



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:04 am BST

PDB ID : 5NX9
Title : Crystal structure of Neanderthal Adenylosuccinate Lyase (ADSL) in complex with its products AMP and fumarate
Authors : Van Laer, B.; Kapp, U.; Soler-Lopez, M.; Leonard, G.; Mueller-Dieckmann, C.
Deposited on : 2017-05-09
Resolution : 2.30 Å(reported)

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

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

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 : 2.11
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) : 2.11

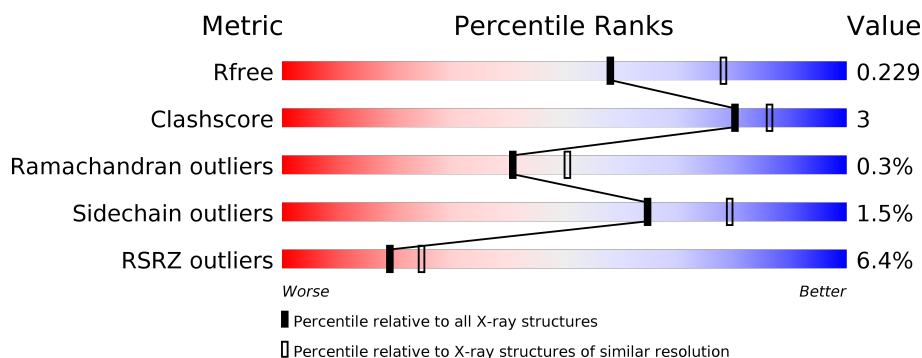
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	487	<div> <div>9%</div> <div>89%</div> <div>7%</div> <div>•</div> </div>
1	B	487	<div> <div>6%</div> <div>93%</div> <div>5%</div> <div>•</div> </div>
1	C	487	<div> <div>8%</div> <div>85%</div> <div>5%</div> <div>9%</div> </div>
1	D	487	<div> <div>2%</div> <div>90%</div> <div>8%</div> <div>•</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15464 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.

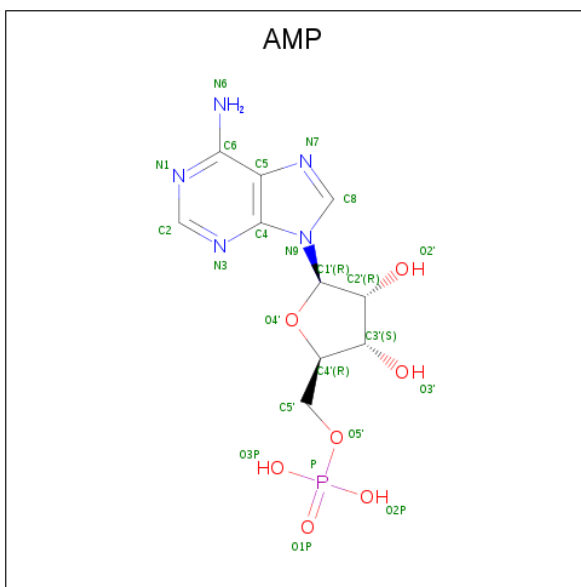
- Molecule 1 is a protein called Adenylosuccinate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	0	0
			3720	2344	662	688	26			
1	B	476	Total	C	N	O	S	0	0	0
			3791	2388	672	703	28			
1	C	441	Total	C	N	O	S	0	0	0
			3530	2228	626	652	24			
1	D	477	Total	C	N	O	S	0	0	0
			3799	2394	673	704	28			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

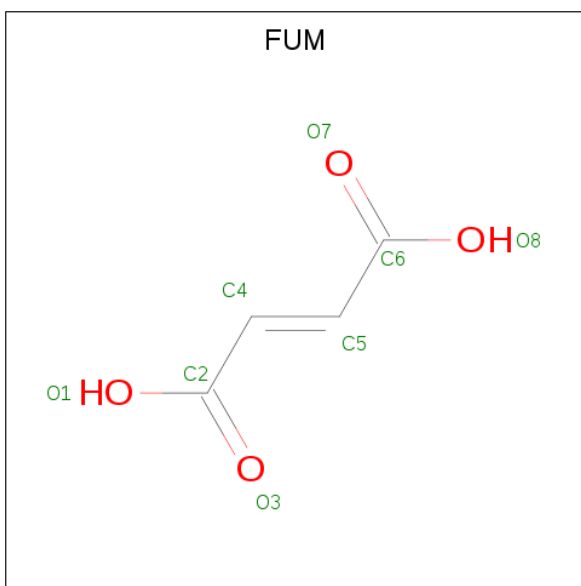
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	2	Total	Cl	0	0
			2	2		
2	D	1	Total	Cl	0	0
			1	1		
2	C	2	Total	Cl	0	0
			2	2		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



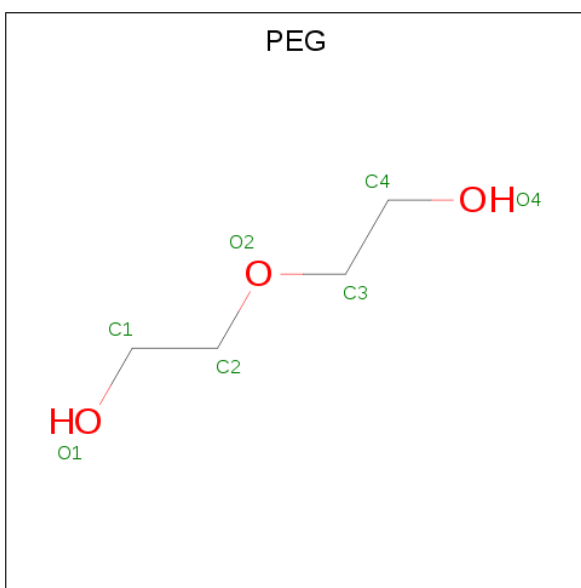
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is FUMARIC ACID (three-letter code: FUM) (formula: C₄H₄O₄).



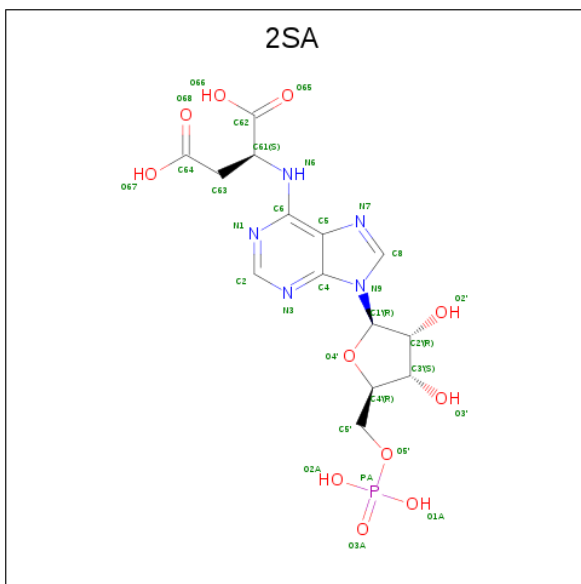
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	4	4		
4	D	1	Total	C	O	0	0
			8	4	4		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



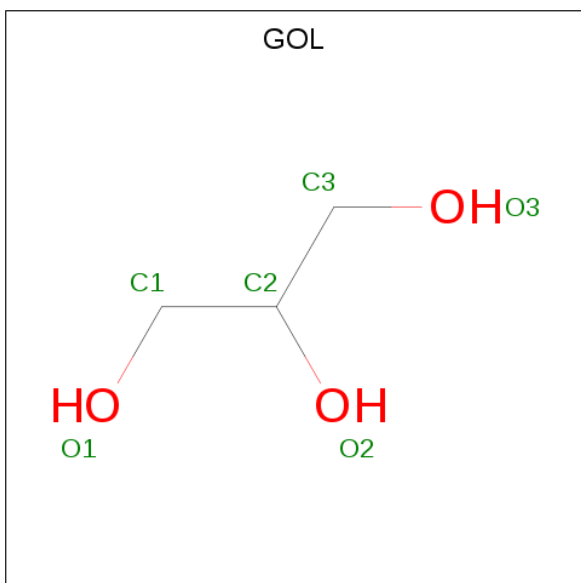
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 2-[9-(3,4-DIHYDROXY-5-PHOSPHONOOXYMETHYL-TETRAHYDRO-FURAN-2-YL)-9H-PURIN-6-YLAMINO]-SUCCINIC ACID (three-letter code: 2SA) (formula: $C_{14}H_{18}N_5O_{11}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			31	14	5	11	1		
6	C	1	Total	C	N	O	P	0	0
			31	14	5	11	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is water.

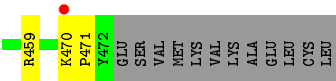
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	99	Total	O	0	0
			99	99		
8	B	98	Total	O	0	0
			98	98		
8	C	98	Total	O	0	0
			98	98		
8	D	102	Total	O	0	0
			102	102		

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

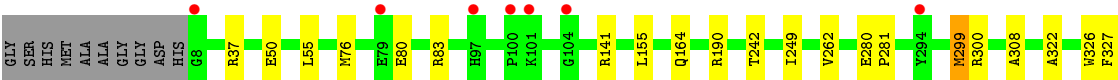
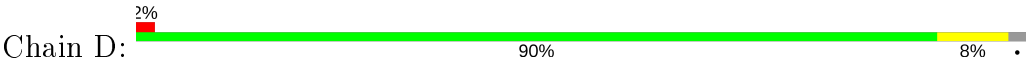
- Chain A:

- Chain B:
-
- Sequence logo for Chain B. The y-axis represents information content in bits (0.00 to 0.10). The x-axis lists amino acids. A color scale at the top indicates conservation levels: 6% (red), 93% (green), and 5% (grey).
- | Position | Amino Acid | Information Content (bits) |
|----------|------------|----------------------------|
| 1 | V390 | 0.08 |
| 2 | K391 | 0.08 |
| 3 | A392 | 0.08 |
| 4 | G393 | 0.08 |
| 5 | G394 | 0.08 |
| 6 | S395 | 0.08 |
| 7 | K396 | 0.08 |
| 8 | Q397 | 0.08 |
| 9 | D398 | 0.08 |
| 10 | C399 | 0.08 |
| 11 | H400 | 0.08 |
| 12 | E401 | 0.08 |
| 13 | D420 | 0.08 |
| 14 | E425 | 0.08 |
| 15 | Y432 | 0.08 |
| 16 | F433 | 0.08 |
| 17 | S434 | 0.08 |
| 18 | P435 | 0.08 |
| 19 | S438 | 0.08 |
| 20 | Q439 | 0.08 |
| 21 | L440 | 0.08 |
| 22 | D441 | 0.08 |
| 23 | H442 | 0.08 |
| 24 | K470 | 0.08 |
| 25 | P471 | 0.08 |
| 26 | K477 | 0.08 |
| 27 | E481 | 0.08 |
| 28 | L482 | 0.08 |
| 29 | C483 | 0.08 |
| 30 | LEU | 0.08 |

- Chain C:
-
- 8% 85% 5% 9%
- GLY SER HIS MET MET ALA ALA GLY GLY ASP ASP GLY S9 Y34 E60 Q63 M76 H93 H126 L155 F160 R190 T242 I249 V262 P281 PHE GLU LYS GLN GLN ILE GLY SER SER ALA MET MET PRO TYR LYS R296 A308 M316 E328 E338
- E343 I351 R372 A381 N364 I385 I386 I387 A388 M389 V390 LYS ALA GLY GLY SER ARG GLN ASP CYS H401 H402 I403 R404 V405 L406 S407 S408 Q408 Q409 A410 D422 L423 L424 E425 R426 L427 Q428 A429 D430 A431 Y432 F433 S434 P435 L436 H437 S438 Q439 L440 D441 H442 L443 L444



● Molecule 1: Adenylosuccinate lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.74Å 107.49Å 209.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.38 – 2.30 48.38 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.38-2.30) 99.5 (48.38-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.193 , 0.227 0.198 , 0.229	Depositor DCC
R_{free} test set	4317 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.6	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	0.95	EDS
Total number of atoms	15464	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: GOL, FUM, CL, 2SA, AMP, PEG

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	0.54	0/3786	0.63	0/5108
1	B	0.56	0/3860	0.65	0/5210
1	C	0.54	0/3594	0.61	0/4855
1	D	0.53	0/3868	0.63	2/5221 (0.0%)
All	All	0.54	0/15108	0.63	2/20394 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	300	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	D	398	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3720	0	3752	22	0
1	B	3791	0	3818	17	0
1	C	3530	0	3552	21	0
1	D	3799	0	3829	24	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
3	A	23	0	12	3	0
3	D	23	0	12	0	0
4	A	8	0	2	3	0
4	D	8	0	2	0	0
5	A	35	0	50	1	0
5	B	7	0	10	1	0
5	C	28	0	40	0	0
5	D	21	0	30	0	0
6	B	31	0	14	0	0
6	C	31	0	14	0	0
7	C	6	0	8	0	0
8	A	99	0	0	0	0
8	B	98	0	0	1	0
8	C	98	0	0	3	0
8	D	102	0	0	1	0
All	All	15464	0	15145	80	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 (80) 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:D:141:ARG:NH1	1:D:476:MET:O	2.14	0.81
1:A:141:ARG:NH1	1:A:476:MET:O	2.12	0.81
1:B:328:GLU:O	1:B:329:ARG:HB2	1.79	0.81
1:D:328:GLU:O	1:D:329:ARG:HB2	1.81	0.81
1:A:328:GLU:O	1:A:329:ARG:HB2	1.82	0.79
1:C:328:GLU:O	1:C:329:ARG:HB2	1.82	0.79
1:A:159:HIS:CE1	1:B:331:LEU:HD13	2.23	0.73
1:B:64:GLU:OE2	1:B:99:CYS:HA	1.90	0.72
1:C:389:MET:HA	1:C:436:ILE:HD11	1.74	0.70
1:D:383:GLU:OE2	1:D:396:ARG:NH2	2.30	0.64
1:D:141:ARG:NH2	1:D:360:GLU:OE2	2.31	0.64
1:A:141:ARG:NH2	1:A:360:GLU:OE2	2.30	0.64
1:B:371:ARG:HD3	1:D:418:GLY:O	1.98	0.63
1:B:37:ARG:CZ	1:B:69:LEU:HB3	2.30	0.61
3:A:503:AMP:N6	4:A:504:FUM:C5	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:VAL:HG11	1:D:351:ILE:HG23	1.86	0.57
1:B:34:TYR:OH	1:B:126:ASN:ND2	2.37	0.57
1:C:262:VAL:HG11	1:C:351:ILE:HG23	1.87	0.56
1:C:34:TYR:OH	1:C:126:ASN:ND2	2.38	0.56
1:A:34:TYR:OH	1:A:126:ASN:ND2	2.37	0.56
1:A:262:VAL:HG11	1:A:351:ILE:HG23	1.89	0.55
1:A:389:MET:HE2	1:A:436:ILE:HG23	1.88	0.55
1:D:242:THR:HG23	1:D:329:ARG:HG3	1.88	0.55
1:C:242:THR:HG23	1:C:329:ARG:HG3	1.89	0.55
1:C:389:MET:CA	1:C:436:ILE:HD11	2.36	0.54
1:D:327:PHE:O	8:D:601:HOH:O	2.18	0.54
1:A:328:GLU:O	1:A:329:ARG:CB	2.55	0.54
1:B:328:GLU:O	1:B:329:ARG:CB	2.54	0.54
1:A:242:THR:HG23	1:A:329:ARG:HG3	1.91	0.53
1:B:375:GLN:NE2	8:B:601:HOH:O	2.23	0.53
1:D:328:GLU:O	1:D:329:ARG:CB	2.56	0.53
1:B:64:GLU:OE1	1:B:101:LYS:HB2	2.09	0.52
1:C:328:GLU:O	1:C:329:ARG:CB	2.57	0.52
1:B:242:THR:HG23	1:B:329:ARG:HG3	1.92	0.50
1:C:424:ILE:HD12	1:C:444:LEU:HD11	1.92	0.50
3:A:503:AMP:HN61	4:A:504:FUM:C5	2.25	0.49
1:A:343:GLU:OE2	1:D:343:GLU:OE1	2.31	0.49
1:C:436:ILE:O	1:C:436:ILE:HG22	2.12	0.49
1:A:137:ARG:NH2	1:A:475:VAL:HG12	2.27	0.49
1:B:52:THR:HG21	5:B:503:PEG:H11	1.95	0.48
1:D:424:ILE:HD11	1:D:444:LEU:HD21	1.96	0.48
1:A:371:ARG:HG2	5:A:509:PEG:H31	1.95	0.48
1:D:280:GLU:HB2	1:D:281:PRO:HD2	1.96	0.48
1:D:262:VAL:HG11	1:D:351:ILE:CG2	2.44	0.47
1:C:296:ARG:NH2	8:C:604:HOH:O	2.48	0.47
1:A:262:VAL:HG11	1:A:351:ILE:CG2	2.45	0.47
1:B:420:ASP:OD1	1:D:371:ARG:NH1	2.47	0.46
1:A:85:ARG:HB3	1:D:299:MET:HE1	1.96	0.46
1:C:262:VAL:HG11	1:C:351:ILE:CG2	2.45	0.46
1:D:80:GLU:OE1	1:D:83:ARG:NH1	2.44	0.46
1:B:37:ARG:NH2	1:B:69:LEU:HD13	2.32	0.45
1:A:389:MET:CE	1:A:436:ILE:HG23	2.48	0.44
1:A:389:MET:HB3	1:A:399:CYS:SG	2.58	0.43
1:A:389:MET:HE2	1:A:436:ILE:CG2	2.48	0.43
1:A:470:LYS:HB3	1:A:471:PRO:HD3	2.01	0.43
1:B:64:GLU:OE1	1:B:101:LYS:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:ALA:N	1:C:351:ILE:HD11	2.34	0.43
1:C:155:LEU:HD22	1:C:372:ARG:HG2	2.00	0.43
1:C:436:ILE:O	1:C:436:ILE:CG2	2.67	0.43
1:C:470:LYS:HB3	1:C:471:PRO:HD3	2.01	0.42
1:D:389:MET:HB3	1:D:399:CYS:SG	2.59	0.42
1:D:155:LEU:HD22	1:D:372:ARG:HG2	2.01	0.42
1:D:249:ILE:HD11	1:D:322:ALA:HB3	2.02	0.42
1:D:50:GLU:HB3	1:D:55:LEU:HD12	2.02	0.41
1:A:308:ALA:N	1:A:351:ILE:HD11	2.34	0.41
1:B:249:ILE:HD11	1:B:322:ALA:HB3	2.03	0.41
1:C:63:GLN:CG	8:C:679:HOH:O	2.68	0.41
1:D:308:ALA:N	1:D:351:ILE:HD11	2.34	0.41
1:D:470:LYS:HB3	1:D:471:PRO:HD3	2.03	0.41
1:D:76:MET:HE2	1:D:76:MET:HB2	1.99	0.41
1:A:249:ILE:HD11	1:A:322:ALA:HB3	2.03	0.41
1:A:21:TYR:HB3	1:A:350:THR:HG21	2.03	0.41
1:B:343:GLU:OE1	1:C:343:GLU:OE2	2.39	0.41
1:B:470:LYS:HB3	1:B:471:PRO:HD3	2.03	0.41
1:C:385:ILE:HD13	1:C:443:LEU:HD13	2.02	0.41
1:A:155:LEU:HD22	1:A:372:ARG:HG2	2.02	0.40
3:A:503:AMP:N6	4:A:504:FUM:C4	2.84	0.40
1:C:160:PHE:HB2	1:D:326:TRP:HE3	1.86	0.40
1:C:63:GLN:HG3	8:C:679:HOH:O	2.21	0.40
1:C:76:MET:HE2	1:C:76:MET:HB2	1.97	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	462/487 (95%)	458 (99%)	3 (1%)	1 (0%)	47 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	474/487 (97%)	469 (99%)	3 (1%)	2 (0%)	34	42
1	C	435/487 (89%)	432 (99%)	2 (0%)	1 (0%)	47	58
1	D	475/487 (98%)	473 (100%)	1 (0%)	1 (0%)	47	58
All	All	1846/1948 (95%)	1832 (99%)	9 (0%)	5 (0%)	41	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	ARG
1	B	9	SER
1	B	329	ARG
1	C	329	ARG
1	D	329	ARG

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	408/422 (97%)	400 (98%)	8 (2%)	55	72
1	B	416/422 (99%)	411 (99%)	5 (1%)	71	84
1	C	388/422 (92%)	383 (99%)	5 (1%)	69	82
1	D	417/422 (99%)	410 (98%)	7 (2%)	60	76
All	All	1629/1688 (96%)	1604 (98%)	25 (2%)	65	79

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	98	CYS
1	A	190	ARG
1	A	299	MET
1	A	329	ARG
1	A	375	GLN

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Mol	Chain	Res	Type
1	A	402	LYS
1	A	430	ASP
1	B	98	CYS
1	B	190	ARG
1	B	329	ARG
1	B	331	LEU
1	B	425	GLU
1	C	60	GLU
1	C	93	HIS
1	C	190	ARG
1	C	329	ARG
1	C	459	ARG
1	D	37	ARG
1	D	164	GLN
1	D	190	ARG
1	D	299	MET
1	D	329	ARG
1	D	371	ARG
1	D	395	SER

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

Mol	Chain	Res	Type
1	A	63	GLN
1	A	439	GLN
1	D	161	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 6 are monoatomic - leaving 20 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	PEG	C	506	-	6,6,6	0.52	0	5,5,5	0.39	0
5	PEG	A	508	-	6,6,6	0.54	0	5,5,5	0.17	0
5	PEG	A	507	-	6,6,6	0.58	0	5,5,5	0.60	0
5	PEG	D	505	-	6,6,6	0.57	0	5,5,5	0.39	0
5	PEG	D	506	-	6,6,6	0.55	0	5,5,5	0.32	0
7	GOL	C	507	-	5,5,5	0.33	0	5,5,5	0.36	0
5	PEG	A	506	-	6,6,6	0.68	0	5,5,5	0.37	0
6	2SA	B	502	-	22,33,33	3.22	6 (27%)	24,49,49	1.76	5 (20%)
5	PEG	A	505	-	6,6,6	0.57	0	5,5,5	0.35	0
3	AMP	A	503	-	22,25,25	1.10	3 (13%)	25,38,38	1.58	6 (24%)
4	FUM	A	504	-	1,7,7	0.58	0	2,8,8	1.22	0
6	2SA	C	501	-	22,33,33	3.27	6 (27%)	24,49,49	1.85	5 (20%)
4	FUM	D	503	-	1,7,7	0.21	0	2,8,8	1.12	0
5	PEG	C	505	-	6,6,6	0.56	0	5,5,5	0.32	0
5	PEG	B	503	-	6,6,6	0.54	0	5,5,5	0.37	0
5	PEG	A	509	-	6,6,6	0.54	0	5,5,5	0.29	0
5	PEG	D	504	-	6,6,6	0.68	0	5,5,5	0.52	0
3	AMP	D	502	-	22,25,25	0.77	1 (4%)	25,38,38	1.40	3 (12%)
5	PEG	C	504	-	6,6,6	0.71	0	5,5,5	0.39	0
5	PEG	C	508	-	6,6,6	0.52	0	5,5,5	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	C	506	-	-	3/4/4/4	-
5	PEG	A	508	-	-	2/4/4/4	-
5	PEG	A	507	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	D	505	-	-	2/4/4/4	-
5	PEG	D	506	-	-	3/4/4/4	-
7	GOL	C	507	-	-	0/4/4/4	-
5	PEG	A	506	-	-	2/4/4/4	-
6	2SA	B	502	-	-	6/12/38/38	0/3/3/3
5	PEG	A	505	-	-	2/4/4/4	-
3	AMP	A	503	-	-	1/6/26/26	0/3/3/3
4	FUM	A	504	-	-	0/0/5/5	-
6	2SA	C	501	-	-	6/12/38/38	0/3/3/3
4	FUM	D	503	-	-	0/0/5/5	-
5	PEG	C	505	-	-	2/4/4/4	-
5	PEG	B	503	-	-	2/4/4/4	-
5	PEG	A	509	-	-	3/4/4/4	-
5	PEG	D	504	-	-	3/4/4/4	-
3	AMP	D	502	-	-	1/6/26/26	0/3/3/3
5	PEG	C	504	-	-	3/4/4/4	-
5	PEG	C	508	-	-	1/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	502	2SA	C3'-C2'	-9.19	1.28	1.53
6	C	501	2SA	C3'-C2'	-8.96	1.28	1.53
6	B	502	2SA	O4'-C1'	7.13	1.51	1.41
6	C	501	2SA	O4'-C1'	7.02	1.50	1.41
6	C	501	2SA	O4'-C4'	-6.79	1.29	1.45
6	B	502	2SA	O4'-C4'	-6.58	1.30	1.45
6	C	501	2SA	C61-N6	4.52	1.52	1.45
6	B	502	2SA	C3'-C4'	4.42	1.64	1.53
6	C	501	2SA	C3'-C4'	4.12	1.63	1.53
6	C	501	2SA	O2'-C2'	3.46	1.51	1.43
3	A	503	AMP	C2'-C1'	-2.38	1.50	1.53
6	B	502	2SA	O2'-C2'	2.34	1.48	1.43
3	A	503	AMP	O4'-C1'	2.28	1.44	1.41
3	D	502	AMP	O4'-C1'	2.12	1.44	1.41
6	B	502	2SA	C2'-C1'	2.12	1.57	1.53
3	A	503	AMP	C2-N3	2.01	1.35	1.32

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	502	2SA	C2-N1-C6	4.53	120.47	116.59
6	C	501	2SA	C2-N1-C6	4.52	120.47	116.59
6	C	501	2SA	N3-C2-N1	-4.27	122.00	128.68
3	D	502	AMP	N3-C2-N1	-3.96	122.48	128.68
3	A	503	AMP	N3-C2-N1	-3.88	122.62	128.68
6	B	502	2SA	N3-C2-N1	-3.79	122.76	128.68
6	B	502	2SA	O4'-C1'-C2'	-3.33	102.05	106.93
3	A	503	AMP	O4'-C1'-C2'	-3.21	102.23	106.93
6	C	501	2SA	C63-C61-N6	-3.02	102.75	108.56
6	C	501	2SA	O4'-C1'-C2'	-3.01	102.53	106.93
3	A	503	AMP	O3P-P-O2P	2.77	118.23	107.64
3	A	503	AMP	C1'-N9-C4	-2.68	121.94	126.64
6	C	501	2SA	C4-C5-N7	-2.36	106.94	109.40
3	D	502	AMP	O2P-P-O5'	-2.24	100.78	106.73
6	B	502	2SA	C4-C5-N7	-2.10	107.21	109.40
3	A	503	AMP	C4-C5-N7	-2.10	107.21	109.40
3	A	503	AMP	O2P-P-O5'	-2.09	101.16	106.73
6	B	502	2SA	C3'-C2'-C1'	2.04	104.05	100.98
3	D	502	AMP	O3P-P-O2P	2.01	115.32	107.64

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	502	2SA	N1-C6-N6-C61
6	B	502	2SA	C5-C6-N6-C61
6	B	502	2SA	C62-C61-N6-C6
6	C	501	2SA	N1-C6-N6-C61
6	C	501	2SA	C5-C6-N6-C61
6	C	501	2SA	C62-C61-N6-C6
6	C	501	2SA	C63-C61-N6-C6
6	C	501	2SA	C62-C61-C63-C64
5	A	505	PEG	O1-C1-C2-O2
5	D	506	PEG	O1-C1-C2-O2
5	A	505	PEG	O2-C3-C4-O4
5	C	504	PEG	O2-C3-C4-O4
5	C	506	PEG	O2-C3-C4-O4
5	A	507	PEG	O1-C1-C2-O2
5	A	509	PEG	O2-C3-C4-O4
5	D	504	PEG	O1-C1-C2-O2
5	D	505	PEG	O1-C1-C2-O2
5	A	506	PEG	O2-C3-C4-O4
5	A	509	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	508	PEG	O1-C1-C2-O2
5	C	505	PEG	O2-C3-C4-O4
5	C	505	PEG	O1-C1-C2-O2
5	A	507	PEG	O2-C3-C4-O4
5	C	504	PEG	O1-C1-C2-O2
5	B	503	PEG	O2-C3-C4-O4
5	A	508	PEG	O2-C3-C4-O4
5	A	506	PEG	O1-C1-C2-O2
5	D	506	PEG	O2-C3-C4-O4
6	B	502	2SA	O4'-C4'-C5'-O5'
5	D	505	PEG	C4-C3-O2-C2
5	C	506	PEG	C1-C2-O2-C3
5	C	508	PEG	O1-C1-C2-O2
5	D	506	PEG	C1-C2-O2-C3
5	A	507	PEG	C1-C2-O2-C3
5	D	504	PEG	C1-C2-O2-C3
5	B	503	PEG	C4-C3-O2-C2
5	C	504	PEG	C4-C3-O2-C2
5	A	509	PEG	C4-C3-O2-C2
5	D	504	PEG	C4-C3-O2-C2
5	C	506	PEG	C4-C3-O2-C2
6	B	502	2SA	C63-C61-N6-C6
6	B	502	2SA	C3'-C4'-C5'-O5'
3	D	502	AMP	O4'-C4'-C5'-O5'
3	A	503	AMP	O4'-C4'-C5'-O5'
6	C	501	2SA	O4'-C4'-C5'-O5'
5	A	507	PEG	C4-C3-O2-C2

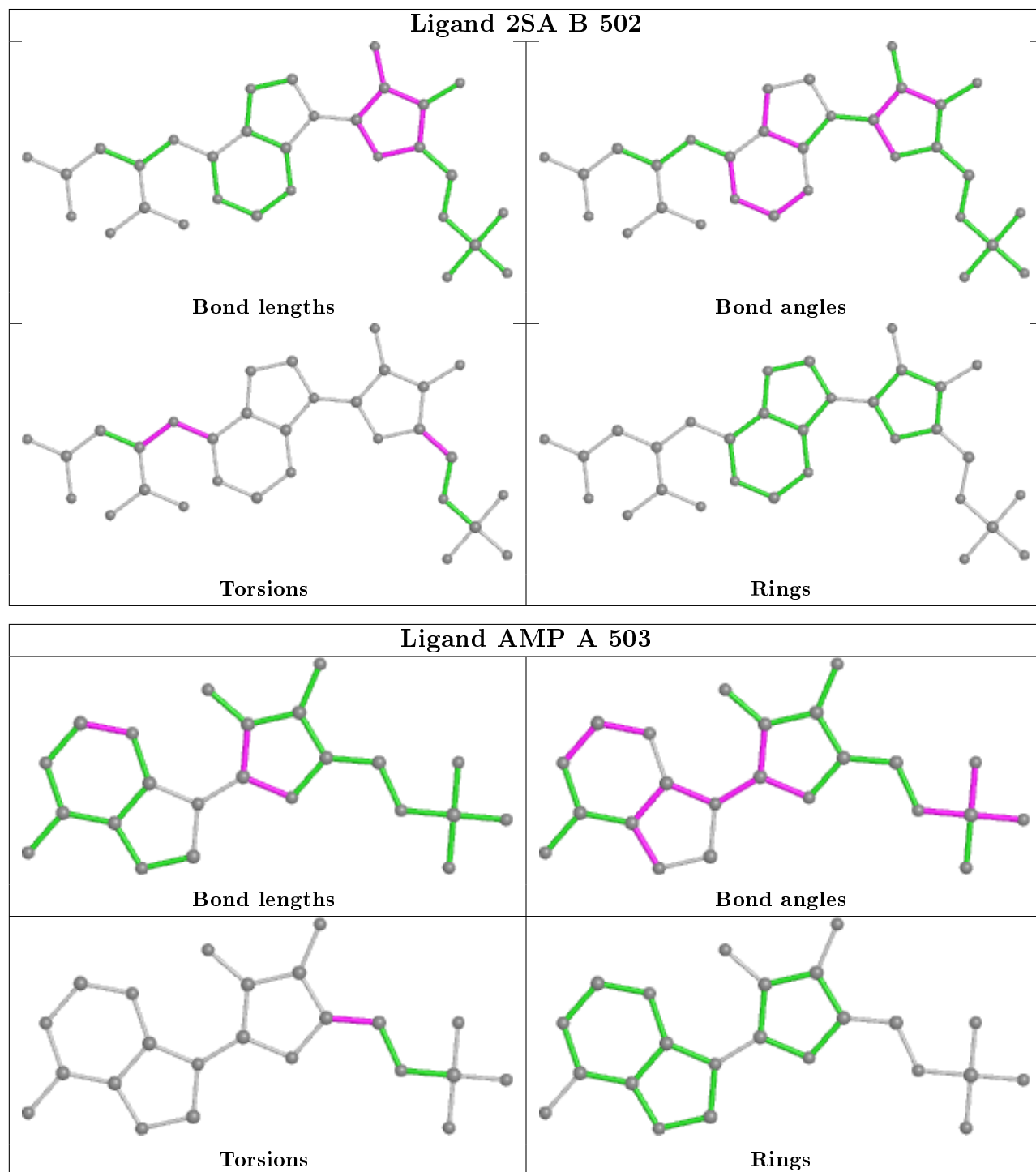
There are no ring outliers.

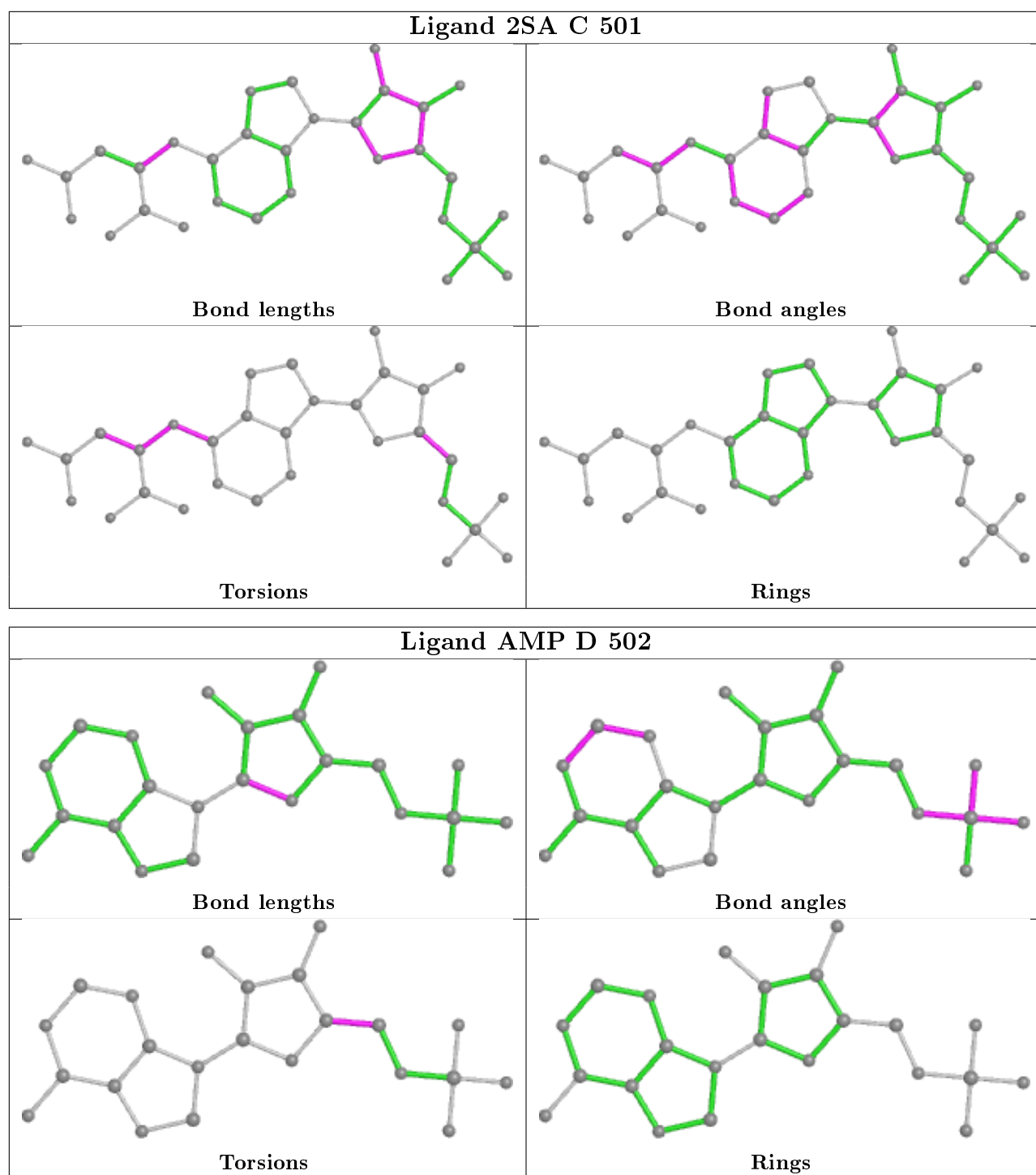
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	AMP	3	0
4	A	504	FUM	3	0
5	B	503	PEG	1	0
5	A	509	PEG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	466/487 (95%)	0.22	44 (9%) 8 11	21, 36, 81, 110	0
1	B	476/487 (97%)	0.07	27 (5%) 23 30	21, 35, 76, 106	0
1	C	441/487 (90%)	0.18	39 (8%) 10 13	21, 34, 91, 130	0
1	D	477/487 (97%)	0.01	9 (1%) 66 73	22, 37, 63, 87	0
All	All	1860/1948 (95%)	0.12	119 (6%) 19 25	21, 35, 77, 130	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	432	TYR	9.3
1	C	436	ILE	7.4
1	C	437	HIS	6.5
1	A	282	PHE	6.0
1	B	392	ALA	6.0
1	C	427	ILE	5.5
1	C	405	VAL	5.5
1	A	431	ALA	5.5
1	C	429	ALA	5.5
1	A	399	CYS	5.4
1	C	438	SER	5.4
1	B	438	SER	5.2
1	C	431	ALA	5.1
1	C	430	ASP	5.0
1	C	435	PRO	5.0
1	C	408	GLN	5.0
1	C	406	LEU	5.0
1	C	386	ILE	4.9
1	A	397	GLN	4.8
1	C	441	ASP	4.8
1	A	429	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	400	HIS	4.7
1	C	389	MET	4.7
1	C	384	ASN	4.6
1	C	434	SER	4.5
1	A	438	SER	4.5
1	B	399	CYS	4.5
1	C	433	PHE	4.3
1	B	442	HIS	4.3
1	A	401	GLU	4.3
1	A	478	VAL	4.3
1	C	426	ARG	4.2
1	C	424	ILE	4.2
1	A	430	ASP	4.2
1	B	435	PRO	4.2
1	A	392	ALA	4.2
1	C	385	ILE	4.1
1	A	394	GLY	4.0
1	B	441	ASP	4.0
1	B	294	TYR	3.9
1	C	428	GLN	3.9
1	A	475	VAL	3.8
1	A	398	ASP	3.8
1	B	389	MET	3.7
1	D	100	PRO	3.6
1	A	393	GLY	3.6
1	C	410	ALA	3.5
1	C	388	ALA	3.5
1	C	387	MET	3.5
1	A	434	SER	3.4
1	A	391	LYS	3.3
1	B	385	ILE	3.3
1	B	391	LYS	3.3
1	A	437	HIS	3.2
1	C	404	ARG	3.2
1	A	432	TYR	3.2
1	C	401	GLU	3.2
1	A	435	PRO	3.1
1	B	387	MET	3.1
1	B	395	SER	3.1
1	C	439	GLN	3.0
1	A	433	PHE	3.0
1	C	440	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	393	GLY	2.9
1	A	479	LYS	2.9
1	C	402	LYS	2.8
1	B	432	TYR	2.8
1	B	390	VAL	2.8
1	C	409	GLN	2.8
1	A	396	ARG	2.8
1	A	72	ILE	2.8
1	D	442	HIS	2.8
1	A	477	LYS	2.8
1	B	282	PHE	2.7
1	B	8	GLY	2.7
1	B	398	ASP	2.6
1	B	434	SER	2.6
1	A	316	MET	2.6
1	B	481	GLU	2.6
1	B	440	LEU	2.5
1	D	97	HIS	2.5
1	D	104	GLY	2.5
1	A	387	MET	2.5
1	A	383	GLU	2.5
1	A	390	VAL	2.5
1	A	285	GLN	2.5
1	D	101	LYS	2.5
1	A	60	GLU	2.5
1	A	395	SER	2.4
1	A	427	ILE	2.4
1	B	401	GLU	2.4
1	A	75	LYS	2.4
1	A	425	GLU	2.4
1	B	396	ARG	2.4
1	B	388	ALA	2.3
1	D	8	GLY	2.3
1	A	315	VAL	2.3
1	D	484	LEU	2.3
1	A	389	MET	2.3
1	A	284	LYS	2.3
1	A	400	HIS	2.3
1	C	316	MET	2.3
1	A	403	ILE	2.3
1	A	68	ASN	2.2
1	C	407	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	422	ASP	2.2
1	D	79	GLU	2.2
1	D	294	TYR	2.2
1	B	397	GLN	2.2
1	A	103	ALA	2.2
1	C	381	ALA	2.1
1	B	60	GLU	2.1
1	A	324	VAL	2.1
1	B	477	LYS	2.1
1	C	425	GLU	2.1
1	A	386	ILE	2.1
1	A	474	SER	2.1
1	C	249	ILE	2.0
1	C	470	LYS	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 carbohydrates 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	PEG	D	505	7/7	0.73	0.30	57,67,74,75	0
7	GOL	C	507	6/6	0.78	0.22	60,63,65,67	0
5	PEG	A	509	7/7	0.80	0.22	63,64,68,71	0
5	PEG	D	506	7/7	0.81	0.15	56,61,68,70	0
5	PEG	A	508	7/7	0.81	0.13	61,65,67,68	0
5	PEG	C	505	7/7	0.84	0.14	64,67,68,68	0
5	PEG	C	504	7/7	0.87	0.11	37,45,47,48	0
5	PEG	A	507	7/7	0.88	0.17	53,55,58,58	0
5	PEG	C	508	7/7	0.89	0.15	51,54,61,67	0

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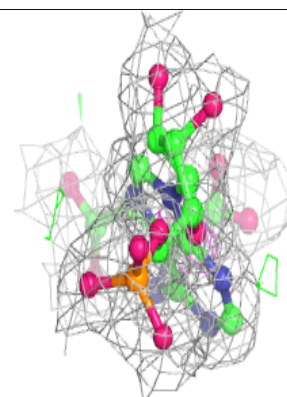
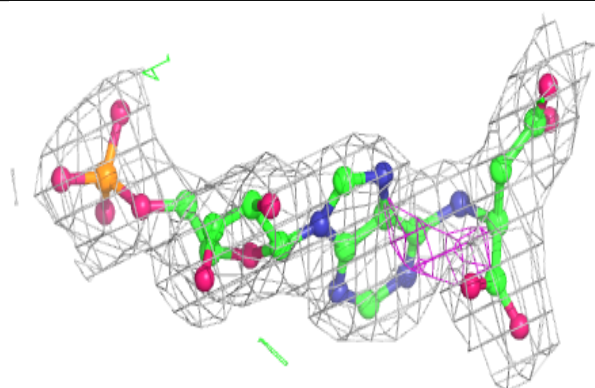
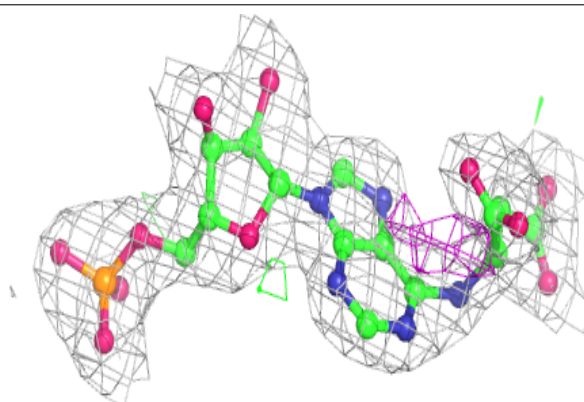
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	PEG	A	506	7/7	0.90	0.13	50,51,57,57	0
5	PEG	B	503	7/7	0.91	0.12	49,53,55,56	0
5	PEG	D	504	7/7	0.92	0.13	46,47,50,51	0
5	PEG	C	506	7/7	0.92	0.15	42,48,63,64	0
5	PEG	A	505	7/7	0.93	0.14	44,48,52,52	0
4	FUM	D	503	8/8	0.94	0.10	33,34,36,38	0
6	2SA	C	501	31/31	0.96	0.11	24,28,48,54	0
4	FUM	A	504	8/8	0.96	0.13	33,35,36,38	0
2	CL	C	502	1/1	0.97	0.10	45,45,45,45	0
2	CL	A	501	1/1	0.97	0.08	49,49,49,49	0
3	AMP	D	502	23/23	0.98	0.09	30,34,38,44	0
6	2SA	B	502	31/31	0.98	0.09	26,31,37,38	0
2	CL	C	503	1/1	0.99	0.11	26,26,26,26	0
3	AMP	A	503	23/23	0.99	0.10	27,29,31,33	0
2	CL	B	501	1/1	1.00	0.09	24,24,24,24	0
2	CL	D	501	1/1	1.00	0.08	35,35,35,35	0
2	CL	A	502	1/1	1.00	0.10	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.

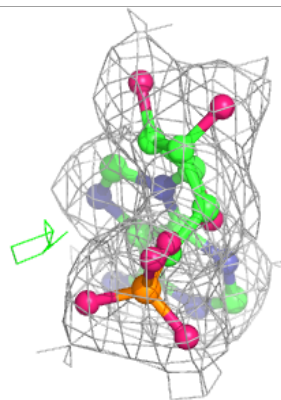
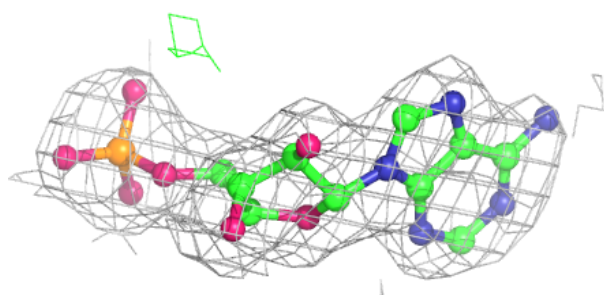
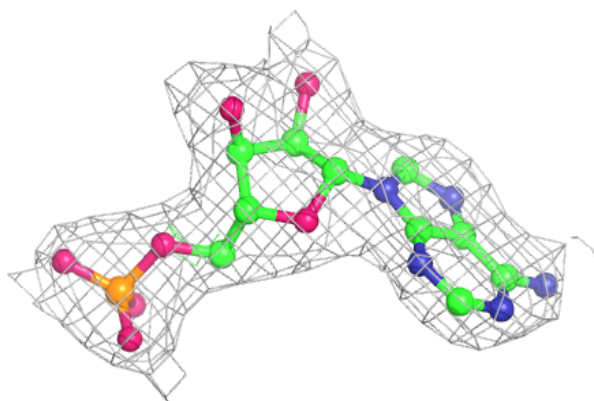
Electron density around 2SA C 501:

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

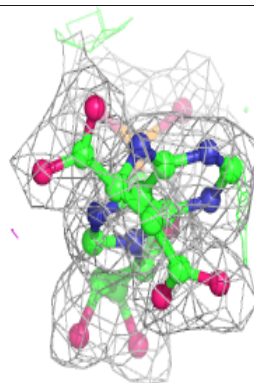
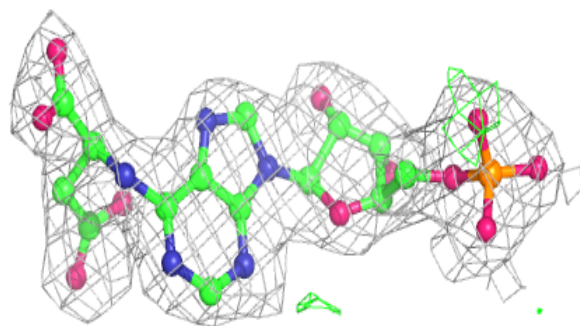
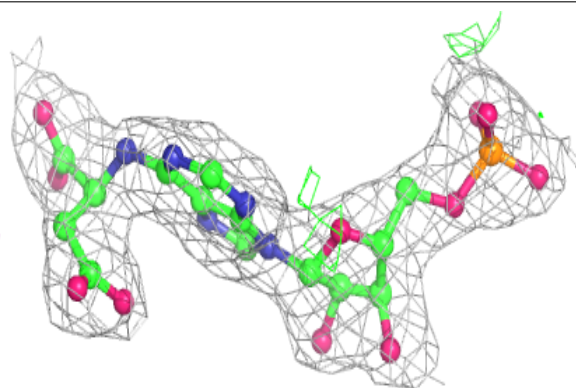


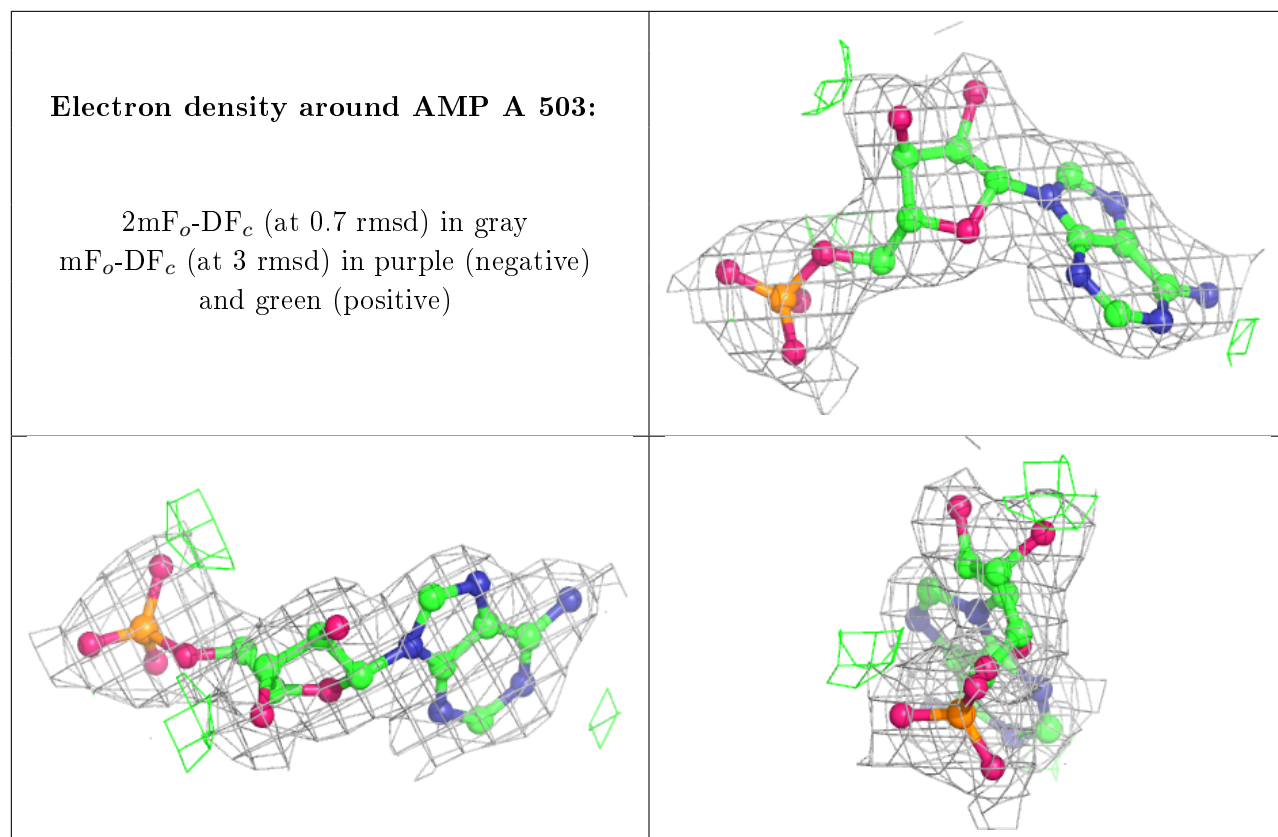
Electron density around AMP D 502:

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

**Electron density around 2SA B 502:**

$2mF_o-DF_c$ (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.