



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:33 AM UTC

PDB ID : 5NX9 / pdb_00005nx9
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 types of validation reports are described at

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

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

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

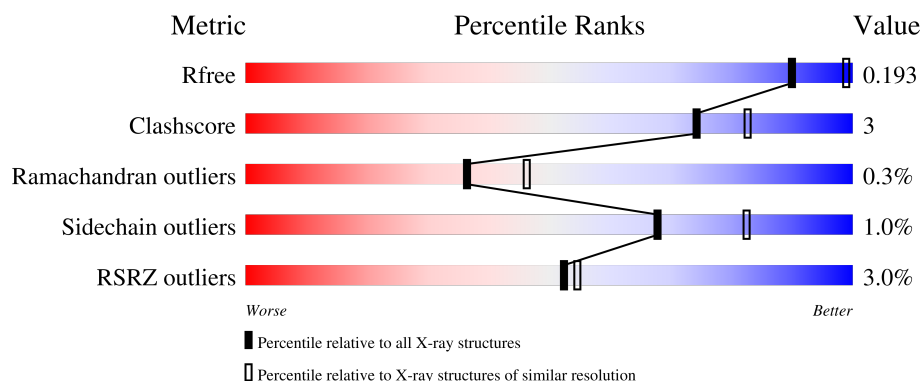
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	487	3% 88% 7% .
1	B	487	3% 91% 6% ..
1	C	487	4% 85% 6% 9%
1	D	487	% 89% 8% ..

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 (CCD ID: CL) (formula: Cl).

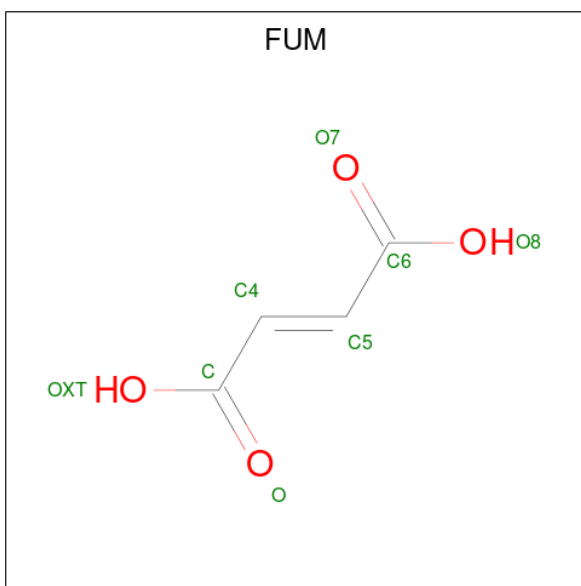
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		
2	B	1	Total	Cl	0	0
			1	1		
2	C	2	Total	Cl	0	0
			2	2		
2	D	1	Total	Cl	0	0
			1	1		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: 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 (CCD ID: FUM) (formula: $C_4H_4O_4$).



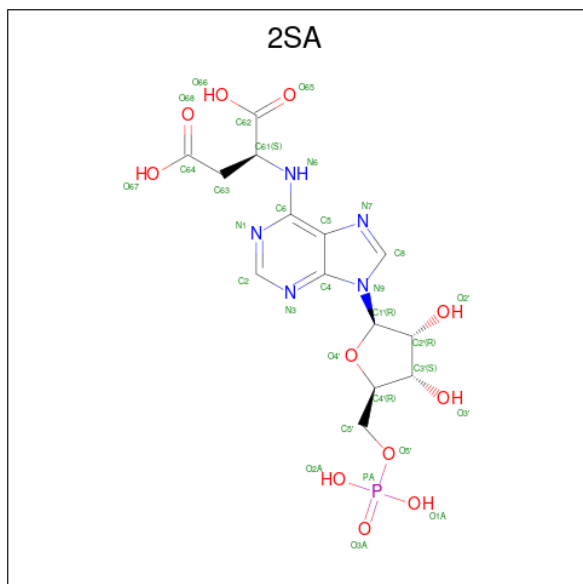
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	4	4		
4	D	1	Total	C	O	0	0
			8	4	4		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



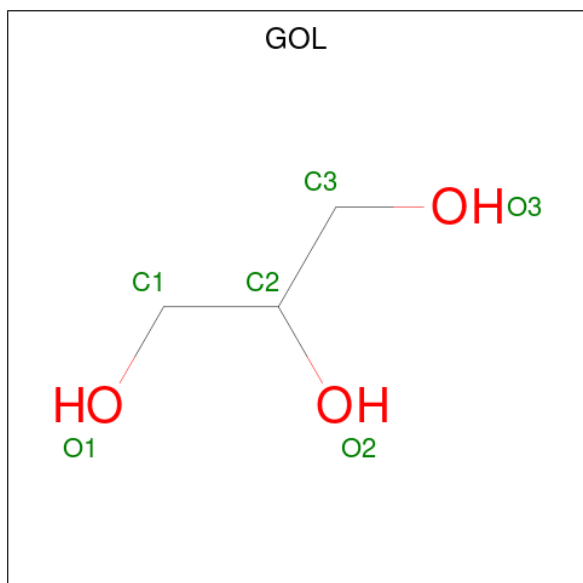
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	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 (CCD ID: 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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

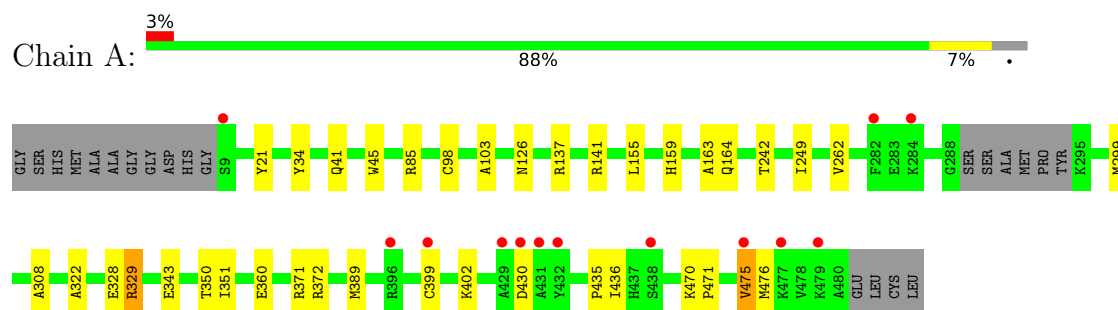
- Molecule 8 is water.

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		

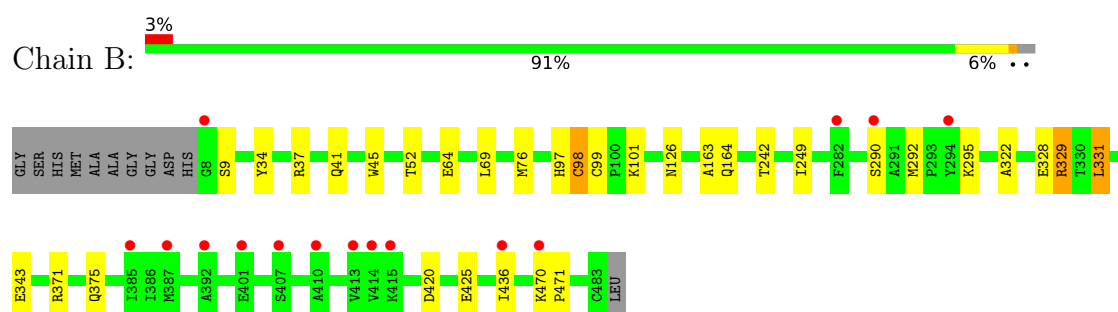
3 Residue-property plots

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.

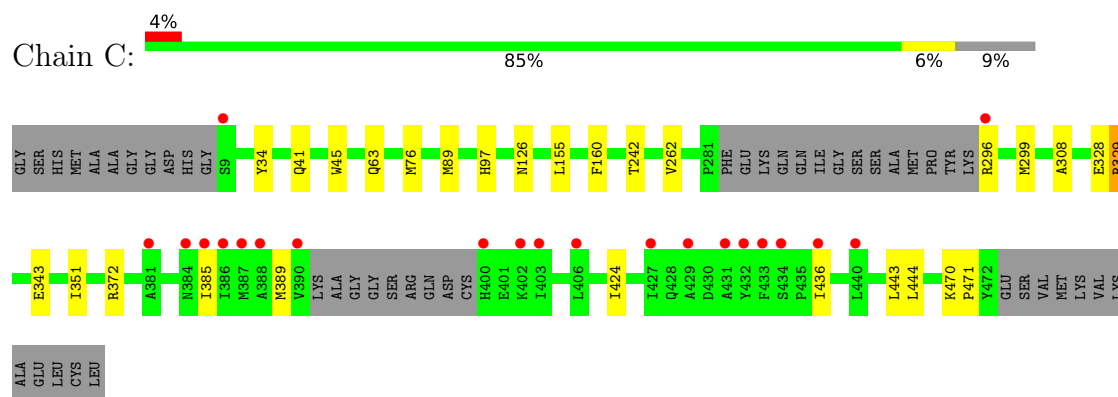
• Molecule 1: Adenylosuccinate lyase



• Molecule 1: Adenylosuccinate lyase

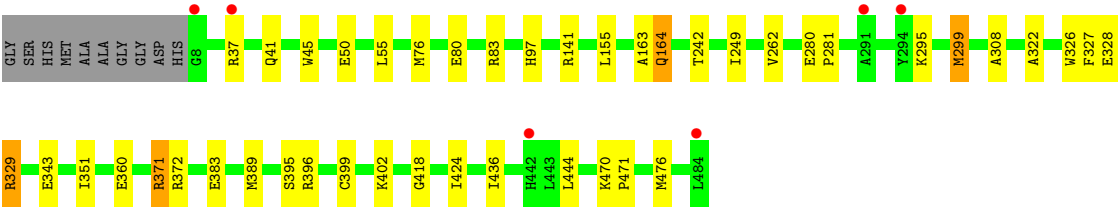


• Molecule 1: Adenylosuccinate lyase



• 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 (Not available) , 0.193	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)	0.36 , 34.6	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: 2SA, PEG, AMP, CL, GOL, FUM

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	0.72	0/3786	0.80	1/5108 (0.0%)
1	B	0.74	0/3860	0.80	1/5210 (0.0%)
1	C	0.72	0/3594	0.77	0/4855
1	D	0.72	0/3868	0.79	0/5221
All	All	0.72	0/15108	0.79	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	A	103	ALA	N-CA-C	-5.85	101.38	110.10
1	B	98	CYS	CB-CA-C	-5.44	101.43	110.68

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	27	0
1	B	3791	0	3818	23	0
1	C	3530	0	3552	24	0
1	D	3799	0	3829	26	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	1	3	0
4	D	8	0	1	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	1	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	15143	95	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 (95) 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:A:389:MET:HE3	1:A:436:ILE:HG12	1.77	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:LYS:NZ	6:C:501:2SA:O68	2.34	0.60
3:A:503:AMP:N6	4:A:504:FUM:C5	2.67	0.57
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: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:A:389:MET:HE2	1:A:389:MET:HA	1.89	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:389:MET:HE1	1:A:435:PRO:HG2	1.90	0.53
1:B:292:MET:HE3	1:B:295:LYS:HD2	1.91	0.53
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:A:389:MET:HE1	1:A:435:PRO:HB2	1.90	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:HG22	1:C:436:ILE:O	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:A:262:VAL:HG11	1:A:351:ILE:CG2	2.45	0.47
1:C:296:ARG:NH2	8:C:604:HOH:O	2.48	0.47
1:B:420:ASP:OD1	1:D:371:ARG:NH1	2.47	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:C:299:MET:O	1:C:299:MET:HE3	2.17	0.45
1:A:389:MET:HE1	1:A:435:PRO:CG	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ARG:NH2	1:B:69:LEU:HD13	2.32	0.45
1:B:290:SER:CB	1:C:89:MET:HE3	2.46	0.45
1:C:76:MET:HE1	1:C:97:HIS:ND1	2.31	0.45
1:A:389:MET:CE	1:A:436:ILE:HG23	2.48	0.44
1:B:41:GLN:HE21	1:B:45:TRP:NE1	2.16	0.44
1:A:85:ARG:HB3	1:D:299:MET:HE1	1.99	0.44
1:A:389:MET:HB3	1:A:399:CYS:SG	2.58	0.43
1:D:41:GLN:HE21	1:D:45:TRP:NE1	2.16	0.43
1:C:41:GLN:HE21	1:C:45:TRP:NE1	2.17	0.43
1:A:41:GLN:HE21	1:A:45:TRP:NE1	2.16	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
1:C:155:LEU:HD22	1:C:372:ARG:HG2	2.00	0.43
1:C:308:ALA:N	1:C:351:ILE:HD11	2.34	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:B:76:MET:HE1	1:B:97:HIS:ND1	2.34	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:B:163:ALA:O	1:B:164:GLN:C	2.63	0.42
1:D:249:ILE:HD11	1:D:322:ALA:HB3	2.02	0.42
1:A:163:ALA:O	1:A:164:GLN:C	2.63	0.41
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:D:76:MET:HE1	1:D:97:HIS:ND1	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:163:ALA:O	1:D:164:GLN:C	2.64	0.41
1:D:308:ALA:N	1:D:351:ILE:HD11	2.34	0.41
1:A:21:TYR:HB3	1:A:350:THR:HG21	2.03	0.41
1:A:249:ILE:HD11	1:A:322:ALA:HB3	2.03	0.41
1:B:343:GLU:OE1	1:C:343:GLU:OE2	2.39	0.41
1:D:470:LYS:HB3	1:D:471:PRO:HD3	2.03	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:63:GLN:HG3	8:C:679:HOH:O	2.21	0.40
1:C:160:PHE:HB2	1:D:326:TRP:HE3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	462/487 (95%)	458 (99%)	3 (1%)	1 (0%)	43	55
1	B	474/487 (97%)	469 (99%)	3 (1%)	2 (0%)	30	38
1	C	435/487 (89%)	432 (99%)	2 (0%)	1 (0%)	43	55
1	D	475/487 (98%)	473 (100%)	1 (0%)	1 (0%)	43	55
All	All	1846/1948 (95%)	1832 (99%)	9 (0%)	5 (0%)	36	46

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%)	403 (99%)	5 (1%)	63	79
1	B	416/422 (99%)	412 (99%)	4 (1%)	68	82
1	C	388/422 (92%)	388 (100%)	0	100	100
1	D	417/422 (99%)	409 (98%)	8 (2%)	50	69
All	All	1629/1688 (96%)	1612 (99%)	17 (1%)	68	82

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	CYS
1	A	299	MET
1	A	402	LYS
1	A	430	ASP
1	A	475	VAL
1	B	98	CYS
1	B	331	LEU
1	B	425	GLU
1	B	436	ILE
1	D	37	ARG
1	D	164	GLN
1	D	295	LYS
1	D	299	MET
1	D	371	ARG
1	D	395	SER
1	D	402	LYS
1	D	436	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	63	GLN
1	A	177	GLN
1	A	184	GLN
1	A	217	HIS
1	A	221	GLN
1	A	439	GLN
1	B	177	GLN
1	C	41	GLN
1	C	177	GLN
1	C	221	GLN
1	D	63	GLN
1	D	93	HIS
1	D	126	ASN
1	D	177	GLN
1	D	285	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 oligosaccharides 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$
4	FUM	D	503	-	7,7,7	1.36	1 (14%)	8,8,8	0.99	0
5	PEG	C	506	-	6,6,6	0.53	0	5,5,5	0.39	0
5	PEG	D	506	-	6,6,6	0.55	0	5,5,5	0.32	0
5	PEG	A	507	-	6,6,6	0.58	0	5,5,5	0.59	0
4	FUM	A	504	-	7,7,7	1.17	1 (14%)	8,8,8	1.03	0
6	2SA	C	501	-	33,33,33	2.88	9 (27%)	47,49,49	2.13	14 (29%)
7	GOL	C	507	-	5,5,5	0.34	0	5,5,5	0.39	0
5	PEG	A	505	-	6,6,6	0.58	0	5,5,5	0.35	0
5	PEG	A	506	-	6,6,6	0.68	0	5,5,5	0.37	0
5	PEG	C	508	-	6,6,6	0.53	0	5,5,5	0.33	0
5	PEG	A	508	-	6,6,6	0.55	0	5,5,5	0.16	0
3	AMP	A	503	-	25,25,25	1.33	4 (16%)	37,38,38	2.04	13 (35%)
5	PEG	C	505	-	6,6,6	0.56	0	5,5,5	0.31	0
5	PEG	D	504	-	6,6,6	0.68	0	5,5,5	0.51	0
6	2SA	B	502	-	33,33,33	2.83	9 (27%)	47,49,49	1.84	13 (27%)
5	PEG	A	509	-	6,6,6	0.55	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMP	D	502	-	25,25,25	1.13	4 (16%)	37,38,38	1.98	10 (27%)
5	PEG	D	505	-	6,6,6	0.57	0	5,5,5	0.39	0
5	PEG	B	503	-	6,6,6	0.55	0	5,5,5	0.37	0
5	PEG	C	504	-	6,6,6	0.71	0	5,5,5	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUM	D	503	-	-	0/5/5/5	-
5	PEG	C	506	-	-	3/4/4/4	-
5	PEG	D	506	-	-	3/4/4/4	-
5	PEG	A	507	-	-	4/4/4/4	-
4	FUM	A	504	-	-	2/5/5/5	-
6	2SA	C	501	-	-	13/22/38/38	0/3/3/3
7	GOL	C	507	-	-	0/4/4/4	-
5	PEG	A	505	-	-	2/4/4/4	-
5	PEG	A	506	-	-	2/4/4/4	-
5	PEG	C	508	-	-	1/4/4/4	-
5	PEG	A	508	-	-	2/4/4/4	-
3	AMP	A	503	-	-	3/10/26/26	0/3/3/3
5	PEG	C	505	-	-	2/4/4/4	-
5	PEG	D	504	-	-	3/4/4/4	-
6	2SA	B	502	-	-	7/22/38/38	0/3/3/3
5	PEG	A	509	-	-	3/4/4/4	-
3	AMP	D	502	-	-	4/10/26/26	0/3/3/3
5	PEG	D	505	-	-	2/4/4/4	-
5	PEG	B	503	-	-	2/4/4/4	-
5	PEG	C	504	-	-	3/4/4/4	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	502	2SA	C3'-C2'	-9.29	1.28	1.53
6	C	501	2SA	C3'-C2'	-9.06	1.28	1.53
6	C	501	2SA	C6-N6	7.11	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	502	2SA	C6-N6	7.04	1.46	1.35
6	C	501	2SA	O4'-C4'	-6.82	1.29	1.45
6	B	502	2SA	O4'-C4'	-6.61	1.30	1.45
6	B	502	2SA	C3'-C4'	4.46	1.64	1.53
6	C	501	2SA	C3'-C4'	4.15	1.63	1.53
6	C	501	2SA	C1'-N9	-4.09	1.35	1.46
6	B	502	2SA	O4'-C1'	3.91	1.51	1.42
6	C	501	2SA	O4'-C1'	3.84	1.50	1.42
6	C	501	2SA	O2'-C2'	3.30	1.51	1.43
3	A	503	AMP	C5-C4	3.26	1.44	1.39
6	B	502	2SA	C1'-N9	-3.24	1.37	1.46
3	D	502	AMP	C5-C4	2.78	1.44	1.39
3	A	503	AMP	C5-N7	-2.56	1.34	1.39
3	A	503	AMP	C4-N9	-2.55	1.32	1.37
6	C	501	2SA	C61-N6	2.55	1.52	1.46
3	D	502	AMP	C4-N9	-2.45	1.32	1.37
3	D	502	AMP	C5-N7	-2.39	1.34	1.39
3	A	503	AMP	C5-C6	2.28	1.47	1.41
6	B	502	2SA	O2'-C2'	2.24	1.48	1.43
6	C	501	2SA	C61-C62	2.21	1.58	1.52
4	A	504	FUM	O8-C6	-2.16	1.24	1.30
6	B	502	2SA	C5-N7	-2.05	1.35	1.39
4	D	503	FUM	O7-C6	2.02	1.28	1.23
6	B	502	2SA	C63-C64	2.01	1.56	1.51
3	D	502	AMP	C8-N7	2.01	1.35	1.31

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	AMP	C5-C4-N3	-5.56	119.06	126.72
6	C	501	2SA	C5-C4-N3	-5.28	119.45	126.72
6	B	502	2SA	C5-C4-N3	-5.15	119.62	126.72
3	A	503	AMP	C5-C4-N3	-4.98	119.85	126.72
6	C	501	2SA	C62-C61-N6	4.96	122.08	110.56
3	D	502	AMP	N3-C4-N9	4.56	134.93	127.17
6	C	501	2SA	O66-C62-O65	-4.51	113.85	124.08
3	A	503	AMP	N3-C4-N9	4.42	134.69	127.17
6	C	501	2SA	N1-C2-N3	-4.35	122.00	128.58
6	B	502	2SA	N3-C4-N9	4.03	134.03	127.17
3	D	502	AMP	N3-C2-N1	-4.03	122.48	128.58
3	D	502	AMP	C2-N3-C4	3.99	121.58	111.83
3	A	503	AMP	N3-C2-N1	-3.94	122.62	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	AMP	C4-N9-C8	3.90	109.83	105.74
6	B	502	2SA	N1-C2-N3	-3.85	122.76	128.58
6	C	501	2SA	C2-N3-C4	3.77	121.03	111.83
3	A	503	AMP	C2-N3-C4	3.66	120.77	111.83
6	C	501	2SA	N3-C4-N9	3.44	133.02	127.17
6	B	502	2SA	C5-N7-C8	3.37	108.75	103.45
3	D	502	AMP	C4-N9-C8	3.20	109.10	105.74
6	C	501	2SA	C4-C5-N7	-3.19	106.94	110.58
6	C	501	2SA	O66-C62-C61	3.11	124.02	113.51
6	C	501	2SA	C6-C5-N7	3.04	135.75	132.43
6	B	502	2SA	C4-C5-N7	-2.95	107.21	110.58
3	A	503	AMP	C4-C5-N7	-2.95	107.21	110.58
6	B	502	2SA	C2-N3-C4	2.91	118.95	111.83
3	A	503	AMP	N9-C8-N7	-2.87	109.87	113.94
6	C	501	2SA	N9-C8-N7	-2.87	109.87	113.94
3	A	503	AMP	O3P-P-O2P	2.78	118.23	107.80
6	B	502	2SA	O66-C62-O65	-2.77	117.80	124.08
3	D	502	AMP	N9-C8-N7	-2.71	110.09	113.94
3	A	503	AMP	C5-N7-C8	2.66	107.63	103.45
6	B	502	2SA	C4-C5-C6	2.60	118.94	116.78
6	C	501	2SA	C5-N7-C8	2.59	107.52	103.45
6	B	502	2SA	N9-C8-N7	-2.51	110.37	113.94
3	D	502	AMP	O2P-P-O5'	-2.26	100.78	106.67
6	B	502	2SA	O66-C62-C61	2.23	121.07	113.51
3	D	502	AMP	C4-C5-N7	-2.23	108.03	110.58
6	C	501	2SA	C4-N9-C8	2.19	108.03	105.74
6	C	501	2SA	O67-C64-C63	2.17	120.76	114.00
3	A	503	AMP	C6-C5-N7	2.16	136.25	132.09
6	B	502	2SA	O4'-C1'-C2'	-2.13	102.05	106.62
3	A	503	AMP	O2P-P-O5'	-2.11	101.16	106.67
3	D	502	AMP	C5-N7-C8	2.11	106.77	103.45
6	B	502	2SA	O67-C64-C63	2.08	120.46	114.00
6	B	502	2SA	C5'-C4'-C3'	-2.05	107.83	115.21
3	A	503	AMP	O4'-C1'-C2'	-2.05	102.23	106.62
6	C	501	2SA	O4'-C1'-N9	2.04	112.01	108.09
3	A	503	AMP	C4-N9-C1'	-2.01	121.94	126.63
3	D	502	AMP	O3P-P-O2P	2.00	115.32	107.80

There are no chirality outliers.

All (61) 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	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
5	A	505	PEG	O1-C1-C2-O2
5	A	509	PEG	O2-C3-C4-O4
5	C	506	PEG	O2-C3-C4-O4
5	A	505	PEG	O2-C3-C4-O4
5	A	507	PEG	O1-C1-C2-O2
5	C	504	PEG	O2-C3-C4-O4
5	D	504	PEG	O1-C1-C2-O2
5	D	506	PEG	O1-C1-C2-O2
5	A	506	PEG	O2-C3-C4-O4
5	A	508	PEG	O1-C1-C2-O2
5	A	509	PEG	O1-C1-C2-O2
5	D	505	PEG	O1-C1-C2-O2
5	A	507	PEG	O2-C3-C4-O4
5	C	505	PEG	O1-C1-C2-O2
5	C	505	PEG	O2-C3-C4-O4
5	C	504	PEG	O1-C1-C2-O2
5	A	508	PEG	O2-C3-C4-O4
5	B	503	PEG	O2-C3-C4-O4
6	C	501	2SA	C62-C61-C63-C64
6	C	501	2SA	N6-C61-C62-O65
6	C	501	2SA	N6-C61-C62-O66
6	C	501	2SA	N6-C61-C63-C64
4	A	504	FUM	C4-C5-C6-O8
5	A	506	PEG	O1-C1-C2-O2
3	A	503	AMP	C2'-C1'-N9-C8
6	B	502	2SA	C2'-C1'-N9-C8
5	D	506	PEG	O2-C3-C4-O4
5	C	506	PEG	C1-C2-O2-C3
5	C	508	PEG	O1-C1-C2-O2
5	D	505	PEG	C4-C3-O2-C2
3	D	502	AMP	C2'-C1'-N9-C8
6	C	501	2SA	C2'-C1'-N9-C8
5	D	506	PEG	C1-C2-O2-C3
6	C	501	2SA	C63-C61-C62-O65
4	A	504	FUM	C4-C5-C6-O7
5	D	504	PEG	C1-C2-O2-C3
5	B	503	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
5	C	504	PEG	C4-C3-O2-C2
5	A	509	PEG	C4-C3-O2-C2
5	A	507	PEG	C1-C2-O2-C3
5	D	504	PEG	C4-C3-O2-C2
6	B	502	2SA	C2'-C1'-N9-C4
6	C	501	2SA	C2'-C1'-N9-C4
6	B	502	2SA	O4'-C4'-C5'-O5'
5	C	506	PEG	C4-C3-O2-C2
6	C	501	2SA	C63-C61-C62-O66
6	C	501	2SA	O4'-C1'-N9-C8
3	A	503	AMP	C2'-C1'-N9-C4
3	A	503	AMP	O4'-C1'-N9-C8
3	D	502	AMP	C2'-C1'-N9-C4
3	D	502	AMP	O4'-C1'-N9-C8
6	B	502	2SA	O4'-C1'-N9-C8
3	D	502	AMP	O4'-C1'-N9-C4
5	A	507	PEG	C4-C3-O2-C2
6	B	502	2SA	C3'-C4'-C5'-O5'

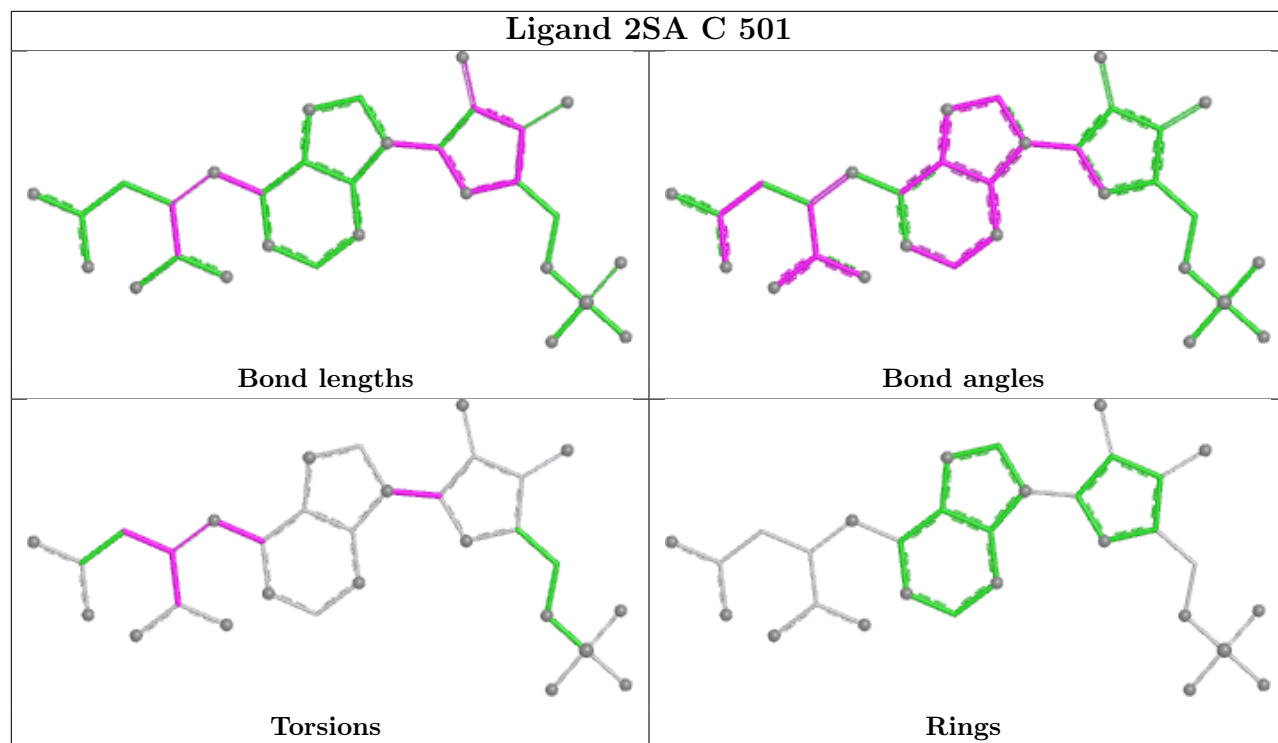
There are no ring outliers.

5 monomers are involved in 6 short contacts:

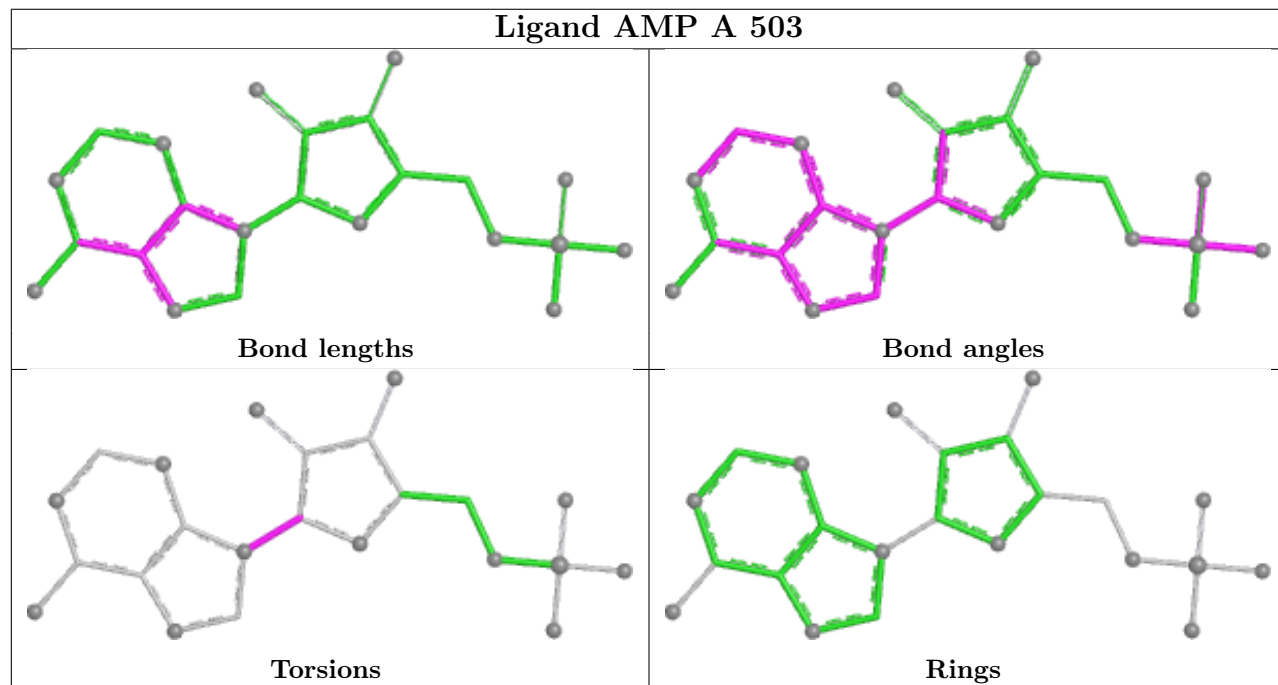
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	FUM	3	0
6	C	501	2SA	1	0
3	A	503	AMP	3	0
5	A	509	PEG	1	0
5	B	503	PEG	1	0

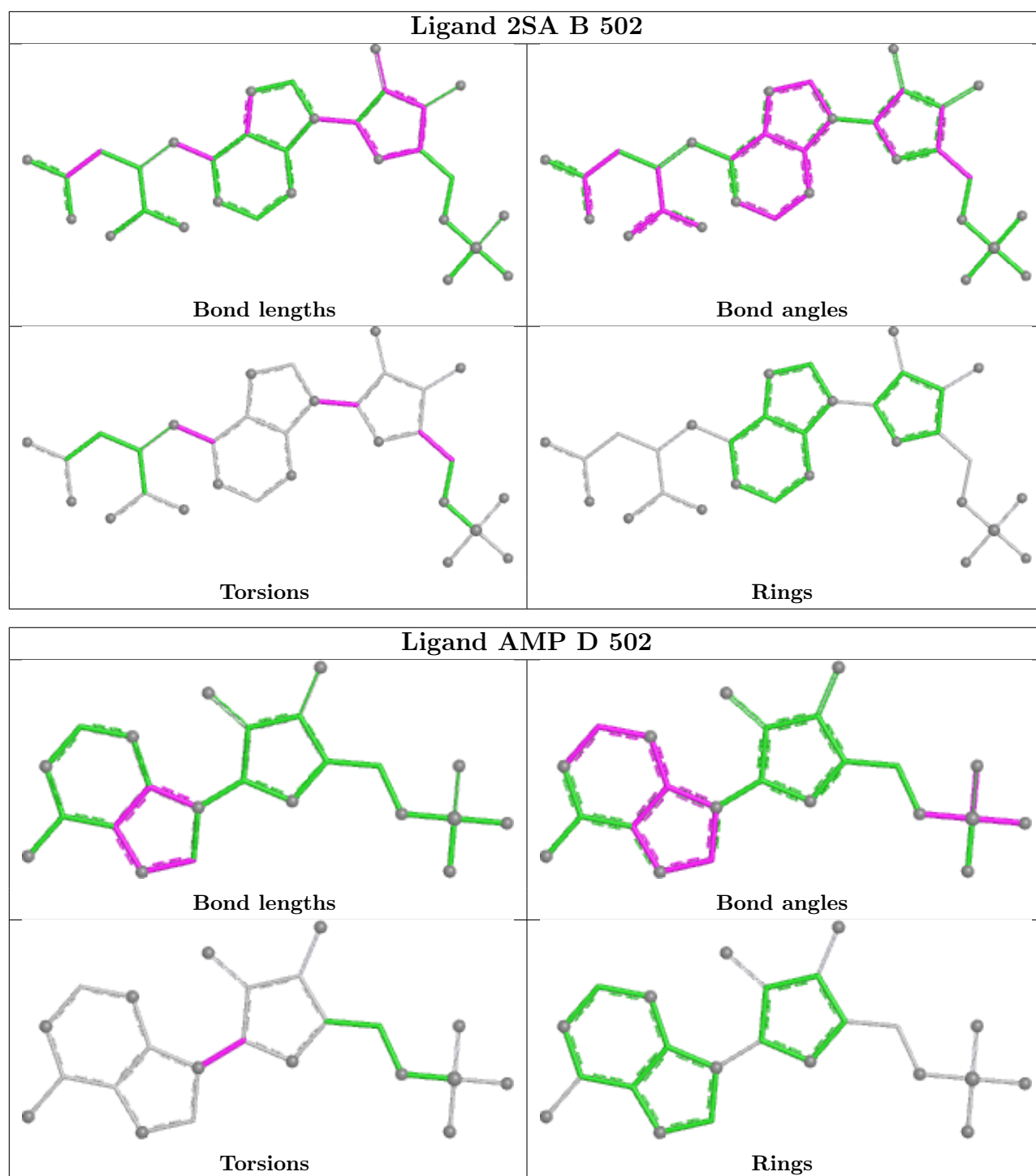
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand 2SA C 501



Ligand AMP A 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	A	466/487 (95%)	0.05	13 (2%) 55 57	21, 36, 81, 110	0
1	B	476/487 (97%)	0.07	15 (3%) 50 52	21, 35, 76, 106	0
1	C	441/487 (90%)	0.03	21 (4%) 35 37	21, 34, 91, 130	0
1	D	477/487 (97%)	-0.04	6 (1%) 75 76	22, 37, 63, 87	0
All	All	1860/1948 (95%)	0.03	55 (2%) 52 54	21, 35, 77, 130	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	PHE	6.6
1	C	432	TYR	4.0
1	C	390	VAL	3.8
1	C	436	ILE	3.8
1	B	282	PHE	3.7
1	C	385	ILE	3.6
1	B	8	GLY	3.6
1	D	484	LEU	3.6
1	C	431	ALA	3.1
1	C	403	ILE	3.1
1	C	386	ILE	3.1
1	D	294	TYR	3.0
1	B	294	TYR	3.0
1	B	414	VAL	2.9
1	A	475	VAL	2.9
1	D	8	GLY	2.8
1	A	431	ALA	2.7
1	C	429	ALA	2.7
1	B	413	VAL	2.7
1	B	290	SER	2.7
1	B	392	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	291	ALA	2.6
1	A	438	SER	2.6
1	A	432	TYR	2.6
1	D	442	HIS	2.6
1	C	427	ILE	2.6
1	C	433	PHE	2.5
1	B	385	ILE	2.4
1	C	400	HIS	2.4
1	B	387	MET	2.4
1	C	387	MET	2.4
1	A	430	ASP	2.3
1	B	436	ILE	2.3
1	A	396	ARG	2.3
1	C	402	LYS	2.3
1	A	399	CYS	2.2
1	B	415	LYS	2.2
1	C	9	SER	2.2
1	C	384	ASN	2.2
1	B	407	SER	2.2
1	C	388	ALA	2.2
1	C	406	LEU	2.1
1	C	440	LEU	2.1
1	B	410	ALA	2.1
1	A	479	LYS	2.1
1	A	429	ALA	2.1
1	A	477	LYS	2.1
1	B	470	LYS	2.1
1	A	9	SER	2.0
1	B	401	GLU	2.0
1	A	284	LYS	2.0
1	C	434	SER	2.0
1	C	381	ALA	2.0
1	C	296	ARG	2.0
1	D	37	ARG	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 ⓘ

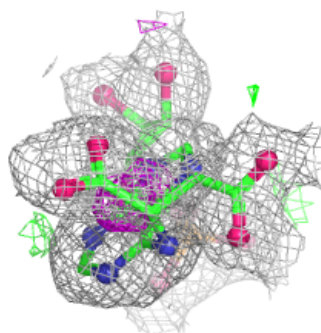
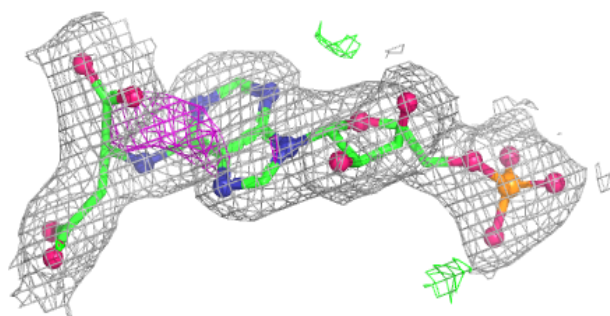
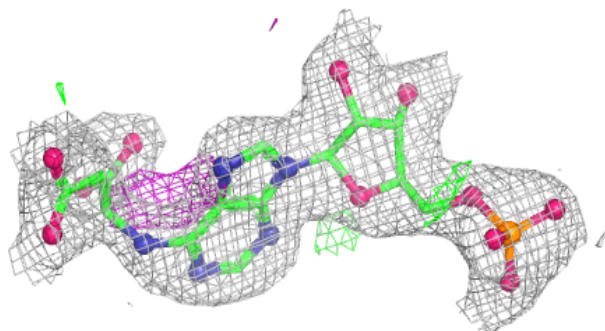
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PEG	D	505	7/7	0.78	0.17	57,67,74,75	0
7	GOL	C	507	6/6	0.82	0.16	60,63,65,67	0
5	PEG	A	509	7/7	0.83	0.18	63,64,68,71	0
5	PEG	C	505	7/7	0.86	0.14	64,67,68,68	0
5	PEG	D	506	7/7	0.87	0.13	56,61,68,70	0
5	PEG	A	508	7/7	0.89	0.12	61,65,67,68	0
5	PEG	A	507	7/7	0.89	0.12	53,55,58,58	0
5	PEG	C	508	7/7	0.90	0.12	51,54,61,67	0
5	PEG	D	504	7/7	0.91	0.11	46,47,50,51	0
5	PEG	C	504	7/7	0.91	0.11	37,45,47,48	0
5	PEG	A	506	7/7	0.91	0.10	50,51,57,57	0
5	PEG	B	503	7/7	0.91	0.10	49,53,55,56	0
5	PEG	C	506	7/7	0.92	0.09	42,48,63,64	0
5	PEG	A	505	7/7	0.92	0.11	44,48,52,52	0
4	FUM	A	504	8/8	0.92	0.11	33,35,36,38	0
4	FUM	D	503	8/8	0.93	0.08	33,34,36,38	0
6	2SA	C	501	31/31	0.96	0.07	24,28,48,54	0
3	AMP	D	502	23/23	0.97	0.05	30,34,38,44	0
6	2SA	B	502	31/31	0.97	0.05	26,31,37,38	0
2	CL	A	501	1/1	0.97	0.08	49,49,49,49	0
2	CL	C	502	1/1	0.97	0.04	45,45,45,45	0
2	CL	D	501	1/1	0.98	0.07	35,35,35,35	0
3	AMP	A	503	23/23	0.98	0.04	27,29,31,33	0
2	CL	C	503	1/1	0.98	0.03	26,26,26,26	0
2	CL	A	502	1/1	0.99	0.04	27,27,27,27	0
2	CL	B	501	1/1	1.00	0.01	24,24,24,24	0

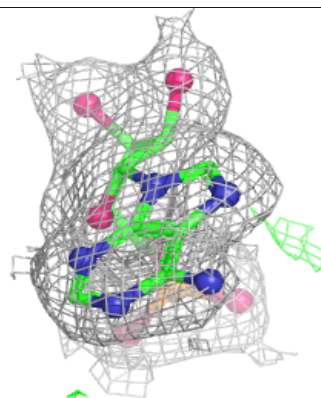
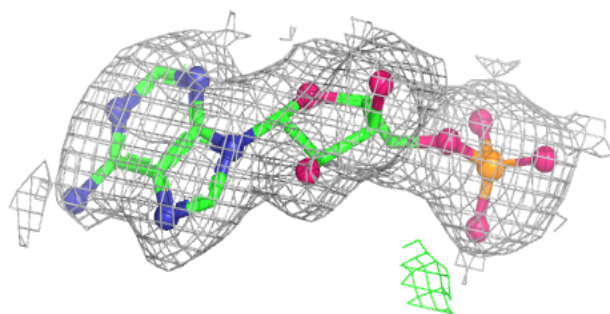
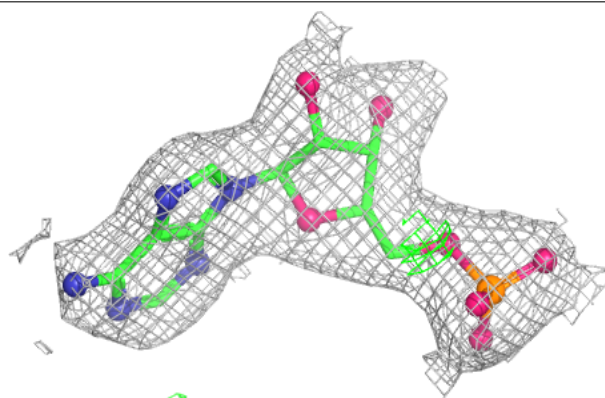
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

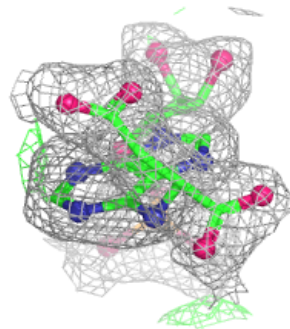
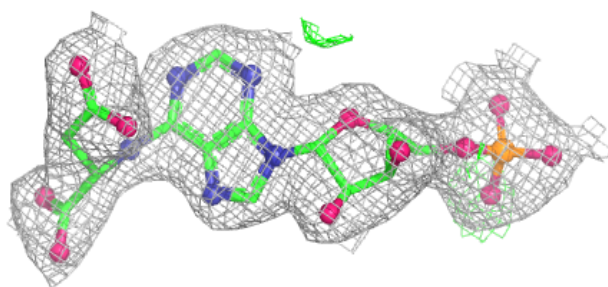
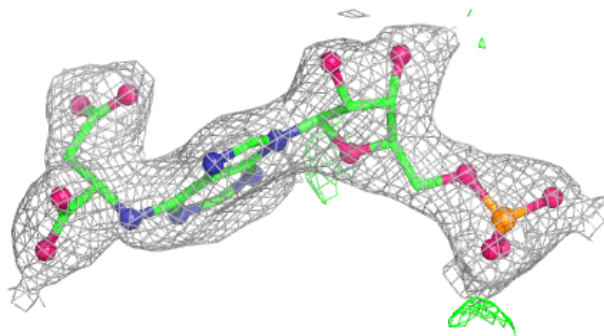
**Electron density around AMP D 502:**

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

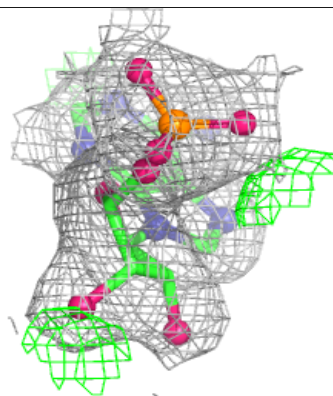
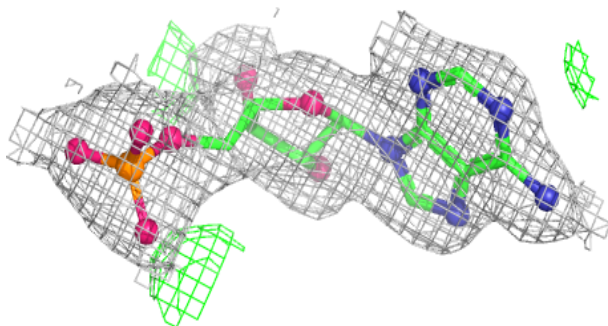
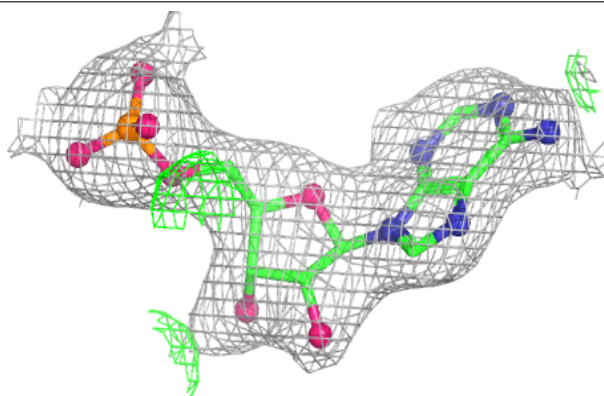


Electron density around 2SA B 502:

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

**Electron density around AMP A 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.