



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 12:53 PM BST

PDB ID : 6OFB
Title : Crystal structure of human glutamine-dependent NAD⁺ synthetase complexed with NaAD⁺, AMP, pyrophosphate, and Mg²⁺
Authors : Chuenchor, W.; Doukov, T.I.; Gerratana, B.
Deposited on : 2019-03-28
Resolution : 2.84 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 : 2.13.1
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) : 2.13.1

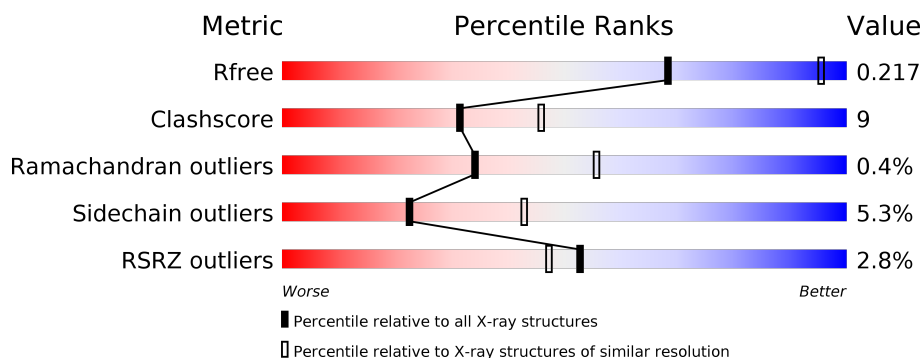
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	707	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>..</div> </div> </div>
1	B	707	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>..</div> </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
4	POP	A	903	-	-	X	-
6	CL	B	907	-	-	X	-
6	CL	B	908	-	-	X	-

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 11222 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.

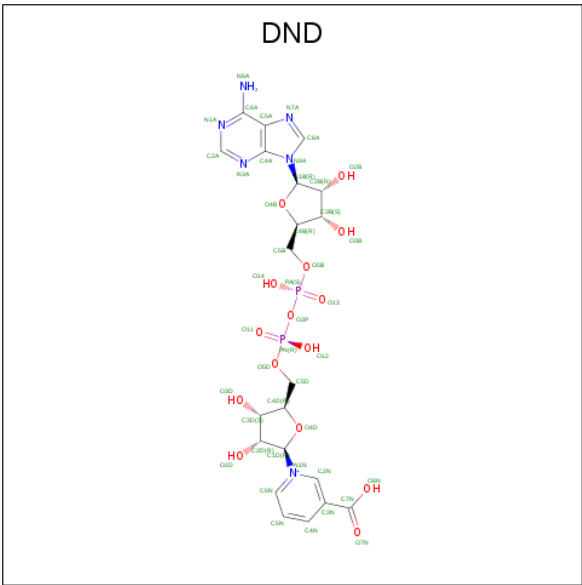
- Molecule 1 is a protein called Glutamine-dependent NAD(+) synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	696	Total	C	N	O	S	0	1	0
			5500	3473	964	1021	42			
1	B	696	Total	C	N	O	S	0	2	0
			5512	3483	966	1021	42			

There are 6 discrepancies between the modelled and reference sequences:

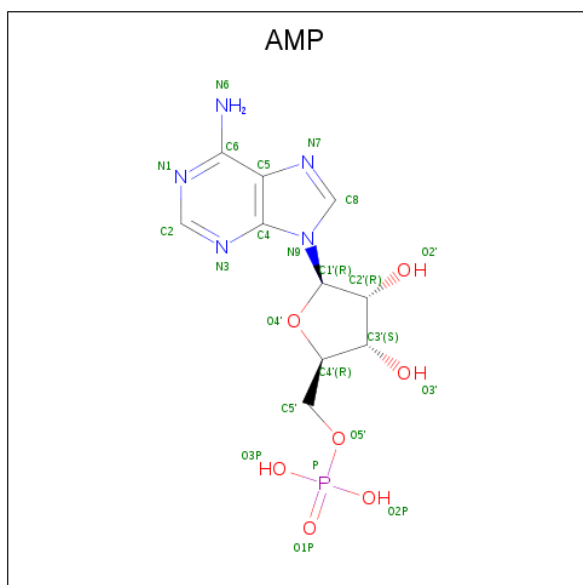
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q6IA69
A	74	LEU	VAL	variant	UNP Q6IA69
A	204	HIS	GLN	variant	UNP Q6IA69
B	0	SER	-	expression tag	UNP Q6IA69
B	74	LEU	VAL	variant	UNP Q6IA69
B	204	HIS	GLN	variant	UNP Q6IA69

- Molecule 2 is NICOTINIC ACID ADENINE DINUCLEOTIDE (three-letter code: DND) (formula: C₂₁H₂₇N₆O₁₅P₂) (labeled as "Ligand of Interest" by author).



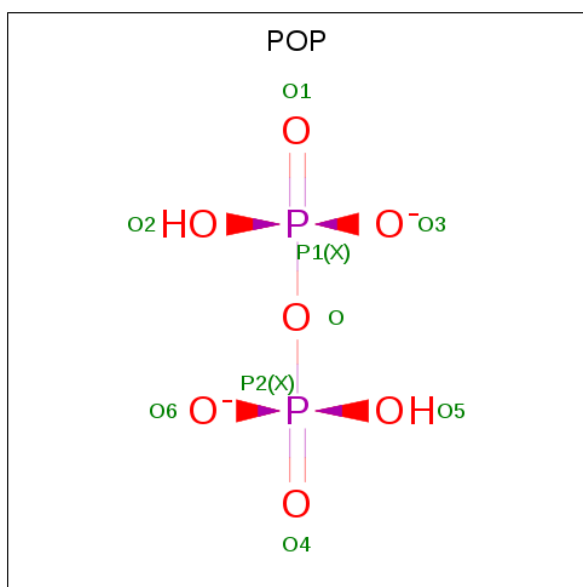
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	6	15	2		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by author).



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

- Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 9 7 2	0	0
4	B	1	Total O P 9 7 2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by author).

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	4	Total Cl 4 4	0	0
6	A	5	Total Cl 5 5	0	0

- Molecule 7 is water.


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	16	Total O 16 16	0	0

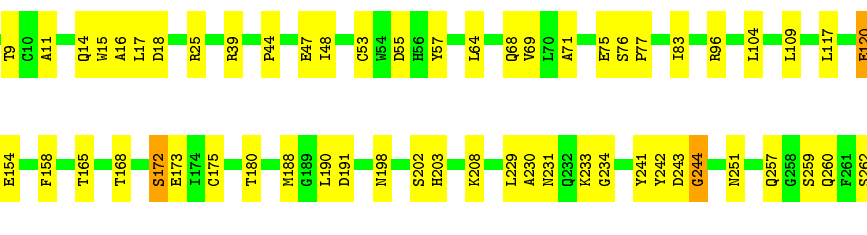
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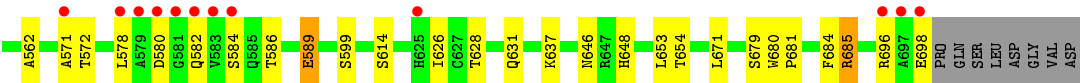
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	31	Total	O	0	0
			31	31		

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.

- Chain A: 



- Chain B:
-
- 29% 75% 22%
- | Category | Value |
|----------|-------|
| SER | A118 |
| GLY | M119 |
| GLY | E120 |
| R3 | Y123 |
| A8 | R124 |
| A11 | E125 |
| L12 | L126 |
| L17 | E127 |
| H15 | M128 |
| H16 | R134 |
| D18 | T138 |
| N22 | Y141 |
| L23 | T147 |
| I26 | L150 |
| Y40 | T151 |
| R41 | K152 |
| L42 | Q153 |
| G43 | F158 |
| P44 | L163 |
| E47 | T168 |
| Y51 | S172 |
| G52 | E173 |
| C53 | I174 |
| H54 | G175 |
| D55 | E176 |
| Y57 | S183 |
| Y58 | P184 |
| L63 | D191 |
| V69 | T197 |
| L70 | N198 |
| A71 | G201 |
| E75 | S202 |
| V86 | T211 |
| N91 | M231 |
| R96 | G234 |
| R100 | C235 |
| L110 | Y241 |
| I111 | Y242 |
| K114 | D243 |
| H115 | G244 |
| A116 | C245 |
| L117 | V266 |
| S259 | T270 |
| Q260 | L275 |
| V266 | L285 |
| S286 | S287 |
| R288 | R294 |
| S293 | R300 |
| R294 | L307 |
| R300 | E311 |
| L307 | D312 |
| E311 | L313 |
| D312 | L314 |
| L313 | E322 |
| L314 | W323 |
| E322 | K324 |
| W323 | S333 |
| K324 | P336 |
| S333 | L340 |
| P336 | F343 |
| L340 | A486 |
| F343 | R487 |
| A486 | I488 |
| R487 | Q489 |
| I488 | A491 |
| Q489 | L511 |
| A491 | A516 |
| L511 | G524 |
| A516 | K528 |
| G524 | Y529 |
| K528 | D530 |
| Y529 | C531 |
| D530 | S532 |
| C531 | S533 |
| S532 | I536 |
| S533 | G540 |
| I536 | L547 |
| G540 | L549 |
| L547 | V387 |
| L549 | S382 |
| V387 | G383 |
| S382 | N384 |
| G383 | E386 |
| N384 | L547 |
| E386 | L549 |



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	102.25Å 198.89Å 219.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.40 – 2.84 37.40 – 2.84	Depositor EDS
% Data completeness (in resolution range)	98.7 (37.40-2.84) 98.7 (37.40-2.84)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.85Å)	Xtriage
Refinement program	PHENIX 1.16_3549, PHENIX 1.16_3549	Depositor
R, R_{free}	0.179 , 0.217 0.180 , 0.217	Depositor DCC
R_{free} test set	2668 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	71.7	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11222	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: DND, MG, AMP, POP, CL

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	0.43	0/5625	0.58	0/7631
1	B	0.44	0/5641	0.59	1/7653 (0.0%)
All	All	0.43	0/11266	0.58	1/15284 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	GLY	N-CA-C	-5.18	100.15	113.10

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	5500	0	5435	103	0
1	B	5512	0	5451	98	0
2	A	44	0	25	2	0
2	B	44	0	25	2	0
3	A	23	0	12	2	0
3	B	23	0	12	2	0
4	A	9	0	0	4	0
4	B	9	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	5	0	0	1	0
6	B	4	0	0	4	0
7	A	16	0	0	2	0
7	B	31	0	0	0	0
All	All	11222	0	10960	200	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 9.

All (200) 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:126:LEU:HD13	1:B:126:LEU:HD13	1.40	1.01
1:A:151:THR:HG23	1:A:153:GLN:HG3	1.44	0.96
1:B:349:GLN:HG2	1:B:511:LEU:HD12	1.51	0.91
1:A:288:ARG:HG2	1:A:289:ASN:H	1.35	0.89
1:A:487:ARG:NH2	2:A:901:DND:O14	2.11	0.82
1:B:63:LEU:HD21	1:B:91:MET:HE3	1.61	0.82
1:B:234:GLY:HA2	1:B:241:TYR:CE1	2.15	0.82
1:A:528:LYS:NZ	1:A:648:HIS:HD2	1.81	0.77
1:A:288:ARG:CG	1:A:289:ASN:H	1.95	0.77
1:A:288:ARG:HG2	1:A:289:ASN:N	2.00	0.77
1:A:120:GLU:OE2	1:B:58:TYR:OH	2.03	0.75
1:A:398:ILE:H	1:A:398:ILE:HD12	1.55	0.72
1:A:173:GLU:O	1:A:198:ASN:HA	1.90	0.72
1:B:100:ARG:HG2	1:B:174:ILE:HD11	1.69	0.72
1:B:390:ASP:O	1:B:394:ILE:HG13	1.90	0.72
1:A:626:ILE:H	1:A:626:ILE:HD12	1.55	0.71
1:B:487:ARG:NH2	2:B:901:DND:O14	2.18	0.69
1:B:63:LEU:HD21	1:B:91:MET:CE	2.21	0.69
1:A:357:SER:OG	4:A:903:POP:O6	2.09	0.69
1:A:14:GLN:OE1	1:A:25:ARG:HD2	1.92	0.69
1:B:429:THR:HG22	1:B:432:ARG:HH12	1.58	0.69
1:A:612:PRO:HD3	1:A:640:PHE:CE1	2.29	0.67
1:B:357:SER:OG	4:B:903:POP:O4	2.11	0.67
1:B:572:THR:HG21	1:B:584:SER:OG	1.95	0.67
1:A:387:VAL:O	1:A:391:VAL:HG23	1.95	0.67
1:B:387:VAL:O	1:B:391:VAL:HG23	1.95	0.67
1:A:528:LYS:HZ1	1:A:648:HIS:HD2	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:HIS:ND1	7:A:1002:HOH:O	2.27	0.66
1:B:349:GLN:HG2	1:B:511:LEU:CD1	2.24	0.65
1:A:151:THR:HG23	1:A:153:GLN:CG	2.26	0.64
1:B:151:THR:HG23	1:B:153:GLN:H	1.63	0.64
1:A:671:LEU:O	1:A:672:ARG:HG2	1.98	0.63
1:B:173:GLU:O	1:B:198:ASN:HA	1.98	0.63
1:A:39:ARG:NH1	1:A:306:ALA:O	2.31	0.63
1:A:616:PHE:CE1	1:A:632:VAL:HG23	2.34	0.62
1:B:118:ALA:HB2	1:B:176:GLU:HG2	1.82	0.62
1:B:117:LEU:HB3	1:B:125:GLU:HB2	1.82	0.61
1:B:653:LEU:HD12	1:B:654:THR:H	1.65	0.61
1:B:243:ASP:HB2	1:B:260:GLN:HG2	1.82	0.60
1:B:548[A]:ARG:NH1	6:B:907:CL:CL	2.70	0.60
1:A:109:LEU:HD13	1:A:303:VAL:HG21	1.83	0.59
1:A:15:TRP:HB3	1:A:18:ASP:HB3	1.84	0.59
1:B:628:THR:OG1	1:B:631:GLN:HG3	2.02	0.59
6:B:907:CL:CL	6:B:908:CL:CL	2.94	0.59
1:A:665:GLU:OE2	1:A:667:ASN:HB2	2.03	0.59
1:B:123:TYR:OH	1:B:202:SER:HA	2.02	0.59
1:A:44:PRO:HD2	1:A:47:GLU:OE2	2.03	0.59
1:A:120:GLU:HA	1:A:120:GLU:OE2	2.02	0.59
1:A:117:LEU:HD12	1:A:126:LEU:HD23	1.84	0.58
1:A:441:HIS:CE1	1:A:504:ARG:HD3	2.38	0.58
1:A:583:VAL:HG22	1:A:584:SER:H	1.69	0.58
1:A:109:LEU:HD13	1:A:303:VAL:CG2	2.33	0.58
1:B:446:ASN:OD1	1:B:448:ASP:HB2	2.05	0.57
1:A:605:ARG:NH2	1:A:672:ARG:HD2	2.20	0.57
1:B:480:ALA:O	1:B:484:VAL:HG23	2.05	0.56
1:B:71:ALA:O	1:B:75:GLU:HG2	2.05	0.56
1:A:234:GLY:HA2	1:A:241:TYR:CE1	2.41	0.56
1:A:15:TRP:CZ2	1:A:346:ARG:HB3	2.40	0.56
1:B:516:ALA:O	1:B:540:GLY:HA2	2.06	0.56
1:B:349:GLN:CG	1:B:511:LEU:HD12	2.31	0.55
1:A:533:SER:HA	1:A:654:THR:OG1	2.07	0.55
1:B:417:TYR:CE2	1:B:419:ALA:HB2	2.42	0.55
1:A:55:ASP:HB2	1:B:671:LEU:O	2.07	0.54
1:B:479:LEU:HD11	2:B:901:DND:H5	1.88	0.54
1:A:231:ASN:HB3	1:A:244:GLY:HA2	1.88	0.54
1:A:530:ASP:OD1	1:A:532:SER:OG	2.19	0.54
1:A:96:ARG:HD2	1:A:128:TRP:O	2.08	0.54
1:B:586:THR:OG1	1:B:589:GLU:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LYS:O	1:A:308:SER:HB2	2.07	0.54
1:B:151:THR:HG23	1:B:153:GLN:N	2.23	0.54
1:A:126:LEU:CD1	1:B:126:LEU:HD13	2.27	0.53
1:A:417:TYR:CE2	1:A:419:ALA:HB2	2.43	0.53
1:B:245:CYS:SG	1:B:260:GLN:HG3	2.48	0.53
1:B:528:LYS:NZ	1:B:648:HIS:HD2	2.06	0.53
1:B:12:LEU:HD22	1:B:266:VAL:HG22	1.91	0.53
1:A:541:GLY:N	7:A:1001:HOH:O	2.21	0.53
1:A:680:TRP:N	1:A:681:PRO:HD3	2.24	0.53
1:B:40:TYR:CE1	1:B:197:THR:HG21	2.43	0.53
1:B:685:ARG:HA	1:B:685:ARG:HH11	1.74	0.52
3:B:902:AMP:H2'	4:B:903:POP:O6	2.10	0.52
1:A:233:LYS:HE2	1:A:262:SER:OG	2.09	0.52
1:A:626:ILE:N	1:A:626:ILE:HD12	2.25	0.51
1:B:11:ALA:HA	1:B:231:ASN:O	2.10	0.51
3:A:902:AMP:H2'	4:A:903:POP:O4	2.10	0.51
1:A:71:ALA:O	1:A:75:GLU:HG2	2.10	0.51
1:B:429:THR:HG22	1:B:432:ARG:NH1	2.25	0.51
1:B:413:LEU:HD12	1:B:414:THR:H	1.75	0.51
1:A:616:PHE:HE1	1:A:632:VAL:HG23	1.75	0.50
1:B:15:TRP:HB3	1:B:18:ASP:HB3	1.93	0.50
1:A:524:GLY:HA3	1:A:646:ASN:HB3	1.93	0.50
1:B:336:PRO:O	1:B:340:LEU:HG	2.11	0.50
1:B:467:LEU:O	1:B:473:GLY:HA3	2.12	0.50
1:B:96:ARG:HD2	1:B:128:TRP:O	2.12	0.50
1:A:53:CYS:HB2	1:A:57:TYR:CZ	2.46	0.49
1:B:15:TRP:CE2	1:B:346:ARG:HD3	2.48	0.49
1:B:482:GLN:HA	1:B:485:GLN:HE21	1.78	0.49
1:A:427:THR:HG22	1:A:430:ARG:NH2	2.28	0.49
1:A:361:ASP:HB2	4:A:903:POP:O5	2.13	0.49
1:B:23:LEU:HD13	1:B:69:VAL:HG13	1.93	0.49
1:B:433:GLU:O	1:B:437:GLN:HG3	2.12	0.49
1:A:83:ILE:HG13	1:A:104:LEU:HD13	1.95	0.48
1:A:9:THR:OG1	1:A:230:ALA:HB2	2.13	0.48
1:B:51:TYR:HD1	1:B:242:TYR:HH	1.61	0.48
1:B:626:ILE:N	1:B:626:ILE:HD12	2.28	0.48
1:B:8:ALA:HB2	1:B:270:THR:HG22	1.95	0.48
1:B:22:ASN:O	1:B:26:ILE:HG13	2.14	0.48
1:A:11:ALA:HA	1:A:231:ASN:O	2.13	0.48
1:A:48:ILE:HG23	1:A:69:VAL:HG11	1.95	0.47
1:B:626:ILE:HD12	1:B:626:ILE:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:GLY:O	1:B:259:SER:O	2.32	0.47
1:A:578:LEU:HD21	1:A:584:SER:N	2.30	0.47
1:A:616:PHE:CD1	1:A:632:VAL:HG23	2.50	0.47
1:A:628:THR:HG23	1:A:631:GLN:OE1	2.14	0.47
6:A:908:CL:CL	6:A:909:CL:CL	3.07	0.46
1:B:43:GLY:HA3	1:B:47:GLU:OE1	2.15	0.46
1:A:670:ASP:OD1	1:A:672:ARG:NH1	2.47	0.46
1:B:360:VAL:O	1:B:363:ALA:HB3	2.16	0.46
1:A:288:ARG:HG2	1:A:289:ASN:CG	2.36	0.46
1:A:616:PHE:CE1	1:A:632:VAL:CG2	2.99	0.46
1:B:44:PRO:HD2	1:B:47:GLU:OE2	2.16	0.46
1:A:281:TYR:O	1:A:284:GLU:HB3	2.16	0.46
1:B:524:GLY:HA3	1:B:646:ASN:HB3	1.98	0.46
1:B:168:THR:HG21	1:B:307:LEU:HD22	1.99	0.45
1:B:680:TRP:N	1:B:681:PRO:HD3	2.32	0.45
1:A:16:ALA:O	1:A:17:LEU:HB2	2.17	0.45
1:A:398:ILE:CD1	1:A:398:ILE:H	2.22	0.45
1:A:628:THR:OG1	1:A:631:GLN:HG3	2.16	0.45
1:B:376:VAL:O	1:B:380:VAL:HG23	2.17	0.45
1:B:360:VAL:HG23	6:B:908:CL:CL	2.53	0.45
1:A:342:ASP:HA	1:A:345:ARG:HG2	1.98	0.44
2:A:901:DND:H7	2:A:901:DND:H10	1.70	0.44
1:A:336:PRO:HB2	1:A:368:LEU:HD13	2.00	0.44
1:A:14:GLN:OE1	1:A:14:GLN:HA	2.17	0.44
1:A:528:LYS:NZ	1:A:648:HIS:CD2	2.73	0.44
1:A:76:SER:HA	1:A:77:PRO:HD3	1.84	0.44
1:B:637:LYS:HE2	1:B:684:PHE:HB3	1.98	0.44
1:A:341:TRP:O	1:A:345:ARG:HG2	2.17	0.44
1:A:457:ILE:O	1:A:461:VAL:HG12	2.18	0.44
1:A:203:HIS:HA	1:A:242:TYR:HA	2.00	0.44
1:A:616:PHE:HE1	1:A:632:VAL:CG2	2.30	0.44
1:B:275:LEU:HA	1:B:275:LEU:HD23	1.73	0.44
1:B:384:ASN:OD1	1:B:386:GLU:HG2	2.17	0.44
1:A:257:GLN:HG3	1:A:323:TRP:CH2	2.53	0.43
1:A:626:ILE:CD1	1:A:626:ILE:H	2.27	0.43
1:B:231:ASN:HD22	1:B:244:GLY:HA2	1.82	0.43
1:B:191:ASP:O	1:B:300:ARG:NH2	2.52	0.43
1:A:165:THR:HB	1:A:305:PHE:O	2.18	0.43
1:B:293:SER:O	1:B:294:ARG:HD2	2.19	0.43
1:A:528:LYS:HZ2	1:A:648:HIS:HD2	1.61	0.43
1:B:572:THR:CG2	1:B:584:SER:OG	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ILE:HA	1:A:317:ILE:HD13	1.90	0.43
1:A:599:SER:O	1:A:603:LYS:HG3	2.18	0.43
1:A:529:TYR:CZ	1:B:533:SER:HB3	2.54	0.43
1:A:141:TYR:HB2	1:A:158:PHE:HB2	2.00	0.42
1:A:244:GLY:O	1:A:259:SER:O	2.37	0.42
1:A:290:LEU:HB3	1:A:291:ALA:H	1.67	0.42
1:A:291:ALA:O	1:A:292:ALA:HB3	2.19	0.42
1:A:243:ASP:HB2	1:A:260:GLN:HG2	2.01	0.42
1:A:533:SER:HB2	1:B:529:TYR:CZ	2.54	0.42
1:B:110:LEU:HG	1:B:111:ILE:N	2.34	0.42
1:B:15:TRP:CZ2	1:B:346:ARG:HB3	2.55	0.42
1:A:64:LEU:O	1:A:68:GLN:HG3	2.20	0.41
1:A:675:LEU:HD21	1:B:346:ARG:HB2	2.00	0.41
1:B:235:CYS:O	1:B:346:ARG:NH1	2.53	0.41
1:B:454:VAL:HG21	1:B:488:ILE:HD11	2.01	0.41
1:B:17:LEU:HD11	1:B:56:HIS:CG	2.55	0.41
1:A:484:VAL:O	1:A:488:ILE:HG12	2.20	0.41
1:B:15:TRP:CD2	1:B:346:ARG:HD3	2.55	0.41
1:B:437:GLN:NE2	1:B:562:ALA:HB2	2.35	0.41
1:A:359:GLY:HA3	4:A:903:POP:O2	2.21	0.41
1:B:114:LYS:HE2	1:B:116:ALA:O	2.20	0.41
1:A:606:LYS:HZ1	1:A:670:ASP:HA	1.85	0.41
1:B:285:ILE:HB	1:B:288:ARG:HB3	2.03	0.41
1:A:604:LEU:HA	1:A:604:LEU:HD23	1.90	0.41
3:A:902:AMP:C8	3:A:902:AMP:O2P	2.74	0.41
1:B:52:GLY:O	1:B:54:TRP:CD1	2.73	0.41
1:A:172:SER:H	1:A:188:MET:HE1	1.86	0.41
1:B:126:LEU:HD23	1:B:126:LEU:HA	1.92	0.41
3:B:902:AMP:C8	3:B:902:AMP:O1P	2.74	0.41
1:A:257:GLN:HG3	1:A:323:TRP:CZ3	2.55	0.41
1:B:175:CYS:HB3	1:B:176:GLU:OE1	2.20	0.41
1:B:571:ALA:HB2	6:B:907:CL:CL	2.58	0.41
1:A:594:THR:OG1	1:A:597:GLU:HG2	2.21	0.41
1:B:100:ARG:HG2	1:B:174:ILE:CD1	2.44	0.41
1:B:147:ILE:O	1:B:151:THR:HG22	2.20	0.41
1:B:15:TRP:HB3	1:B:18:ASP:CB	2.51	0.41
1:B:243:ASP:N	1:B:243:ASP:OD1	2.47	0.41
1:B:343:PHE:CE1	1:B:536:ILE:HG21	2.56	0.41
1:A:495:LEU:HD13	1:B:484:VAL:CG2	2.50	0.41
1:A:168:THR:HG21	1:A:307:LEU:HD22	2.02	0.40
1:A:315:ALA:HA	1:A:316:PRO:HD3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:TYR:HA	1:A:533:SER:OG	2.22	0.40
1:A:15:TRP:HB3	1:A:18:ASP:CB	2.51	0.40
1:A:243:ASP:HB2	1:A:260:GLN:CG	2.52	0.40
1:A:406:ARG:NH1	1:A:436:GLN:O	2.51	0.40
1:B:141:TYR:HB2	1:B:158:PHE:HB2	2.02	0.40
1:B:183:SER:HA	1:B:184:PRO:HD3	1.91	0.40
1:B:356:LEU:HD22	1:B:415:THR:HG21	2.04	0.40
1:B:42:LEU:HD22	1:B:197:THR:HB	2.03	0.40
1:B:547:LEU:HA	1:B:547:LEU:HD23	1.91	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	695/707 (98%)	656 (94%)	35 (5%)	4 (1%)	25	46
1	B	696/707 (98%)	658 (94%)	36 (5%)	2 (0%)	41	61
All	All	1391/1414 (98%)	1314 (94%)	71 (5%)	6 (0%)	34	56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	244	GLY
1	A	244	GLY
1	B	313	LEU
1	A	175	CYS
1	A	251	ASN
1	A	285	ILE

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	600/608 (99%)	564 (94%)	36 (6%)	19	37
1	B	601/608 (99%)	573 (95%)	28 (5%)	26	50
All	All	1201/1216 (99%)	1137 (95%)	64 (5%)	22	43

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	120	GLU
1	A	124	ARG
1	A	150	LEU
1	A	151	THR
1	A	154	GLU
1	A	172	SER
1	A	180	THR
1	A	190	LEU
1	A	191	ASP
1	A	202	SER
1	A	208	LYS
1	A	229	LEU
1	A	288	ARG
1	A	289	ASN
1	A	311	GLU
1	A	313	LEU
1	A	322	GLU
1	A	324	LYS
1	A	343	PHE
1	A	378	GLU
1	A	412	ILE
1	A	422	ASN
1	A	436	GLN
1	A	475	SER
1	A	553	PHE
1	A	557	ARG

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Mol	Chain	Res	Type
1	A	578	LEU
1	A	582	GLN
1	A	584	SER
1	A	590	ASP
1	A	599	SER
1	A	614	SER
1	A	641	SER
1	A	672	ARG
1	A	679	SER
1	B	41	ARG
1	B	86	VAL
1	B	120	GLU
1	B	128	TRP
1	B	138	THR
1	B	150	LEU
1	B	163	LEU
1	B	172	SER
1	B	211	THR
1	B	286	SER
1	B	288	ARG
1	B	311	GLU
1	B	314	LEU
1	B	322	GLU
1	B	324	LYS
1	B	333	SER
1	B	381	ARG
1	B	386	GLU
1	B	578	LEU
1	B	580	ASP
1	B	582	GLN
1	B	589	GLU
1	B	599	SER
1	B	614	SER
1	B	679	SER
1	B	685	ARG
1	B	696	ARG
1	B	698	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN

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Mol	Chain	Res	Type
1	A	349	GLN
1	A	441	HIS
1	A	483	ASN
1	A	582	GLN
1	A	585	GLN
1	A	648	HIS
1	A	658	HIS
1	B	122	ASN
1	B	137	HIS
1	B	185	HIS
1	B	483	ASN
1	B	485	GLN
1	B	585	GLN
1	B	648	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 11 are monoatomic - leaving 6 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	POP	B	903	5	6,8,8	0.79	0	13,13,13	0.96	0
3	AMP	A	902	-	22,25,25	0.72	0	25,38,38	1.40	2 (8%)
4	POP	A	903	5	6,8,8	0.82	0	13,13,13	1.16	0
3	AMP	B	902	-	22,25,25	0.71	0	25,38,38	1.40	2 (8%)
2	DND	B	901	-	40,48,48	0.94	3 (7%)	47,73,73	1.16	2 (4%)
2	DND	A	901	-	40,48,48	0.94	3 (7%)	47,73,73	1.16	2 (4%)

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	POP	B	903	5	-	0/6/6/6	-
3	AMP	A	902	-	-	0/6/26/26	0/3/3/3
4	POP	A	903	5	-	0/6/6/6	-
3	AMP	B	902	-	-	0/6/26/26	0/3/3/3
2	DND	B	901	-	-	13/22/62/62	0/5/5/5
2	DND	A	901	-	-	13/22/62/62	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	DND	C3N-C7N	2.69	1.50	1.47
2	A	901	DND	C3N-C7N	2.64	1.50	1.47
2	A	901	DND	O4B-C1B	2.50	1.44	1.41
2	B	901	DND	O4B-C1B	2.48	1.44	1.41
2	B	901	DND	C2A-N3A	2.14	1.35	1.32
2	A	901	DND	C2A-N3A	2.13	1.35	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	AMP	N3-C2-N1	-4.49	121.67	128.68
3	B	902	AMP	N3-C2-N1	-4.46	121.71	128.68
2	B	901	DND	N3A-C2A-N1A	-3.66	122.96	128.68
2	A	901	DND	N3A-C2A-N1A	-3.63	123.00	128.68
3	B	902	AMP	O3P-P-O5'	-2.84	99.18	106.73
3	A	902	AMP	O3P-P-O5'	-2.83	99.20	106.73
2	A	901	DND	C3D-C2D-C1D	2.12	104.17	100.98
2	B	901	DND	C3D-C2D-C1D	2.11	104.15	100.98

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	DND	C5D-O5D-PN-O11
2	A	901	DND	O4D-C1D-N1N-C6N
2	A	901	DND	O4D-C1D-N1N-C2N
2	A	901	DND	C2D-C1D-N1N-C2N
2	B	901	DND	C5D-O5D-PN-O11
2	B	901	DND	O4D-C1D-N1N-C6N
2	B	901	DND	O4D-C1D-N1N-C2N
2	B	901	DND	C2D-C1D-N1N-C2N
2	A	901	DND	O4B-C4B-C5B-O5B
2	B	901	DND	O4B-C4B-C5B-O5B
2	A	901	DND	C3B-C4B-C5B-O5B
2	B	901	DND	C3B-C4B-C5B-O5B
2	A	901	DND	C4B-C5B-O5B-PA
2	B	901	DND	C4B-C5B-O5B-PA
2	A	901	DND	PN-O3P-PA-O5B
2	B	901	DND	PN-O3P-PA-O5B
2	A	901	DND	C5D-O5D-PN-O3P
2	B	901	DND	C5D-O5D-PN-O3P
2	A	901	DND	C5D-O5D-PN-O12
2	B	901	DND	C5D-O5D-PN-O12
2	A	901	DND	PN-O3P-PA-O13
2	B	901	DND	PN-O3P-PA-O13
2	B	901	DND	O4D-C4D-C5D-O5D
2	A	901	DND	O4D-C4D-C5D-O5D
2	A	901	DND	C2D-C1D-N1N-C6N
2	B	901	DND	C2D-C1D-N1N-C6N

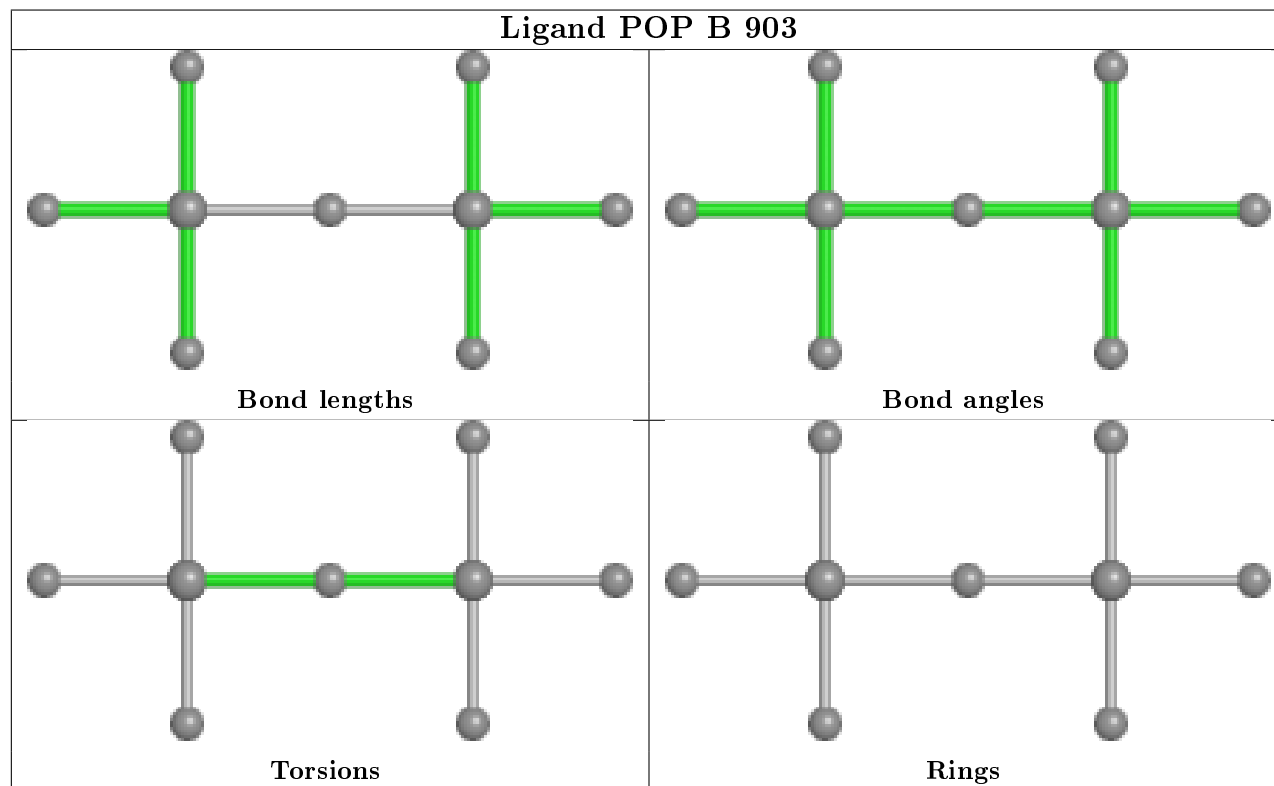
There are no ring outliers.

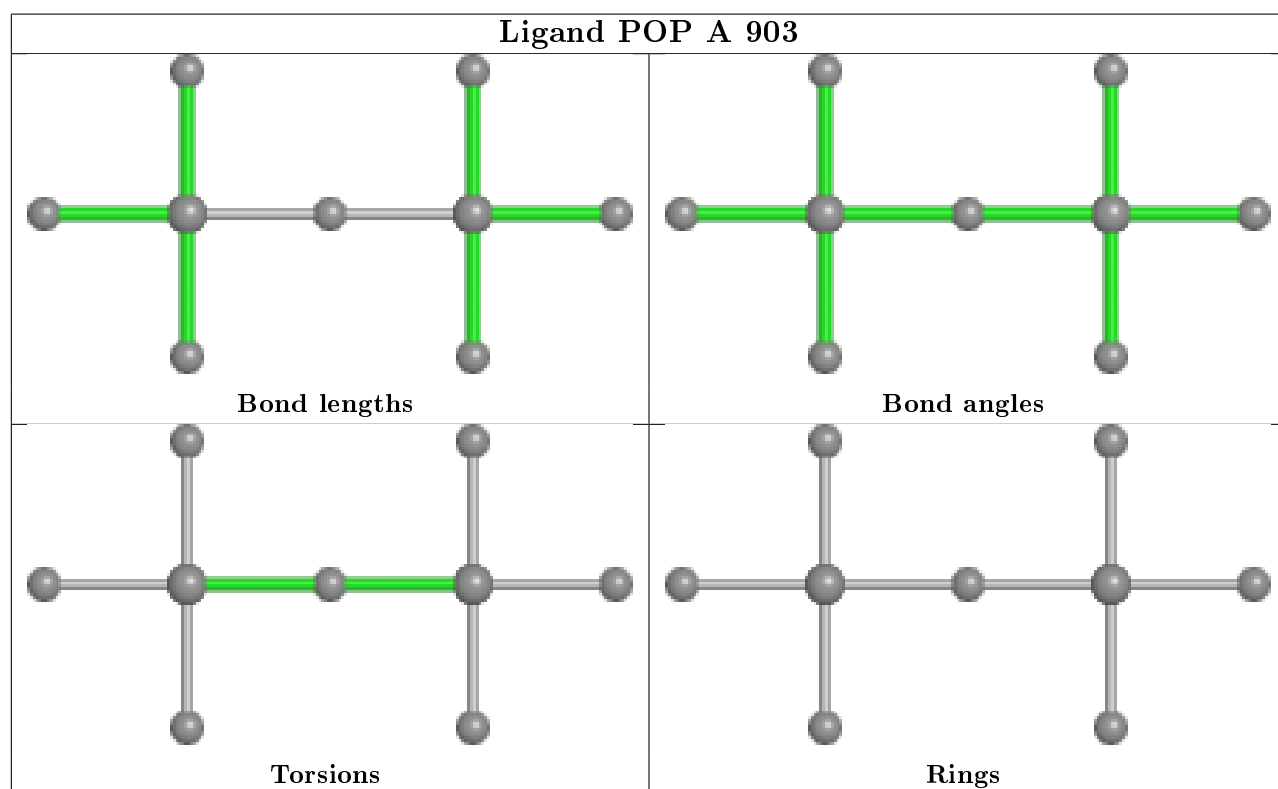
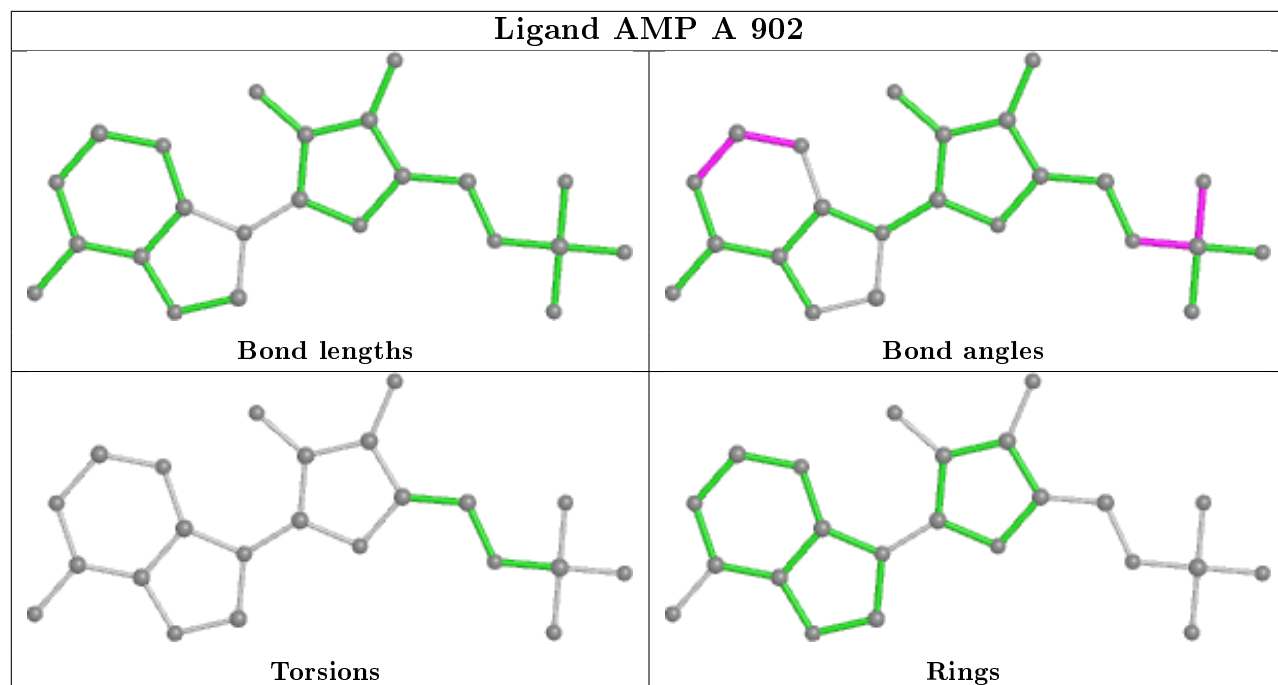
6 monomers are involved in 12 short contacts:

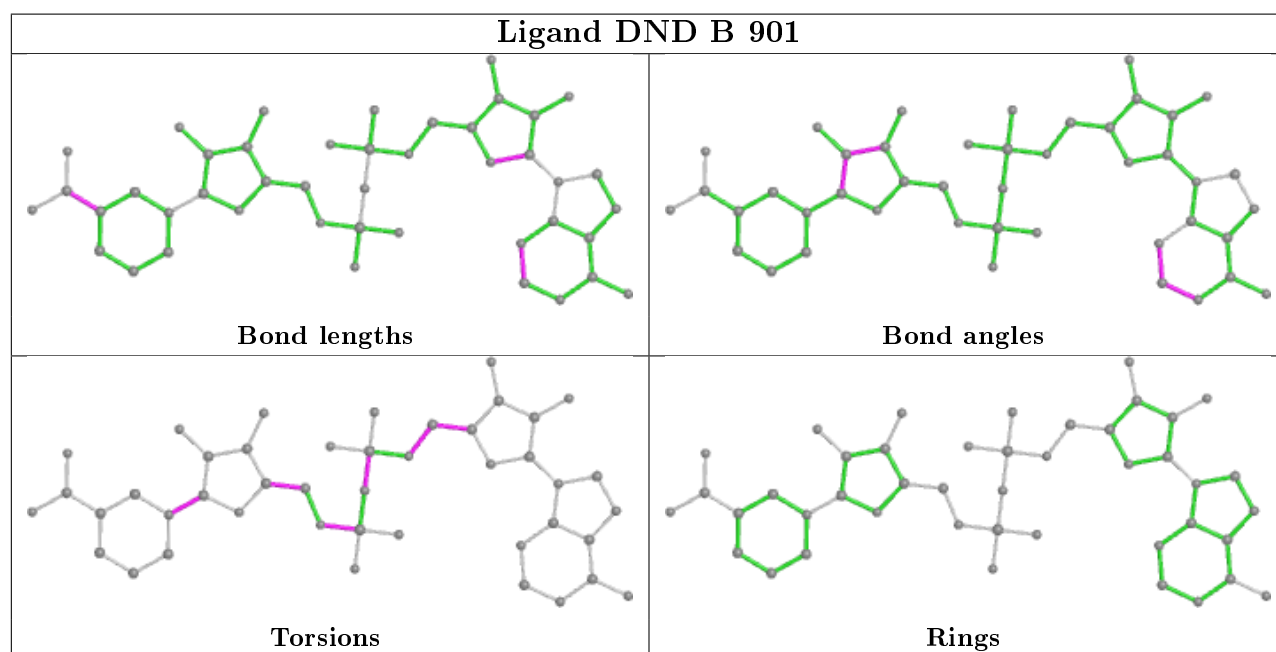
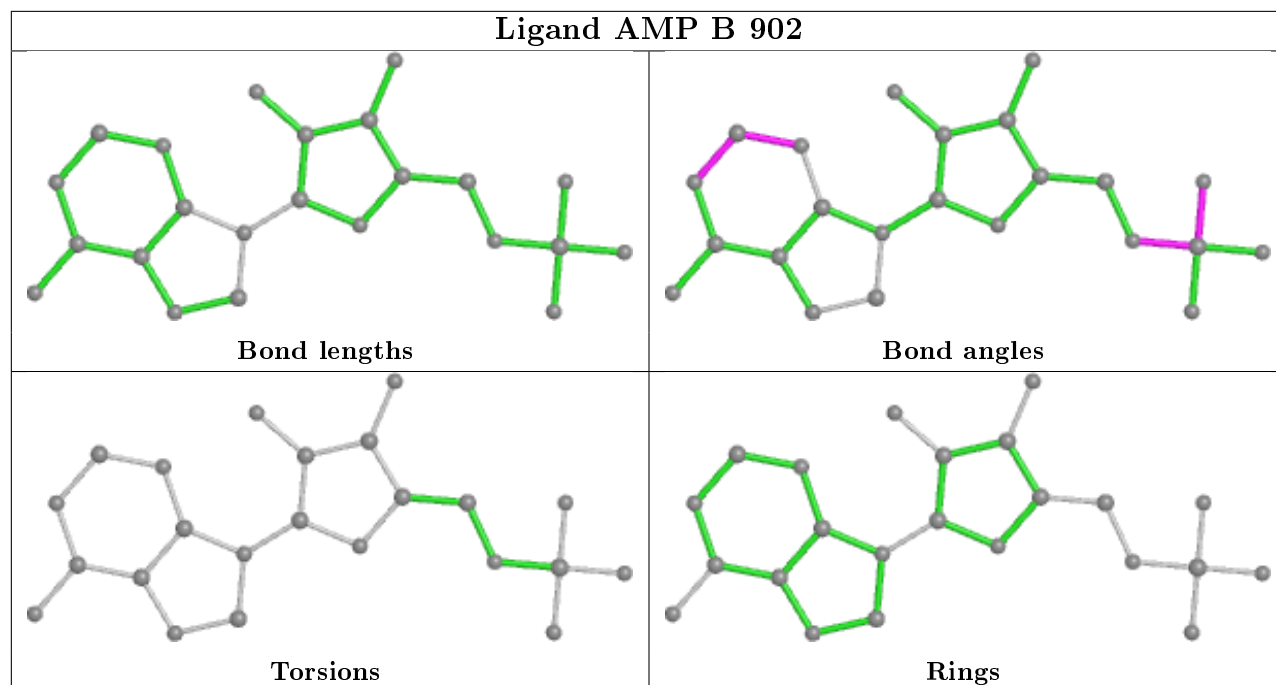
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	903	POP	2	0
3	A	902	AMP	2	0
4	A	903	POP	4	0
3	B	902	AMP	2	0
2	B	901	DND	2	0
2	A	901	DND	2	0

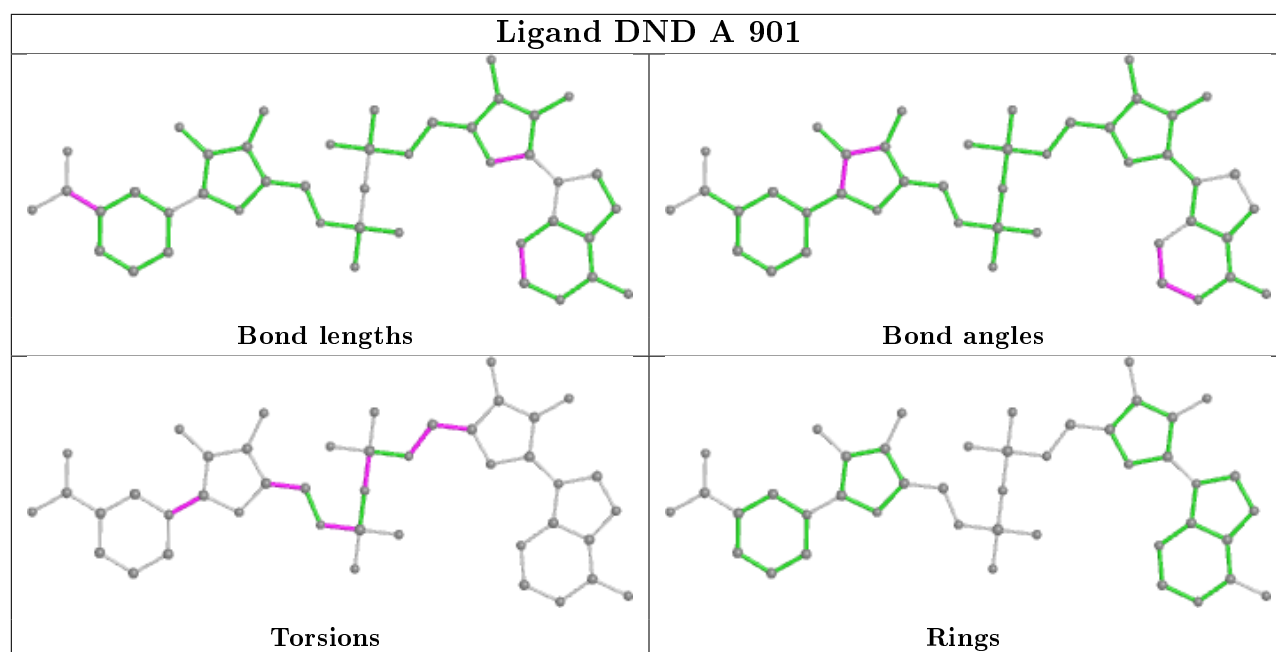
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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	696/707 (98%)	-0.20	22 (3%) 47 41	46, 68, 116, 168	0
1	B	696/707 (98%)	-0.27	17 (2%) 59 54	49, 66, 104, 158	0
All	All	1392/1414 (98%)	-0.24	39 (2%) 53 47	46, 68, 108, 168	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	579	ALA	6.5
1	A	580	ASP	5.9
1	B	581	GLY	5.9
1	A	313	LEU	5.4
1	B	582	GLN	4.9
1	A	578	LEU	4.5
1	B	580	ASP	4.5
1	A	314	LEU	4.1
1	A	581	GLY	4.0
1	A	697	ALA	3.8
1	A	627	CYS	3.7
1	B	579	ALA	3.6
1	A	582	GLN	3.6
1	A	698	GLU	3.5
1	B	313	LEU	3.3
1	A	584	SER	3.3
1	A	583	VAL	3.3
1	B	697	ALA	3.1
1	B	571	ALA	3.1
1	A	402	PRO	3.0
1	B	698	GLU	3.0
1	A	310	HIS	2.9
1	B	533	SER	2.8
1	A	288	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	696	ARG	2.7
1	B	531	CYS	2.7
1	A	470	ALA	2.5
1	A	571	ALA	2.4
1	A	629	PRO	2.4
1	B	134	ARG	2.3
1	B	578	LEU	2.3
1	A	289	ASN	2.3
1	A	620	LEU	2.2
1	A	472	GLY	2.1
1	B	584	SER	2.1
1	B	382	SER	2.1
1	B	625	HIS	2.1
1	B	583	VAL	2.1
1	A	626	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å ²)	Q<0.9
5	MG	A	904	1/1	0.59	0.32	113,113,113,113	0
2	DND	A	901	44/44	0.75	0.38	102,171,233,251	0
2	DND	B	901	44/44	0.78	0.34	102,171,233,251	0
6	CL	A	909	1/1	0.80	0.09	105,105,105,105	0
3	AMP	A	902	23/23	0.82	0.28	133,144,202,203	0
3	AMP	B	902	23/23	0.83	0.30	133,144,202,203	0
4	POP	A	903	9/9	0.88	0.23	102,110,193,243	0
5	MG	B	904	1/1	0.89	0.28	107,107,107,107	0

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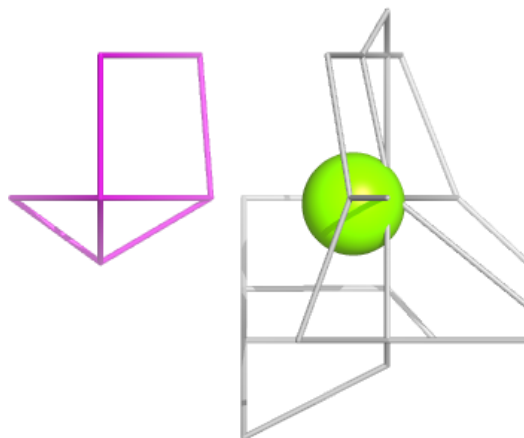
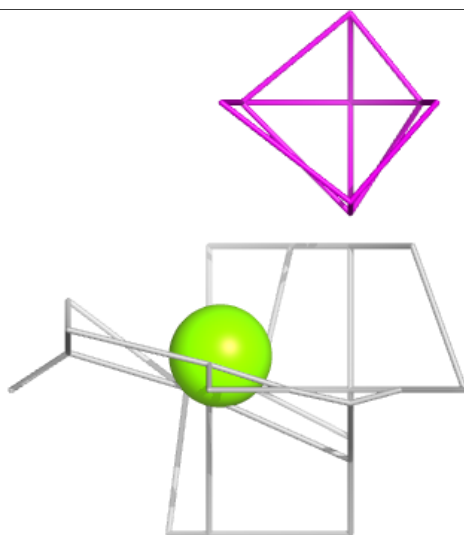
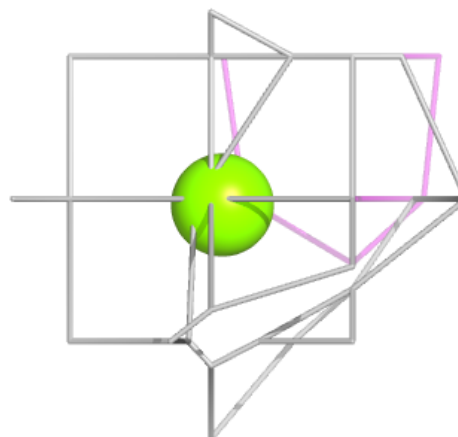
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	CL	B	905	1/1	0.93	0.12	71,71,71,71	0
6	CL	A	906	1/1	0.93	0.17	63,63,63,63	0
6	CL	B	908	1/1	0.94	0.07	110,110,110,110	0
6	CL	A	908	1/1	0.96	0.09	84,84,84,84	0
4	POP	B	903	9/9	0.96	0.19	82,101,198,248	0
6	CL	B	906	1/1	0.97	0.26	58,58,58,58	0
6	CL	B	907	1/1	0.97	0.08	98,98,98,98	0
6	CL	A	905	1/1	0.97	0.42	74,74,74,74	0
6	CL	A	907	1/1	0.97	0.27	64,64,64,64	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.

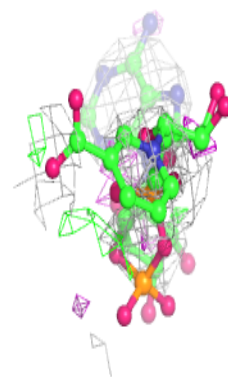
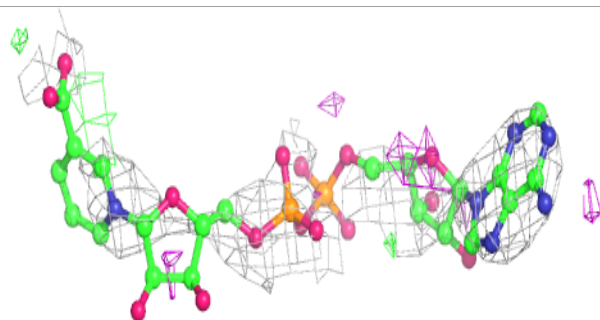
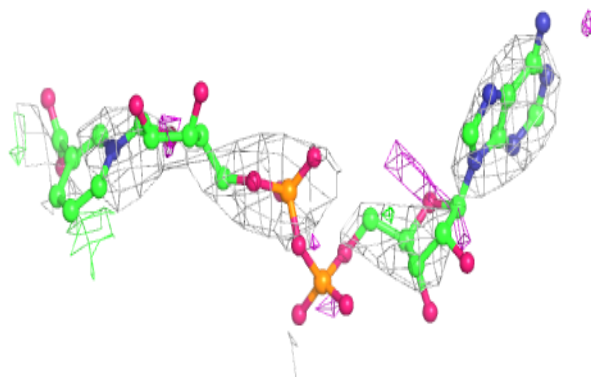
Electron density around MG A 904:

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

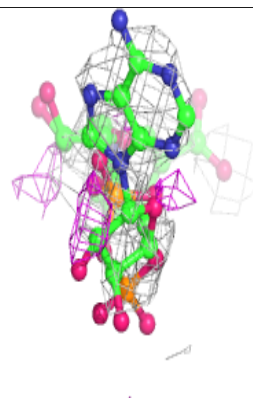
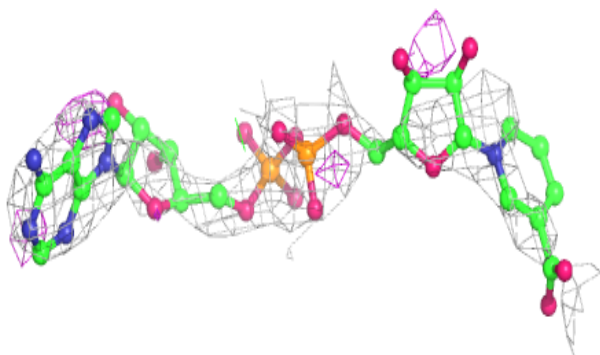
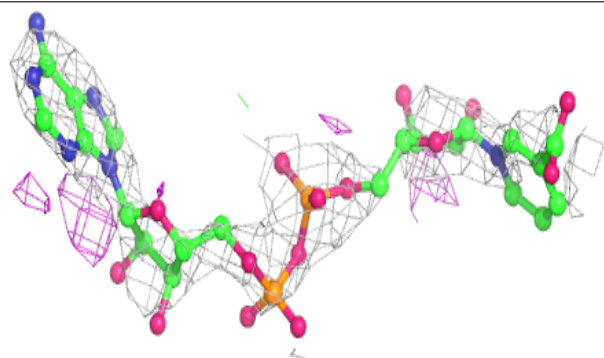


Electron density around DND A 901:

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

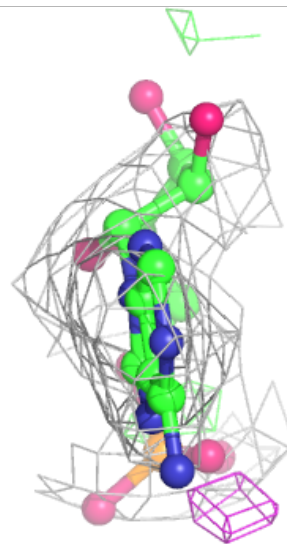
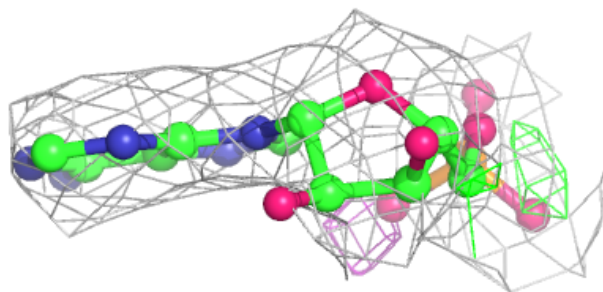
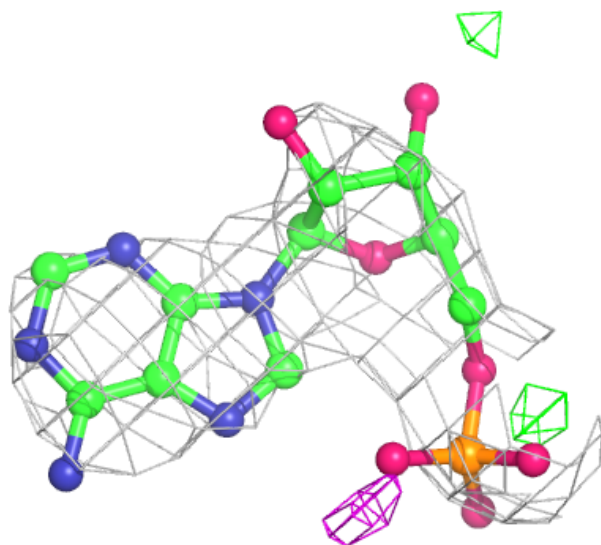
**Electron density around DND B 901:**

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



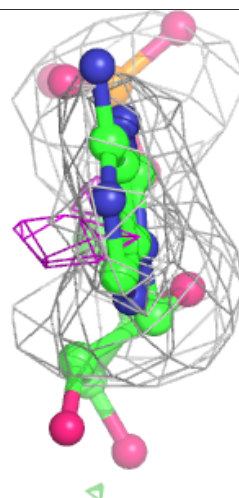
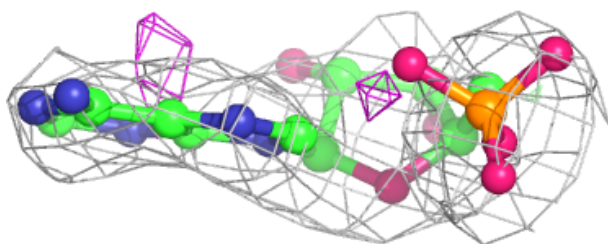
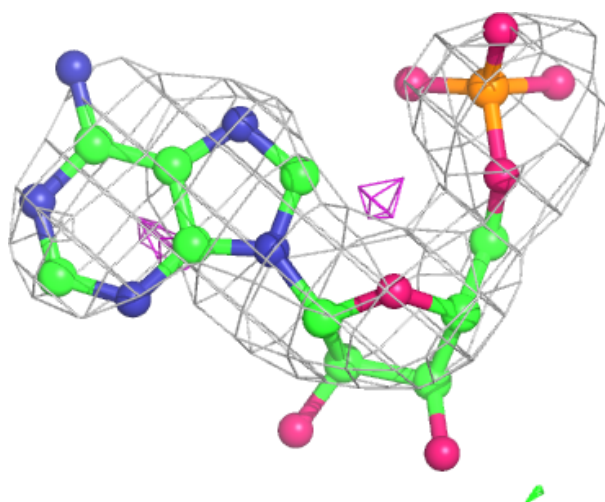
Electron density around AMP A 902:

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



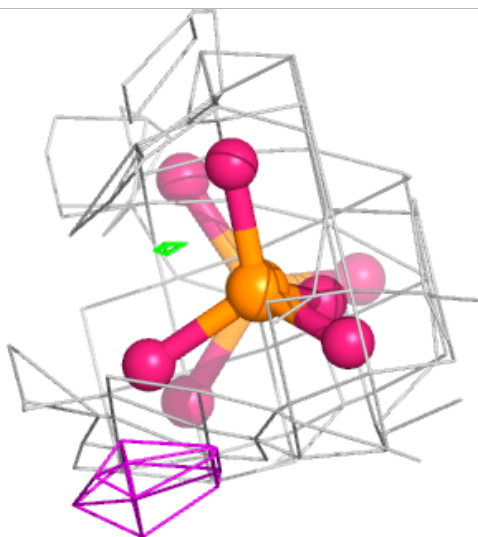
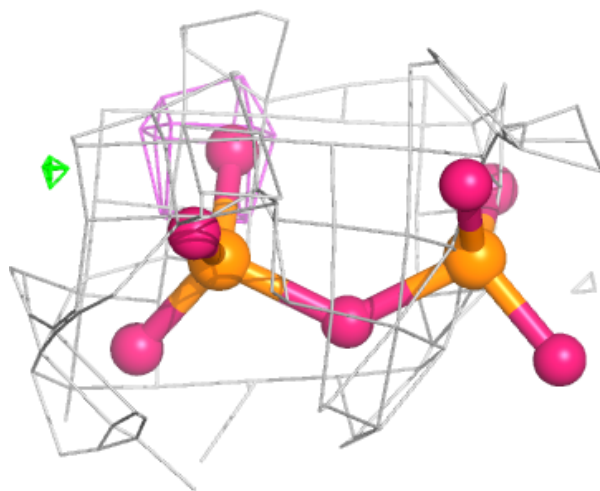
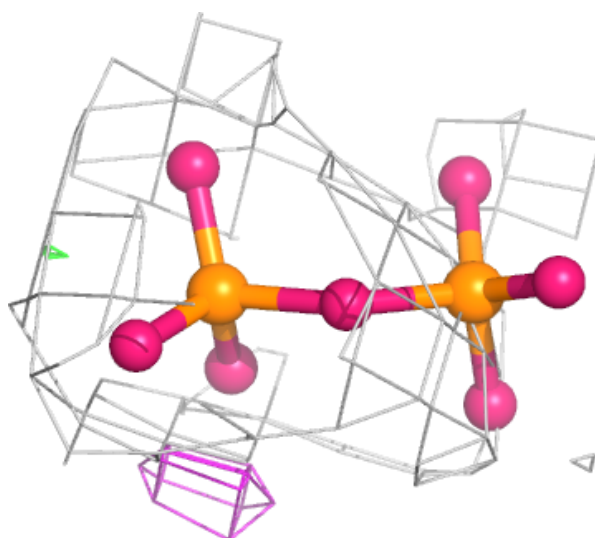
Electron density around AMP B 902:

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



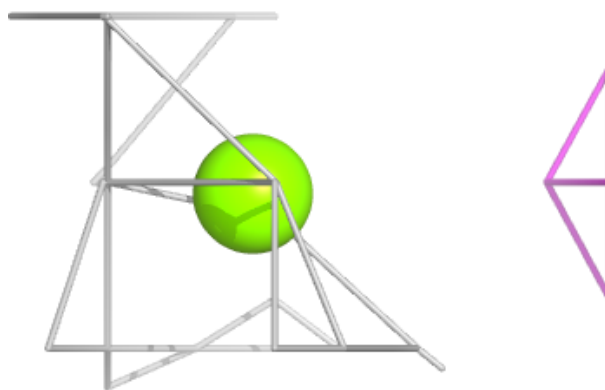
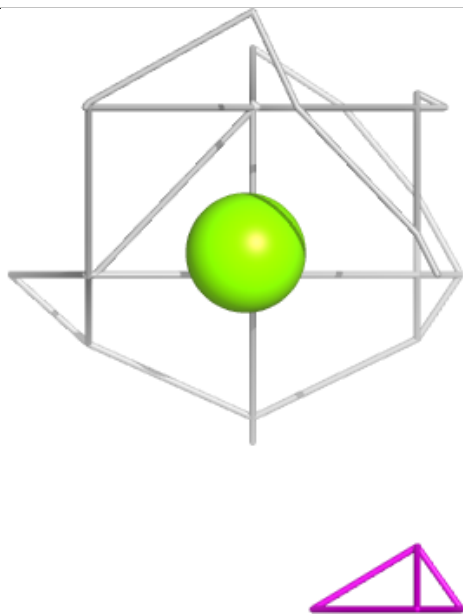
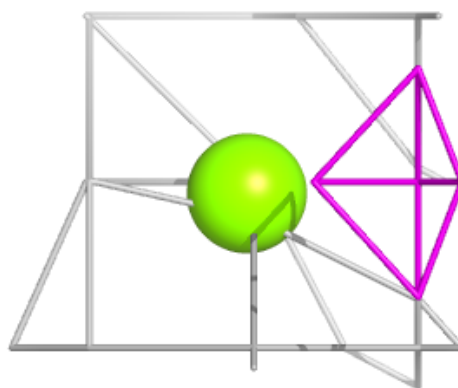
Electron density around POP A 903:

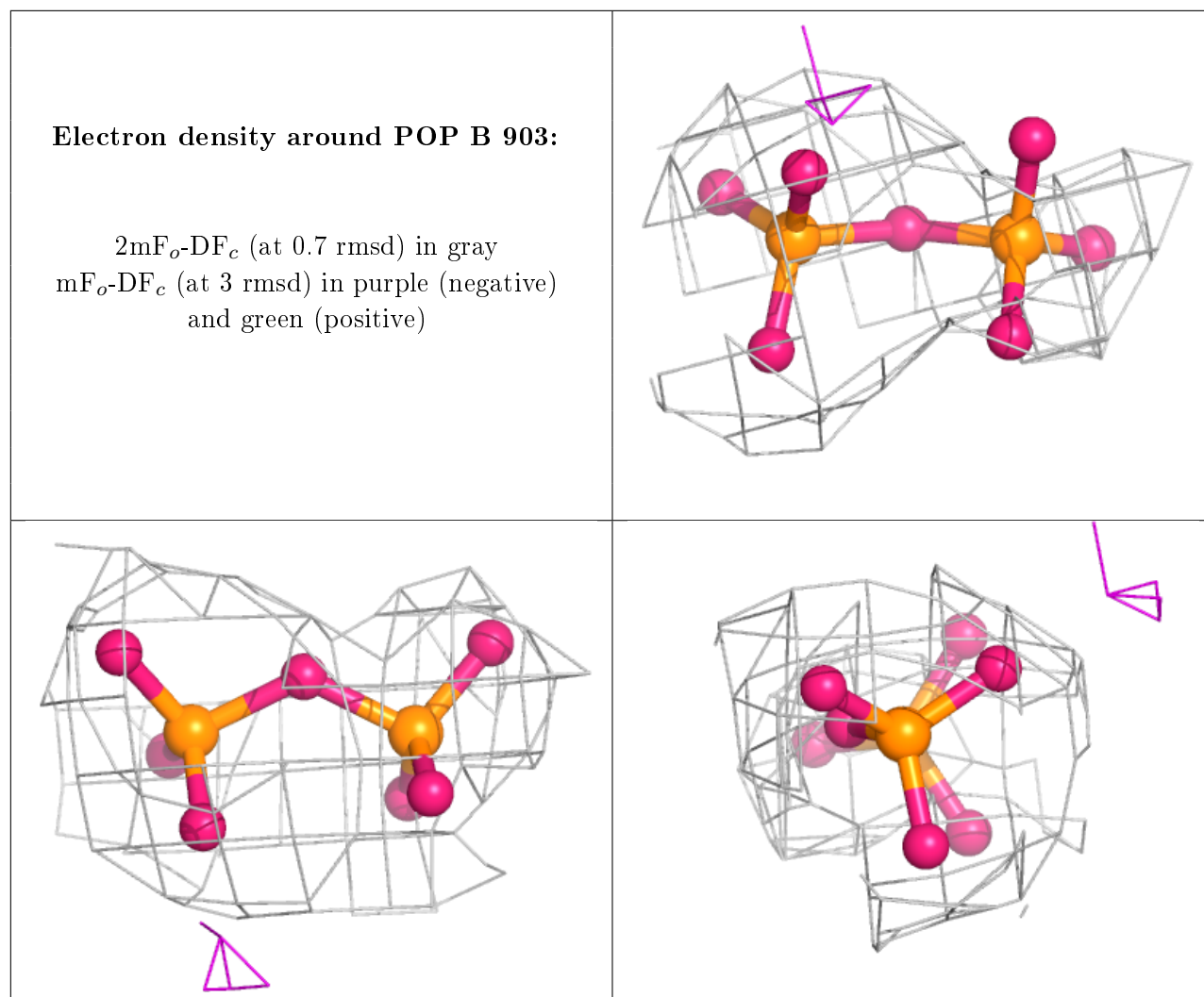
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG B 904:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.