Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2023 – 04:31 pm BST

PDB ID	:	8AJW
Title	:	Crystal structure of the Q65N mutant of S-adenosyl-L-homocysteine hydrolase from Pseudomonas aeruginosa cocrystallized with adenosine in the presence of K+ cations
Authors	:	Drozdzal, P.; Wozniak, K.; Malecki, P.; Gawel, M.; Komorowska, M.; Brzezinski, K.
Deposited on	:	2022-07-28
Resolution	:	1.82 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 (i) 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 (1)) were used in the production of this report:

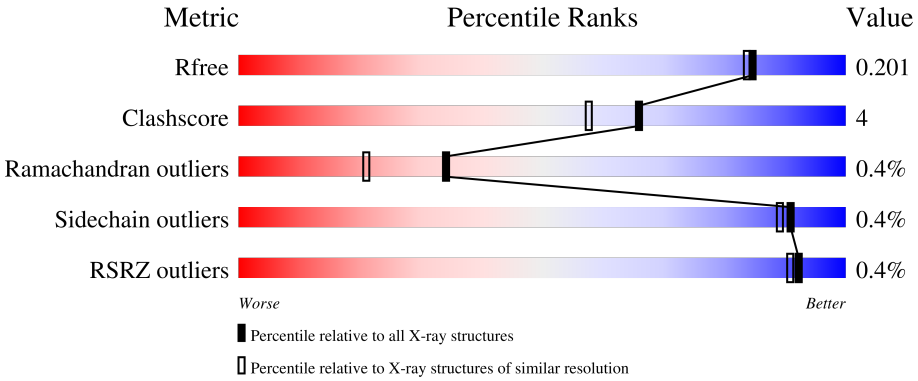
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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 <=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	AAA	472	89% 8%
1	BBB	472	% 91% 7%
1	CCC	472	92% 6%
1	DDD	472	91% 7%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16154 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.

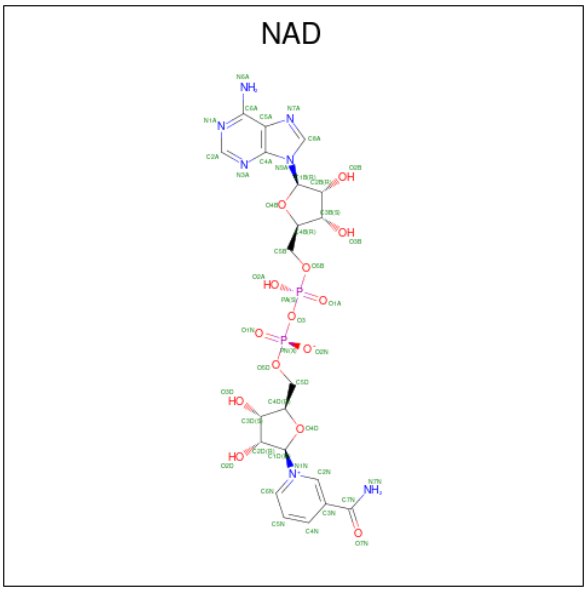
- Molecule 1 is a protein called S-adenosyl-L-homocysteine hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	461	Total	C	N	O	S	0	16	0
			3659	2305	637	694	23			
1	BBB	465	Total	C	N	O	S	18	10	0
			3626	2283	629	691	23			
1	CCC	461	Total	C	N	O	S	8	16	0
			3656	2308	634	691	23			
1	DDD	461	Total	C	N	O	S	9	10	0
			3605	2272	624	686	23			

There are 16 discrepancies between the modelled and reference sequences:

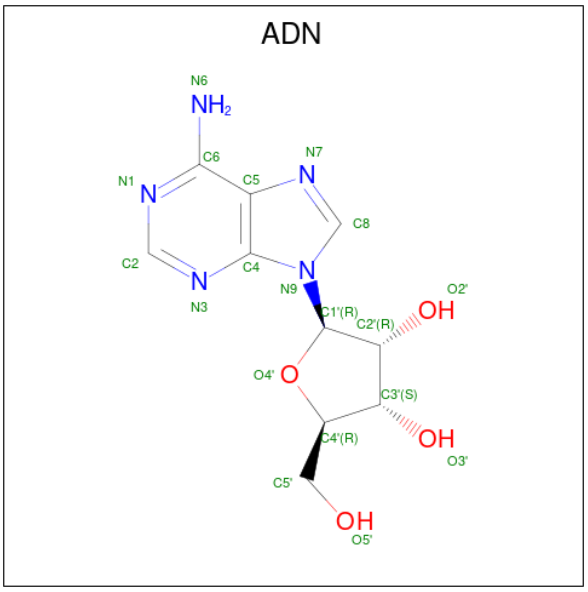
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-2	SER	-	expression tag	UNP Q9I685
AAA	-1	ASN	-	expression tag	UNP Q9I685
AAA	0	ALA	-	expression tag	UNP Q9I685
AAA	65	ASN	GLN	engineered mutation	UNP Q9I685
BBB	-2	SER	-	expression tag	UNP Q9I685
BBB	-1	ASN	-	expression tag	UNP Q9I685
BBB	0	ALA	-	expression tag	UNP Q9I685
BBB	65	ASN	GLN	engineered mutation	UNP Q9I685
CCC	-2	SER	-	expression tag	UNP Q9I685
CCC	-1	ASN	-	expression tag	UNP Q9I685
CCC	0	ALA	-	expression tag	UNP Q9I685
CCC	65	ASN	GLN	engineered mutation	UNP Q9I685
DDD	-2	SER	-	expression tag	UNP Q9I685
DDD	-1	ASN	-	expression tag	UNP Q9I685
DDD	0	ALA	-	expression tag	UNP Q9I685
DDD	65	ASN	GLN	engineered mutation	UNP Q9I685

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



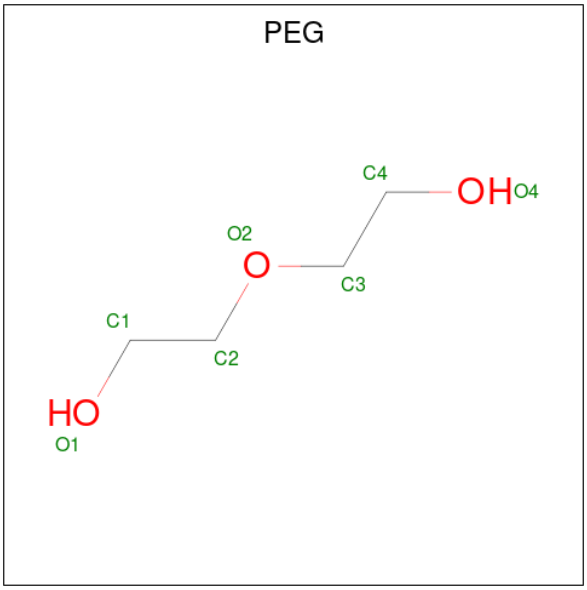
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	BBB	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	CCC	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	DDD	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is ADENOSINE (three-letter code: ADN) (formula: $C_{10}H_{13}N_5O_4$) (labeled as "Ligand of Interest" by depositor).



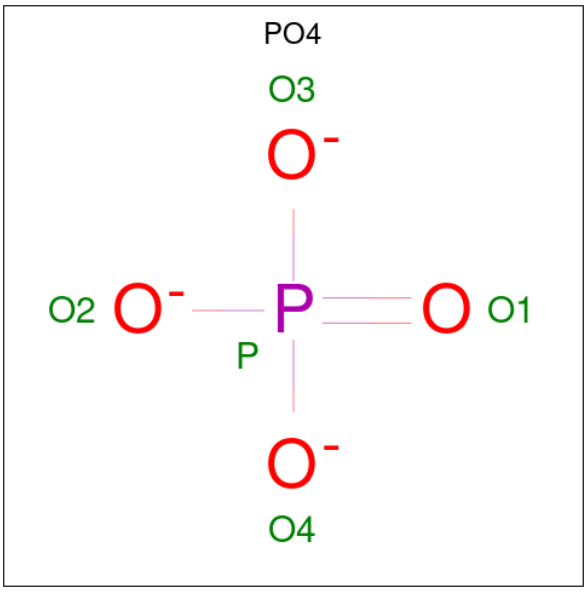
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	0	1
			19	10	5	4		
3	BBB	1	Total	C	N	O	0	1
			19	10	5	4		
3	CCC	1	Total	C	N	O	0	1
			19	10	5	4		
3	DDD	1	Total	C	N	O	0	1
			19	10	5	4		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total O P 5 4 1	0	0
5	BBB	1	Total O P 5 4 1	0	0
5	CCC	1	Total O P 5 4 1	0	0
5	DDD	1	Total O P 5 4 1	0	0

- Molecule 6 is water.

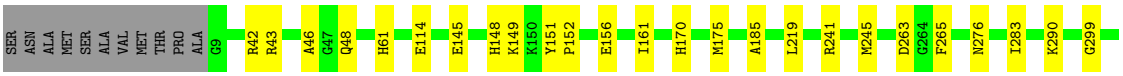
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	412	Total O 415 415	0	8
6	BBB	312	Total O 313 313	0	2
6	CCC	304	Total O 305 305	1	2
6	DDD	296	Total O 296 296	0	3

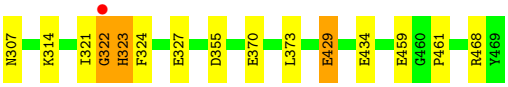
3 Residue-property plots (i)

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: S-adenosyl-L-homocysteine hydrolase

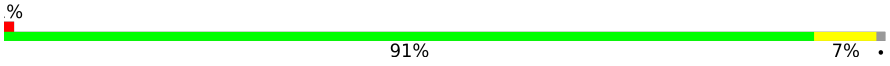
Chain AAA:

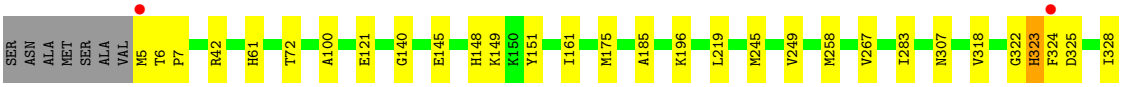


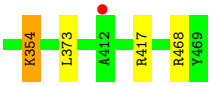


• Molecule 1: S-adenosyl-L-homocysteine hydrolase

Chain BBB:

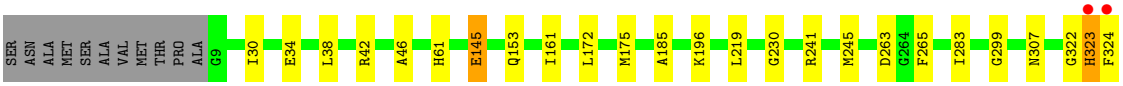


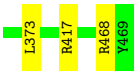




• Molecule 1: S-adenosyl-L-homocysteine hydrolase

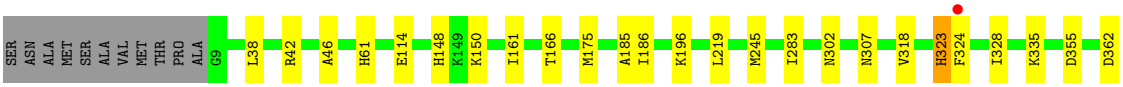
Chain CCC:

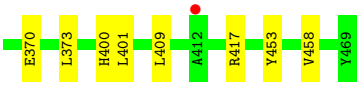




• Molecule 1: S-adenosyl-L-homocysteine hydrolase

Chain DDD:




E370
L373
H400
L401
L409
A412
R417
Y453
V458
Y469

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.50Å 133.62Å 100.86Å 90.00° 103.18° 90.00°	Depositor
Resolution (Å)	79.13 – 1.82 79.13 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.7 (79.13-1.82) 99.7 (79.13-1.82)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.160 , 0.194 0.169 , 0.201	Depositor DCC
R_{free} test set	1285 reflections (0.75%)	wwPDB-VP
Wilson B-factor (Å^2)	31.2	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	16154	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADN, PO4, PEG, NAD

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	AAA	0.83	4/3733 (0.1%)	0.74	0/5045
1	BBB	0.82	2/3701 (0.1%)	0.75	1/5003 (0.0%)
1	CCC	0.80	3/3742 (0.1%)	0.73	0/5054
1	DDD	0.79	3/3680 (0.1%)	0.72	0/4973
All	All	0.81	12/14856 (0.1%)	0.74	1/20075 (0.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	323	HIS	C-O	9.50	1.41	1.23
1	AAA	434	GLU	CD-OE2	9.19	1.35	1.25
1	AAA	156	GLU	CD-OE2	-6.72	1.18	1.25
1	AAA	370	GLU	CD-OE1	-6.55	1.18	1.25
1	CCC	323[A]	HIS	C-O	5.86	1.34	1.23
1	CCC	323[B]	HIS	C-O	5.86	1.34	1.23
1	CCC	34	GLU	CD-OE1	5.72	1.31	1.25
1	AAA	429	GLU	CD-OE1	5.57	1.31	1.25
1	BBB	324	PHE	C-O	5.55	1.33	1.23
1	DDD	150	LYS	CG-CD	-5.36	1.34	1.52
1	DDD	323	HIS	C-O	5.18	1.33	1.23
1	DDD	370	GLU	CD-OE1	-5.11	1.20	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	7	PRO	N-CA-CB	6.13	110.66	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	3659	0	3657	43	0
1	BBB	3626	0	3620	21	0
1	CCC	3656	0	3679	33	0
1	DDD	3605	0	3616	22	0
2	AAA	44	0	26	3	0
2	BBB	44	0	26	0	0
2	CCC	44	0	26	3	0
2	DDD	44	0	26	2	0
3	AAA	19	0	3	1	0
3	BBB	19	0	3	0	0
3	CCC	19	0	3	0	0
3	DDD	19	0	3	0	0
4	AAA	7	0	10	1	0
5	AAA	5	0	0	0	0
5	BBB	5	0	0	0	0
5	CCC	5	0	0	0	0
5	DDD	5	0	0	0	0
6	AAA	415	0	0	9	0
6	BBB	313	0	0	3	0
6	CCC	305	0	0	5	0
6	DDD	296	0	0	9	0
All	All	16154	0	14698	117	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 (117) 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:AAA:276[B]:ASN:OD1	6:AAA:601:HOH:O	1.64	1.14
1:AAA:324[A]:PHE:HB3	6:AAA:922:HOH:O	1.53	1.04
1:CCC:323[B]:HIS:CG	1:CCC:324[B]:PHE:H	1.78	1.01
1:CCC:323[B]:HIS:ND1	1:CCC:324[B]:PHE:HD2	1.63	0.95
1:DDD:114:GLU:HG3	6:DDD:798:HOH:O	1.67	0.94
1:CCC:323[B]:HIS:HD1	1:CCC:324[B]:PHE:HD2	0.96	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:323:HIS:HA	1:BBB:373:LEU:HD21	1.55	0.89
1:DDD:324:PHE:HB3	6:DDD:848:HOH:O	1.73	0.87
1:CCC:323[A]:HIS:HA	1:CCC:373:LEU:HD21	1.60	0.83
1:CCC:323[B]:HIS:CG	1:CCC:324[B]:PHE:N	2.46	0.83
1:CCC:323[B]:HIS:ND1	1:CCC:324[B]:PHE:CD2	2.43	0.81
1:AAA:323[B]:HIS:HA	1:AAA:373:LEU:HD21	1.67	0.77
1:AAA:459:GLU:OE1	4:AAA:503:PEG:H22	1.83	0.77
1:AAA:323[A]:HIS:ND1	1:AAA:324[A]:PHE:HD2	1.84	0.76
1:DDD:362:ASP:OD2	6:DDD:601:HOH:O	2.04	0.74
1:AAA:323[A]:HIS:HD1	1:AAA:324[A]:PHE:HD2	1.34	0.72
1:CCC:323[B]:HIS:HB3	2:CCC:501:NAD:O3D	1.92	0.70
1:CCC:322[A]:GLY:O	1:CCC:373:LEU:HD23	1.94	0.67
1:CCC:322[A]:GLY:O	1:CCC:373:LEU:CD2	2.42	0.67
1:AAA:323[A]:HIS:ND1	1:AAA:324[A]:PHE:CD2	2.61	0.66
1:AAA:322[A]:GLY:O	1:AAA:327:GLU:OE2	2.14	0.66
1:BBB:322:GLY:O	1:BBB:373:LEU:HD23	1.96	0.66
1:AAA:241[B]:ARG:HD2	6:AAA:875:HOH:O	1.96	0.66
1:BBB:354:LYS:HE3	6:BBB:706:HOH:O	1.95	0.65
1:CCC:153:GLN:HB2	6:CCC:792[A]:HOH:O	1.96	0.64
1:CCC:30:ILE:HG23	6:DDD:702:HOH:O	1.98	0.64
1:AAA:48:GLN:NE2	6:AAA:604:HOH:O	2.32	0.63
1:BBB:322:GLY:O	1:BBB:373:LEU:CD2	2.47	0.63
1:CCC:322[B]:GLY:O	1:CCC:323[B]:HIS:CD2	2.52	0.62
1:CCC:299:GLY:HA2	1:CCC:323[B]:HIS:CD2	2.36	0.61
1:CCC:323[B]:HIS:CD2	1:CCC:324[B]:PHE:H	2.17	0.60
1:CCC:241[B]:ARG:HD2	6:CCC:817:HOH:O	2.02	0.59
1:AAA:323[B]:HIS:CA	1:AAA:373:LEU:HD21	2.34	0.58
1:AAA:43[A]:ARG:NH2	6:AAA:606:HOH:O	2.35	0.57
1:CCC:241[B]:ARG:HD3	1:CCC:265:PHE:CE1	2.38	0.57
1:AAA:322[B]:GLY:O	1:AAA:373:LEU:CD2	2.53	0.56
1:DDD:373:LEU:HD13	6:DDD:607:HOH:O	2.04	0.56
1:DDD:409:LEU:HD21	1:DDD:417:ARG:NH2	2.20	0.56
1:AAA:323[A]:HIS:HB3	2:AAA:501:NAD:O3D	2.05	0.56
1:AAA:290:LYS:HD3	6:CCC:851:HOH:O	2.06	0.56
1:DDD:324:PHE:CB	6:DDD:848:HOH:O	2.42	0.55
1:BBB:196:LYS:HE3	1:CCC:468:ARG:HB2	1.89	0.55
1:AAA:321[B]:ILE:O	1:AAA:322[B]:GLY:O	2.26	0.54
1:AAA:241[B]:ARG:NH1	1:AAA:263:ASP:O	2.34	0.54
1:AAA:148:HIS:CD2	1:AAA:175:MET:HE1	2.43	0.54
1:AAA:322[B]:GLY:O	2:AAA:501:NAD:H2N	2.08	0.53
1:AAA:323[A]:HIS:HE1	1:DDD:453:TYR:OH	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:323:HIS:CD2	1:DDD:324:PHE:CG	2.96	0.53
1:BBB:161:ILE:O	1:BBB:185:ALA:HA	2.09	0.53
1:BBB:283:ILE:HG13	1:BBB:307:ASN:HB3	1.92	0.52
1:AAA:323[A]:HIS:HD2	1:AAA:327:GLU:OE2	1.94	0.51
1:CCC:161:ILE:O	1:CCC:185:ALA:HA	2.11	0.51
1:CCC:283:ILE:HG13	1:CCC:307:ASN:HB3	1.92	0.51
1:DDD:161:ILE:O	1:DDD:185:ALA:HA	2.09	0.51
1:CCC:241[B]:ARG:NH1	1:CCC:263:ASP:O	2.40	0.50
1:CCC:322[B]:GLY:O	1:CCC:323[B]:HIS:HD2	1.93	0.50
1:DDD:400:HIS:HB2	6:DDD:841:HOH:O	2.12	0.50
1:CCC:323[B]:HIS:HB3	2:CCC:501:NAD:HO3N	1.78	0.49
1:BBB:219:LEU:O	1:BBB:245:MET:HG2	2.12	0.49
1:AAA:161:ILE:O	1:AAA:185:ALA:HA	2.13	0.48
1:CCC:323[B]:HIS:CE1	1:CCC:324[B]:PHE:HB2	2.47	0.48
1:AAA:322[B]:GLY:O	1:AAA:373:LEU:HD22	2.12	0.48
1:CCC:219:LEU:O	1:CCC:245:MET:HG2	2.14	0.48
1:AAA:468:ARG:HB2	1:DDD:196[B]:LYS:HE3	1.96	0.48
1:DDD:148:HIS:CD2	1:DDD:175:MET:HE2	2.49	0.47
1:DDD:219:LEU:O	1:DDD:245:MET:HG2	2.14	0.47
1:AAA:323[B]:HIS:HD2	1:AAA:324[B]:PHE:CZ	2.33	0.47
1:AAA:241[B]:ARG:HD3	1:AAA:265:PHE:CE1	2.50	0.47
1:CCC:417:ARG:NH1	6:CCC:611:HOH:O	2.47	0.47
1:BBB:5:MET:CB	6:BBB:728:HOH:O	2.63	0.47
1:AAA:323[A]:HIS:CE1	1:AAA:324[A]:PHE:HD2	2.33	0.46
1:DDD:283:ILE:HG13	1:DDD:307:ASN:HB3	1.96	0.46
1:BBB:258[A]:MET:C	1:BBB:258[A]:MET:SD	2.94	0.46
1:AAA:219:LEU:O	1:AAA:245:MET:HG2	2.15	0.46
1:BBB:42:ARG:HG3	1:BBB:72:THR:HG23	1.99	0.45
1:AAA:323[A]:HIS:H	1:AAA:373:LEU:HD21	1.82	0.44
1:BBB:148:HIS:CD2	1:BBB:175:MET:HE1	2.52	0.44
1:DDD:323:HIS:HB3	2:DDD:501:NAD:O3D	2.18	0.44
1:DDD:458:VAL:HG11	6:DDD:626:HOH:O	2.18	0.44
1:BBB:323:HIS:CA	1:BBB:373:LEU:HD21	2.39	0.43
1:AAA:149:LYS:NZ	6:AAA:625:HOH:O	2.51	0.43
1:AAA:283:ILE:HG13	1:AAA:307:ASN:HB3	2.00	0.43
1:AAA:114:GLU:HG2	6:AAA:1004:HOH:O	2.18	0.43
1:BBB:318:VAL:HG12	1:BBB:328:ILE:HD13	2.01	0.43
1:AAA:145:GLU:OE2	1:AAA:149:LYS:HE2	2.19	0.42
1:AAA:314:LYS:NZ	6:AAA:626:HOH:O	2.52	0.42
1:BBB:145:GLU:OE2	1:BBB:149:LYS:HE2	2.19	0.42
1:BBB:325:ASP:C	6:BBB:610:HOH:O	2.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:38:LEU:HD12	1:CCC:38:LEU:HA	1.94	0.42
1:DDD:335:LYS:HD3	6:DDD:845:HOH:O	2.18	0.42
1:AAA:429:GLU:OE1	1:AAA:461:PRO:HA	2.20	0.42
1:DDD:318:VAL:HG12	1:DDD:328:ILE:HD13	2.02	0.42
1:DDD:42:ARG:O	1:DDD:46:ALA:HB2	2.19	0.42
1:AAA:299:GLY:HA2	1:AAA:323[A]:HIS:CD2	2.55	0.41
1:BBB:468:ARG:HB2	1:CCC:196[B]:LYS:HE3	2.02	0.41
1:CCC:42:ARG:O	1:CCC:46:ALA:HB2	2.20	0.41
1:CCC:172:LEU:HD23	1:CCC:175:MET:CE	2.50	0.41
1:CCC:323[A]:HIS:CA	1:CCC:373:LEU:HD21	2.38	0.41
1:DDD:38:LEU:HD12	1:DDD:38:LEU:HA	1.93	0.41
1:AAA:323[B]:HIS:ND1	3:AAA:502[B]:ADN:O5'	2.52	0.41
1:CCC:145:GLU:HG3	6:CCC:853:HOH:O	2.20	0.41
1:CCC:323[B]:HIS:CE1	1:CCC:324[B]:PHE:HD2	2.32	0.41
1:AAA:170:HIS:HE1	6:AAA:890:HOH:O	2.01	0.41
1:AAA:114:GLU:H	1:AAA:114:GLU:CD	2.22	0.41
1:BBB:5:MET:HA	1:BBB:100:ALA:HA	2.02	0.41
1:AAA:148:HIS:CD2	1:AAA:175:MET:CE	3.03	0.41
1:BBB:249:VAL:O	1:BBB:267:VAL:HA	2.21	0.41
1:AAA:151:TYR:N	1:AAA:152:PRO:CD	2.84	0.41
1:DDD:323:HIS:CD2	1:DDD:324:PHE:CD2	3.08	0.41
1:AAA:148:HIS:CG	1:AAA:175:MET:HE3	2.55	0.41
1:DDD:186:ILE:HG12	1:DDD:401:LEU:HD11	2.03	0.41
1:CCC:230:GLY:HA3	2:CCC:501:NAD:O5B	2.21	0.40
1:BBB:140:GLY:HA3	1:BBB:323:HIS:NE2	2.36	0.40
1:BBB:121[A]:GLU:OE1	1:BBB:151:TYR:OH	2.28	0.40
1:AAA:42:ARG:O	1:AAA:46:ALA:HB2	2.21	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	AAA	473/472 (100%)	460 (97%)	9 (2%)	4 (1%)	19 7
1	BBB	471/472 (100%)	460 (98%)	9 (2%)	2 (0%)	34 21
1	CCC	474/472 (100%)	460 (97%)	13 (3%)	1 (0%)	47 33
1	DDD	467/472 (99%)	453 (97%)	12 (3%)	2 (0%)	34 21
All	All	1885/1888 (100%)	1833 (97%)	43 (2%)	9 (0%)	34 15

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	322[A]	GLY
1	AAA	322[B]	GLY
1	DDD	355	ASP
1	AAA	355	ASP
1	AAA	61	HIS
1	BBB	6	THR
1	BBB	61	HIS
1	CCC	61	HIS
1	DDD	61	HIS

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	AAA	390/385 (101%)	388 (100%)	2 (0%)	88 87
1	BBB	385/385 (100%)	383 (100%)	2 (0%)	88 87
1	CCC	391/385 (102%)	390 (100%)	1 (0%)	92 91
1	DDD	385/385 (100%)	382 (99%)	3 (1%)	81 77
All	All	1551/1540 (101%)	1543 (100%)	8 (0%)	91 87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	323[A]	HIS
1	AAA	323[B]	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BBB	354	LYS
1	BBB	417	ARG
1	CCC	145	GLU
1	DDD	166[A]	THR
1	DDD	166[B]	THR
1	DDD	302	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PO4	CCC	503	-	4,4,4	0.80	0	6,6,6	0.44	0
4	PEG	AAA	503	-	6,6,6	0.34	0	5,5,5	0.24	0
5	PO4	BBB	503	-	4,4,4	1.05	0	6,6,6	0.54	0
5	PO4	AAA	504	-	4,4,4	0.70	0	6,6,6	0.42	0
5	PO4	DDD	503	-	4,4,4	0.34	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAD	CCC	501	-	42,48,48	0.81	1 (2%)	50,73,73	0.92	2 (4%)
2	NAD	AAA	501	-	42,48,48	1.07	1 (2%)	50,73,73	0.93	3 (6%)
2	NAD	DDD	501	-	42,48,48	0.84	2 (4%)	50,73,73	0.92	2 (4%)
2	NAD	BBB	501	-	42,48,48	1.20	3 (7%)	50,73,73	0.91	3 (6%)

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	PEG	AAA	503	-	-	1/4/4/4	-
2	NAD	CCC	501	-	-	5/26/62/62	0/5/5/5
2	NAD	AAA	501	-	-	5/26/62/62	0/5/5/5
2	NAD	DDD	501	-	-	5/26/62/62	0/5/5/5
2	NAD	BBB	501	-	-	5/26/62/62	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	501	NAD	C2N-N1N	5.94	1.42	1.35
2	AAA	501	NAD	C2N-N1N	5.21	1.41	1.35
2	CCC	501	NAD	C2N-N1N	3.29	1.39	1.35
2	DDD	501	NAD	C2N-N1N	2.85	1.38	1.35
2	BBB	501	NAD	C8A-N7A	-2.40	1.30	1.34
2	BBB	501	NAD	O4D-C1D	2.04	1.43	1.41
2	DDD	501	NAD	C8A-N7A	-2.03	1.31	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	DDD	501	NAD	C6N-N1N-C2N	-2.95	119.29	121.97
2	AAA	501	NAD	C6N-N1N-C2N	-2.92	119.31	121.97
2	BBB	501	NAD	C6N-N1N-C2N	-2.77	119.45	121.97
2	CCC	501	NAD	C5A-C6A-N6A	2.68	124.42	120.35
2	CCC	501	NAD	PN-O3-PA	-2.65	123.74	132.83
2	BBB	501	NAD	O4D-C1D-C2D	-2.34	103.50	106.93
2	AAA	501	NAD	O4D-C1D-C2D	-2.27	103.61	106.93
2	DDD	501	NAD	C5A-C6A-N6A	2.27	123.80	120.35
2	BBB	501	NAD	C5A-C6A-N6A	2.13	123.58	120.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AAA	501	NAD	O4B-C1B-C2B	-2.12	103.83	106.93

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	501	NAD	O4D-C1D-N1N-C2N
2	AAA	501	NAD	O4D-C1D-N1N-C6N
2	AAA	501	NAD	C2D-C1D-N1N-C2N
2	AAA	501	NAD	C2D-C1D-N1N-C6N
2	BBB	501	NAD	O4D-C1D-N1N-C2N
2	BBB	501	NAD	O4D-C1D-N1N-C6N
2	BBB	501	NAD	C2D-C1D-N1N-C2N
2	BBB	501	NAD	C2D-C1D-N1N-C6N
2	CCC	501	NAD	O4D-C1D-N1N-C2N
2	CCC	501	NAD	O4D-C1D-N1N-C6N
2	CCC	501	NAD	C2D-C1D-N1N-C2N
2	CCC	501	NAD	C2D-C1D-N1N-C6N
2	DDD	501	NAD	O4D-C1D-N1N-C2N
2	DDD	501	NAD	O4D-C1D-N1N-C6N
2	DDD	501	NAD	C2D-C1D-N1N-C2N
2	DDD	501	NAD	C2D-C1D-N1N-C6N
4	AAA	503	PEG	C1-C2-O2-C3
2	AAA	501	NAD	O4B-C4B-C5B-O5B
2	BBB	501	NAD	O4B-C4B-C5B-O5B
2	CCC	501	NAD	O4B-C4B-C5B-O5B
2	DDD	501	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

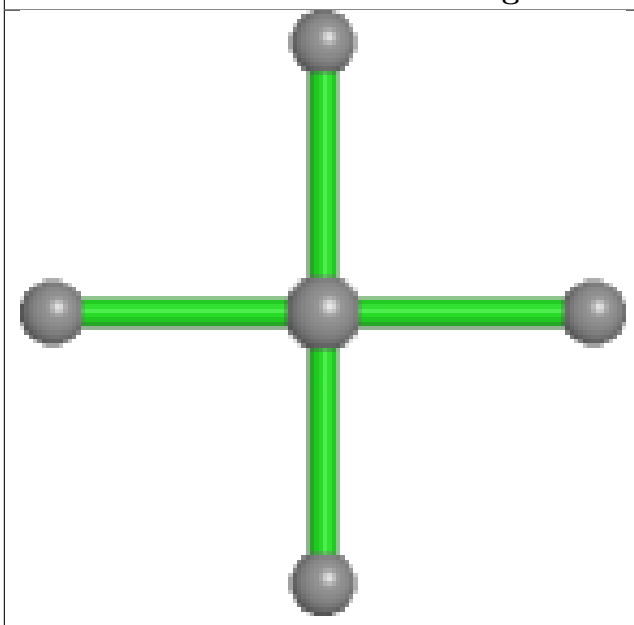
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	503	PEG	1	0
2	CCC	501	NAD	3	0
2	AAA	501	NAD	3	0
2	DDD	501	NAD	2	0

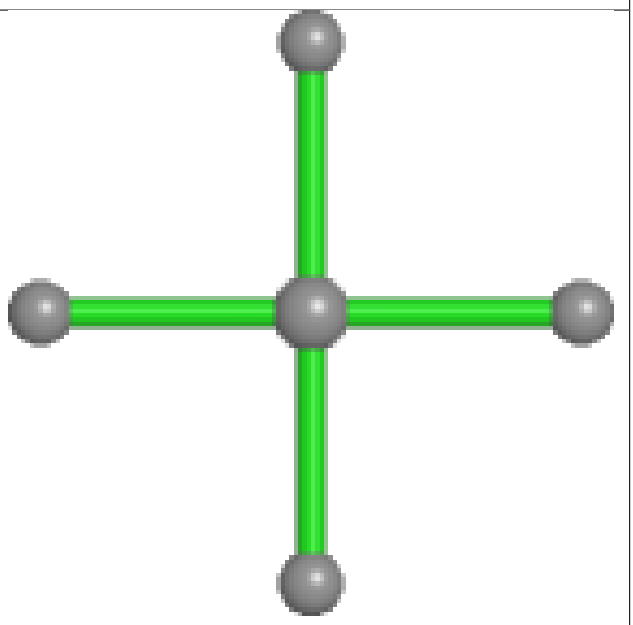
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

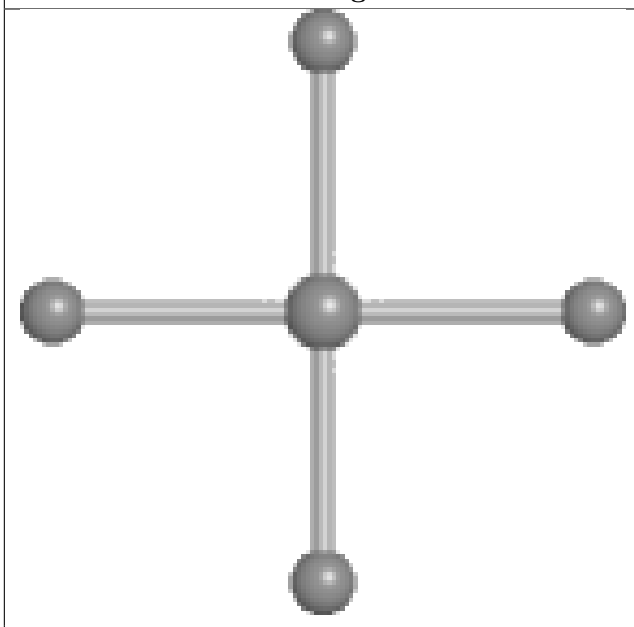
Ligand PO4 CCC 503



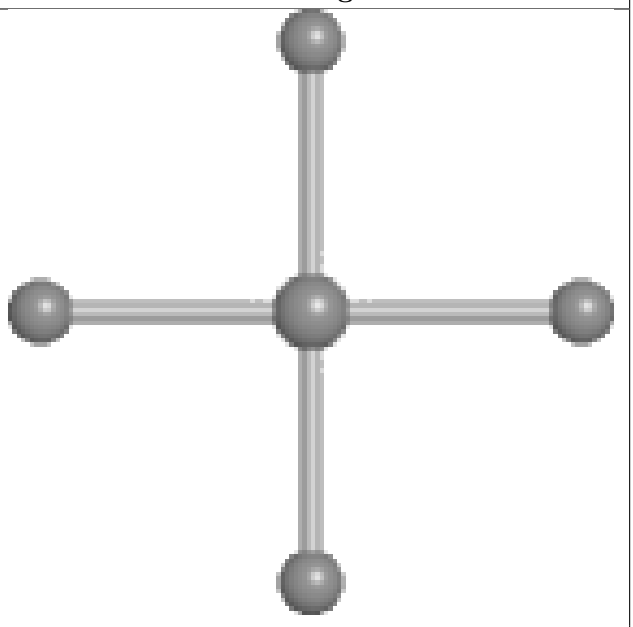
Bond lengths



Bond angles

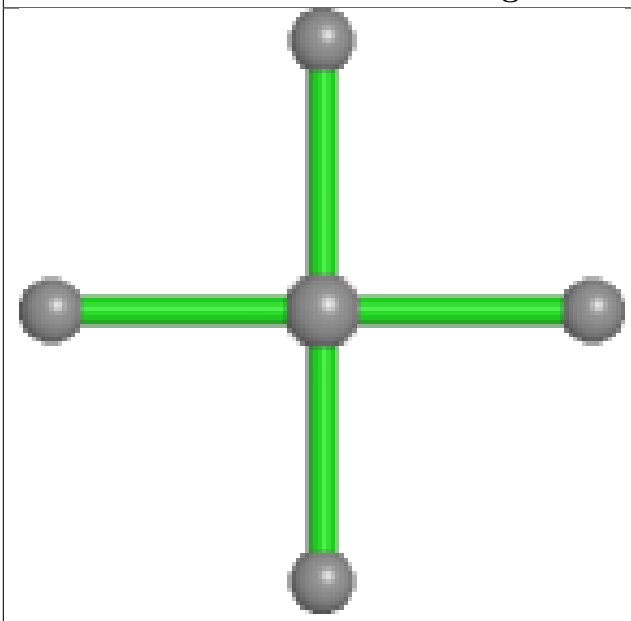


Torsions

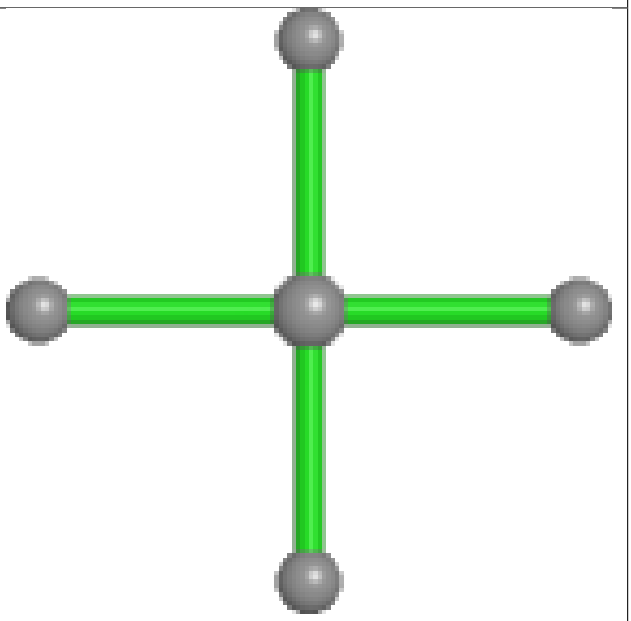


Rings

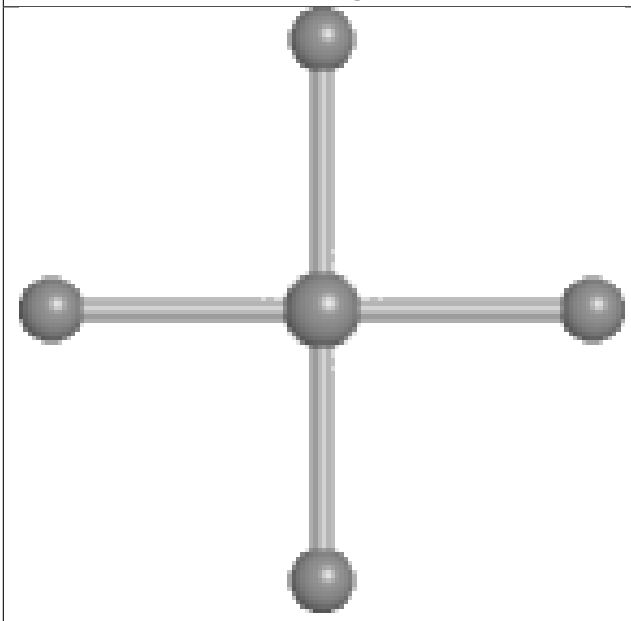
Ligand PO4 BBB 503



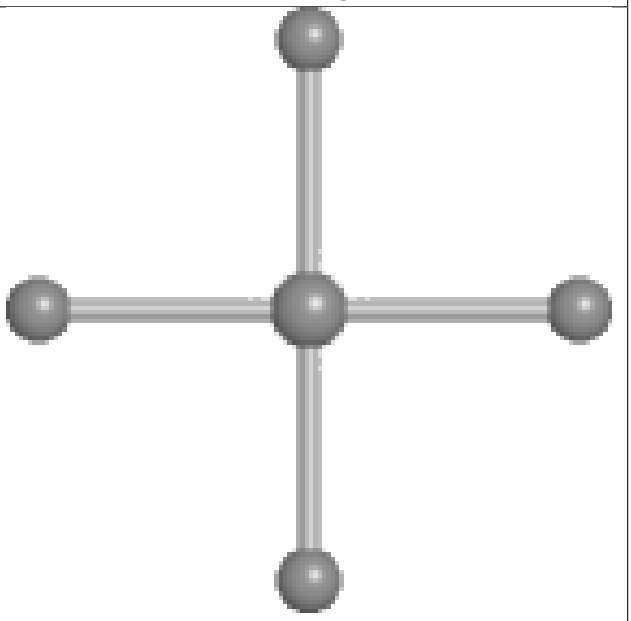
Bond lengths



Bond angles

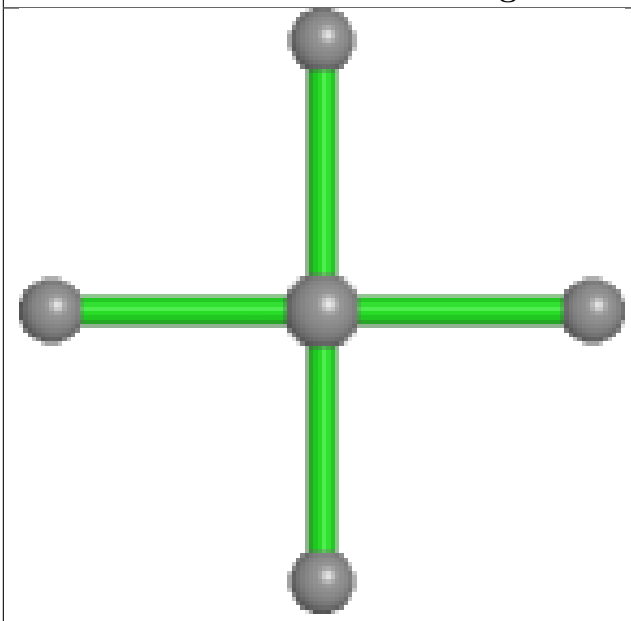


Torsions

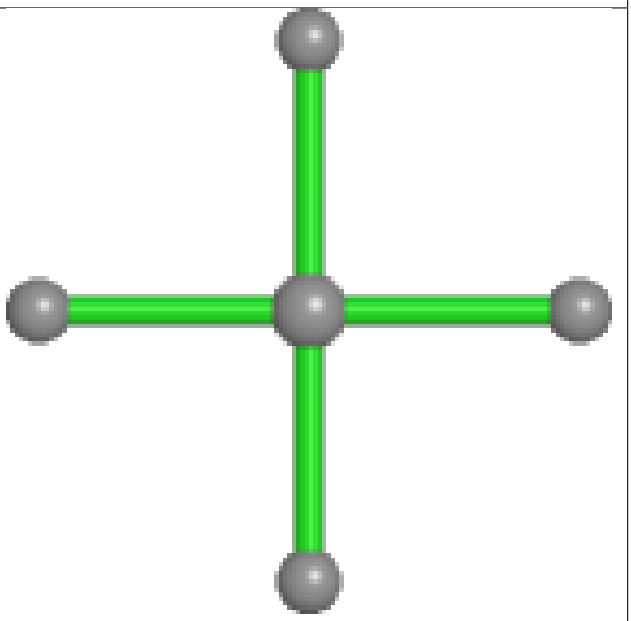


Rings

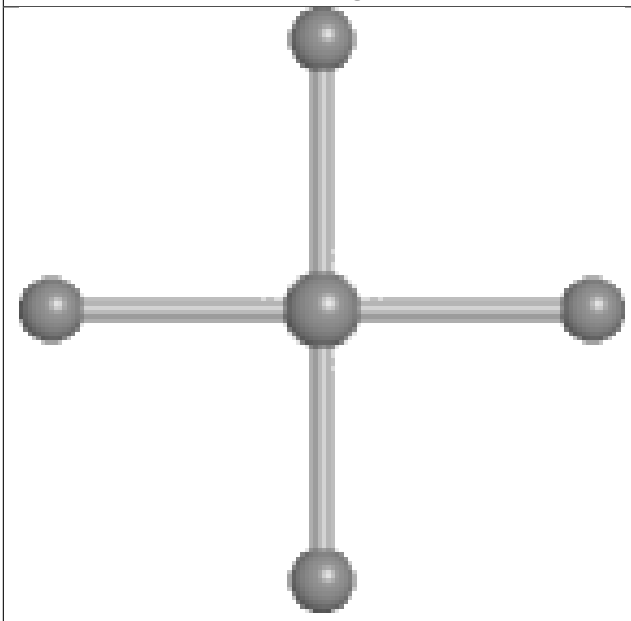
Ligand PO4 AAA 504



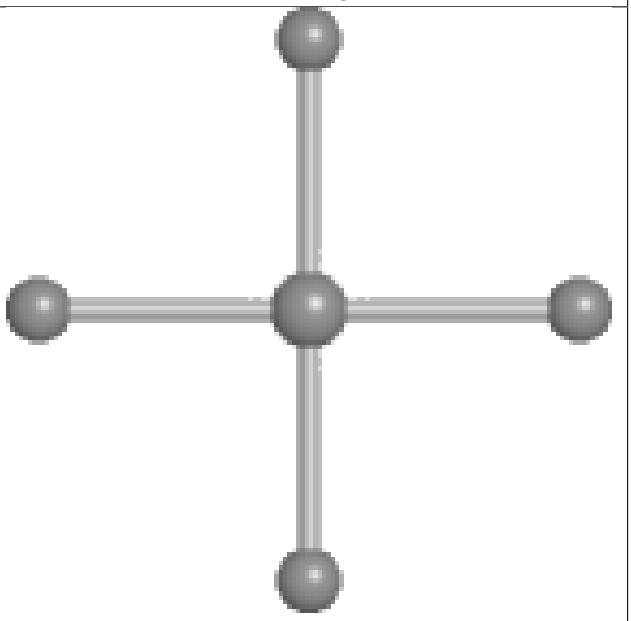
Bond lengths



Bond angles

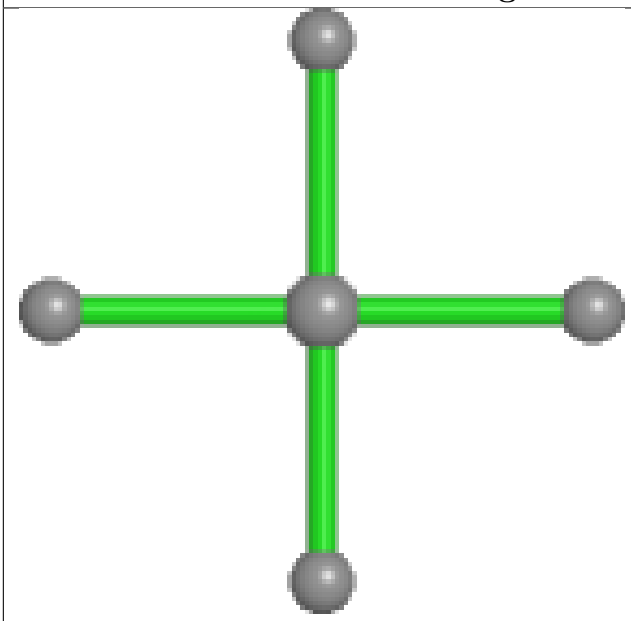


Torsions

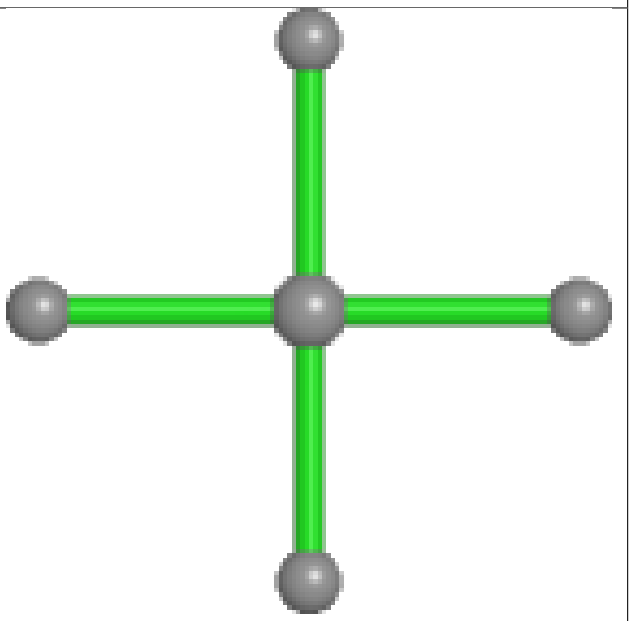


Rings

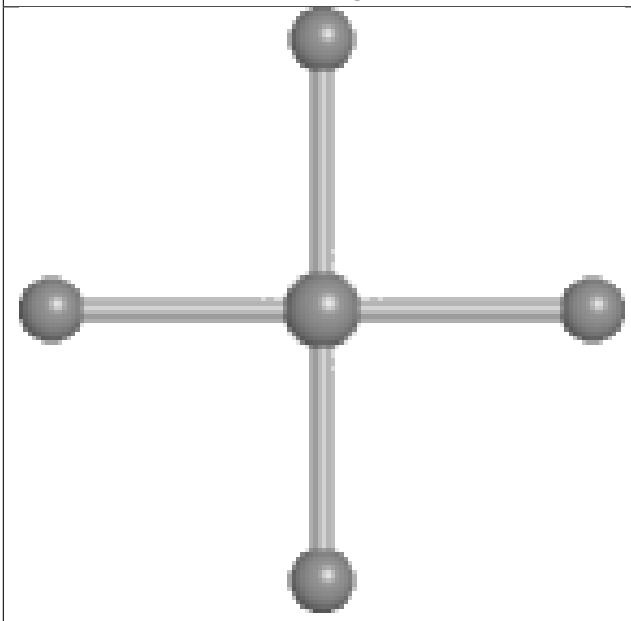
Ligand PO4 DDD 503



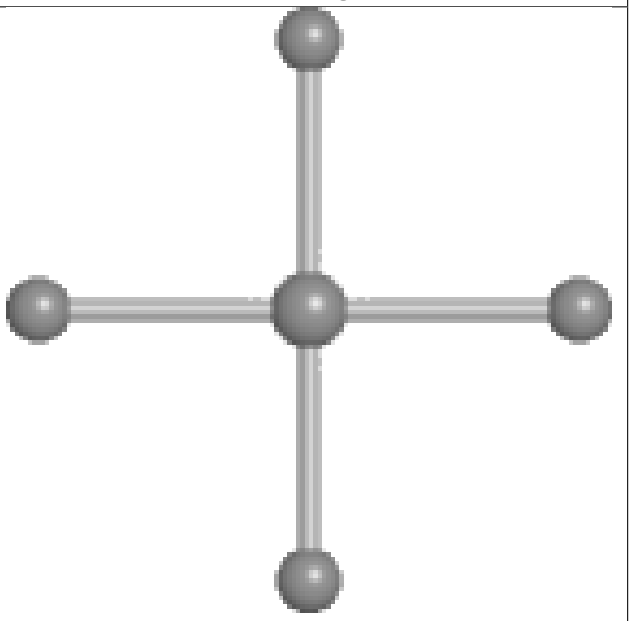
Bond lengths



Bond angles

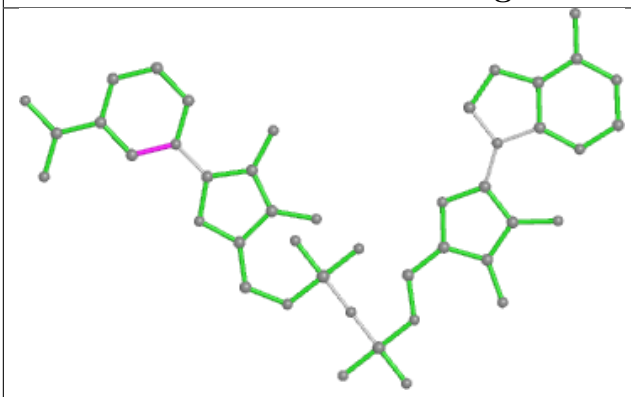


Torsions

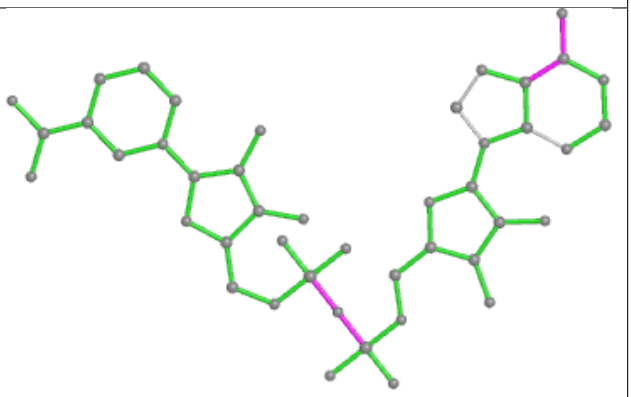


Rings

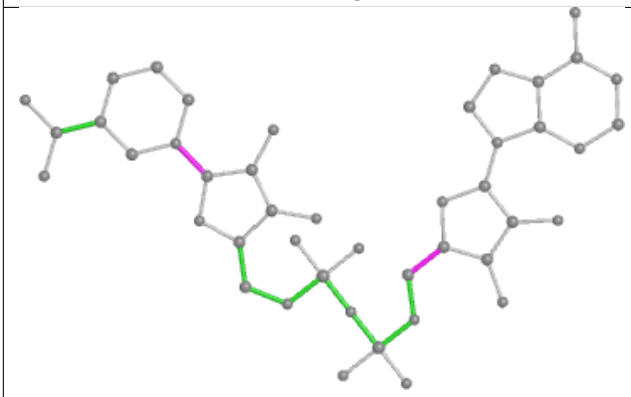
Ligand NAD CCC 501



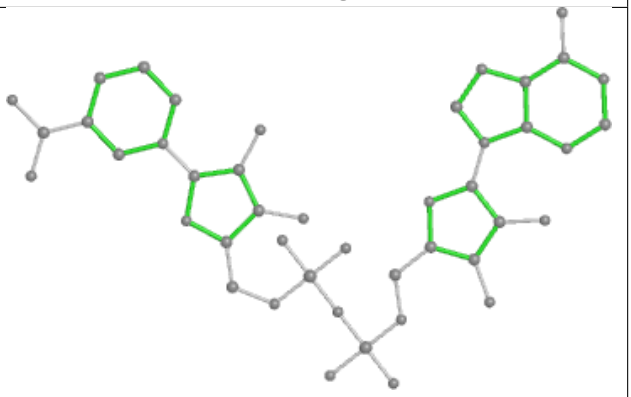
Bond lengths



Bond angles

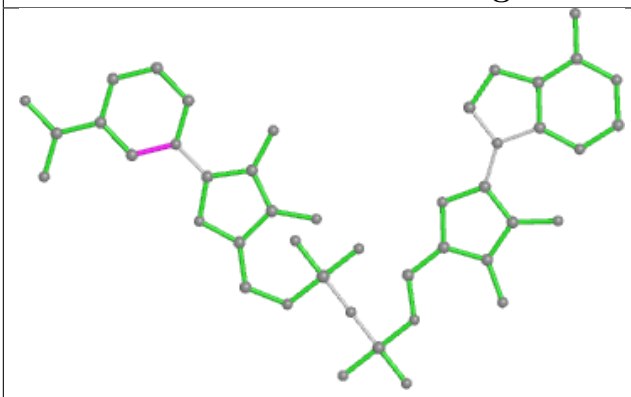


Torsions

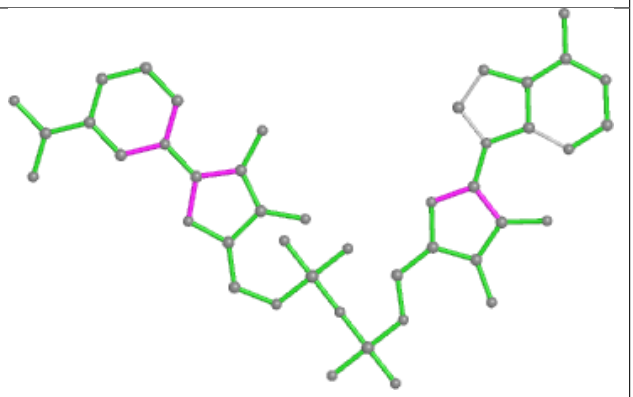


Rings

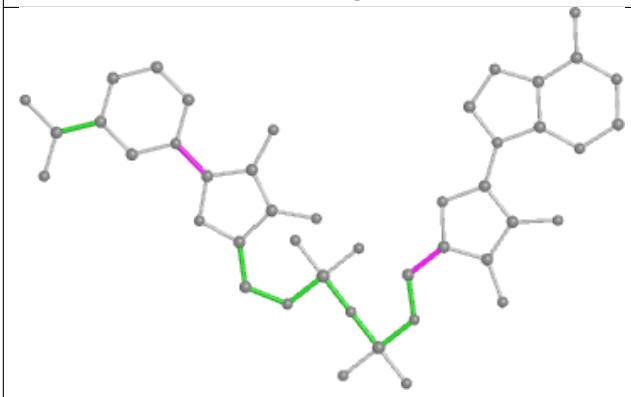
Ligand NAD AAA 501



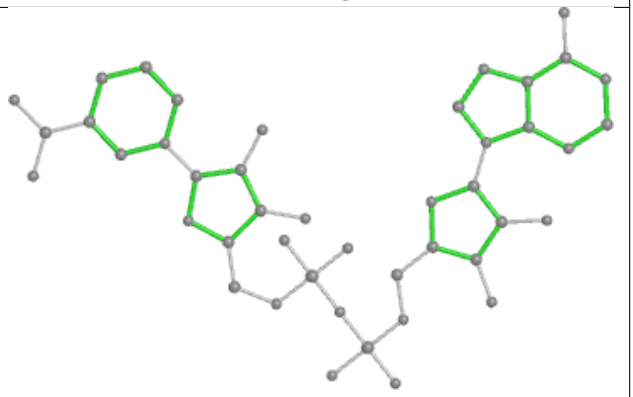
Bond lengths



Bond angles

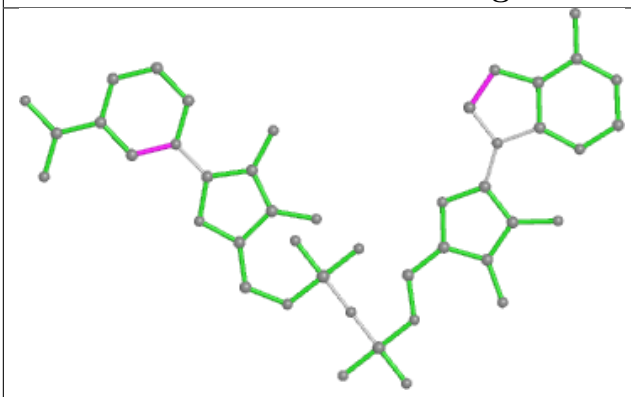


Torsions

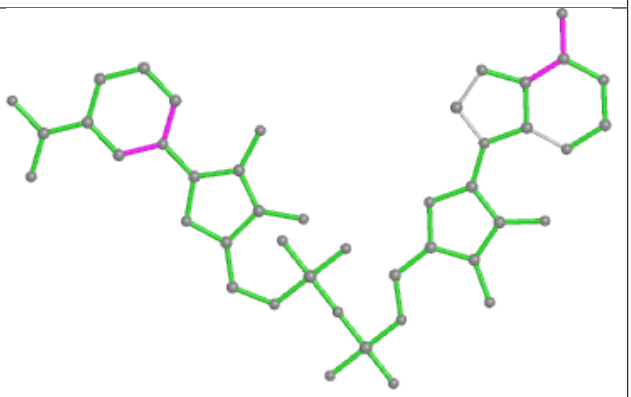


Rings

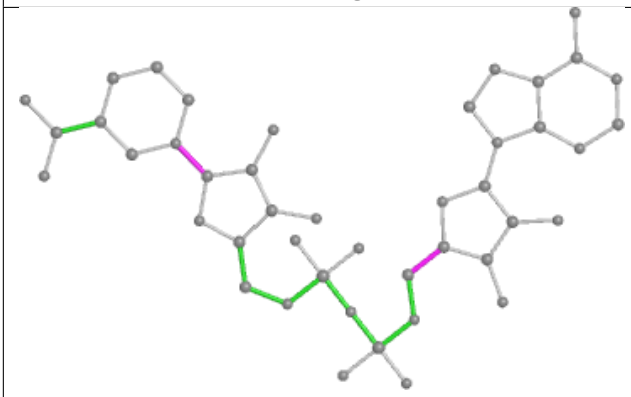
Ligand NAD DDD 501



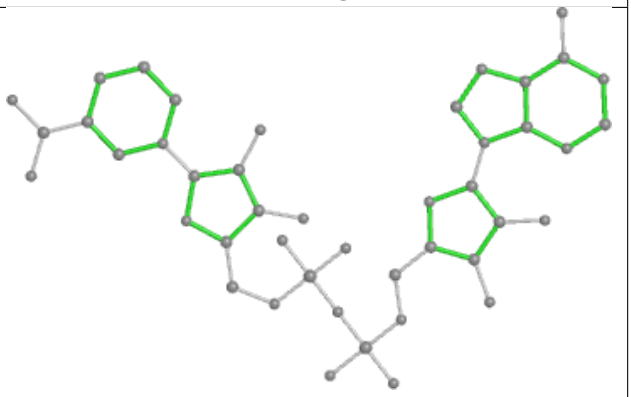
Bond lengths



Bond angles

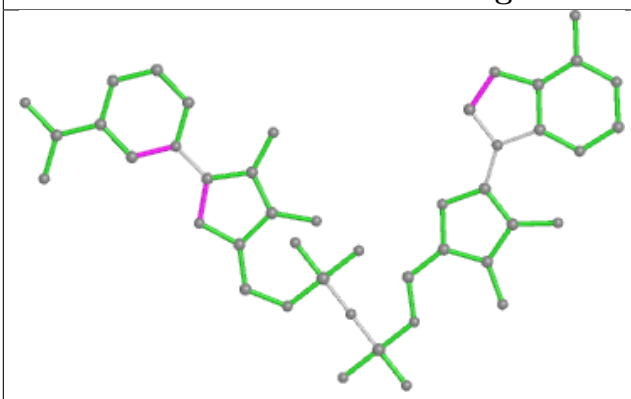


Torsions

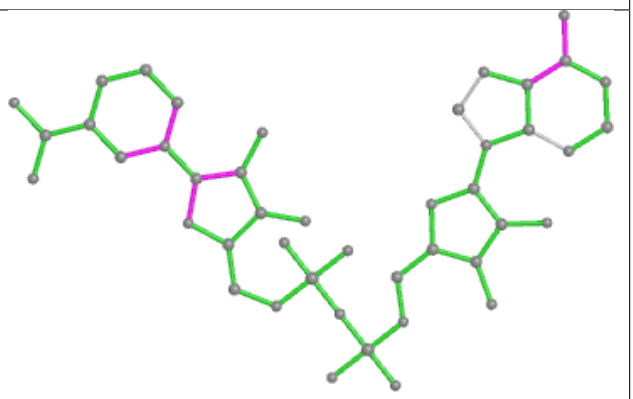


Rings

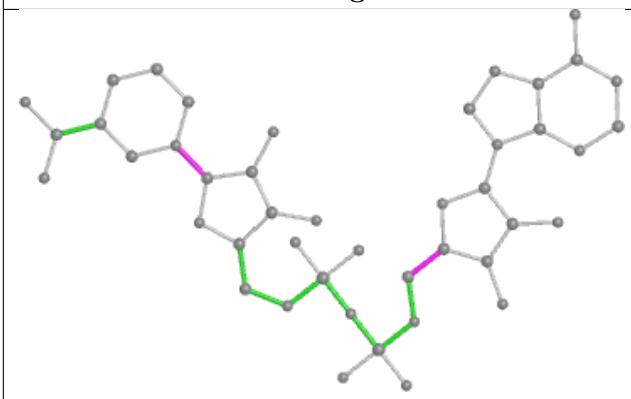
Ligand NAD BBB 501



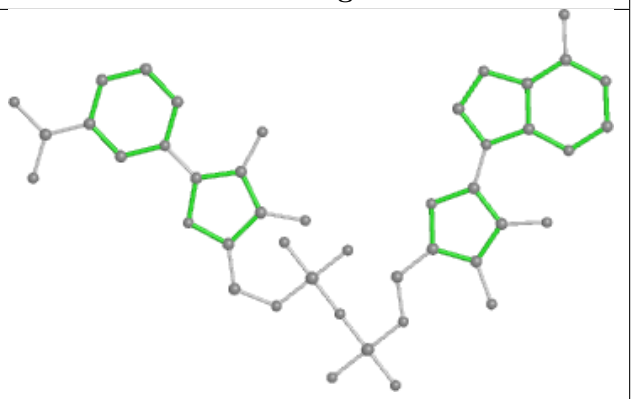
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	AAA	461/472 (97%)	-0.63	1 (0%)	95	93	23, 32, 50, 74	10 (2%)
1	BBB	465/472 (98%)	-0.58	3 (0%)	89	88	23, 35, 59, 97	14 (3%)
1	CCC	461/472 (97%)	-0.59	2 (0%)	92	91	26, 38, 57, 79	10 (2%)
1	DDD	461/472 (97%)	-0.48	2 (0%)	92	91	24, 39, 65, 104	17 (3%)
All	All	1848/1888 (97%)	-0.57	8 (0%)	92	91	23, 36, 59, 104	51 (2%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	324	PHE	4.6
1	BBB	5	MET	3.8
1	CCC	324[A]	PHE	2.9
1	DDD	412	ALA	2.7
1	AAA	322[A]	GLY	2.7
1	BBB	412	ALA	2.5
1	CCC	323[A]	HIS	2.1
1	DDD	324	PHE	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 monosaccharides in this entry.

6.4 Ligands (i)

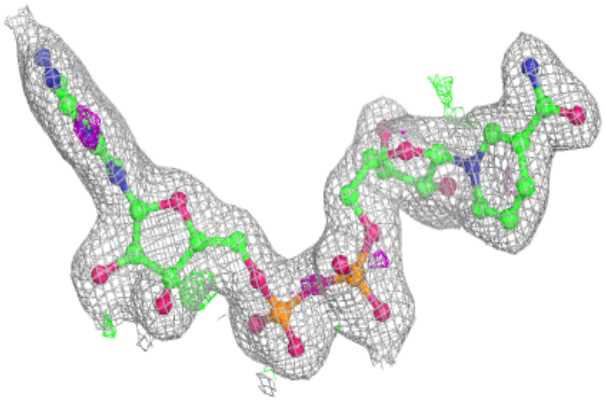
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

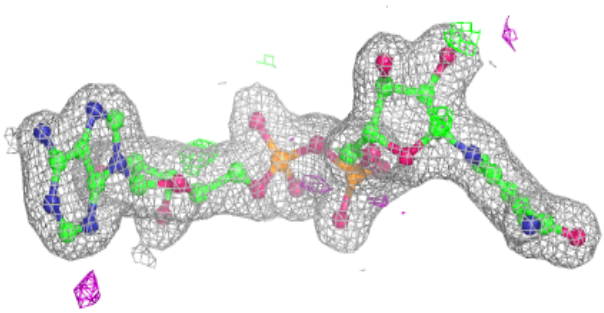
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADN	BBB	502[B]	19/19	0.91	0.11	30,36,41,42	1
3	ADN	CCC	502[B]	19/19	0.92	0.09	30,34,42,45	1
3	ADN	DDD	502[B]	19/19	0.92	0.10	28,33,39,44	1
4	PEG	AAA	503	7/7	0.92	0.12	35,42,51,53	0
3	ADN	AAA	502[B]	19/19	0.95	0.09	23,29,37,38	1
2	NAD	CCC	501	44/44	0.97	0.07	29,33,37,41	0
2	NAD	DDD	501	44/44	0.98	0.07	22,28,32,33	0
2	NAD	BBB	501	44/44	0.98	0.07	23,27,31,32	0
2	NAD	AAA	501	44/44	0.98	0.07	23,27,30,35	0
5	PO4	BBB	503	5/5	0.98	0.11	35,37,47,53	0
5	PO4	CCC	503	5/5	0.98	0.07	37,39,45,50	0
5	PO4	DDD	503	5/5	0.98	0.12	49,50,56,58	0
5	PO4	AAA	504	5/5	0.99	0.09	37,38,42,52	0

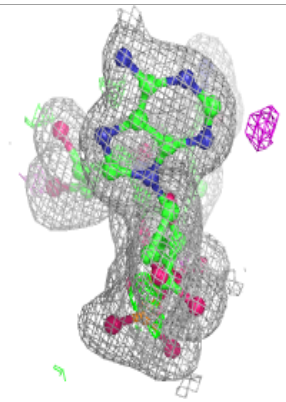
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD CCC 501:

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

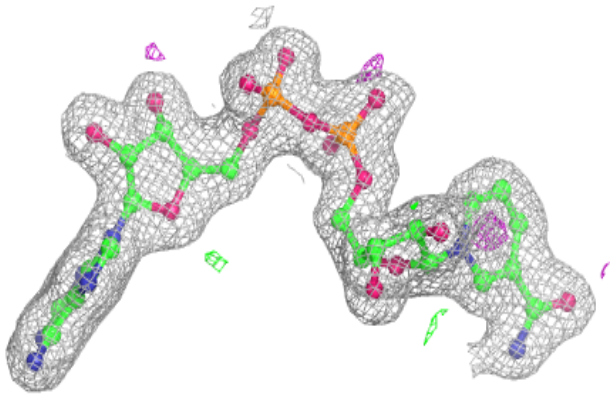


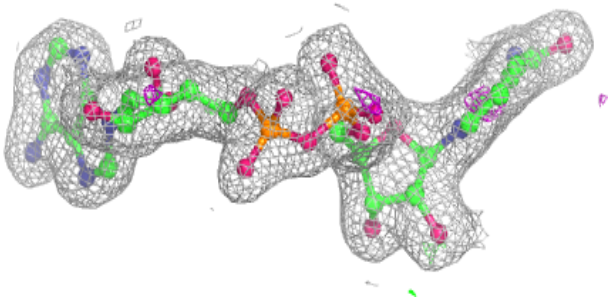


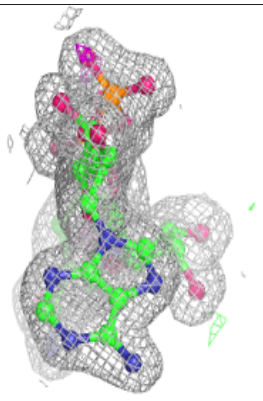


Electron density around NAD DDD 501:

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

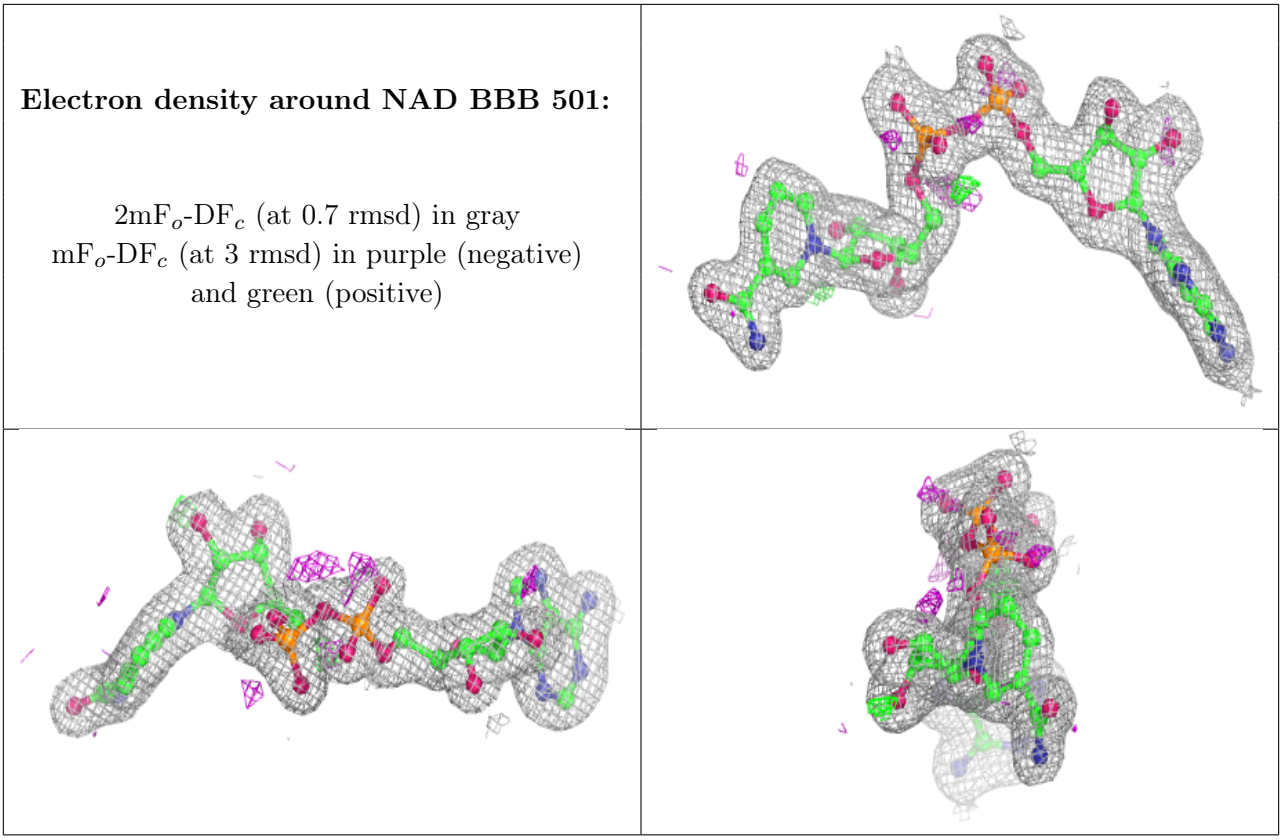






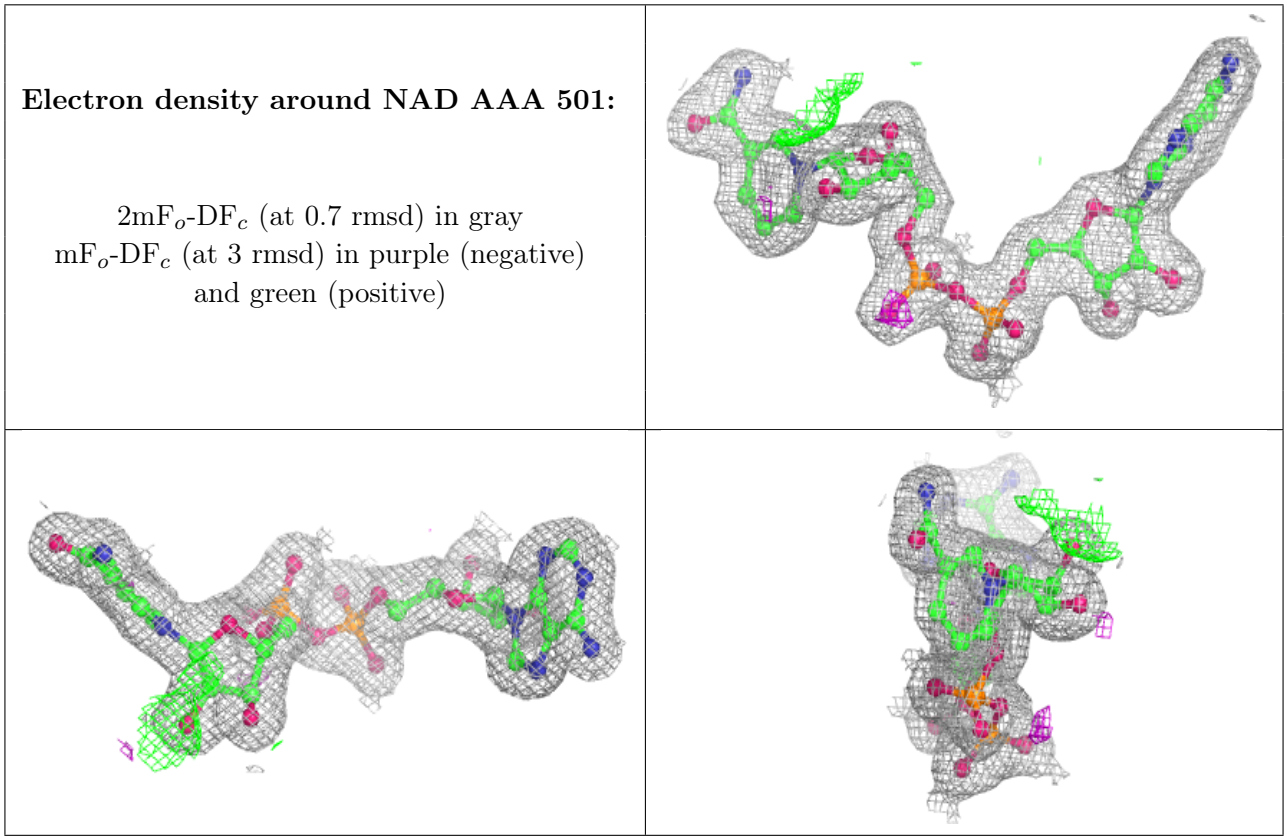
Electron density around NAD BBB 501:

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



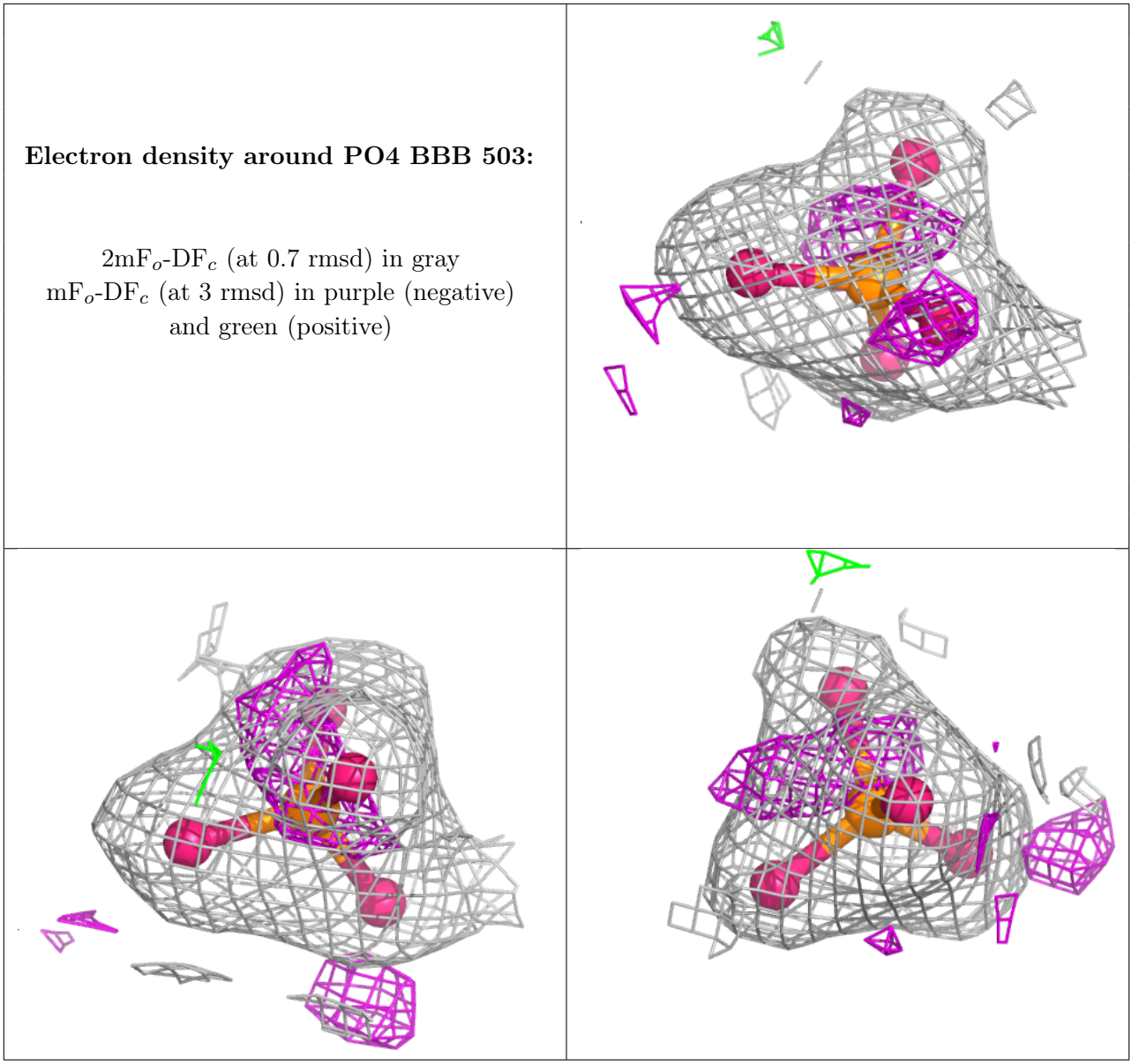
Electron density around NAD AAA 501:

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



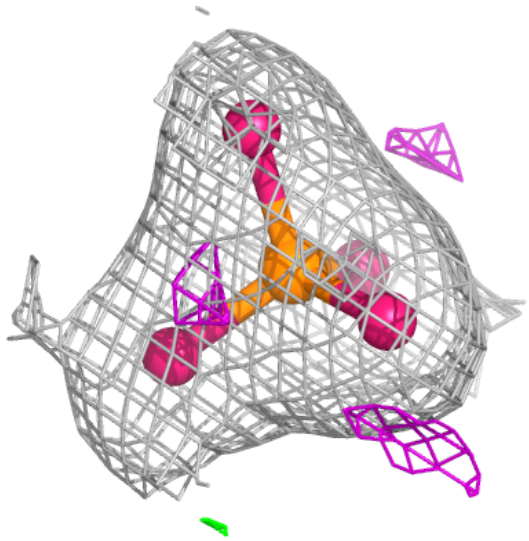
Electron density around PO4 BBB 503:

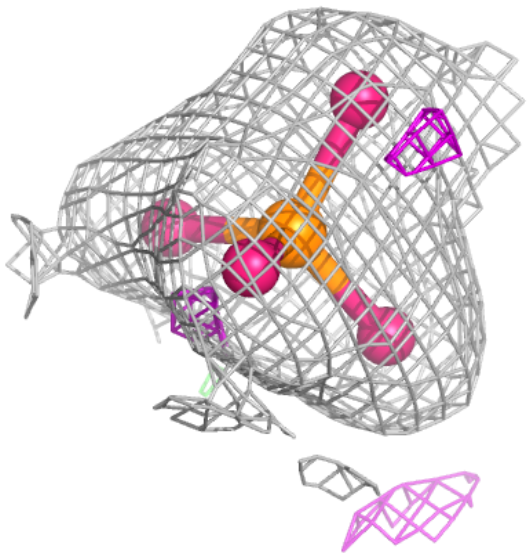
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

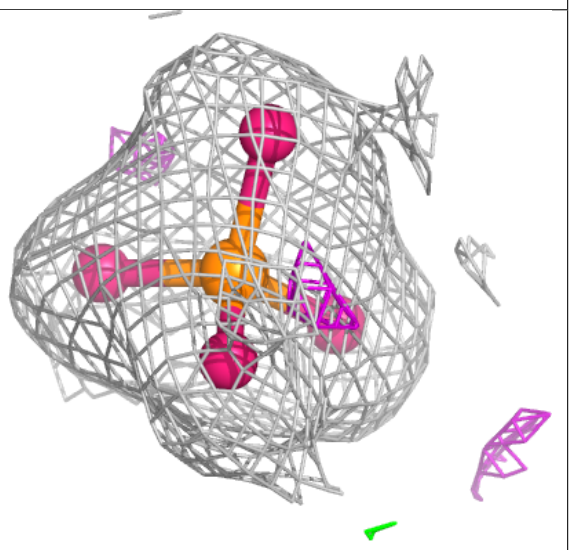


Electron density around PO4 CCC 503:

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

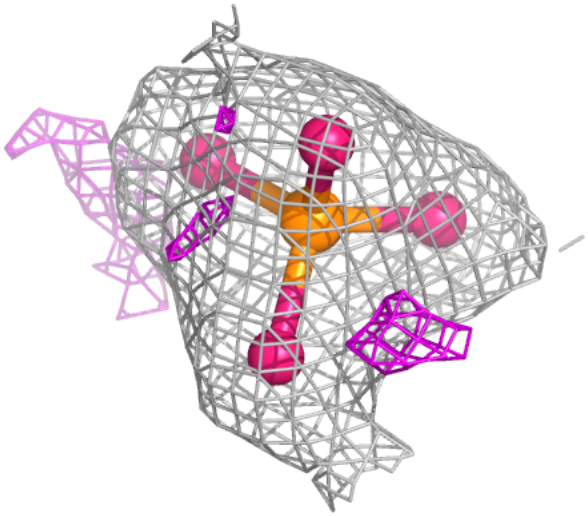


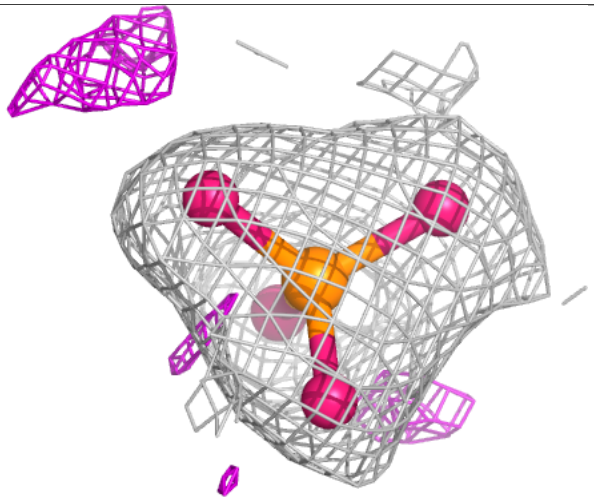


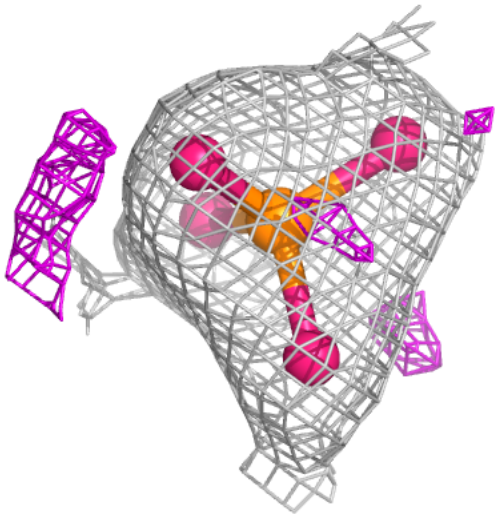


Electron density around PO4 DDD 503:

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

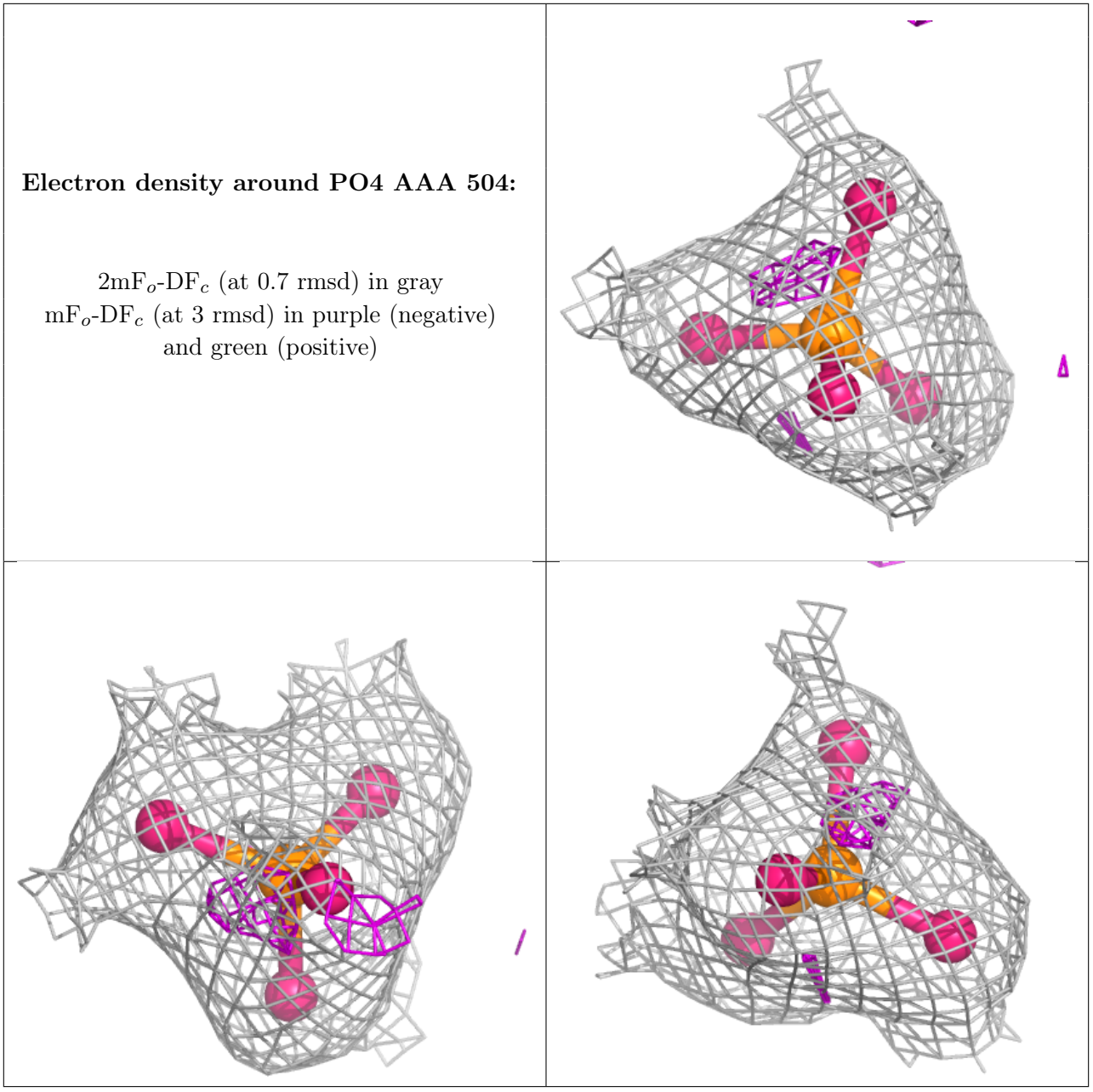






Electron density around PO4 AAA 504:

$2mF_o$-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.