



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 01:54 AM JST

PDB ID : 7EDZ
Title : Crystal Structure of human PPCS in complex with P-HoPan and AMPPNP
Authors : Sharma, N.; Mostert, K.J.; Strauss, E.; Anand, R.
Deposited on : 2021-03-17
Resolution : 1.95 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

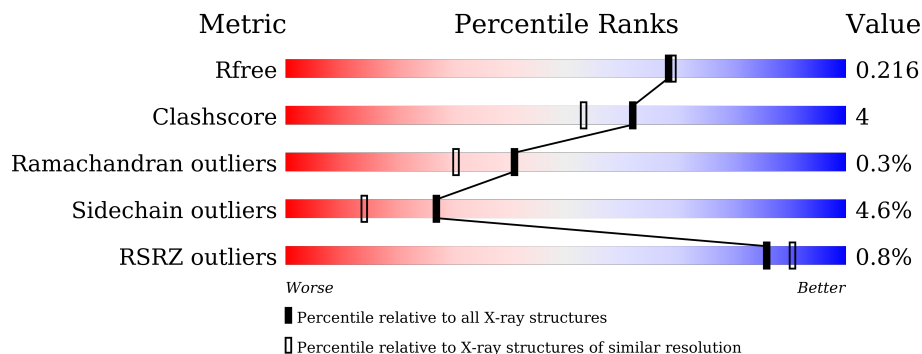
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	311	
1	B	311	
1	C	311	
1	D	311	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	404	-	-	X	-
6	GOL	C	406	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10128 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.

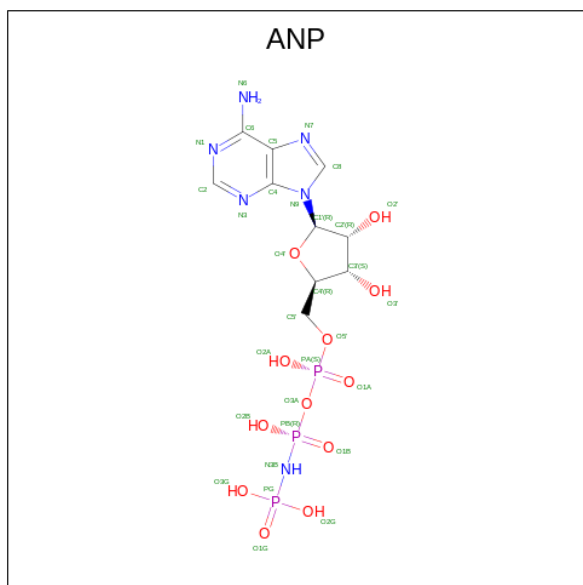
- Molecule 1 is a protein called Phosphopantothenate--cysteine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	305	Total 2358	C 1522	N 403	O 427	S 6	0	3	0
1	C	304	Total 2339	C 1509	N 403	O 422	S 5	0	2	0
1	B	306	Total 2348	C 1513	N 407	O 423	S 5	0	3	0
1	A	305	Total 2347	C 1516	N 408	O 418	S 5	0	3	0

There are 8 discrepancies between the modelled and reference sequences:

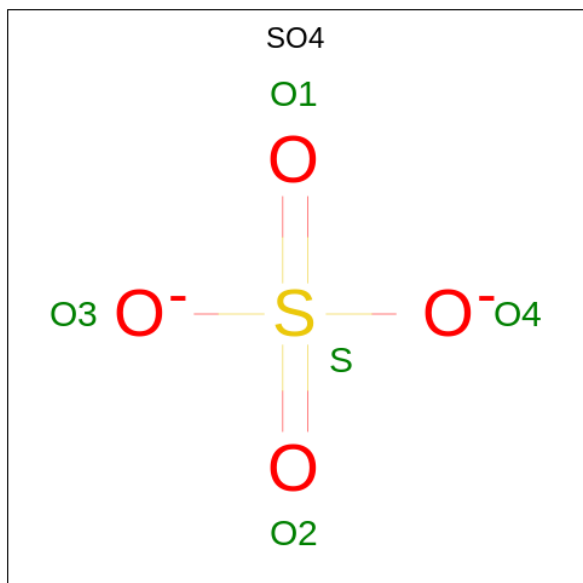
Chain	Residue	Modelled	Actual	Comment	Reference
D	146	VAL	ALA	variant	UNP Q9HAB8
D	268	LEU	PHE	variant	UNP Q9HAB8
C	146	VAL	ALA	variant	UNP Q9HAB8
C	268	LEU	PHE	variant	UNP Q9HAB8
B	146	VAL	ALA	variant	UNP Q9HAB8
B	268	LEU	PHE	variant	UNP Q9HAB8
A	146	VAL	ALA	variant	UNP Q9HAB8
A	268	LEU	PHE	variant	UNP Q9HAB8

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

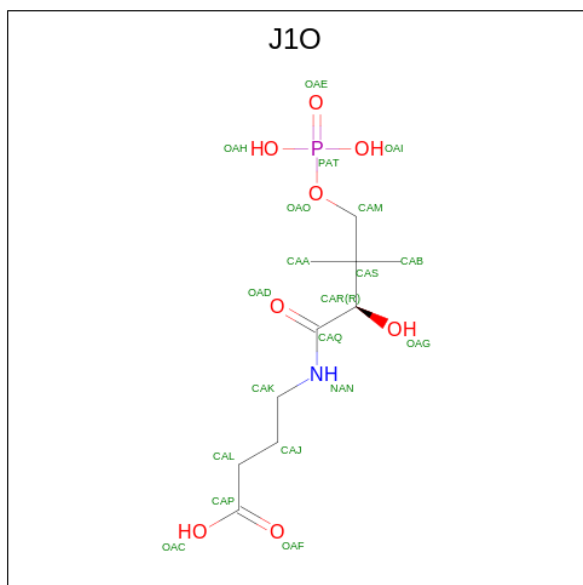


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

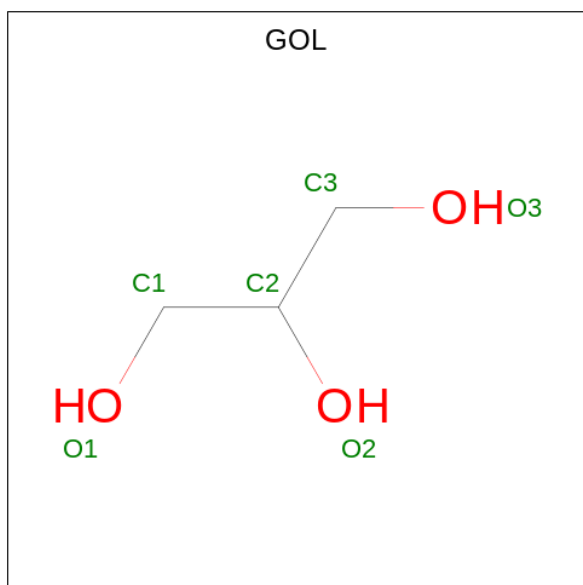
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is 4-[[[(2R)-3,3-dimethyl-2-oxidanyl-4-phosphonoxy-butanoyl]amino]butanoic acid (three-letter code: J1O) (formula: C₁₀H₂₀NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	D	1	Total	C	N	O	P	0	0
			20	10	1	8	1		
5	C	1	Total	C	N	O	P	0	0
			20	10	1	8	1		
5	B	1	Total	C	N	O	P	0	0
			20	10	1	8	1		
5	A	1	Total	C	N	O	P	0	0
			20	10	1	8	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

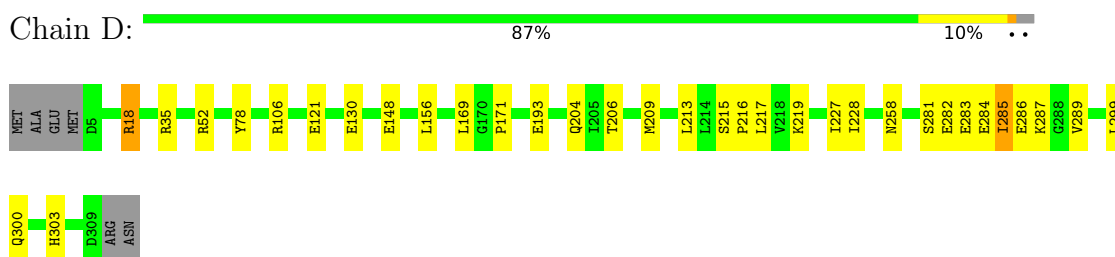
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	117	Total O 117 117	0	0
7	C	114	Total O 114 114	0	0
7	B	101	Total O 101 101	0	0
7	A	121	Total O 121 121	0	0

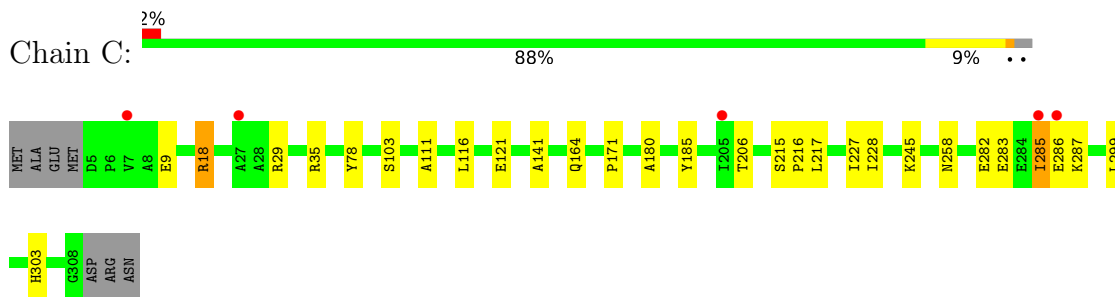
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

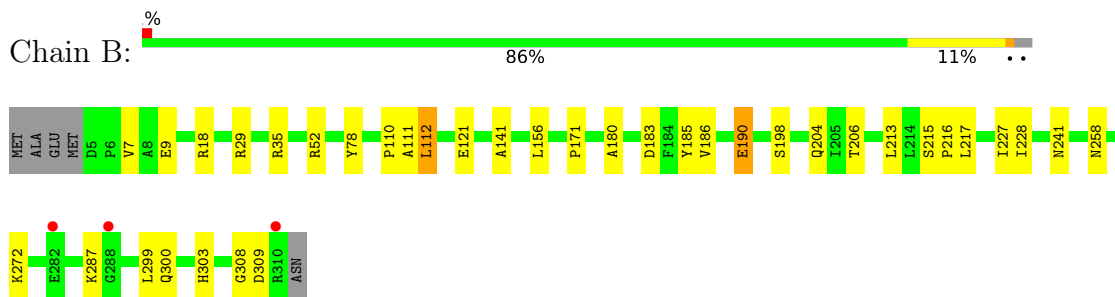
- Molecule 1: Phosphopantothenate--cysteine ligase



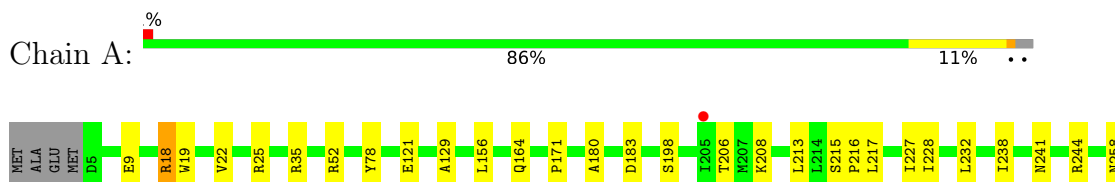
- Molecule 1: Phosphopantothenate--cysteine ligase

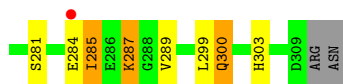


- Molecule 1: Phosphopantothenate--cysteine ligase



- Molecule 1: Phosphopantothenate--cysteine ligase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	100.00Å 100.00Å 146.90Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	36.72 – 1.95 36.72 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.2 (36.72-1.95) 97.2 (36.72-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.176 , 0.206 0.187 , 0.216	Depositor DCC
R_{free} test set	5169 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtrriage
Anisotropy	0.031	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 26.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.447 for k,h,-l 0.440 for -k,-h,-l 0.439 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10128	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% 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: ANP, GOL, MG, J1O, SO4

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	1.00	3/2412 (0.1%)	0.96	0/3281
1	B	1.01	2/2413 (0.1%)	0.94	0/3285
1	C	0.99	0/2401	0.92	0/3267
1	D	0.97	0/2423	0.94	0/3294
All	All	0.99	5/9649 (0.1%)	0.94	0/13127

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	52[A]	ARG	CA-C	5.70	1.67	1.52
1	B	52[B]	ARG	CA-C	5.70	1.67	1.52
1	A	52[A]	ARG	CA-C	5.50	1.67	1.52
1	A	52[B]	ARG	CA-C	5.50	1.67	1.52
1	A	232	LEU	C-N	-5.28	1.22	1.34

There are no bond angle outliers.

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	2347	0	2378	31	0
1	B	2348	0	2355	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2339	0	2357	17	0
1	D	2358	0	2385	18	0
2	A	31	0	13	0	0
2	B	31	0	13	0	0
2	C	31	0	13	0	0
2	D	31	0	13	0	0
3	A	10	0	0	0	0
3	B	10	0	0	1	0
3	C	10	0	0	0	0
3	D	15	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	20	0	0	1	0
5	B	20	0	0	1	0
5	C	20	0	0	1	0
5	D	20	0	0	0	0
6	A	12	0	16	9	0
6	B	12	0	16	4	0
6	C	6	0	8	4	0
7	A	121	0	0	2	0
7	B	101	0	0	2	0
7	C	114	0	0	0	0
7	D	117	0	0	2	0
All	All	10128	0	9567	85	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 4.

All (85) 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:244:ARG:HH11	6:A:404:GOL:H11	1.02	1.08
1:B:272:LYS:HE3	7:B:564:HOH:O	1.55	1.04
1:A:18:ARG:HG2	1:A:18:ARG:HH11	1.22	1.02
1:A:244:ARG:NH1	6:A:404:GOL:H11	1.73	1.01
1:A:164:GLN:HG3	7:A:578:HOH:O	1.65	0.94
1:D:18:ARG:HG2	1:D:18:ARG:HH11	1.31	0.92
1:C:111:ALA:HB2	6:C:406:GOL:H11	1.52	0.88
1:A:241:ASN:CB	6:A:404:GOL:H2	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ARG:HH11	1:C:18:ARG:HG2	1.49	0.76
1:A:241:ASN:HB2	6:A:404:GOL:H2	1.69	0.73
1:C:111:ALA:CB	6:C:406:GOL:H11	2.20	0.71
1:A:241:ASN:CA	6:A:404:GOL:H2	2.21	0.70
1:B:111:ALA:H	6:B:406:GOL:H2	1.57	0.70
1:A:241:ASN:HA	6:A:404:GOL:H2	1.73	0.69
1:B:308:GLY:HA2	7:B:581:HOH:O	1.92	0.68
1:A:241:ASN:HB2	6:A:404:GOL:C2	2.24	0.67
1:A:18:ARG:HH11	1:A:18:ARG:CG	2.06	0.64
1:C:116:LEU:HD13	6:C:406:GOL:H12	1.77	0.64
1:C:111:ALA:H	6:C:406:GOL:H32	1.63	0.63
1:D:209[B]:MET:HE2	7:D:607:HOH:O	1.98	0.62
1:D:18:ARG:HH11	1:D:18:ARG:CG	2.06	0.61
1:B:7:VAL:HG12	1:B:7:VAL:O	2.03	0.59
1:C:18:ARG:HG2	1:C:18:ARG:NH1	2.16	0.56
1:C:29[A]:ARG:NH1	1:C:141:ALA:O	2.37	0.55
6:B:406:GOL:H11	1:A:129:ALA:CB	2.37	0.55
6:B:406:GOL:H11	1:A:129:ALA:HB2	1.88	0.54
1:B:18:ARG:NH1	3:B:404:SO4:O2	2.39	0.54
1:B:29[B]:ARG:NH2	1:B:141:ALA:O	2.39	0.54
1:D:215:SER:HB2	1:D:216:PRO:CD	2.38	0.53
1:C:215:SER:HB2	1:C:216:PRO:CD	2.38	0.53
1:A:215:SER:HB2	1:A:216:PRO:CD	2.38	0.53
1:A:284:GLU:HB3	1:A:289:VAL:CG2	2.38	0.53
1:B:215:SER:HB2	1:B:216:PRO:CD	2.39	0.53
1:D:284:GLU:HB3	1:D:289:VAL:CG2	2.39	0.52
1:A:287:LYS:HG3	1:A:287:LYS:O	2.10	0.52
1:C:171:PRO:O	1:C:303:HIS:HE1	1.93	0.52
1:B:9:GLU:OE1	1:B:185:TYR:OH	2.25	0.51
1:D:52:ARG:HH21	1:D:52:ARG:HG3	1.74	0.51
1:A:18:ARG:HG2	1:A:18:ARG:NH1	2.02	0.50
1:D:18:ARG:CG	1:D:18:ARG:NH1	2.73	0.49
1:B:171:PRO:O	1:B:303:HIS:HE1	1.96	0.49
1:D:171:PRO:O	1:D:303:HIS:HE1	1.96	0.49
1:A:228:ILE:HD13	1:A:299:LEU:HD13	1.95	0.48
1:B:7:VAL:HG22	1:B:213:LEU:HD11	1.96	0.48
1:A:171:PRO:O	1:A:303:HIS:HE1	1.97	0.48
1:D:228:ILE:HD13	1:D:299:LEU:HD13	1.96	0.47
1:B:228:ILE:HD13	1:B:299:LEU:HD13	1.97	0.47
1:A:19:TRP:CE2	6:A:405:GOL:H31	2.50	0.47
1:D:52:ARG:NH2	1:D:193:GLU:HG3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:TYR:OH	1:D:303:HIS:HD2	1.99	0.46
1:C:228:ILE:HD13	1:C:299:LEU:HD13	1.97	0.46
1:C:282:GLU:O	1:C:285:ILE:HG22	2.16	0.45
1:A:78:TYR:OH	1:A:303:HIS:HD2	1.99	0.45
1:A:19:TRP:CD2	6:A:405:GOL:H31	2.50	0.45
1:B:183:ASP:HB3	1:A:198:SER:HB3	1.99	0.45
1:B:110:PRO:O	1:B:112:LEU:HD22	2.17	0.44
1:B:78:TYR:OH	1:B:303:HIS:HD2	2.00	0.44
1:D:217:LEU:CD2	1:D:227:ILE:HD13	2.47	0.44
1:A:217:LEU:CD2	1:A:227:ILE:HD13	2.47	0.43
1:C:217:LEU:CD2	1:C:227:ILE:HD13	2.48	0.43
1:B:180:ALA:HA	5:B:402:J1O:CAP	2.49	0.43
1:B:217:LEU:CD2	1:B:227:ILE:HD13	2.48	0.43
1:C:78:TYR:OH	1:C:303:HIS:HD2	2.01	0.43
1:C:180:ALA:HA	5:C:402:J1O:CAP	2.49	0.43
1:B:241:ASN:HB2	6:B:405:GOL:H2	1.99	0.43
1:A:281:SER:O	1:A:285:ILE:HG13	2.19	0.43
1:A:180:ALA:HA	5:A:402:J1O:CAP	2.49	0.43
1:C:215:SER:HB2	1:C:216:PRO:HD3	2.00	0.42
1:A:215:SER:HB2	1:A:216:PRO:HD3	2.01	0.42
1:B:215:SER:HB2	1:B:216:PRO:HD3	2.02	0.42
1:A:22:VAL:HG22	1:A:25:ARG:NH2	2.35	0.42
1:A:156:LEU:HD22	1:A:213:LEU:HD12	2.02	0.42
1:A:300:GLN:NE2	7:A:508:HOH:O	2.53	0.41
1:A:18:ARG:CG	1:A:18:ARG:NH1	2.73	0.41
1:D:148:GLU:HG3	7:D:584:HOH:O	2.19	0.41
1:D:215:SER:HB2	1:D:216:PRO:HD3	2.02	0.41
1:C:217:LEU:HD23	1:C:217:LEU:C	2.40	0.41
1:C:9:GLU:OE2	1:C:185:TYR:OH	2.24	0.41
1:B:186:VAL:CG1	1:B:190:GLU:HG2	2.51	0.41
1:B:156:LEU:HD22	1:B:213:LEU:HD12	2.03	0.41
1:B:198:SER:HB3	1:A:183:ASP:HB3	2.03	0.41
1:D:52:ARG:NH2	1:D:193:GLU:OE2	2.52	0.40
1:D:281:SER:O	1:D:285:ILE:HG13	2.21	0.40
1:D:169:LEU:HD12	1:D:169:LEU:N	2.36	0.40
1:D:156:LEU:HD22	1:D:213:LEU:HD12	2.04	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	306/311 (98%)	299 (98%)	6 (2%)	1 (0%)	41	30
1	B	307/311 (99%)	300 (98%)	6 (2%)	1 (0%)	41	30
1	C	304/311 (98%)	299 (98%)	4 (1%)	1 (0%)	41	30
1	D	306/311 (98%)	299 (98%)	6 (2%)	1 (0%)	41	30
All	All	1223/1244 (98%)	1197 (98%)	22 (2%)	4 (0%)	41	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	287	LYS
1	A	287	LYS
1	D	287	LYS
1	C	287	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	240/249 (96%)	230 (96%)	10 (4%)	30	17
1	B	239/249 (96%)	230 (96%)	9 (4%)	33	21
1	C	240/249 (96%)	228 (95%)	12 (5%)	24	11
1	D	244/249 (98%)	229 (94%)	15 (6%)	18	7
All	All	963/996 (97%)	917 (95%)	46 (5%)	27	12

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	18	ARG
1	D	35	ARG
1	D	106	ARG
1	D	121	GLU
1	D	130[A]	GLU
1	D	130[B]	GLU
1	D	204	GLN
1	D	206	THR
1	D	219	LYS
1	D	258	ASN
1	D	282	GLU
1	D	283	GLU
1	D	285	ILE
1	D	286	GLU
1	D	300	GLN
1	C	18	ARG
1	C	35	ARG
1	C	103	SER
1	C	121	GLU
1	C	164[A]	GLN
1	C	164[B]	GLN
1	C	206	THR
1	C	245	LYS
1	C	258	ASN
1	C	283	GLU
1	C	285	ILE
1	C	286	GLU
1	B	35	ARG
1	B	112	LEU
1	B	121	GLU
1	B	190	GLU
1	B	204	GLN
1	B	206	THR
1	B	258	ASN
1	B	300	GLN
1	B	309	ASP
1	A	9	GLU
1	A	18	ARG
1	A	35	ARG
1	A	121	GLU
1	A	206	THR
1	A	208	LYS

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Mol	Chain	Res	Type
1	A	238	ILE
1	A	258	ASN
1	A	285	ILE
1	A	300	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	157	HIS
1	D	164	GLN
1	D	204	GLN
1	D	241	ASN
1	D	303	HIS
1	C	157	HIS
1	C	241	ASN
1	C	303	HIS
1	B	157	HIS
1	B	164	GLN
1	B	204	GLN
1	B	303	HIS
1	A	99	GLN
1	A	157	HIS
1	A	164	GLN
1	A	300	GLN
1	A	303	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

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 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
2	ANP	D	401	4	29,33,33	2.05	7 (24%)	31,52,52	1.94	7 (22%)
5	J1O	B	402	-	16,19,19	1.88	5 (31%)	25,27,27	2.14	8 (32%)
6	GOL	B	406	-	5,5,5	0.34	0	5,5,5	0.89	0
3	SO4	D	406	-	4,4,4	0.34	0	6,6,6	0.55	0
2	ANP	A	401	4	29,33,33	2.07	8 (27%)	31,52,52	2.11	4 (12%)
2	ANP	C	401	4	29,33,33	1.85	5 (17%)	31,52,52	2.07	9 (29%)
3	SO4	B	404	-	4,4,4	0.12	0	6,6,6	0.56	0
6	GOL	A	404	-	5,5,5	0.26	0	5,5,5	0.88	0
3	SO4	B	407	-	4,4,4	0.45	0	6,6,6	0.26	0
2	ANP	B	401	4	29,33,33	1.70	10 (34%)	31,52,52	2.00	7 (22%)
6	GOL	C	406	-	5,5,5	0.13	0	5,5,5	0.51	0
3	SO4	A	406	-	4,4,4	0.49	0	6,6,6	0.26	0
3	SO4	D	402	-	4,4,4	0.43	0	6,6,6	0.61	0
3	SO4	C	405	-	4,4,4	0.18	0	6,6,6	0.48	0
3	SO4	A	407	-	4,4,4	0.41	0	6,6,6	0.33	0
3	SO4	D	404	-	4,4,4	0.44	0	6,6,6	0.42	0
5	J1O	D	405	-	16,19,19	1.85	5 (31%)	25,27,27	1.80	5 (20%)
5	J1O	C	402	-	16,19,19	1.33	2 (12%)	25,27,27	2.31	11 (44%)
3	SO4	C	404	-	4,4,4	0.43	0	6,6,6	0.19	0
6	GOL	A	405	-	5,5,5	0.24	0	5,5,5	0.38	0
6	GOL	B	405	-	5,5,5	0.59	0	5,5,5	0.77	0
5	J1O	A	402	-	16,19,19	1.31	2 (12%)	25,27,27	1.90	8 (32%)

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
6	GOL	A	404	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	D	401	4	-	2/14/38/38	0/3/3/3
5	J1O	B	402	-	-	4/24/24/24	-
5	J1O	D	405	-	-	3/24/24/24	-
6	GOL	B	406	-	-	4/4/4/4	-
2	ANP	B	401	4	-	3/14/38/38	0/3/3/3
2	ANP	A	401	4	-	3/14/38/38	0/3/3/3
5	J1O	C	402	-	-	5/24/24/24	-
6	GOL	C	406	-	-	0/4/4/4	-
6	GOL	A	405	-	-	0/4/4/4	-
2	ANP	C	401	4	-	3/14/38/38	0/3/3/3
6	GOL	B	405	-	-	4/4/4/4	-
5	J1O	A	402	-	-	3/24/24/24	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	ANP	PB-O3A	6.55	1.67	1.59
2	A	401	ANP	PG-O1G	6.49	1.56	1.46
2	C	401	ANP	PG-O1G	5.61	1.55	1.46
5	D	405	J1O	CAL-CAP	4.88	1.61	1.50
5	B	402	J1O	PAT-OAE	4.17	1.64	1.50
2	B	401	ANP	O4'-C1'	3.90	1.46	1.41
2	C	401	ANP	PG-N3B	3.86	1.73	1.63
2	A	401	ANP	O4'-C1'	3.81	1.46	1.41
2	A	401	ANP	C2-N3	3.79	1.38	1.32
2	D	401	ANP	PG-O1G	3.51	1.51	1.46
2	D	401	ANP	O4'-C1'	3.36	1.45	1.41
2	D	401	ANP	C2-N3	3.28	1.37	1.32
2	C	401	ANP	O4'-C1'	3.25	1.45	1.41
2	B	401	ANP	C2-N3	3.23	1.37	1.32
5	D	405	J1O	PAT-OAI	3.15	1.67	1.54
5	B	402	J1O	CAL-CAP	3.05	1.57	1.50
5	C	402	J1O	CAL-CAP	2.89	1.57	1.50
2	D	401	ANP	C4-N3	-2.79	1.31	1.35
5	B	402	J1O	PAT-OAH	2.73	1.65	1.54
2	D	401	ANP	PG-N3B	2.65	1.70	1.63
5	C	402	J1O	OAG-CAR	-2.65	1.37	1.42
5	B	402	J1O	OAF-CAP	2.55	1.30	1.22
2	B	401	ANP	C2'-C1'	-2.55	1.49	1.53
2	A	401	ANP	PB-O3A	2.54	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	405	J1O	OAG-CAR	-2.50	1.37	1.42
2	B	401	ANP	PG-N3B	2.45	1.69	1.63
2	C	401	ANP	PG-O3G	-2.44	1.50	1.56
2	A	401	ANP	C5-C4	2.44	1.47	1.40
2	B	401	ANP	C4-N3	-2.43	1.32	1.35
2	A	401	ANP	PG-N3B	2.41	1.69	1.63
5	A	402	J1O	CAA-CAS	2.40	1.59	1.53
5	B	402	J1O	PAT-OAI	-2.39	1.45	1.54
5	D	405	J1O	OAF-CAP	2.39	1.30	1.22
2	B	401	ANP	PB-O1B	2.37	1.49	1.46
2	C	401	ANP	C4-N3	-2.36	1.32	1.35
5	A	402	J1O	CAL-CAP	2.33	1.56	1.50
2	A	401	ANP	PB-O2B	-2.32	1.50	1.56
2	B	401	ANP	PG-O1G	2.27	1.49	1.46
2	A	401	ANP	C2-N1	2.13	1.37	1.33
2	B	401	ANP	PG-O2G	-2.12	1.51	1.56
2	B	401	ANP	PB-O2B	-2.10	1.51	1.56
2	D	401	ANP	PB-N3B	2.07	1.68	1.63
2	B	401	ANP	PG-O3G	-2.07	1.51	1.56
5	D	405	J1O	CAJ-CAK	2.06	1.59	1.51

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	ANP	O1G-PG-N3B	-8.16	99.76	111.77
2	B	401	ANP	O1G-PG-N3B	-7.06	101.38	111.77
2	C	401	ANP	O1G-PG-N3B	-6.89	101.63	111.77
5	B	402	J1O	CAA-CAS-CAR	6.55	120.17	108.82
5	C	402	J1O	CAA-CAS-CAR	6.45	120.00	108.82
2	D	401	ANP	O1G-PG-N3B	-6.32	102.46	111.77
5	D	405	J1O	CAA-CAS-CAR	5.26	117.94	108.82
5	A	402	J1O	CAA-CAS-CAR	4.92	117.35	108.82
2	C	401	ANP	N3-C2-N1	-4.44	121.74	128.68
5	C	402	J1O	OAI-PAT-OAE	4.39	127.85	110.68
2	A	401	ANP	N3-C2-N1	-4.29	121.97	128.68
2	D	401	ANP	O2B-PB-O1B	4.14	118.59	109.92
5	D	405	J1O	OAG-CAR-CAS	4.11	119.92	110.25
5	B	402	J1O	OAI-PAT-OAE	3.86	125.80	110.68
2	A	401	ANP	N6-C6-N1	3.63	126.11	118.57
5	A	402	J1O	OAF-CAP-CAL	-3.62	111.47	123.08
2	B	401	ANP	C5-C6-N6	-3.55	114.96	120.35
5	A	402	J1O	OAI-PAT-OAE	3.36	123.83	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	402	J1O	OAF-CAP-CAL	-3.29	112.52	123.08
2	B	401	ANP	N3-C2-N1	-3.26	123.58	128.68
2	A	401	ANP	C5-C6-N6	-3.19	115.51	120.35
2	B	401	ANP	N6-C6-N1	3.13	125.06	118.57
5	C	402	J1O	OAH-PAT-OAE	-2.98	99.03	110.68
2	D	401	ANP	O2G-PG-O3G	2.97	115.55	107.64
2	C	401	ANP	C3'-C2'-C1'	2.97	105.45	100.98
5	A	402	J1O	OAO-PAT-OAE	2.94	114.71	106.47
2	C	401	ANP	O1B-PB-N3B	-2.84	107.58	111.77
5	B	402	J1O	CAJ-CAK-NAN	-2.83	104.11	112.21
5	B	402	J1O	OAG-CAR-CAS	2.80	116.85	110.25
2	D	401	ANP	N3-C2-N1	-2.71	124.45	128.68
2	D	401	ANP	C5-C6-N6	-2.69	116.26	120.35
5	B	402	J1O	OAI-PAT-OAO	2.68	113.85	106.73
5	B	402	J1O	OAO-PAT-OAE	-2.64	99.08	106.47
5	C	402	J1O	OAG-CAR-CAS	2.62	116.41	110.25
5	C	402	J1O	OAH-PAT-OAO	-2.61	99.80	106.73
5	D	405	J1O	OAD-CAQ-CAR	-2.57	113.22	121.06
5	C	402	J1O	OAD-CAQ-CAR	-2.54	113.31	121.06
2	D	401	ANP	N6-C6-N1	2.52	123.81	118.57
2	C	401	ANP	O4'-C1'-C2'	-2.48	103.31	106.93
5	B	402	J1O	OAH-PAT-OAE	-2.46	101.05	110.68
5	D	405	J1O	CAJ-CAK-NAN	-2.46	105.18	112.21
2	D	401	ANP	O2G-PG-O1G	-2.45	107.30	113.45
2	C	401	ANP	C5-C6-N6	-2.41	116.69	120.35
5	A	402	J1O	OAC-CAP-CAL	2.38	121.67	114.03
2	C	401	ANP	N6-C6-N1	2.32	123.40	118.57
2	C	401	ANP	O5'-C5'-C4'	2.30	116.91	108.99
5	B	402	J1O	CAB-CAS-CAA	-2.30	104.49	109.17
5	C	402	J1O	CAJ-CAK-NAN	-2.29	105.65	112.21
5	D	405	J1O	OAH-PAT-OAE	2.29	119.63	110.68
5	C	402	J1O	OAO-PAT-OAE	2.28	112.87	106.47
2	C	401	ANP	O2B-PB-O1B	2.25	114.65	109.92
5	A	402	J1O	OAI-PAT-OAO	-2.18	100.92	106.73
2	B	401	ANP	O4'-C1'-C2'	-2.14	103.81	106.93
2	B	401	ANP	O3G-PG-O1G	2.13	118.80	113.45
5	C	402	J1O	OAC-CAP-CAL	2.10	120.77	114.03
5	C	402	J1O	CAB-CAS-CAA	-2.09	104.90	109.17
5	A	402	J1O	CAJ-CAK-NAN	-2.08	106.25	112.21
5	A	402	J1O	OAG-CAR-CAS	2.02	115.00	110.25
2	B	401	ANP	O3'-C3'-C2'	-2.00	105.34	111.82

There are no chirality outliers.

All (38) torsion outliers are listed below:

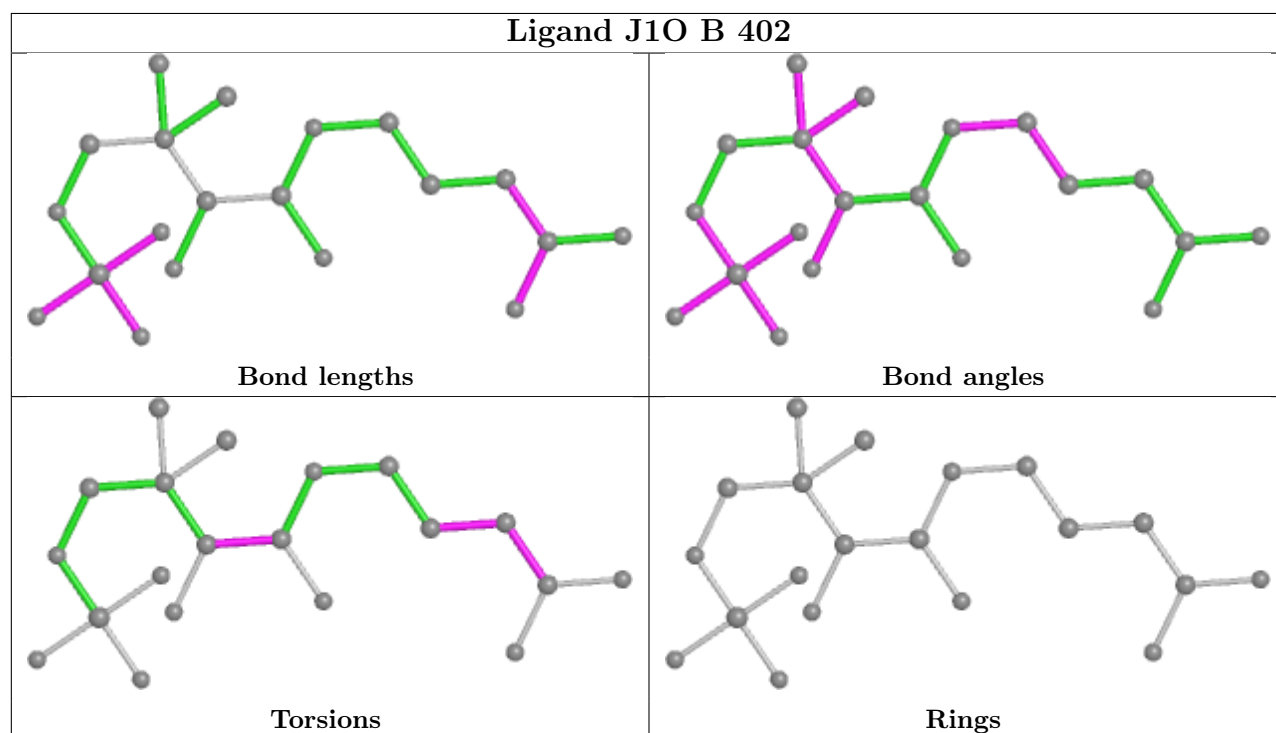
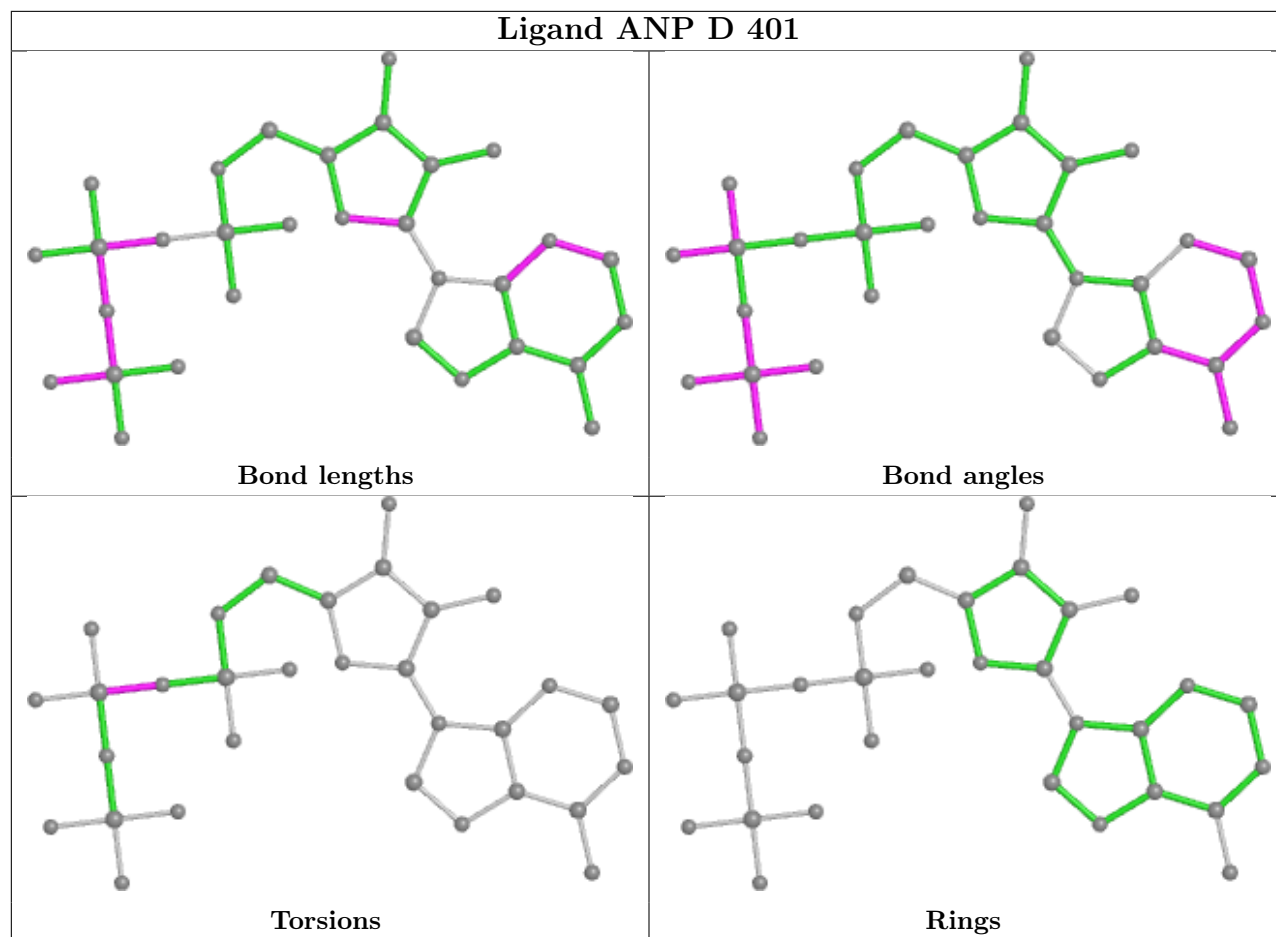
Mol	Chain	Res	Type	Atoms
2	D	401	ANP	PA-O3A-PB-O1B
2	D	401	ANP	PA-O3A-PB-O2B
2	C	401	ANP	PB-N3B-PG-O1G
2	C	401	ANP	PA-O3A-PB-O1B
2	C	401	ANP	PA-O3A-PB-O2B
2	B	401	ANP	PB-N3B-PG-O1G
2	B	401	ANP	PA-O3A-PB-O1B
2	B	401	ANP	PA-O3A-PB-O2B
2	A	401	ANP	PB-N3B-PG-O1G
2	A	401	ANP	PA-O3A-PB-O1B
2	A	401	ANP	PA-O3A-PB-O2B
6	B	406	GOL	C1-C2-C3-O3
6	A	404	GOL	O1-C1-C2-C3
6	A	404	GOL	C1-C2-C3-O3
6	A	404	GOL	O2-C2-C3-O3
5	B	402	J1O	CAK-CAJ-CAL-CAP
5	A	402	J1O	CAK-CAJ-CAL-CAP
6	B	405	GOL	O1-C1-C2-C3
6	B	406	GOL	O1-C1-C2-C3
6	B	405	GOL	O1-C1-C2-O2
6	B	406	GOL	O2-C2-C3-O3
6	A	404	GOL	O1-C1-C2-O2
5	C	402	J1O	CAK-CAJ-CAL-CAP
5	B	402	J1O	OAD-CAQ-CAR-OAG
5	D	405	J1O	CAK-CAJ-CAL-CAP
6	B	405	GOL	O2-C2-C3-O3
5	C	402	J1O	OAD-CAQ-CAR-OAG
6	B	406	GOL	O1-C1-C2-O2
5	C	402	J1O	CAJ-CAL-CAP-OAC
5	D	405	J1O	CAJ-CAL-CAP-OAC
5	A	402	J1O	CAJ-CAL-CAP-OAC
5	C	402	J1O	NAN-CAQ-CAR-CAS
5	D	405	J1O	CAJ-CAL-CAP-OAF
5	C	402	J1O	CAJ-CAL-CAP-OAF
5	B	402	J1O	CAJ-CAL-CAP-OAF
5	B	402	J1O	CAJ-CAL-CAP-OAC
5	A	402	J1O	CAJ-CAL-CAP-OAF
6	B	405	GOL	C1-C2-C3-O3

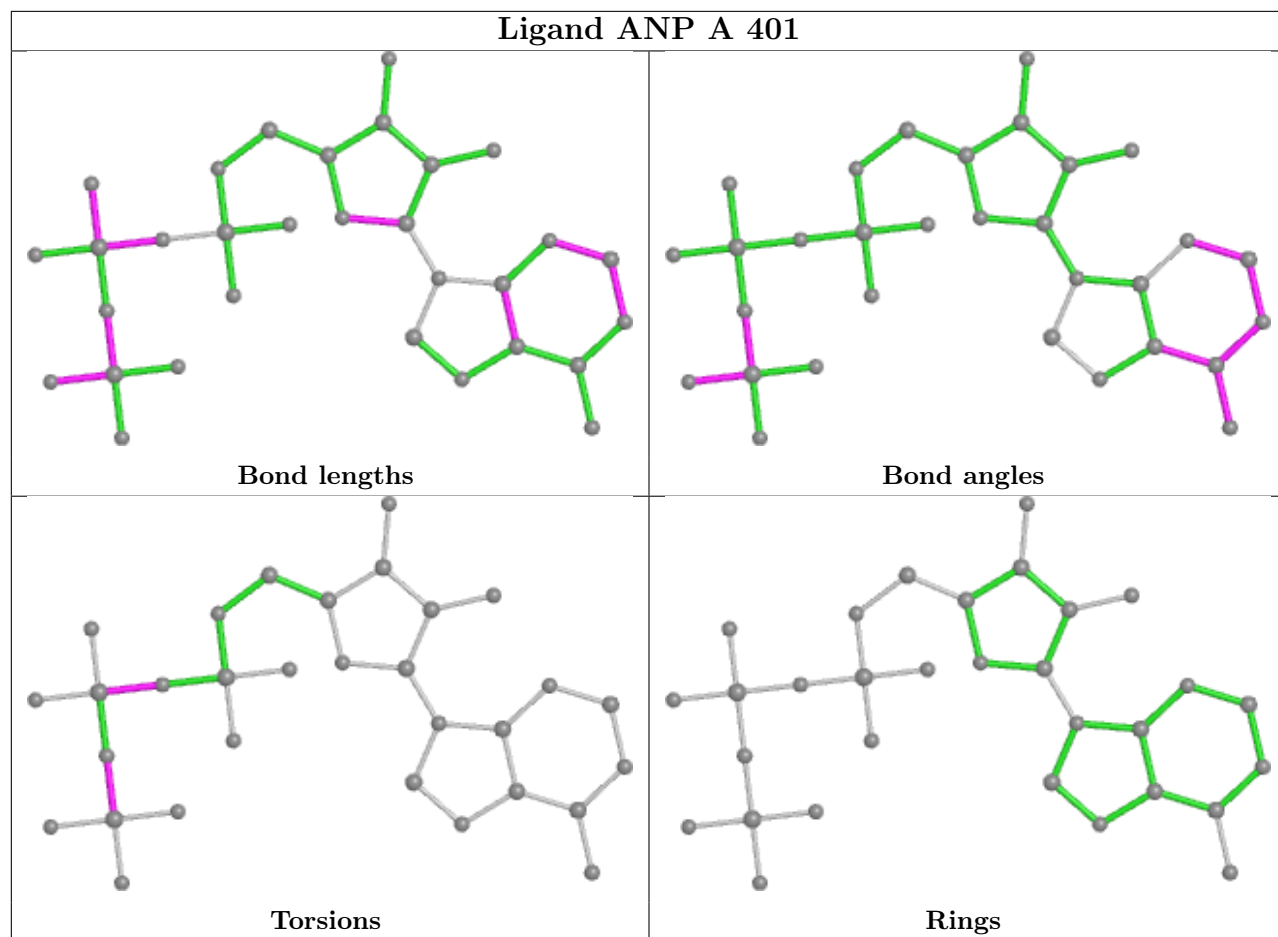
There are no ring outliers.

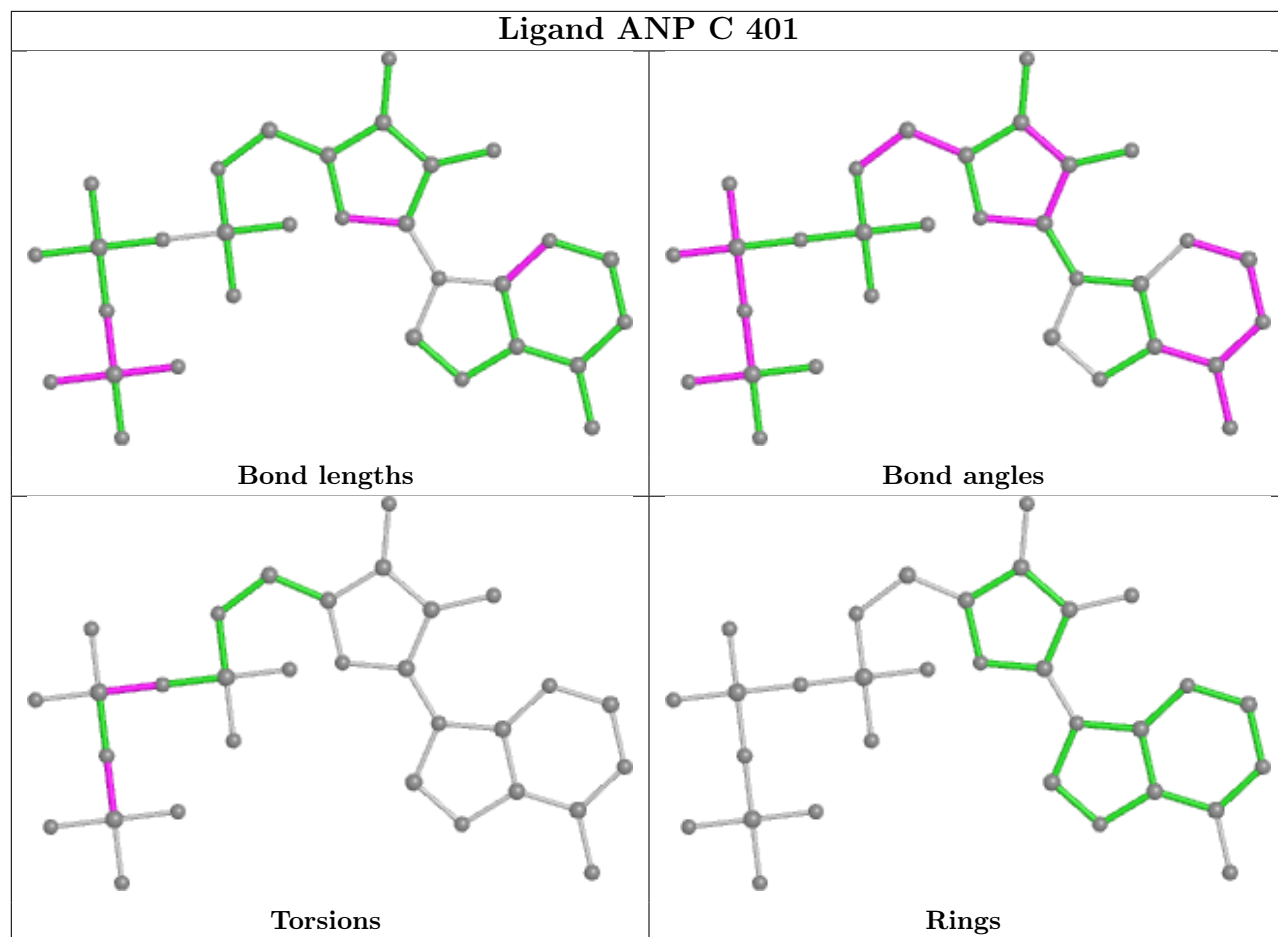
9 monomers are involved in 21 short contacts:

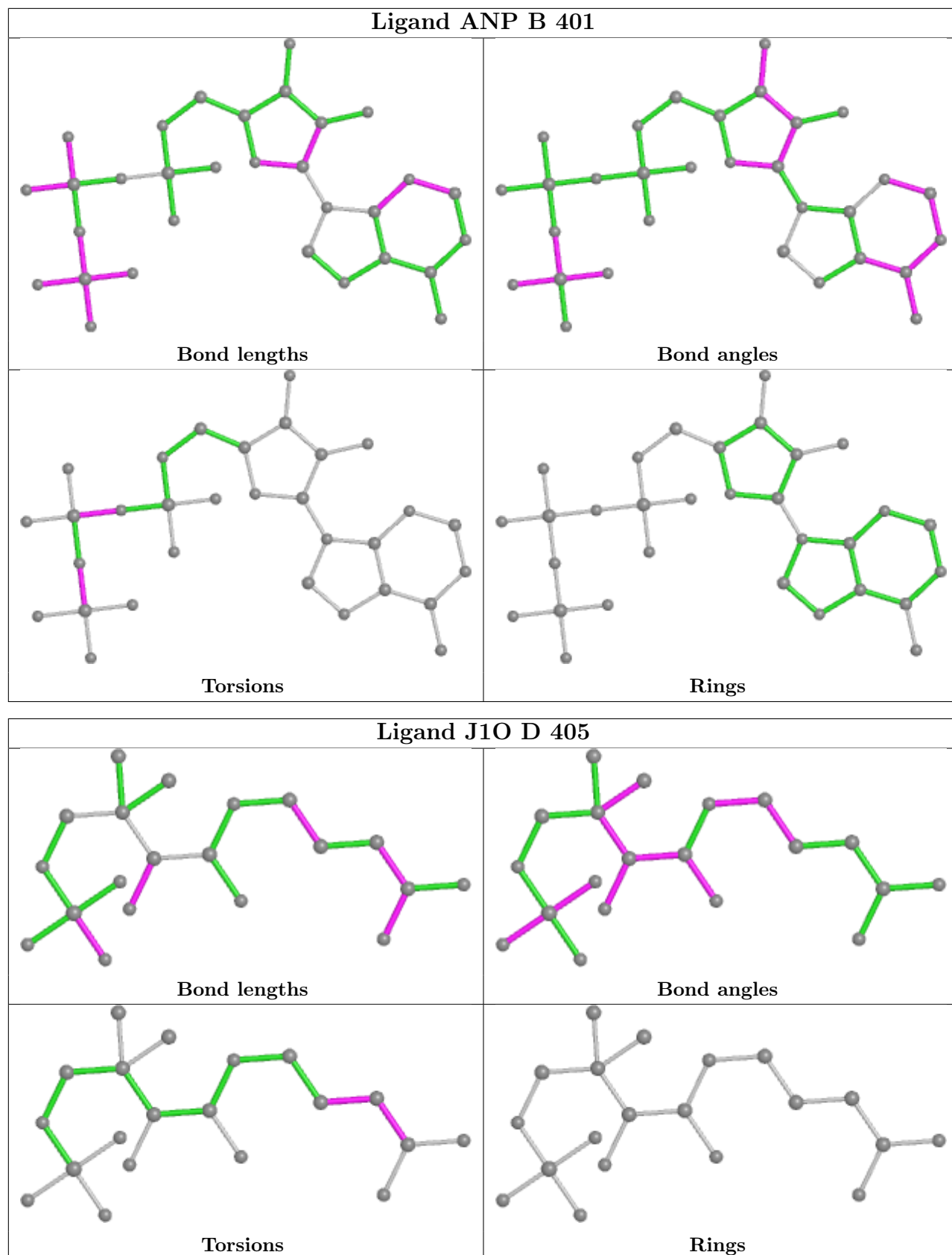
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	402	J1O	1	0
6	B	406	GOL	3	0
3	B	404	SO4	1	0
6	A	404	GOL	7	0
6	C	406	GOL	4	0
5	C	402	J1O	1	0
6	A	405	GOL	2	0
6	B	405	GOL	1	0
5	A	402	J1O	1	0

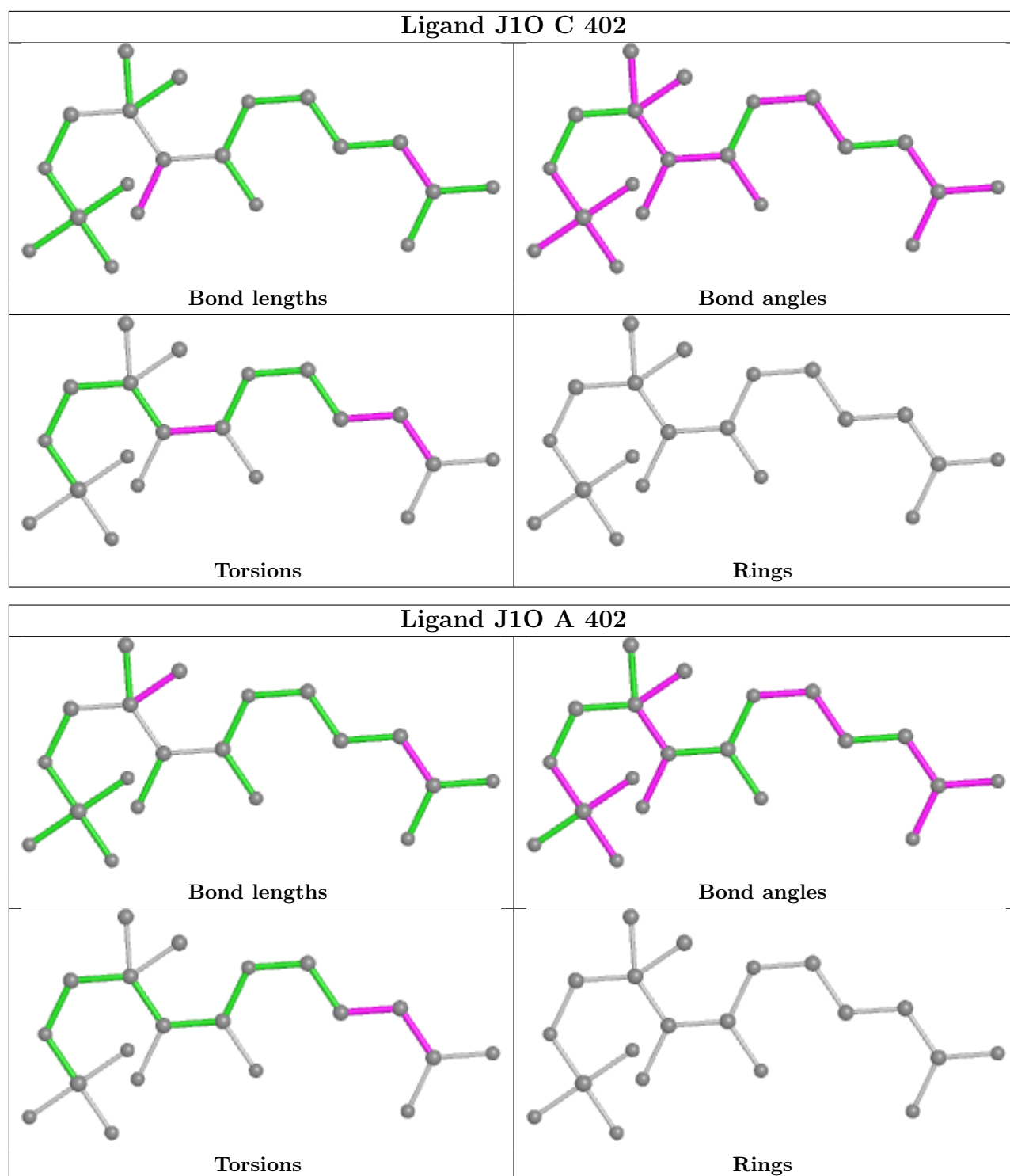
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	305/311 (98%)	0.04	2 (0%) 87 92	22, 34, 61, 106	0
1	B	306/311 (98%)	0.01	3 (0%) 82 87	22, 34, 61, 102	0
1	C	304/311 (97%)	0.11	5 (1%) 72 79	23, 34, 60, 107	0
1	D	305/311 (98%)	-0.00	0 100 100	23, 34, 61, 102	0
All	All	1220/1244 (98%)	0.04	10 (0%) 86 90	22, 34, 62, 107	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	310	ARG	3.9
1	B	288	GLY	2.6
1	A	205	ILE	2.5
1	A	284	GLU	2.5
1	B	282	GLU	2.4
1	C	205	ILE	2.2
1	C	27	ALA	2.2
1	C	7	VAL	2.2
1	C	285	ILE	2.0
1	C	286	GLU	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](#)

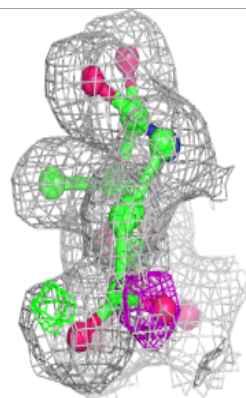
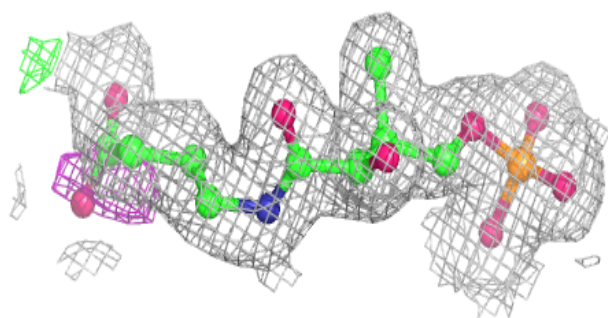
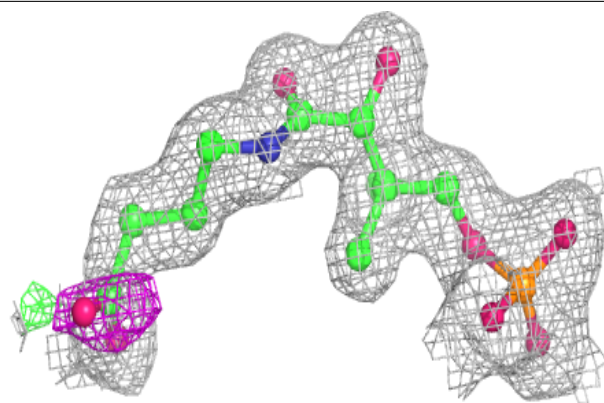
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	B	405	6/6	0.70	0.17	67,75,77,79	0
6	GOL	B	406	6/6	0.70	0.29	54,60,64,65	0
6	GOL	A	405	6/6	0.71	0.18	63,67,69,77	0
3	SO4	D	404	5/5	0.73	0.28	92,96,109,112	0
3	SO4	B	404	5/5	0.77	0.23	87,91,100,103	0
3	SO4	C	405	5/5	0.78	0.20	90,96,107,110	0
3	SO4	C	404	5/5	0.79	0.26	108,112,117,121	0
3	SO4	A	407	5/5	0.82	0.12	98,114,118,128	0
6	GOL	A	404	6/6	0.83	0.23	61,74,76,79	0
6	GOL	C	406	6/6	0.83	0.18	65,67,68,72	0
3	SO4	A	406	5/5	0.92	0.12	75,79,90,97	0
4	MG	D	403	1/1	0.93	0.09	28,28,28,28	0
3	SO4	B	407	5/5	0.93	0.20	77,78,82,94	0
3	SO4	D	406	5/5	0.94	0.16	67,74,78,90	0
5	J1O	D	405	20/20	0.96	0.12	23,26,51,69	0
5	J1O	C	402	20/20	0.97	0.10	22,25,48,48	2
5	J1O	B	402	20/20	0.97	0.11	22,25,48,49	2
5	J1O	A	402	20/20	0.97	0.12	23,26,40,45	2
4	MG	A	403	1/1	0.97	0.05	25,25,25,25	0
2	ANP	A	401	31/31	0.98	0.09	21,24,28,30	0
4	MG	B	403	1/1	0.98	0.08	24,24,24,24	0
2	ANP	D	401	31/31	0.98	0.08	21,24,28,29	0
2	ANP	B	401	31/31	0.98	0.09	22,25,29,32	0
4	MG	C	403	1/1	0.99	0.08	24,24,24,24	0
3	SO4	D	402	5/5	0.99	0.18	42,47,48,52	0
2	ANP	C	401	31/31	0.99	0.09	21,24,27,30	0

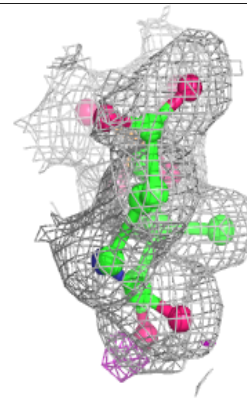
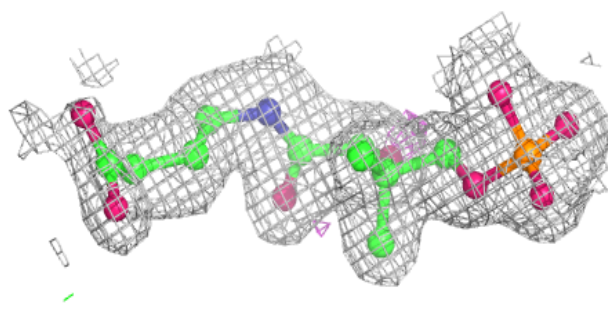
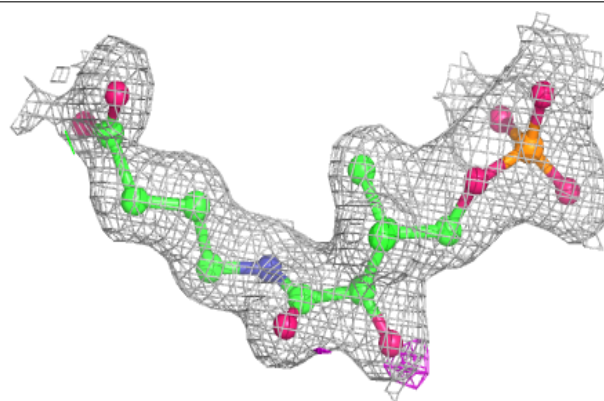
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around J1O D 405:

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

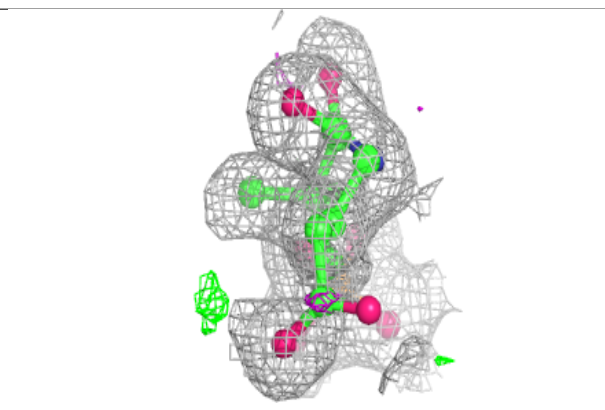
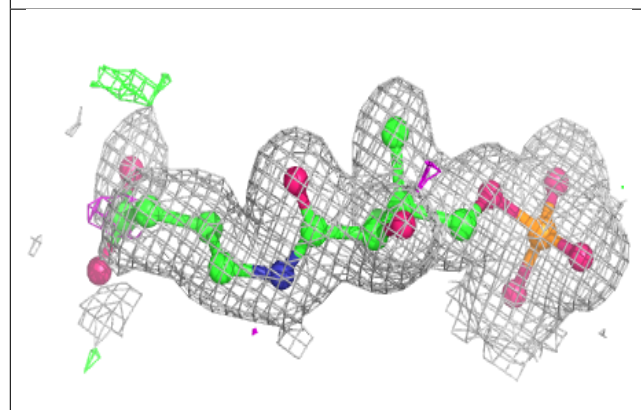
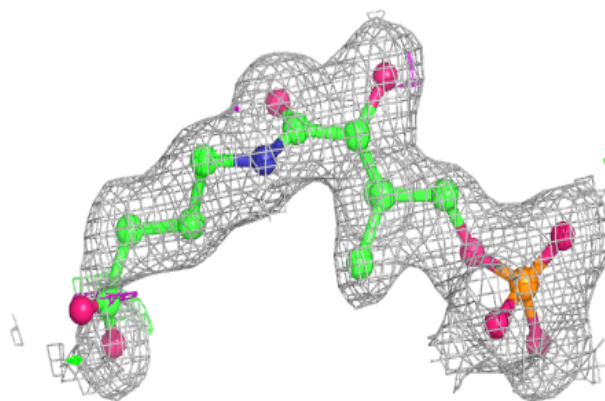
**Electron density around J1O C 402:**

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

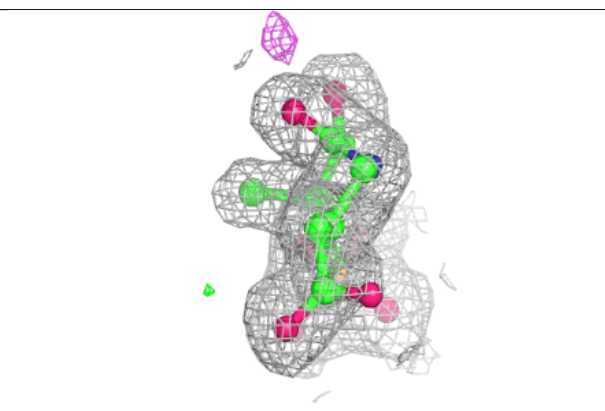
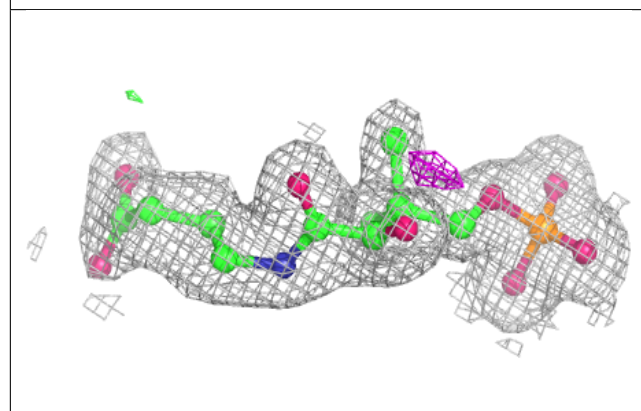
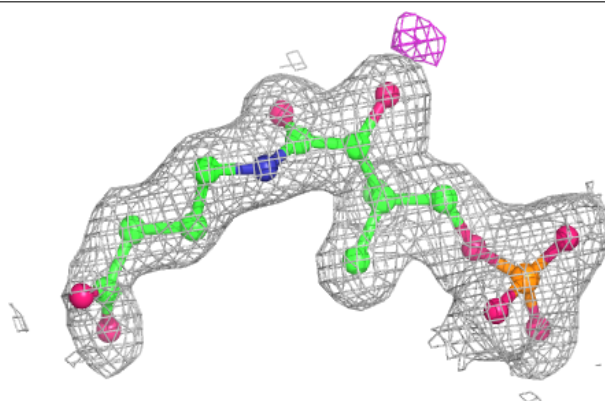


Electron density around J1O B 402:

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

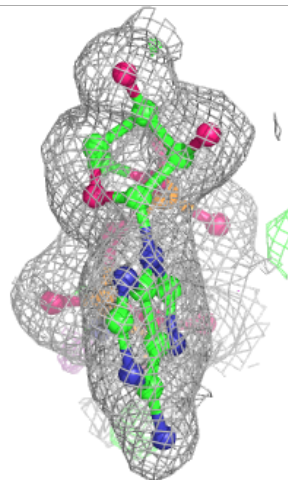
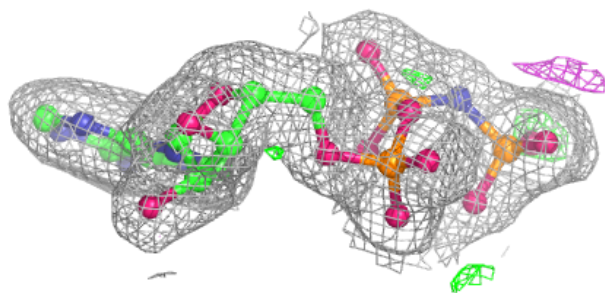
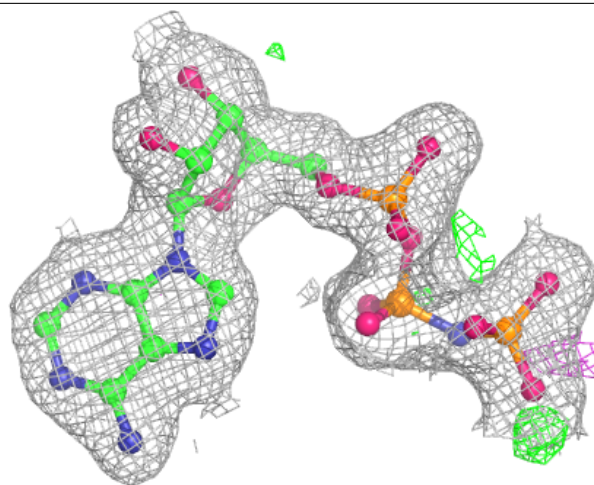
**Electron density around J1O A 402:**

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



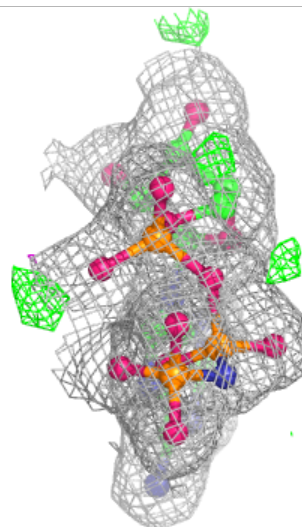
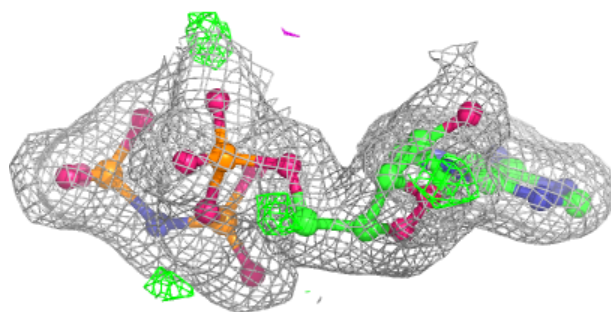
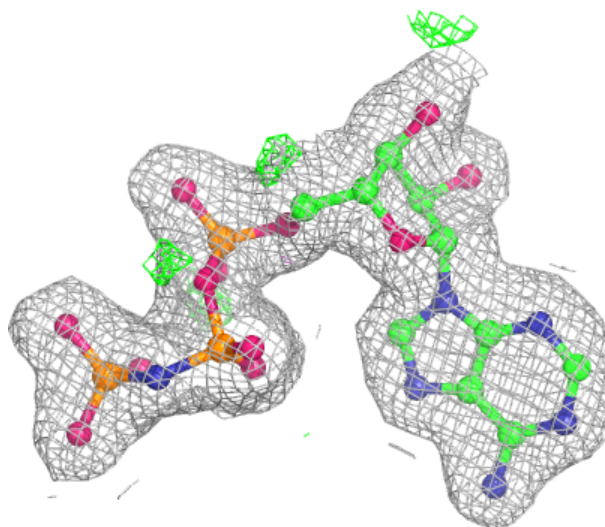
Electron density around ANP A 401:

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



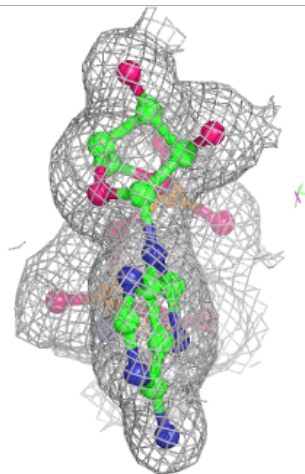
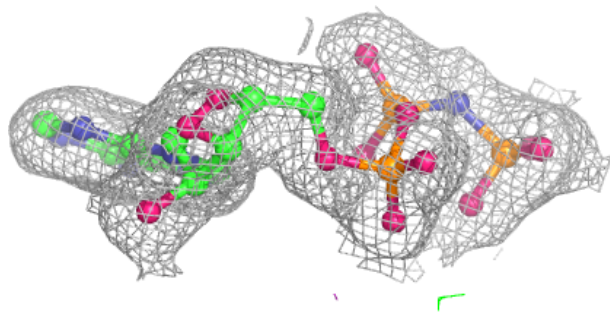
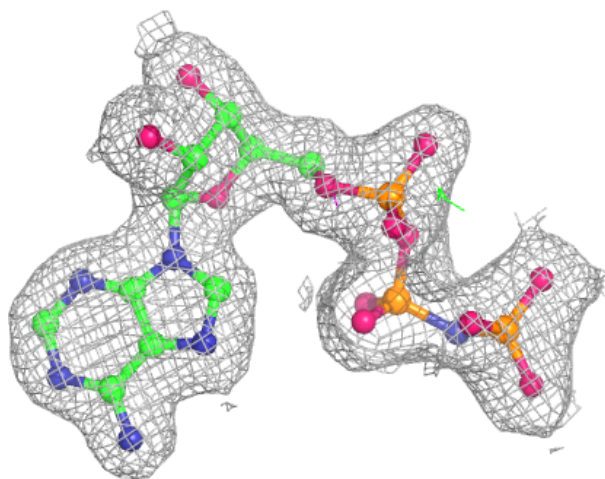
Electron density around ANP D 401:

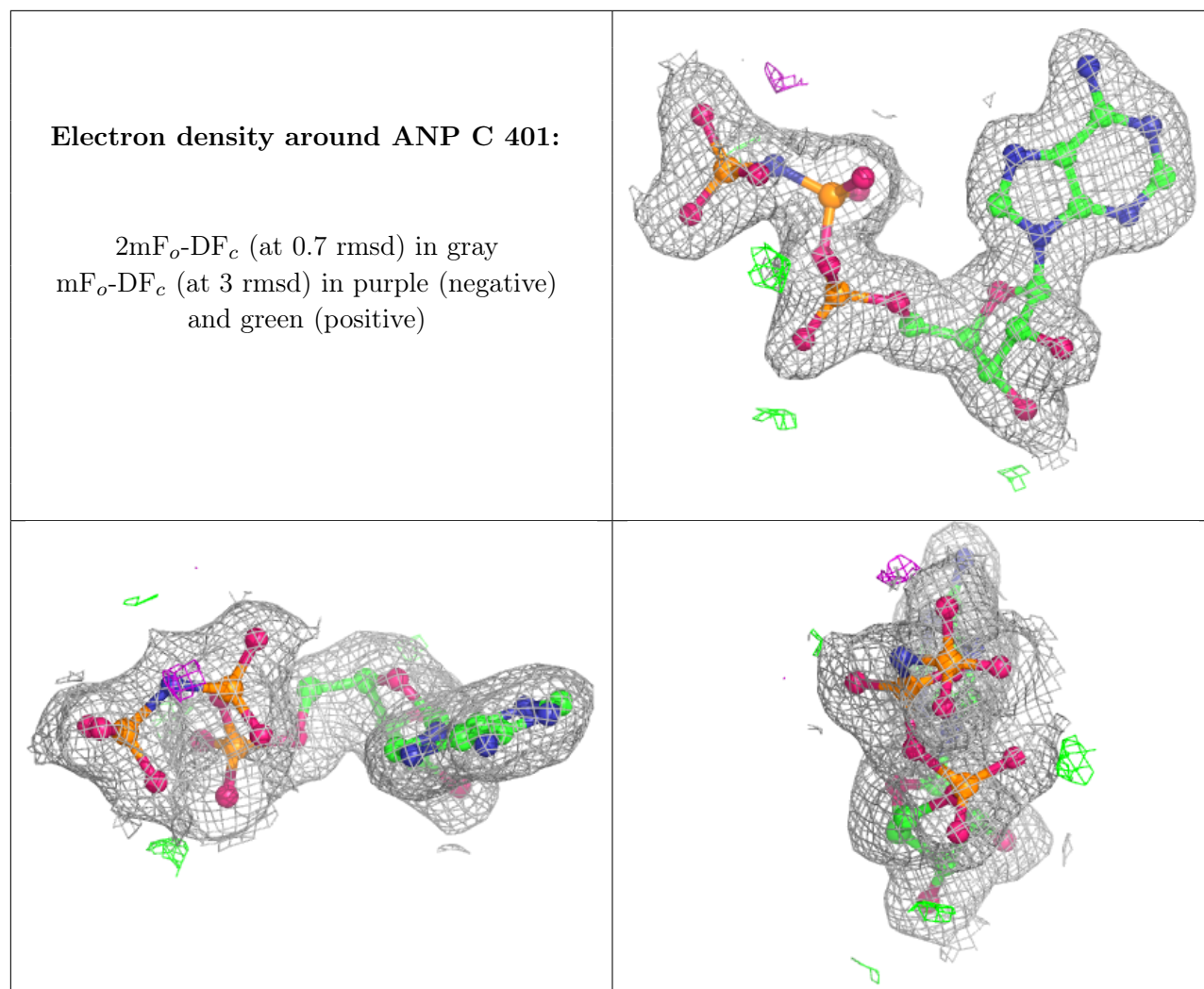
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ANP B 401:

$2mF_o-DF_c$ (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.