Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2024 – 12:42 pm GMT

PDB ID	:	8CFB
Title	:	Crystal structure of S-adenosyl-L-homocysteine hydrolase from P. aeruginosa in complex with F2X-Entry library fragment D02
Authors	:	Malecki, P.H.; Gawel, M.; Stepniewska, M.; Brzezinski, K.
Deposited on	:	2023-02-03
Resolution	:	2.07 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:

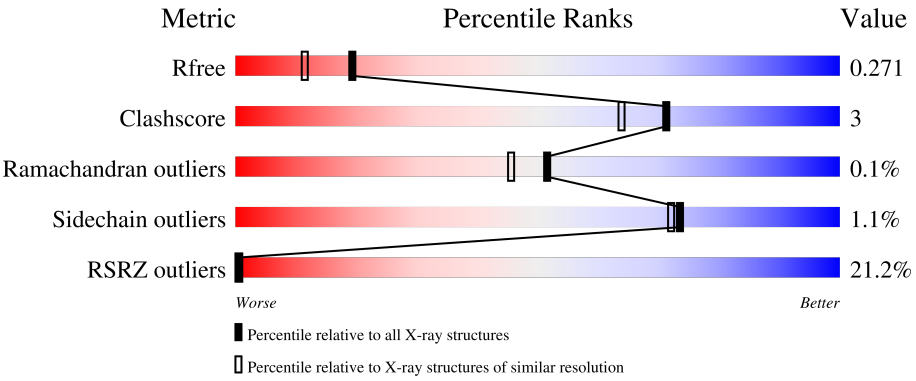
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	A	472	10% 91% 7% ·
1	B	472	20% 87% 10% ·
1	C	472	31% 85% 12% ··
1	D	472	22% 89% 9% ·

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 15122 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.

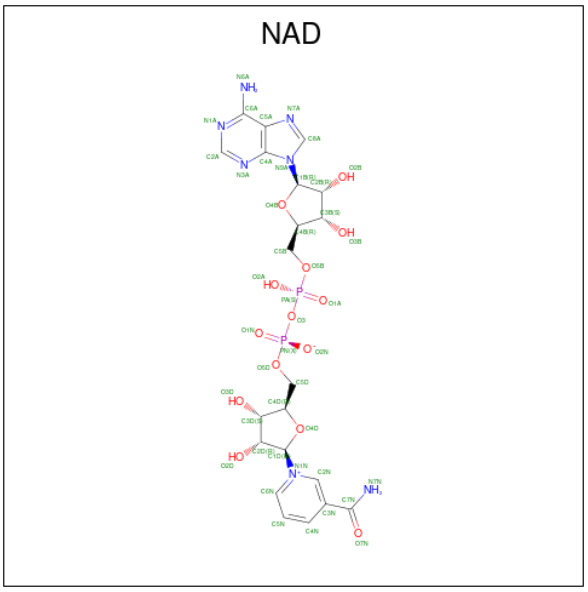
- Molecule 1 is a protein called Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	2	0
			3570	2250	618	680	22			
1	B	461	Total	C	N	O	S	0	4	0
			3577	2256	619	680	22			
1	C	462	Total	C	N	O	S	0	3	0
			3576	2255	619	680	22			
1	D	461	Total	C	N	O	S	0	2	0
			3565	2247	616	680	22			

There are 12 discrepancies between the modelled and reference sequences:

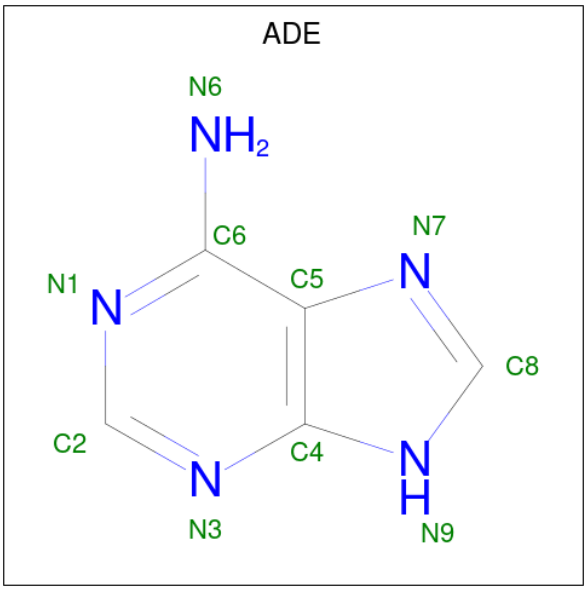
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9I685
A	-1	ASN	-	expression tag	UNP Q9I685
A	0	ALA	-	expression tag	UNP Q9I685
B	-2	SER	-	expression tag	UNP Q9I685
B	-1	ASN	-	expression tag	UNP Q9I685
B	0	ALA	-	expression tag	UNP Q9I685
C	-2	SER	-	expression tag	UNP Q9I685
C	-1	ASN	-	expression tag	UNP Q9I685
C	0	ALA	-	expression tag	UNP Q9I685
D	-2	SER	-	expression tag	UNP Q9I685
D	-1	ASN	-	expression tag	UNP Q9I685
D	0	ALA	-	expression tag	UNP Q9I685

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



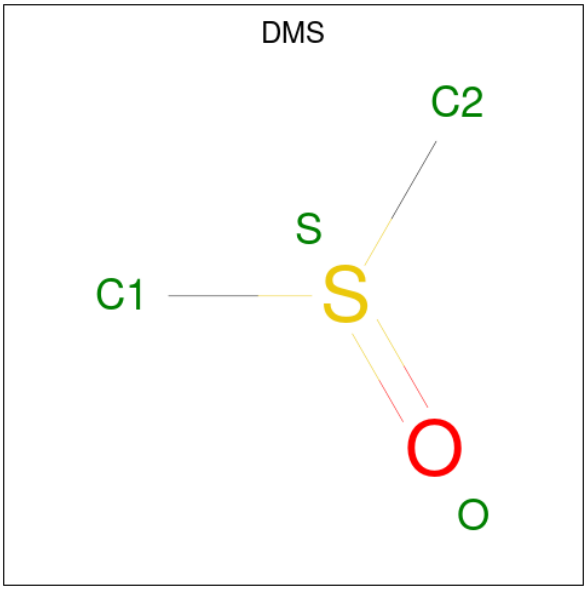
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is ADENINE (three-letter code: ADE) (formula: $C_5H_5N_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 10 5 5	0	0
3	B	1	Total C N 10 5 5	0	0
3	C	1	Total C N 10 5 5	0	0
3	D	1	Total C N 10 5 5	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).

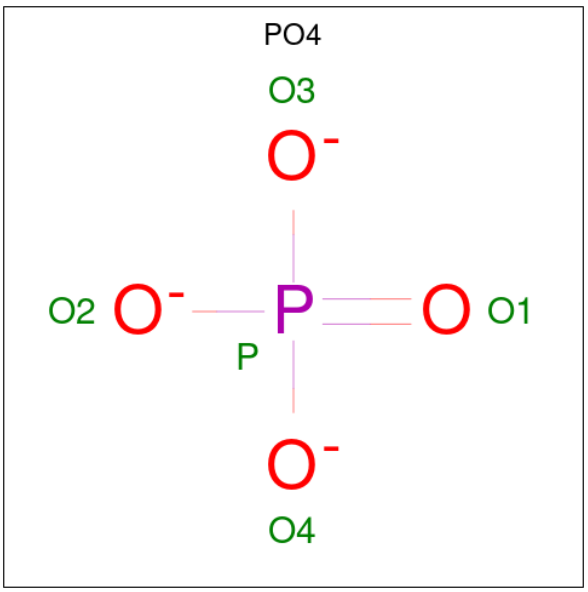


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0
5	B	1	Total K 1 1	0	0
5	C	1	Total K 1 1	0	0
5	D	1	Total K 1 1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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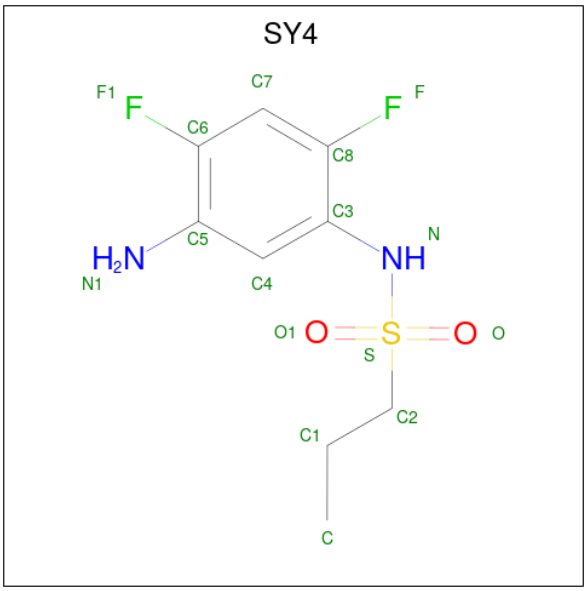
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total O P 5 4 1	0	0
6	D	1	Total O P 5 4 1	0	0

- Molecule 7 is {N}-[5-azanyl-2,4-bis(fluoranyl)phenyl]propane-1-sulfonamide (three-letter code: SY4) (formula: $C_9H_{12}F_2N_2O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C F N O S 16 9 2 2 2 1	0	0

- Molecule 8 is water.

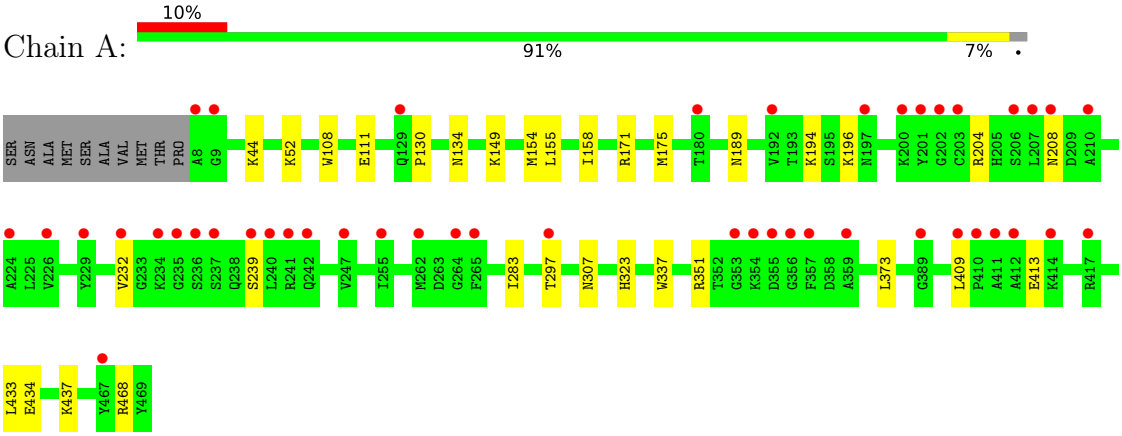
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	233	Total O 235 235	0	2
8	B	118	Total O 118 118	0	0
8	C	47	Total O 47 47	0	0
8	D	118	Total O 119 119	0	1

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.

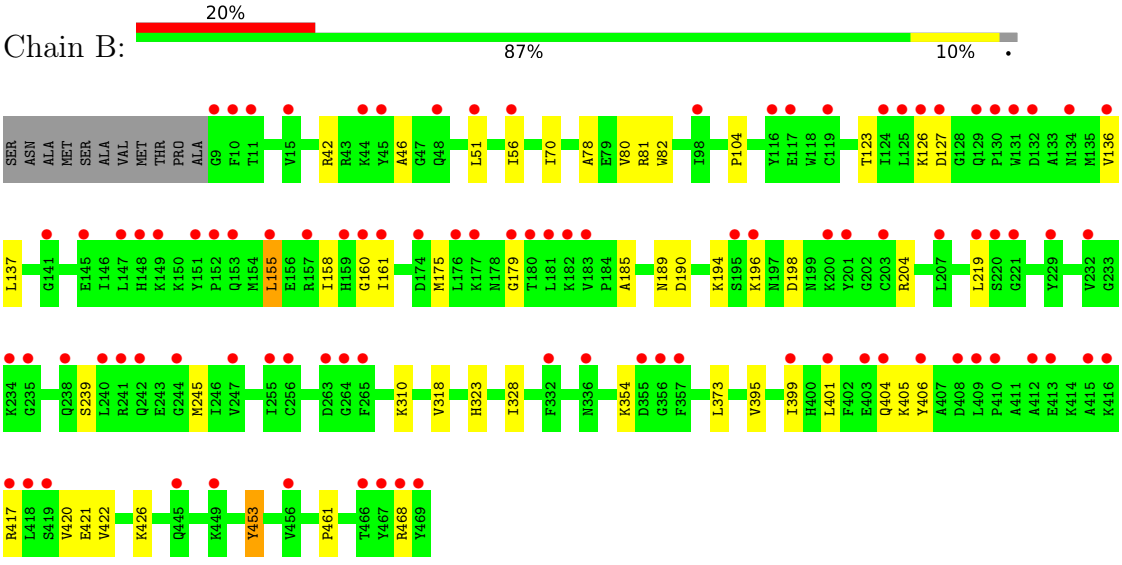
• Molecule 1: Adenosylhomocysteinase

Chain A:



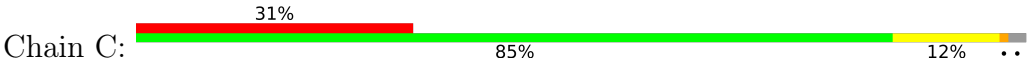
• Molecule 1: Adenosylhomocysteinase

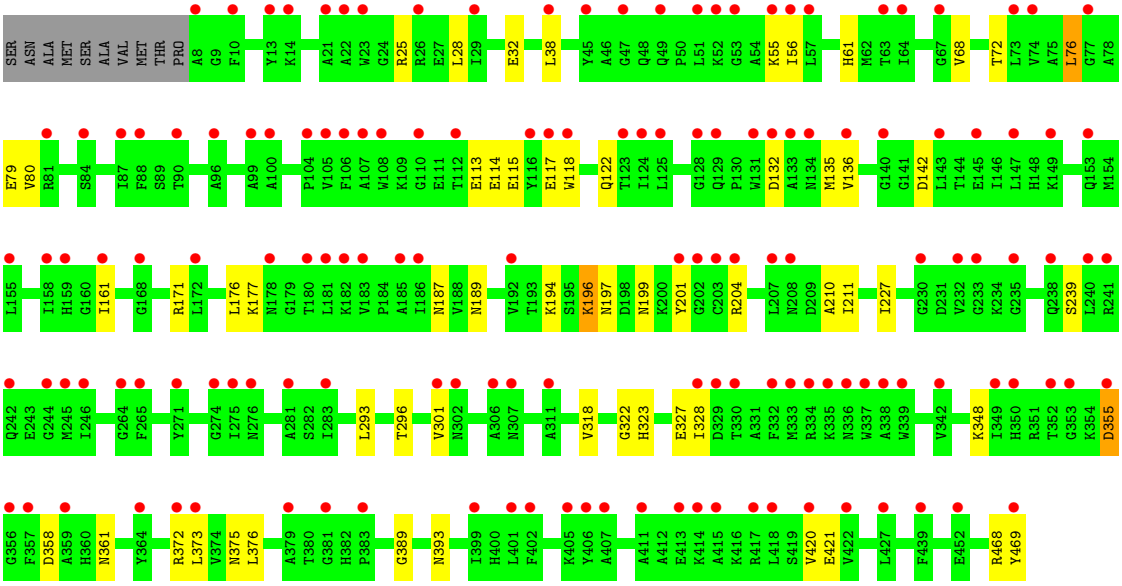
Chain B:



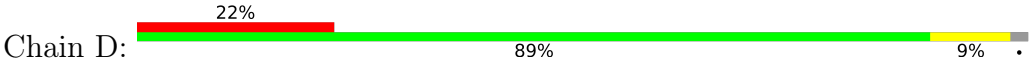
• Molecule 1: Adenosylhomocysteinase

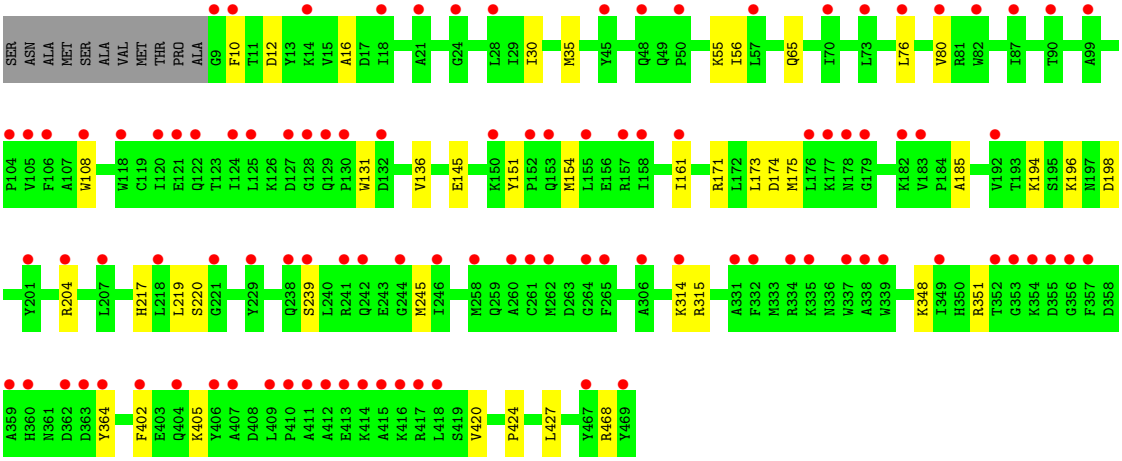
Chain C:





• Molecule 1: Adenosylhomocysteinase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	175.97Å 103.68Å 109.20Å 90.00° 99.99° 90.00°	Depositor
Resolution (Å)	32.64 – 2.07 48.60 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.0 (32.64-2.07) 99.1 (48.60-2.07)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.19.2-4158	Depositor
R, R_{free}	0.235 , 0.271 0.236 , 0.271	Depositor DCC
R_{free} test set	2100 reflections (1.79%)	wwPDB-VP
Wilson B-factor (Å^2)	46.2	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15122	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: SY4, PO4, ADE, K, NAD, DMS

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	0.25	0/3636	0.47	0/4916
1	B	0.25	0/3649	0.48	0/4932
1	C	0.25	0/3645	0.48	0/4927
1	D	0.25	0/3631	0.47	0/4909
All	All	0.25	0/14561	0.47	0/19684

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3570	0	3576	18	0
1	B	3577	0	3592	30	0
1	C	3576	0	3589	35	0
1	D	3565	0	3570	23	0
2	A	44	0	26	1	0
2	B	44	0	26	1	0
2	C	44	0	26	2	0
2	D	44	0	26	1	0
3	A	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	4	0	0
3	C	10	0	4	0	0
3	D	10	0	4	0	0
4	A	4	0	6	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	15	0	0	0	0
6	B	15	0	0	0	0
6	C	20	0	0	1	0
6	D	25	0	0	1	0
7	A	16	0	0	2	0
8	A	235	0	0	0	0
8	B	118	0	0	1	0
8	C	47	0	0	0	0
8	D	119	0	0	0	0
All	All	15122	0	14453	101	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (101) 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:C:204:ARG:HA	1:C:239:SER:HB2	1.71	0.71
1:A:189:ASN:HA	1:A:194:LYS:HD2	1.75	0.69
1:C:211:ILE:HD13	1:C:293:LEU:HD11	1.77	0.65
1:C:204:ARG:NH2	1:D:220:SER:OG	2.31	0.64
1:B:404:GLN:HB3	1:B:417:ARG:HH12	1.63	0.64
1:B:404:GLN:HB3	1:B:417:ARG:NH1	2.14	0.63
1:B:204:ARG:HA	1:B:239:SER:HB2	1.81	0.63
1:D:145:GLU:OE1	1:D:171:ARG:NH2	2.33	0.62
1:B:51:LEU:HB3	1:B:78:ALA:HB2	1.82	0.62
1:D:204:ARG:HA	1:D:239:SER:HB2	1.84	0.59
1:B:160:GLY:HA3	1:B:401:LEU:HD13	1.83	0.59
1:B:56:ILE:HB	1:B:80:VAL:HG12	1.87	0.57
1:C:189:ASN:HA	1:C:194:LYS:HD2	1.86	0.57
1:D:351:ARG:NH2	6:D:504:PO4:O2	2.38	0.57
1:B:196[B]:LYS:NZ	1:C:469:TYR:OXT	2.38	0.57
1:C:227:ILE:HD13	1:C:296:THR:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:HIS:HA	1:B:373:LEU:HD21	1.88	0.56
1:C:348:LYS:HD2	1:D:30:ILE:HD11	1.88	0.55
1:C:55:LYS:NZ	1:C:79:GLU:OE1	2.37	0.54
1:D:16:ALA:HB2	1:D:108:TRP:HB2	1.90	0.54
1:B:189:ASN:HA	1:B:194:LYS:HD2	1.88	0.54
1:A:204:ARG:HA	1:A:239:SER:HB2	1.89	0.53
1:D:35:MET:HE2	1:D:65:GLN:HG3	1.90	0.53
1:C:323:HIS:HA	1:C:373:LEU:HD21	1.90	0.53
1:C:25:ARG:NH1	6:C:504:PO4:O2	2.43	0.52
1:D:171:ARG:O	1:D:175:MET:HG3	2.10	0.52
1:B:426:LYS:HG2	1:B:461:PRO:HG3	1.91	0.52
1:A:44:LYS:HD2	7:A:508:SY4:O1	2.11	0.51
1:C:187:ASN:N	1:C:421:GLU:O	2.31	0.50
1:B:453:TYR:CE2	1:C:301:VAL:HB	2.48	0.49
1:A:283:ILE:HG13	1:A:307:ASN:HB3	1.94	0.49
1:B:453:TYR:HE2	1:C:301:VAL:HB	1.78	0.49
1:D:219:LEU:O	1:D:245:MET:HG2	2.13	0.49
1:C:136:VAL:HB	1:C:161:ILE:HG12	1.94	0.48
1:D:56:ILE:HB	1:D:80:VAL:HG12	1.95	0.48
1:C:114:GLU:HG2	1:C:115:GLU:N	2.29	0.48
1:B:81:ARG:NH1	1:B:123:THR:O	2.46	0.48
1:C:113:GLU:OE2	1:C:372:ARG:NH2	2.47	0.48
1:C:142:ASP:OD1	1:C:171:ARG:NH2	2.47	0.48
1:A:208[A]:ASN:ND2	1:A:239:SER:OG	2.46	0.48
1:C:389:GLY:O	1:C:393:ASN:ND2	2.40	0.48
1:C:197:ASN:HA	1:C:201:TYR:HD2	1.79	0.47
1:C:55:LYS:HD2	1:C:132:ASP:O	2.15	0.47
1:D:136:VAL:HB	1:D:161:ILE:HG12	1.97	0.47
1:D:185:ALA:HB3	1:D:420:VAL:HG22	1.97	0.47
1:B:136:VAL:HB	1:B:161:ILE:HG12	1.97	0.46
1:C:118:TRP:O	1:C:122:GLN:HG2	2.16	0.46
1:C:56:ILE:HB	1:C:80:VAL:HG12	1.96	0.46
1:B:70:ILE:HG23	1:B:80:VAL:HG21	1.96	0.45
1:B:395:VAL:O	1:B:399:ILE:HG12	2.16	0.45
1:D:402:PHE:O	1:D:405:LYS:HD2	2.16	0.45
1:B:81:ARG:HG2	1:B:104:PRO:HG2	1.99	0.45
1:B:404:GLN:O	1:B:406:TYR:N	2.49	0.45
1:B:155:LEU:HA	1:B:158:ILE:HD12	1.98	0.45
1:C:176:LEU:HD22	1:C:420:VAL:HG23	1.99	0.45
1:C:210:ALA:HB2	1:C:375:ASN:HA	1.99	0.45
1:A:468:ARG:HB2	1:D:196:LYS:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LYS:O	1:B:198:ASP:N	2.49	0.45
1:C:199:ASN:OD1	2:C:501:NAD:H5N	2.17	0.44
1:D:194:LYS:HD2	1:D:198:ASP:HB3	1.99	0.44
1:D:10:PHE:CZ	1:D:12:ASP:HB3	2.52	0.44
1:A:409:LEU:HB3	1:A:413:GLU:HB2	2.00	0.44
1:B:42:ARG:O	1:B:46:ALA:HB2	2.17	0.44
1:A:232:VAL:HG12	1:A:297:THR:HB	2.00	0.44
1:A:434:GLU:HG3	7:A:508:SY4:N1	2.32	0.44
1:C:322:GLY:HA3	1:C:327:GLU:OE2	2.18	0.43
1:C:358:ASP:HB3	1:C:361:ASN:HB2	1.99	0.43
1:C:318:VAL:HG12	1:C:328:ILE:HD13	1.99	0.43
1:D:151:TYR:HB3	1:D:154:MET:HE3	2.00	0.43
1:A:337:TRP:CD1	1:A:351:ARG:HA	2.54	0.43
1:B:82:TRP:HH2	1:B:137:LEU:HD13	1.83	0.43
1:C:61:HIS:CE1	1:C:376:LEU:HD13	2.54	0.43
1:B:190:ASP:O	1:C:468:ARG:NH1	2.44	0.43
1:D:315:ARG:HG2	1:D:364:TYR:CZ	2.54	0.43
1:D:348:LYS:HD2	1:D:364:TYR:CD1	2.54	0.43
1:C:72:THR:O	1:C:76:LEU:HD22	2.18	0.43
1:B:185:ALA:HB3	1:B:420:VAL:HG22	2.02	0.42
1:A:155:LEU:HA	1:A:158:ILE:HD12	2.01	0.42
1:C:38:LEU:HD23	1:C:68:VAL:HG12	2.00	0.42
1:C:355:ASP:OD1	1:C:355:ASP:N	2.51	0.42
2:D:501:NAD:H2D	2:D:501:NAD:H6N	1.81	0.42
2:A:501:NAD:H2D	2:A:501:NAD:H6N	1.81	0.42
1:B:219:LEU:O	1:B:245:MET:HG2	2.19	0.42
2:C:501:NAD:H2D	2:C:501:NAD:H6N	1.83	0.42
1:A:171:ARG:O	1:A:175:MET:HG3	2.19	0.42
2:B:501:NAD:H2D	2:B:501:NAD:H6N	1.78	0.41
1:D:154:MET:HE2	1:D:154:MET:HB2	1.88	0.41
1:A:130:PRO:HB3	1:A:154:MET:SD	2.60	0.41
1:A:433:LEU:HG	1:A:437:LYS:HE3	2.02	0.41
1:B:126:LYS:HG2	1:B:127:ASP:OD1	2.20	0.41
1:A:134:ASN:HA	1:A:158:ILE:HA	2.01	0.41
1:B:175:MET:O	1:B:179:GLY:N	2.54	0.41
1:B:310:LYS:NZ	8:B:611:HOH:O	2.53	0.41
1:A:108:TRP:O	1:A:111:GLU:HG3	2.20	0.41
1:A:196:LYS:HE3	1:D:468:ARG:HB2	2.02	0.41
1:B:468:ARG:HB2	1:C:196[A]:LYS:NZ	2.35	0.41
1:D:424:PRO:HD2	1:D:427:LEU:HD12	2.03	0.41
1:B:318:VAL:HG12	1:B:328:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:HIS:HA	1:A:373:LEU:HD21	2.02	0.41
1:D:55:LYS:HB3	1:D:131:TRP:CH2	2.56	0.41
1:C:28:LEU:O	1:C:32:GLU:HG3	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	A	462/472 (98%)	454 (98%)	8 (2%)	0	100	100
1	B	463/472 (98%)	444 (96%)	17 (4%)	2 (0%)	34	25
1	C	463/472 (98%)	452 (98%)	11 (2%)	0	100	100
1	D	461/472 (98%)	451 (98%)	10 (2%)	0	100	100
All	All	1849/1888 (98%)	1801 (97%)	46 (2%)	2 (0%)	51	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	405	LYS
1	B	422	VAL

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	379/385 (98%)	377 (100%)	2 (0%)	88 89
1	B	381/385 (99%)	377 (99%)	4 (1%)	76 75
1	C	380/385 (99%)	373 (98%)	7 (2%)	59 55
1	D	379/385 (98%)	373 (98%)	6 (2%)	62 59
All	All	1519/1540 (99%)	1500 (99%)	19 (1%)	73 67

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	149	LYS
1	B	155	LEU
1	B	354	LYS
1	B	421	GLU
1	B	453	TYR
1	C	76	LEU
1	C	117	GLU
1	C	135	MET
1	C	177	LYS
1	C	196[A]	LYS
1	C	196[B]	LYS
1	C	355	ASP
1	D	76	LEU
1	D	173	LEU
1	D	174[A]	ASP
1	D	174[B]	ASP
1	D	217	HIS
1	D	314	LYS

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)

Of 29 ligands modelled in this entry, 4 are monoatomic - leaving 25 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	$\#\|Z\| > 2$
6	PO4	B	506	-	4,4,4	0.93	0	6,6,6	0.41	0
6	PO4	B	504	-	4,4,4	0.92	0	6,6,6	0.41	0
2	NAD	C	501	-	42,48,48	0.54	0	50,73,73	0.61	1 (2%)
6	PO4	A	506	-	4,4,4	0.88	0	6,6,6	0.51	0
7	SY4	A	508	-	15,16,16	1.60	4 (26%)	18,23,23	3.51	9 (50%)
6	PO4	D	505	-	4,4,4	0.92	0	6,6,6	0.44	0
6	PO4	D	506	-	4,4,4	0.90	0	6,6,6	0.46	0
6	PO4	A	505	-	4,4,4	0.90	0	6,6,6	0.45	0
6	PO4	A	507	-	4,4,4	0.89	0	6,6,6	0.56	0
2	NAD	D	501	-	42,48,48	0.54	0	50,73,73	0.61	1 (2%)
2	NAD	A	501	-	42,48,48	0.55	0	50,73,73	0.66	1 (2%)
6	PO4	D	508	-	4,4,4	0.91	0	6,6,6	0.40	0
6	PO4	C	505	-	4,4,4	0.94	0	6,6,6	0.41	0
6	PO4	C	507	-	4,4,4	0.92	0	6,6,6	0.38	0
3	ADE	B	502	-	9,11,11	0.96	0	7,15,15	1.11	1 (14%)
6	PO4	D	507	-	4,4,4	0.90	0	6,6,6	0.47	0
6	PO4	D	504	-	4,4,4	0.94	0	6,6,6	0.42	0
6	PO4	C	504	-	4,4,4	0.92	0	6,6,6	0.39	0
6	PO4	B	505	-	4,4,4	0.94	0	6,6,6	0.43	0
2	NAD	B	501	-	42,48,48	0.54	0	50,73,73	0.60	1 (2%)
4	DMS	A	503	-	3,3,3	0.66	0	3,3,3	0.60	0
6	PO4	C	506	-	4,4,4	0.92	0	6,6,6	0.42	0
3	ADE	A	502	-	9,11,11	0.96	0	7,15,15	1.11	1 (14%)
3	ADE	C	502	-	9,11,11	0.94	0	7,15,15	1.10	0
3	ADE	D	502	-	9,11,11	0.95	0	7,15,15	1.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	C	501	-	-	5/26/62/62	0/5/5/5
7	SY4	A	508	-	-	1/9/9/9	0/1/1/1
3	ADE	B	502	-	-	-	0/2/2/2
2	NAD	B	501	-	-	5/26/62/62	0/5/5/5
3	ADE	D	502	-	-	-	0/2/2/2
3	ADE	A	502	-	-	-	0/2/2/2
2	NAD	D	501	-	-	5/26/62/62	0/5/5/5
3	ADE	C	502	-	-	-	0/2/2/2
2	NAD	A	501	-	-	5/26/62/62	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	508	SY4	S-N	3.93	1.70	1.62
7	A	508	SY4	O-S	2.47	1.47	1.43
7	A	508	SY4	O1-S	2.29	1.46	1.43
7	A	508	SY4	C5-N1	2.28	1.45	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	508	SY4	O1-S-O	-12.20	101.68	119.35
7	A	508	SY4	C7-C6-C5	-3.80	120.21	123.34
7	A	508	SY4	C7-C8-C3	-3.70	119.98	123.50
7	A	508	SY4	C4-C3-C8	2.94	120.46	117.75
7	A	508	SY4	O-S-C2	2.71	112.19	107.86
7	A	508	SY4	O1-S-C2	2.61	112.02	107.86
2	A	501	NAD	C5A-C6A-N6A	2.41	124.01	120.35
2	B	501	NAD	C5A-C6A-N6A	2.32	123.88	120.35
2	D	501	NAD	C5A-C6A-N6A	2.31	123.87	120.35
2	C	501	NAD	C5A-C6A-N6A	2.31	123.86	120.35
7	A	508	SY4	C3-N-S	-2.20	118.34	123.59
7	A	508	SY4	C2-S-N	2.11	109.78	106.77
7	A	508	SY4	O-S-N	2.09	112.36	107.28
3	A	502	ADE	C5-C6-N6	2.02	123.43	120.35
3	B	502	ADE	C5-C6-N6	2.02	123.43	120.35

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	O4D-C1D-N1N-C2N
2	A	501	NAD	O4D-C1D-N1N-C6N
2	A	501	NAD	C2D-C1D-N1N-C2N
2	A	501	NAD	C2D-C1D-N1N-C6N
2	B	501	NAD	O4D-C1D-N1N-C2N
2	B	501	NAD	O4D-C1D-N1N-C6N
2	B	501	NAD	C2D-C1D-N1N-C2N
2	B	501	NAD	C2D-C1D-N1N-C6N
2	C	501	NAD	O4D-C1D-N1N-C2N
2	C	501	NAD	O4D-C1D-N1N-C6N
2	C	501	NAD	C2D-C1D-N1N-C2N
2	C	501	NAD	C2D-C1D-N1N-C6N
2	D	501	NAD	O4D-C1D-N1N-C2N
2	D	501	NAD	O4D-C1D-N1N-C6N
2	D	501	NAD	C2D-C1D-N1N-C2N
2	D	501	NAD	C2D-C1D-N1N-C6N
7	A	508	SY4	C1-C2-S-O1
2	A	501	NAD	O4B-C4B-C5B-O5B
2	C	501	NAD	O4B-C4B-C5B-O5B
2	D	501	NAD	O4B-C4B-C5B-O5B
2	B	501	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

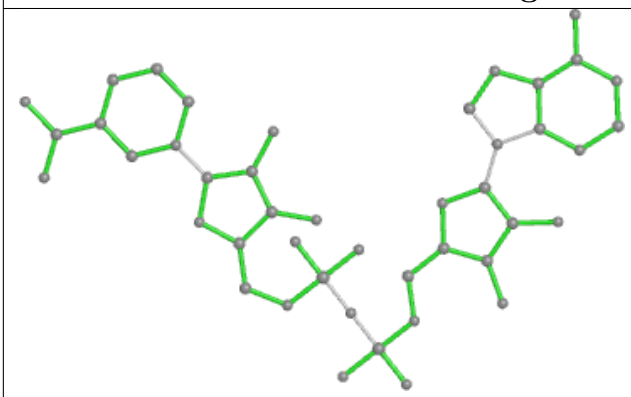
7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	NAD	2	0
7	A	508	SY4	2	0
2	D	501	NAD	1	0
2	A	501	NAD	1	0
6	D	504	PO4	1	0
6	C	504	PO4	1	0
2	B	501	NAD	1	0

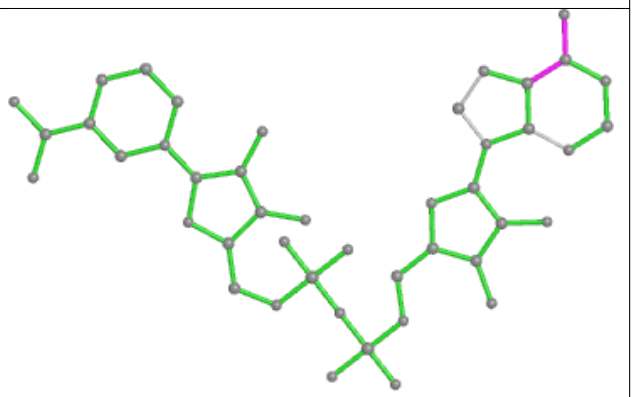
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

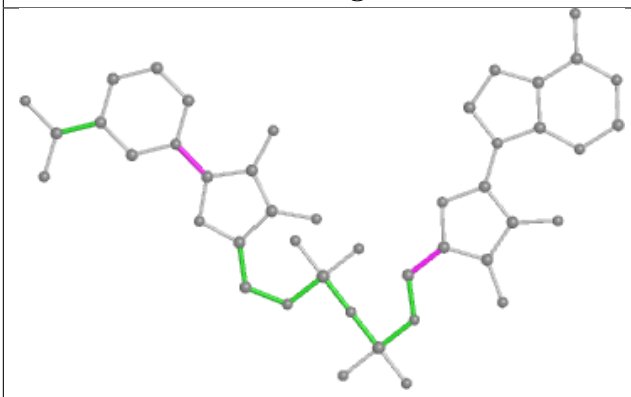
Ligand NAD C 501



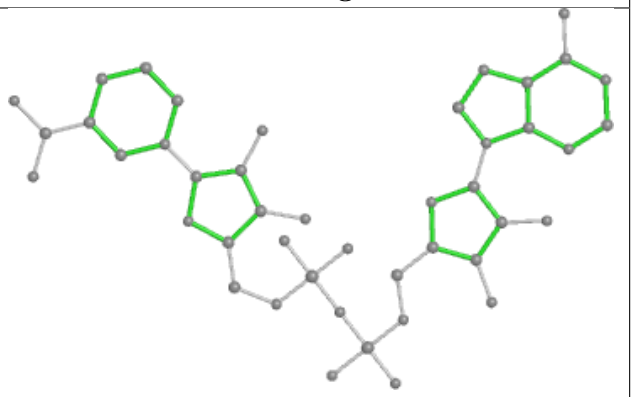
Bond lengths



Bond angles

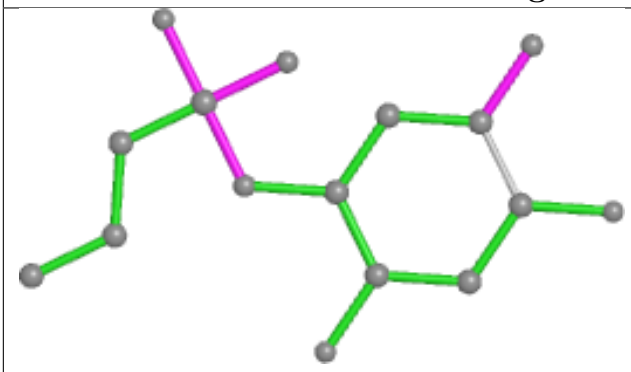


Torsions

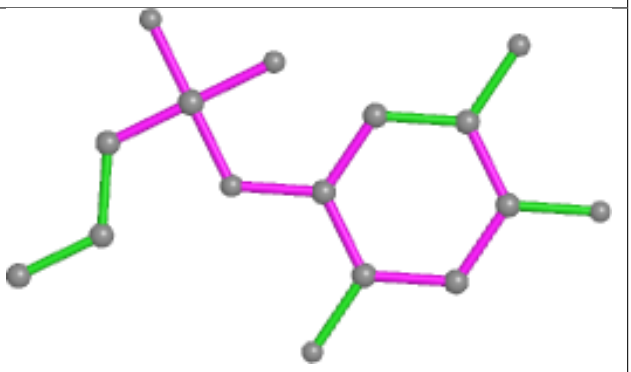


Rings

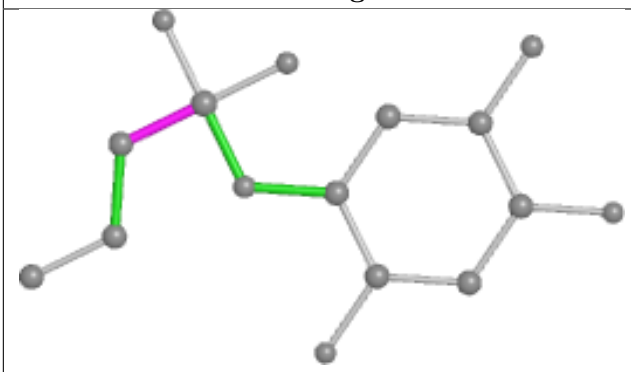
Ligand SY4 A 508



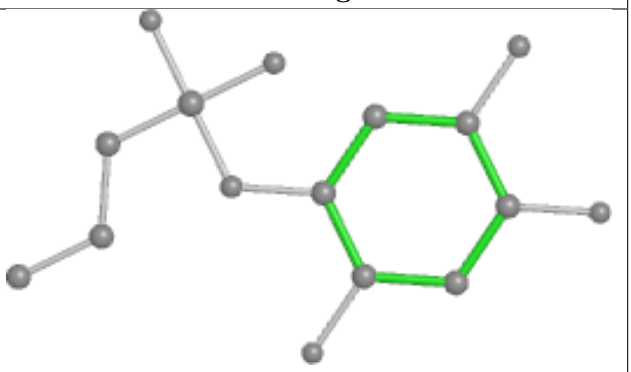
Bond lengths



Bond angles

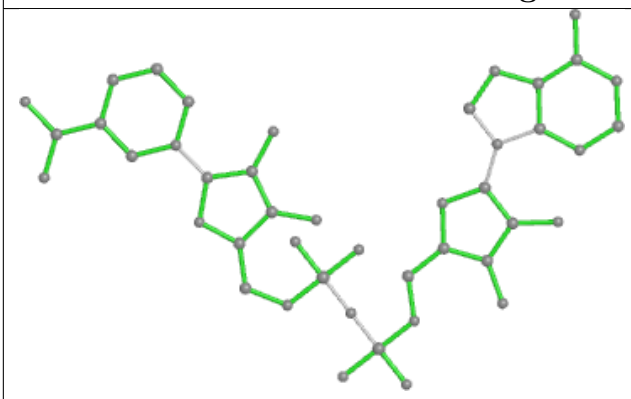


Torsions

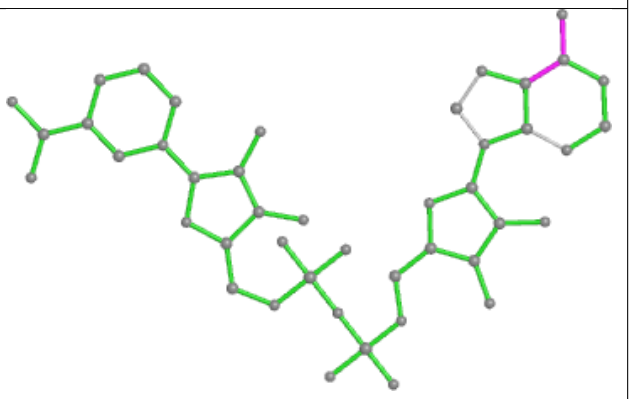


Rings

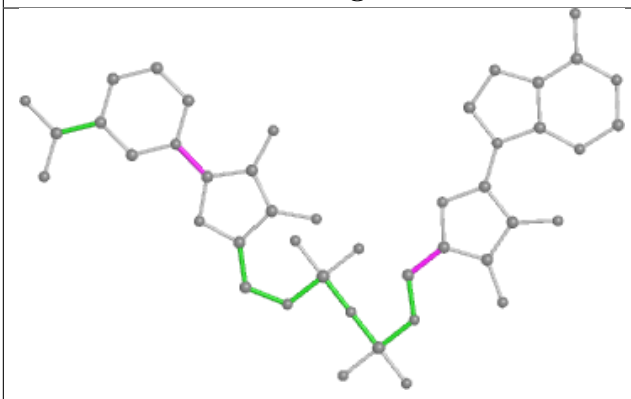
Ligand NAD D 501



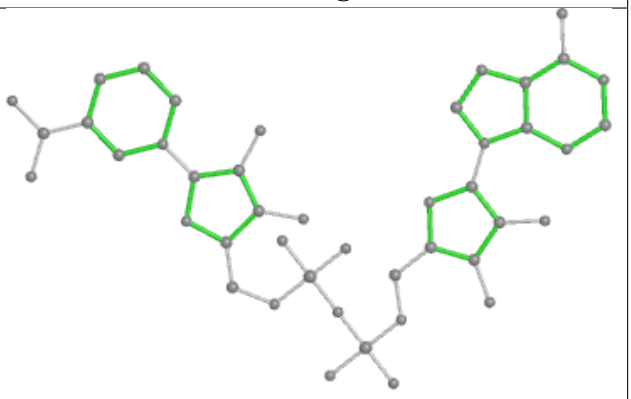
Bond lengths



Bond angles

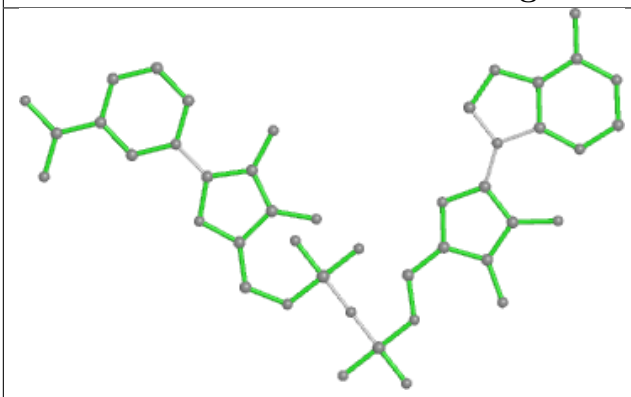


Torsions

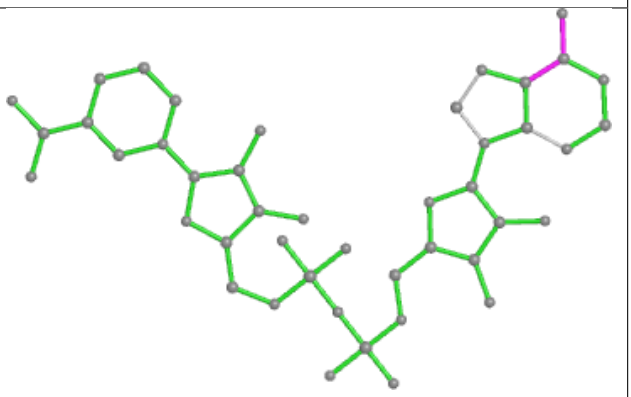


Rings

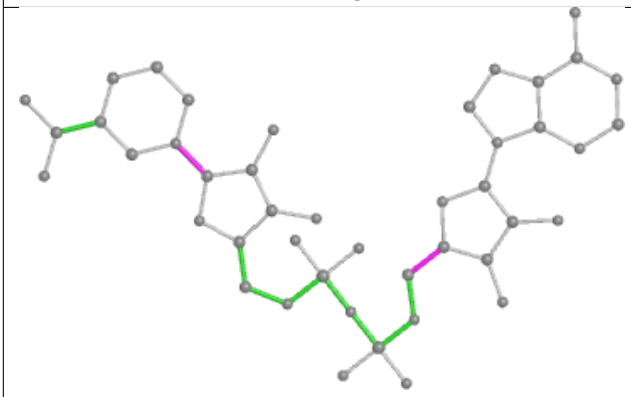
Ligand NAD A 501



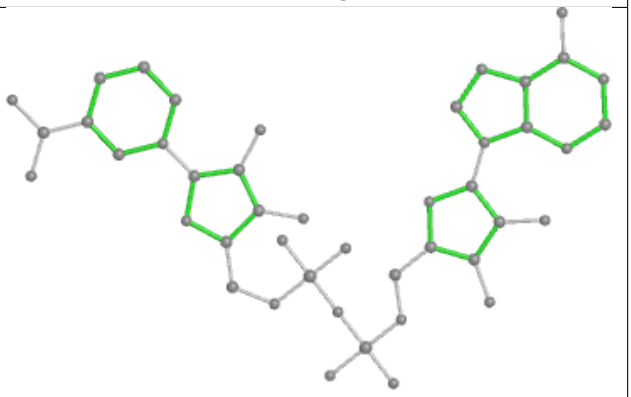
Bond lengths



Bond angles

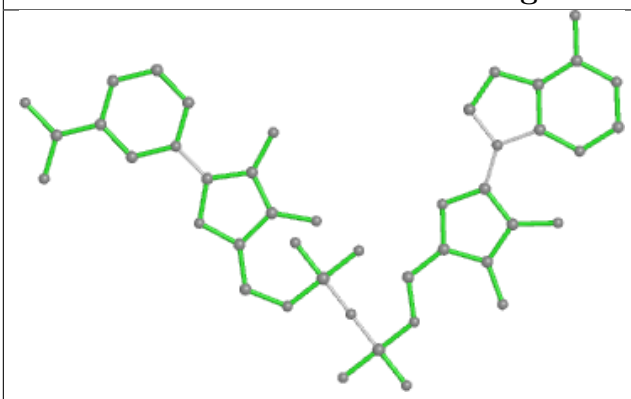


Torsions

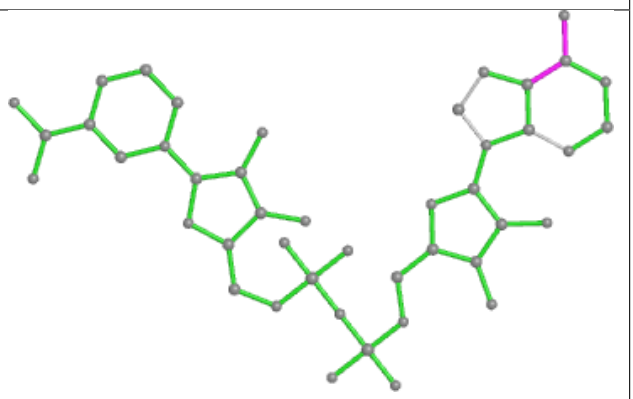


Rings

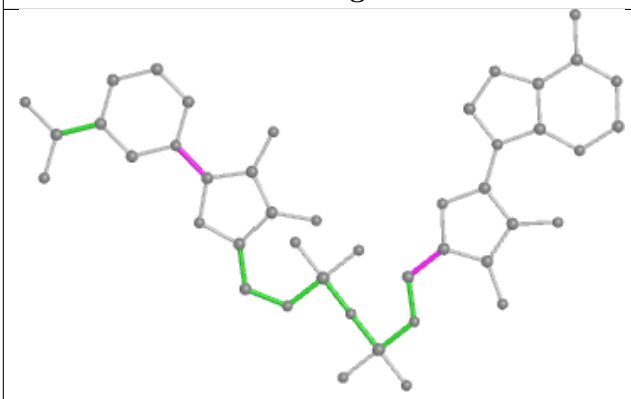
Ligand NAD B 501



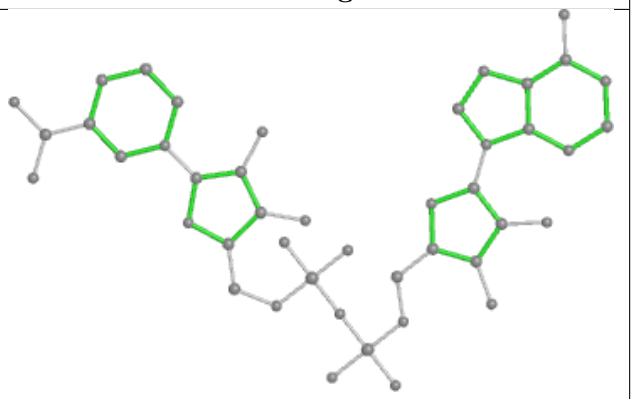
Bond lengths



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	A	462/472 (97%)	0.50	46 (9%) 7 7	38, 50, 69, 104	0
1	B	461/472 (97%)	1.12	95 (20%) 1 0	41, 72, 126, 163	0
1	C	462/472 (97%)	1.68	147 (31%) 0 0	60, 94, 126, 166	0
1	D	461/472 (97%)	1.22	103 (22%) 0 0	39, 74, 110, 164	0
All	All	1846/1888 (97%)	1.13	391 (21%) 0 0	38, 72, 120, 166	0

All (391) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	409	LEU	10.3
1	D	411	ALA	8.8
1	C	356	GLY	8.8
1	B	406	TYR	8.6
1	B	160	GLY	8.1
1	B	181	LEU	7.8
1	D	10	PHE	7.7
1	D	412	ALA	7.5
1	B	416	LYS	7.5
1	D	410	PRO	7.2
1	C	158	ILE	7.0
1	B	155	LEU	6.8
1	D	416	LYS	6.5
1	B	179	GLY	6.4
1	B	409	LEU	6.3
1	C	352	THR	6.3
1	C	415	ALA	6.0
1	D	9	GLY	5.9
1	C	118	TRP	5.9
1	D	359	ALA	5.6
1	C	131	TRP	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	406	TYR	5.5
1	B	417	ARG	5.4
1	B	176	LEU	5.2
1	D	417	ARG	5.1
1	B	412	ALA	5.0
1	C	155	LEU	5.0
1	B	130	PRO	5.0
1	C	406	TYR	4.9
1	B	125	LEU	4.9
1	B	10	PHE	4.9
1	B	9	GLY	4.9
1	C	143	LEU	4.8
1	B	401	LEU	4.7
1	C	418	LEU	4.7
1	C	407	ALA	4.7
1	B	124	ILE	4.7
1	C	307	ASN	4.6
1	C	10	PHE	4.6
1	C	332	PHE	4.6
1	C	357	PHE	4.5
1	A	232	VAL	4.5
1	B	182	LYS	4.5
1	C	180	THR	4.5
1	C	153	GLN	4.4
1	D	339	TRP	4.4
1	D	121	GLU	4.4
1	C	411	ALA	4.4
1	D	335	LYS	4.3
1	C	53	GLY	4.3
1	D	155	LEU	4.3
1	D	158	ILE	4.3
1	C	401	LEU	4.3
1	D	415	ALA	4.2
1	D	418	LEU	4.2
1	C	405	LYS	4.2
1	A	359	ALA	4.2
1	C	182	LYS	4.2
1	C	67	GLY	4.2
1	D	150	LYS	4.2
1	C	353	GLY	4.2
1	B	147	LEU	4.1
1	C	338	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	128	GLY	4.1
1	A	357	PHE	4.0
1	C	88	PHE	4.0
1	C	181	LEU	4.0
1	B	136	VAL	4.0
1	C	124	ILE	4.0
1	B	48	GLN	4.0
1	C	359	ALA	4.0
1	D	24	GLY	4.0
1	B	152	PRO	3.9
1	C	201	TYR	3.9
1	C	417	ARG	3.9
1	C	349	ILE	3.9
1	C	337	TRP	3.8
1	D	125	LEU	3.8
1	C	52	LYS	3.8
1	B	11	THR	3.8
1	C	100	ALA	3.8
1	D	120	ILE	3.8
1	D	130	PRO	3.8
1	C	110	GLY	3.8
1	C	364	TYR	3.8
1	D	349	ILE	3.8
1	A	192	VAL	3.7
1	C	335	LYS	3.7
1	C	104	PRO	3.7
1	C	413	GLU	3.7
1	C	276	ASN	3.7
1	C	159	HIS	3.6
1	C	55	LYS	3.6
1	A	410	PRO	3.6
1	B	413	GLU	3.6
1	D	338	ALA	3.6
1	C	414	LYS	3.6
1	A	409	LEU	3.6
1	C	47	GLY	3.6
1	B	157	ARG	3.6
1	C	302	ASN	3.6
1	C	372	ARG	3.6
1	B	408	ASP	3.5
1	D	176	LEU	3.5
1	B	469	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	129	GLN	3.5
1	B	180	THR	3.5
1	C	161	ILE	3.4
1	C	22	ALA	3.4
1	B	241	ARG	3.4
1	B	264	GLY	3.4
1	D	127	ASP	3.4
1	C	99	ALA	3.4
1	C	132	ASP	3.4
1	C	112	THR	3.4
1	D	82	TRP	3.4
1	C	183	VAL	3.4
1	A	262	MET	3.4
1	D	182	LYS	3.4
1	C	38	LEU	3.4
1	C	452	GLU	3.4
1	B	131	TRP	3.3
1	C	469	TYR	3.3
1	B	183	VAL	3.3
1	C	74	VAL	3.3
1	C	420	VAL	3.3
1	B	45	TYR	3.3
1	D	106	PHE	3.3
1	D	334	ARG	3.3
1	C	105	VAL	3.3
1	B	415	ALA	3.3
1	C	168	GLY	3.3
1	B	174	ASP	3.3
1	B	357	PHE	3.3
1	D	192	VAL	3.3
1	D	337	TRP	3.2
1	C	342	VAL	3.2
1	C	336	ASN	3.2
1	D	152	PRO	3.2
1	A	264	GLY	3.2
1	C	57	LEU	3.2
1	D	314	LYS	3.2
1	B	356	GLY	3.2
1	D	118	TRP	3.2
1	C	87	ILE	3.2
1	D	128	GLY	3.2
1	C	56	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	178	ASN	3.2
1	A	354	LYS	3.2
1	C	355	ASP	3.2
1	A	229	TYR	3.1
1	A	240	LEU	3.1
1	D	356	GLY	3.1
1	D	18	ILE	3.1
1	C	311	ALA	3.1
1	B	141	GLY	3.1
1	A	207	LEU	3.1
1	B	468	ARG	3.1
1	B	51	LEU	3.1
1	D	57	LEU	3.1
1	B	445	GLN	3.0
1	B	98	ILE	3.0
1	C	106	PHE	3.0
1	C	192	VAL	3.0
1	D	229	TYR	3.0
1	C	84	SER	3.0
1	B	129	GLN	3.0
1	D	218	LEU	3.0
1	D	258[A]	MET	3.0
1	A	353	GLY	3.0
1	C	330	THR	3.0
1	D	355	ASP	3.0
1	B	177	LYS	2.9
1	C	274	GLY	2.9
1	D	45	TYR	2.9
1	D	129	GLN	2.9
1	C	240	LEU	2.9
1	A	356	GLY	2.9
1	B	151	TYR	2.9
1	D	354	LYS	2.9
1	C	96	ALA	2.9
1	B	399	ILE	2.9
1	C	204	ARG	2.9
1	B	355	ASP	2.9
1	B	116	TYR	2.9
1	C	149	LYS	2.9
1	B	153	GLN	2.9
1	B	410	PRO	2.9
1	B	265	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	242	GLN	2.9
1	C	242	GLN	2.9
1	C	383	PRO	2.9
1	D	261	CYS	2.9
1	C	108	TRP	2.8
1	A	202	GLY	2.8
1	B	235	GLY	2.8
1	C	178	ASN	2.8
1	B	201	TYR	2.8
1	D	28	LEU	2.8
1	C	134	ASN	2.8
1	C	264	GLY	2.8
1	C	14	LYS	2.8
1	D	407	ALA	2.8
1	C	123	THR	2.8
1	C	402	PHE	2.8
1	A	203	CYS	2.8
1	A	467	TYR	2.8
1	D	201	TYR	2.8
1	A	210	ALA	2.7
1	C	235	GLY	2.7
1	B	418	LEU	2.7
1	B	232	VAL	2.7
1	C	244	GLY	2.7
1	D	265	PHE	2.7
1	B	403	GLU	2.7
1	B	247	VAL	2.7
1	B	263	ASP	2.7
1	B	404	GLN	2.7
1	D	153	GLN	2.7
1	B	207	LEU	2.7
1	D	73	LEU	2.7
1	D	157	ARG	2.7
1	B	145	GLU	2.7
1	D	469	TYR	2.7
1	B	203	CYS	2.7
1	C	334	ARG	2.7
1	C	90	THR	2.7
1	D	241	ARG	2.7
1	D	353	GLY	2.6
1	D	104	PRO	2.6
1	D	357	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	389	GLY	2.6
1	C	140	GLY	2.6
1	D	179	GLY	2.6
1	C	21	ALA	2.6
1	B	149	LYS	2.6
1	B	219	LEU	2.6
1	C	81	ARG	2.6
1	C	13	TYR	2.6
1	C	232	VAL	2.6
1	D	364	TYR	2.6
1	C	23	TRP	2.6
1	A	224	ALA	2.6
1	C	133	ALA	2.6
1	D	414	LYS	2.6
1	C	241	ARG	2.6
1	B	159	HIS	2.6
1	D	90	THR	2.6
1	D	105	VAL	2.6
1	C	116	TYR	2.6
1	C	117	GLU	2.6
1	D	306	ALA	2.6
1	B	117	GLU	2.6
1	B	126	LYS	2.5
1	D	360	HIS	2.5
1	C	63	THR	2.5
1	C	145	GLU	2.5
1	C	275	ILE	2.5
1	C	339	TRP	2.5
1	D	21	ALA	2.5
1	A	355	ASP	2.5
1	C	73	LEU	2.5
1	C	77	GLY	2.5
1	A	411	ALA	2.5
1	C	185	ALA	2.5
1	D	362	ASP	2.5
1	C	350	HIS	2.5
1	A	197	ASN	2.5
1	D	50	PRO	2.5
1	A	237	SER	2.5
1	C	379	ALA	2.5
1	C	208[A]	ASN	2.4
1	A	242	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	333	MET	2.4
1	A	234	LYS	2.4
1	C	203	CYS	2.4
1	C	399	ILE	2.4
1	A	412	ALA	2.4
1	C	107	ALA	2.4
1	B	466	THR	2.4
1	A	235	GLY	2.4
1	D	207	LEU	2.4
1	B	456	VAL	2.4
1	D	260	ALA	2.4
1	C	45	TYR	2.4
1	C	230	GLY	2.4
1	D	264	GLY	2.4
1	B	15	VAL	2.4
1	A	200	LYS	2.4
1	B	419	SER	2.4
1	A	201	TYR	2.4
1	B	467	TYR	2.4
1	C	125	LEU	2.3
1	C	147	LEU	2.3
1	C	49	GLN	2.3
1	C	238	GLN	2.3
1	A	236	SER	2.3
1	C	271	TYR	2.3
1	D	467	TYR	2.3
1	D	48	GLN	2.3
1	D	76	LEU	2.3
1	C	283	ILE	2.3
1	C	328	ILE	2.3
1	D	87	ILE	2.3
1	B	148	HIS	2.3
1	C	172	LEU	2.3
1	B	221	GLY	2.3
1	B	244	GLY	2.3
1	D	183	VAL	2.3
1	D	244	GLY	2.3
1	A	8	ALA	2.3
1	B	234	LYS	2.3
1	C	29	ILE	2.3
1	A	9	GLY	2.3
1	C	207	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	221	GLY	2.3
1	A	265	PHE	2.3
1	D	238	GLN	2.3
1	C	186	ILE	2.3
1	D	161	ILE	2.3
1	D	404	GLN	2.3
1	D	331	ALA	2.3
1	B	44	LYS	2.3
1	B	449	LYS	2.3
1	B	119	CYS	2.3
1	C	329	ASP	2.2
1	B	200	LYS	2.2
1	D	132	ASP	2.2
1	B	240	LEU	2.2
1	C	373	LEU	2.2
1	B	134	ASN	2.2
1	A	297	THR	2.2
1	A	417	ARG	2.2
1	C	427	LEU	2.2
1	C	301	VAL	2.2
1	D	332	PHE	2.2
1	B	220	SER	2.2
1	B	132	ASP	2.2
1	B	238	GLN	2.2
1	D	204	ARG	2.2
1	B	56	ILE	2.2
1	B	336	ASN	2.2
1	C	8	ALA	2.2
1	B	256	CYS	2.2
1	A	255	ILE	2.2
1	B	161	ILE	2.2
1	D	70	ILE	2.2
1	C	51	LEU	2.2
1	A	241	ARG	2.2
1	A	414	LYS	2.2
1	D	122	GLN	2.2
1	D	413	GLU	2.2
1	C	202	GLY	2.2
1	C	233	GLY	2.2
1	A	226	VAL	2.1
1	C	26	ARG	2.1
1	B	127	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	229	TYR	2.1
1	D	262	MET	2.1
1	A	239	SER	2.1
1	C	281	ALA	2.1
1	B	255	ILE	2.1
1	D	246	ILE	2.1
1	A	129	GLN	2.1
1	D	242	GLN	2.1
1	C	136	VAL	2.1
1	C	381	GLY	2.1
1	C	245	MET	2.1
1	D	239	SER	2.1
1	D	402	PHE	2.1
1	D	352	THR	2.1
1	D	14	LYS	2.1
1	A	208[A]	ASN	2.1
1	C	306	ALA	2.1
1	D	177	LYS	2.1
1	B	195	SER	2.1
1	C	439	PHE	2.1
1	D	108	TRP	2.1
1	A	206	SER	2.0
1	D	124	ILE	2.0
1	A	180	THR	2.0
1	D	80	VAL	2.0
1	B	332	PHE	2.0
1	A	247	VAL	2.0
1	C	265	PHE	2.0
1	B	196[A]	LYS	2.0
1	C	64	ILE	2.0
1	C	246	ILE	2.0
1	D	99	ALA	2.0
1	C	422	VAL	2.0
1	D	363	ASP	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, 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.

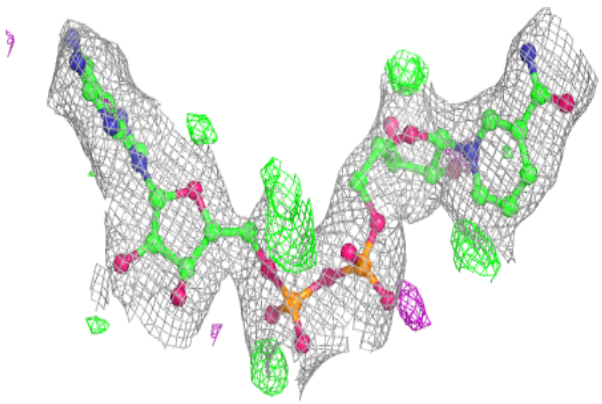
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PO4	C	504	5/5	0.72	0.22	86,91,99,101	0
6	PO4	C	507	5/5	0.80	0.28	76,83,90,93	5
6	PO4	C	506	5/5	0.83	0.26	75,79,84,87	5
2	NAD	C	501	44/44	0.85	0.20	58,75,80,84	0
4	DMS	A	503	4/4	0.85	0.30	59,68,69,72	4
6	PO4	B	506	5/5	0.85	0.24	62,70,72,76	5
6	PO4	C	505	5/5	0.86	0.24	81,81,86,88	0
3	ADE	C	502	10/10	0.87	0.17	78,82,86,87	0
7	SY4	A	508	16/16	0.87	0.17	45,51,68,69	0
2	NAD	B	501	44/44	0.90	0.16	56,64,68,75	0
6	PO4	D	507	5/5	0.91	0.17	53,57,61,65	5
6	PO4	A	505	5/5	0.92	0.17	56,58,63,66	5
6	PO4	D	508	5/5	0.92	0.17	52,54,60,62	5
6	PO4	D	505	5/5	0.92	0.15	91,94,98,100	0
6	PO4	D	506	5/5	0.93	0.15	64,66,72,73	5
5	K	C	503	1/1	0.93	0.11	64,64,64,64	0
3	ADE	B	502	10/10	0.94	0.16	56,59,61,62	0
2	NAD	D	501	44/44	0.95	0.13	44,52,64,65	0
6	PO4	A	506	5/5	0.95	0.14	55,57,58,59	0
3	ADE	A	502	10/10	0.95	0.18	38,43,45,46	0
3	ADE	D	502	10/10	0.96	0.15	63,66,69,70	0
6	PO4	A	507	5/5	0.96	0.18	45,45,50,58	0
6	PO4	B	505	5/5	0.96	0.21	60,61,63,71	5
2	NAD	A	501	44/44	0.96	0.17	37,45,51,52	0
6	PO4	D	504	5/5	0.96	0.37	68,73,77,77	5
5	K	D	503	1/1	0.97	0.10	54,54,54,54	0
5	K	B	503	1/1	0.98	0.05	48,48,48,48	0
6	PO4	B	504	5/5	0.98	0.23	71,72,75,79	0
5	K	A	504	1/1	0.99	0.10	40,40,40,40	0

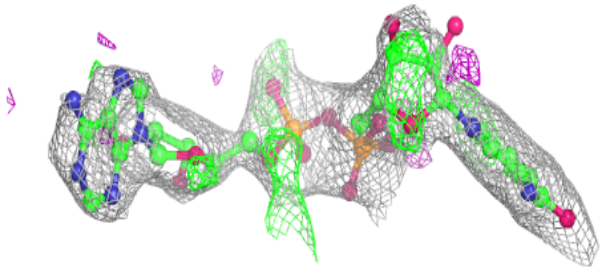
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

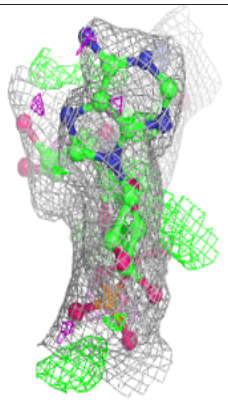
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAD C 501:

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

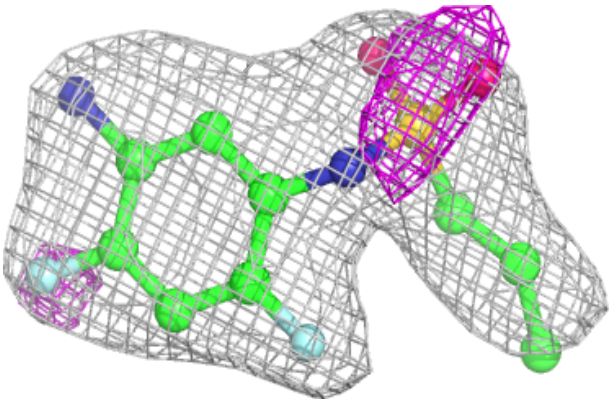


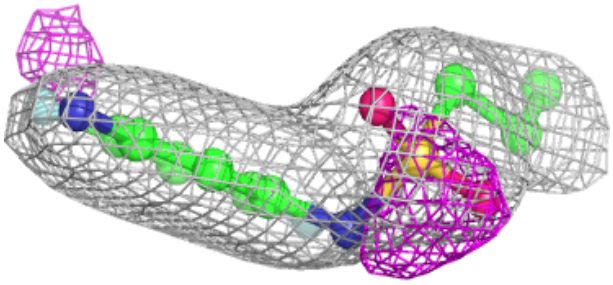


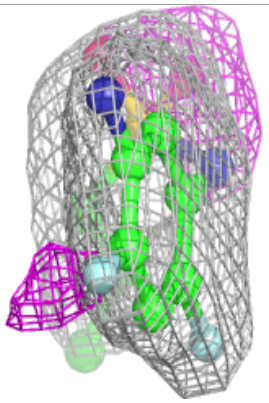


Electron density around SY4 A 508:

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

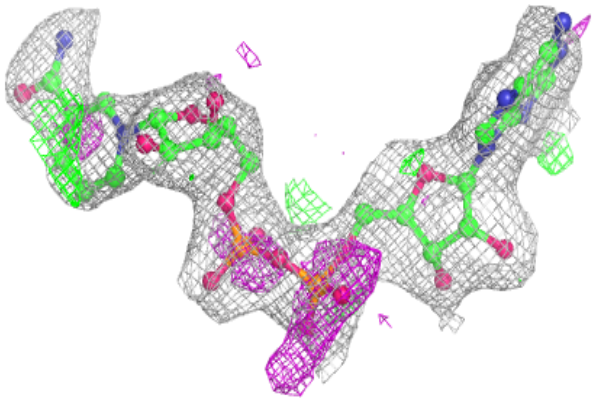


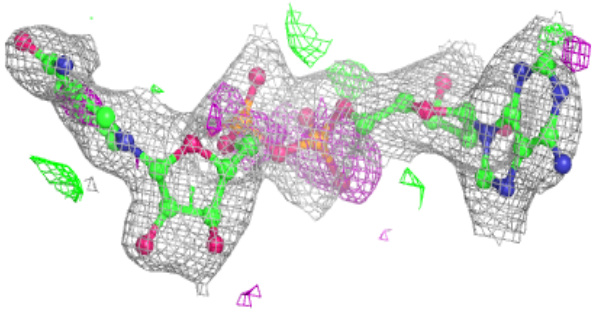


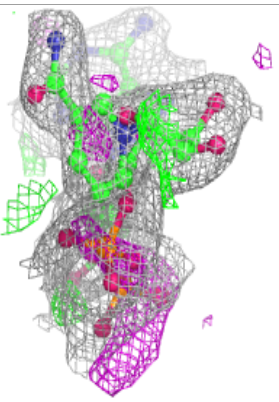


Electron density around NAD B 501:

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

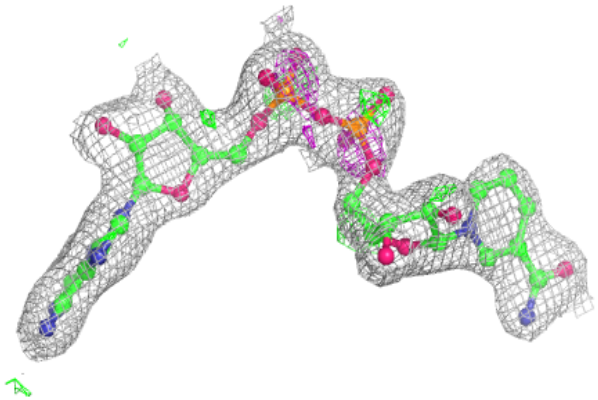


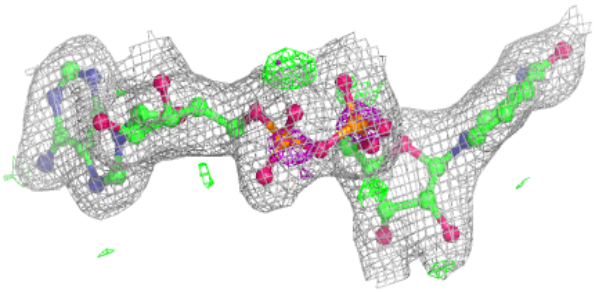


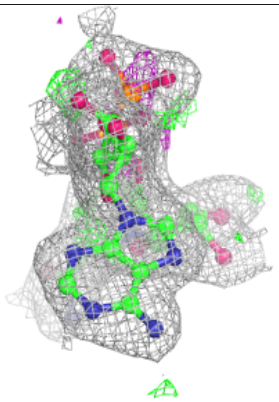


Electron density around NAD D 501:

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

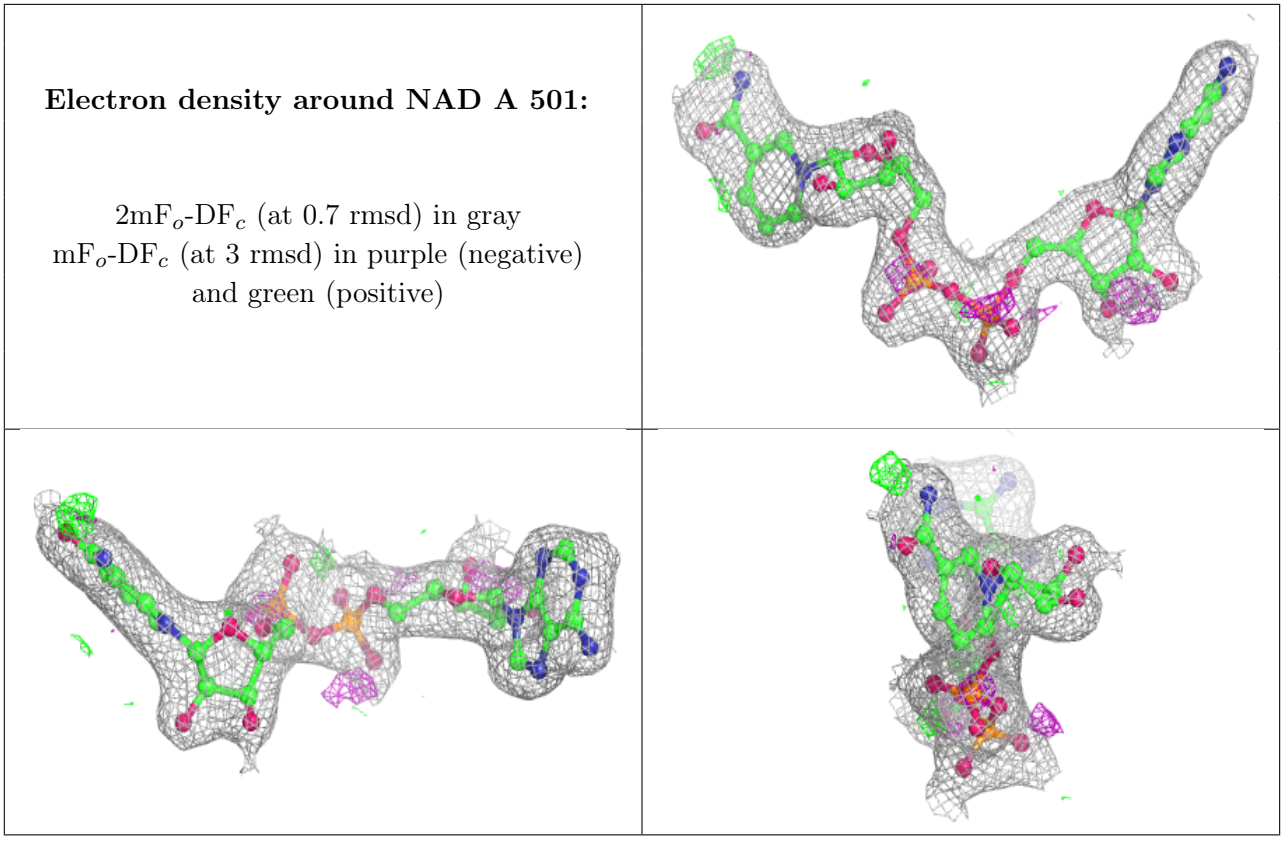






Electron density around NAD A 501:

$2mF_o$-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.