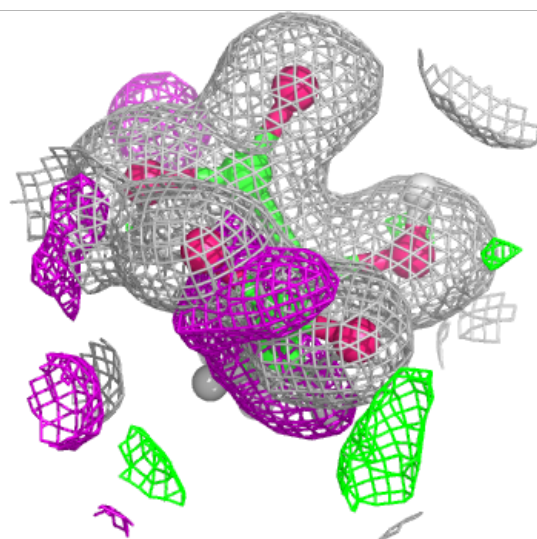
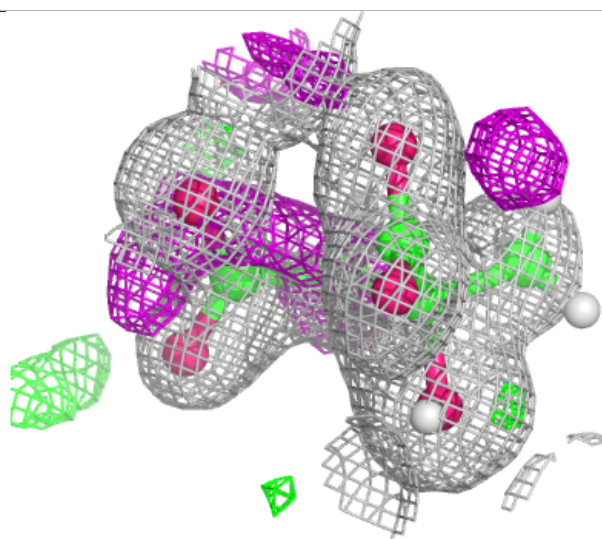
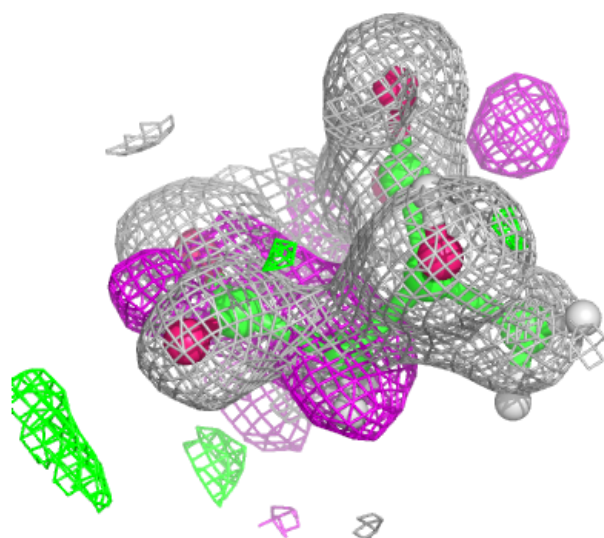
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	S2G	B	202	10/10	0.80	0.15	18,32,41,44	0
8	S2G	D	201	10/10	0.81	0.15	18,32,41,44	0
5	A1H6S	A	505	10/10	0.96	0.09	13,22,34,42	0
5	A1H6S	C	505	10/10	0.96	0.07	13,19,25,26	0
6	MES	A	506	12/12	0.98	0.06	18,23,33,35	0
6	MES	C	506	12/12	0.98	0.06	16,24,30,34	0
7	CL	B	201	1/1	0.98	0.10	21,21,21,21	0
3	ANP	A	501	31/31	0.98	0.06	11,17,21,24	0
3	ANP	C	501	31/31	0.98	0.05	12,15,20,26	0
4	MG	A	503	1/1	0.99	0.05	13,13,13,13	0
4	MG	A	504	1/1	0.99	0.06	13,13,13,13	0
4	MG	C	502	1/1	0.99	0.04	12,12,12,12	0
4	MG	C	503	1/1	0.99	0.04	13,13,13,13	0
4	MG	C	504	1/1	0.99	0.03	14,14,14,14	0
4	MG	A	502	1/1	0.99	0.03	13,13,13,13	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.

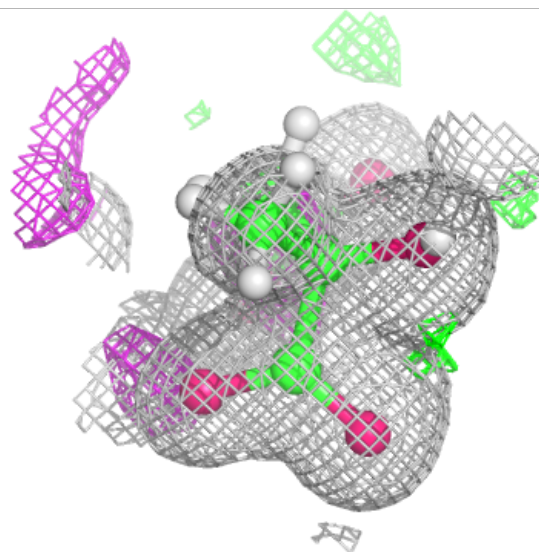
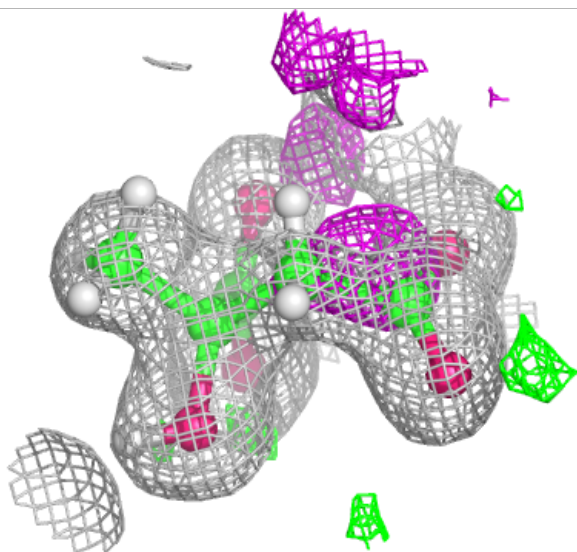
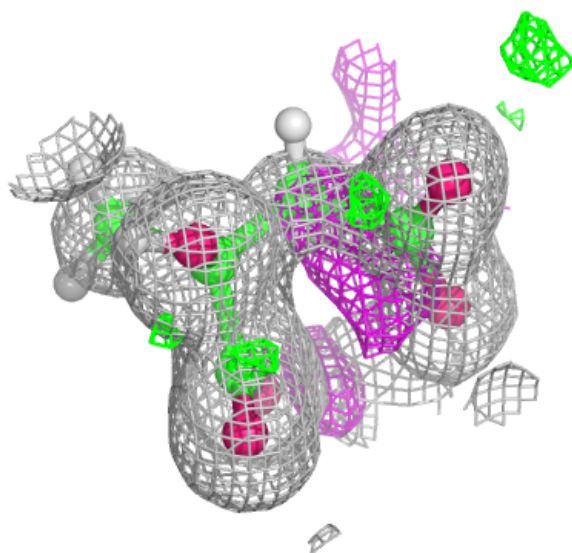
Electron density around A1H6S A 505:

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



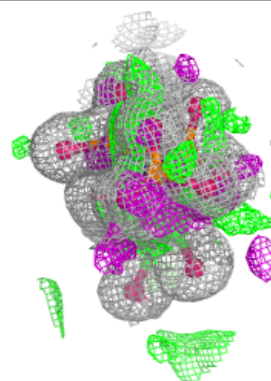
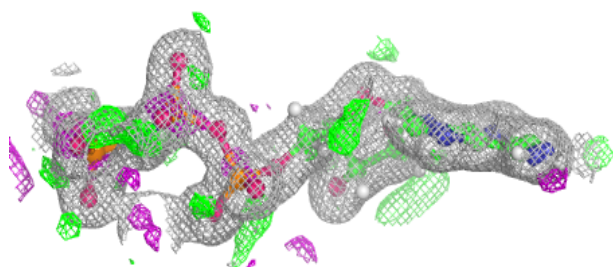
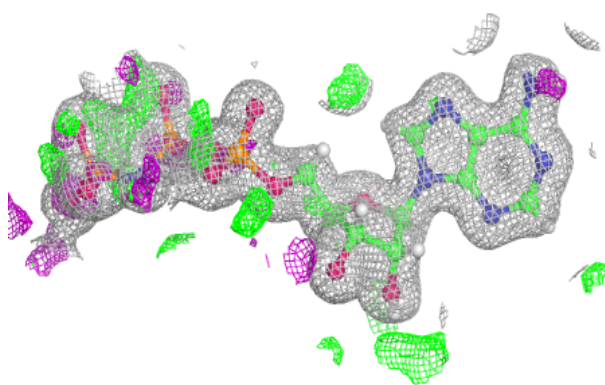
Electron density around A1H6S C 505:

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

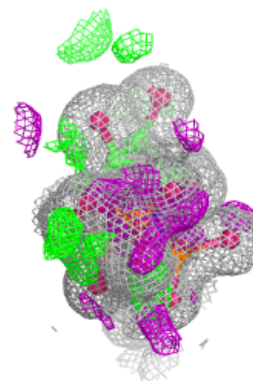
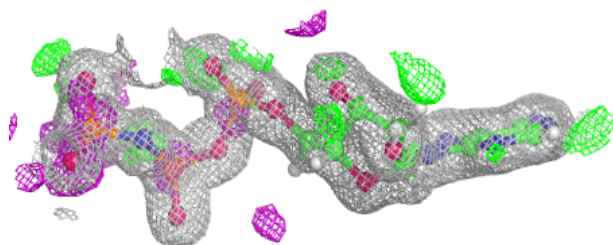
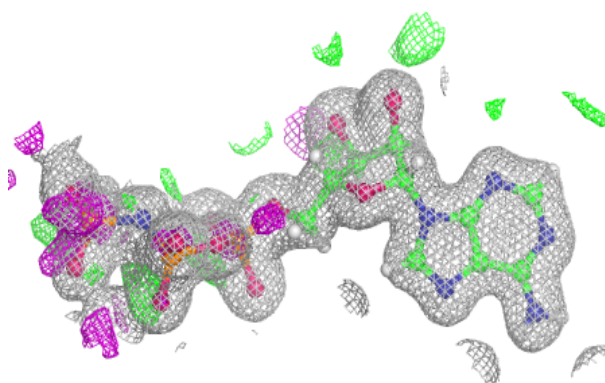


Electron density around ANP A 501:

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

**Electron density around ANP C 501:**

$2mF_o-DF_c$ (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.