Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:23 PM UTC

PDB ID	:	7O4V / pdb_00007o4v
Title	:	Structure of Mycobacterium tuberculosis beta-oxidation trifunctional enzyme in complex with oxidized nicotinamide adenine dinucleotide
Authors	:	Dalwani, S.; Wierenga, R.K.; Venkatesan, R.
Deposited on	:	2021-04-07
Resolution	:	2.42 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

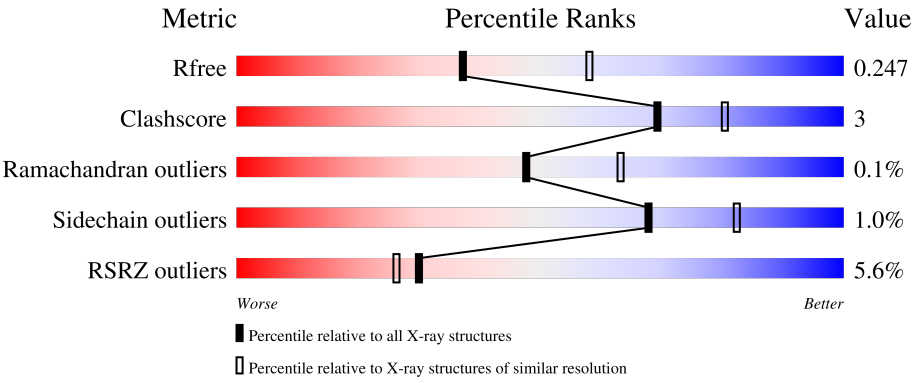
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.42 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	736	4% 89% 9%
1	B	736	6% 91% 8%
2	C	403	8% 89% 11%
2	D	403	7% 91% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	806	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17045 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 3-hydroxyacyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	729	Total	C	N	O	S	0	0	0
			5416	3425	933	1037	21			
1	A	729	Total	C	N	O	S	0	0	0
			5420	3428	934	1037	21			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	initiating methionine	UNP O53872
B	-14	GLY	-	expression tag	UNP O53872
B	-13	SER	-	expression tag	UNP O53872
B	-12	SER	-	expression tag	UNP O53872
B	-11	HIS	-	expression tag	UNP O53872
B	-10	HIS	-	expression tag	UNP O53872
B	-9	HIS	-	expression tag	UNP O53872
B	-8	HIS	-	expression tag	UNP O53872
B	-7	HIS	-	expression tag	UNP O53872
B	-6	HIS	-	expression tag	UNP O53872
B	-5	SER	-	expression tag	UNP O53872
B	-4	GLN	-	expression tag	UNP O53872
B	-3	ASP	-	expression tag	UNP O53872
B	-2	PRO	-	expression tag	UNP O53872
B	-1	ASN	-	expression tag	UNP O53872
B	0	SER	-	expression tag	UNP O53872
A	-15	MET	-	initiating methionine	UNP O53872
A	-14	GLY	-	expression tag	UNP O53872
A	-13	SER	-	expression tag	UNP O53872
A	-12	SER	-	expression tag	UNP O53872
A	-11	HIS	-	expression tag	UNP O53872
A	-10	HIS	-	expression tag	UNP O53872
A	-9	HIS	-	expression tag	UNP O53872
A	-8	HIS	-	expression tag	UNP O53872
A	-7	HIS	-	expression tag	UNP O53872

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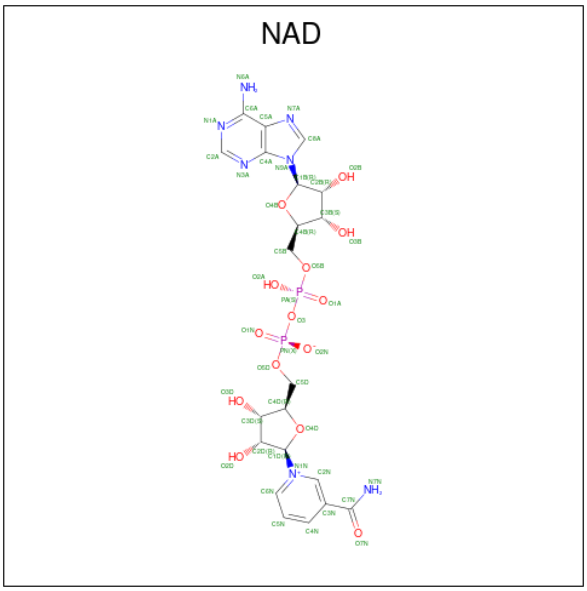
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	HIS	-	expression tag	UNP O53872
A	-5	SER	-	expression tag	UNP O53872
A	-4	GLN	-	expression tag	UNP O53872
A	-3	ASP	-	expression tag	UNP O53872
A	-2	PRO	-	expression tag	UNP O53872
A	-1	ASN	-	expression tag	UNP O53872
A	0	SER	-	expression tag	UNP O53872

- Molecule 2 is a protein called Putative acyltransferase Rv0859.

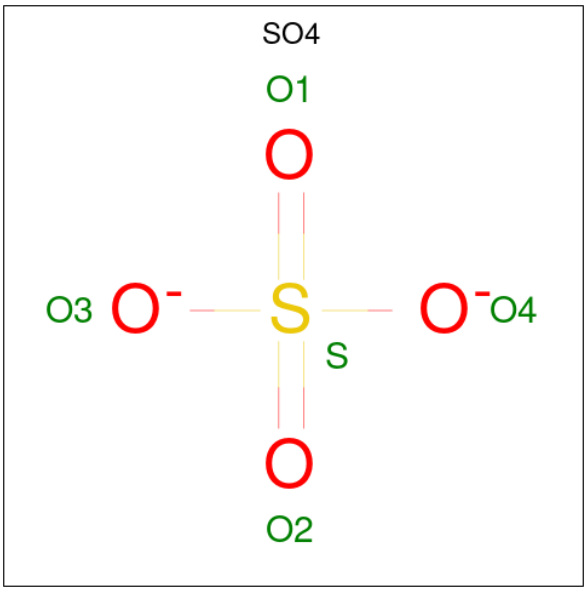
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	401	Total	C	N	O	S	0	0	0
			2955	1845	524	570	16			
2	C	401	Total	C	N	O	S	0	0	0
			2952	1843	524	570	15			

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

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

- Molecule 5 is water.

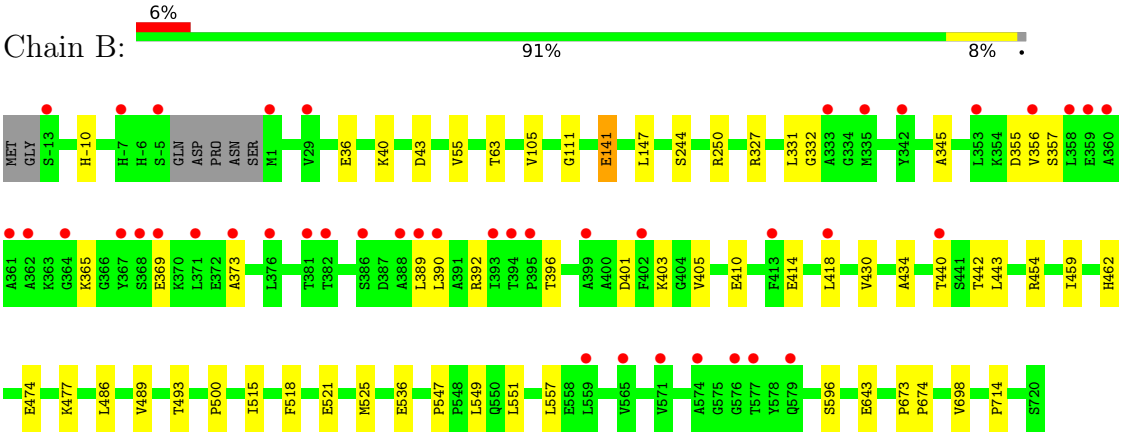
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	19	Total O 19 19	0	0
5	D	29	Total O 29 29	0	0
5	C	21	Total O 21 21	0	0
5	A	20	Total O 20 20	0	0

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.

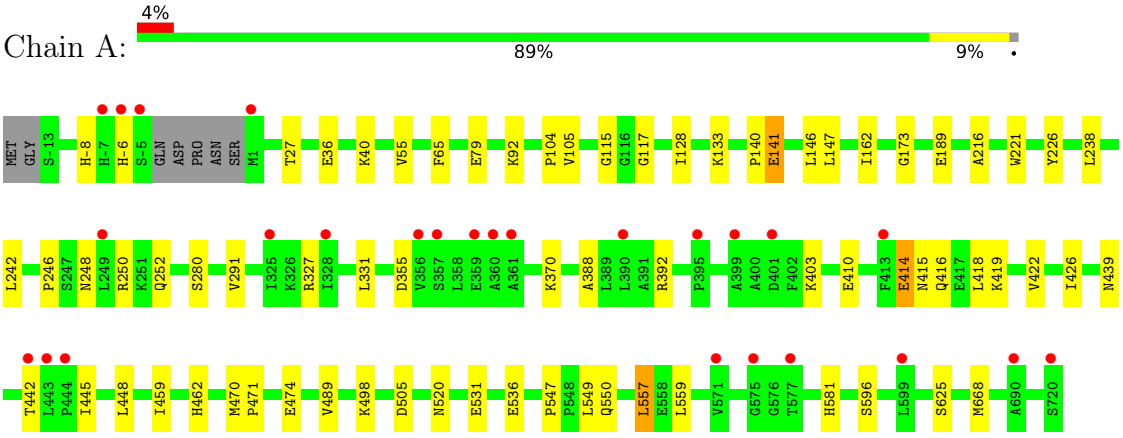
• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

Chain B:



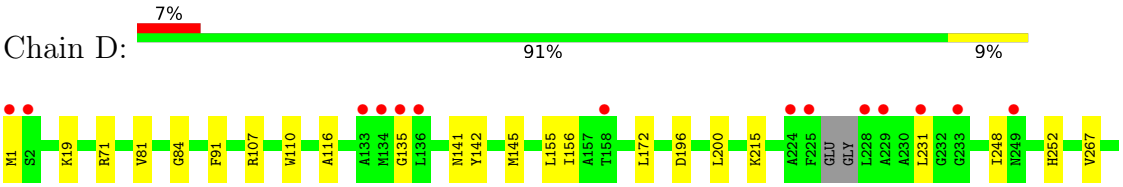
• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

Chain A:



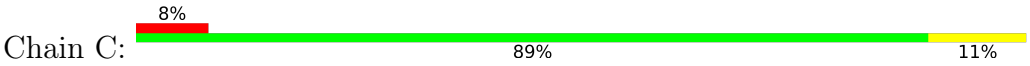
• Molecule 2: Putative acyltransferase Rv0859

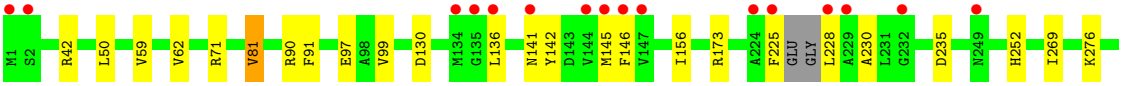
Chain D:

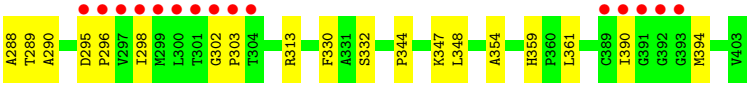




• Molecule 2: Putative acyltransferase Rv0859







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	243.75Å 133.24Å 115.60Å 90.00° 110.14° 90.00°	Depositor
Resolution (Å)	72.92 – 2.42 72.92 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.3 (72.92-2.42) 99.3 (72.92-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.214 , 0.244 0.217 , 0.247	Depositor DCC
R_{free} test set	6528 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	67.0	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17045	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: NAD, 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	0.09	0/5523	0.27	0/7477
1	B	0.10	0/5519	0.28	0/7473
2	C	0.09	0/2995	0.29	0/4055
2	D	0.09	0/2998	0.28	0/4058
All	All	0.09	0/17035	0.28	0/23063

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	5420	0	5442	41	0
1	B	5416	0	5431	34	0
2	C	2952	0	2974	29	0
2	D	2955	0	2981	25	0
3	A	44	0	26	3	0
3	B	44	0	26	3	0
4	A	25	0	0	2	0
4	B	20	0	0	0	0
4	C	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	40	0	0	0	0
5	A	20	0	0	0	0
5	B	19	0	0	0	0
5	C	21	0	0	0	0
5	D	29	0	0	1	0
All	All	17045	0	16880	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 3.

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:B:365:LYS:NZ	1:B:390:LEU:O	2.20	0.73
1:A:327:ARG:NH1	1:A:403:LYS:O	2.25	0.69
1:B:434:ALA:O	1:B:454:ARG:NH2	2.27	0.67
2:C:289:THR:O	2:C:313:ARG:NH1	2.29	0.66
1:B:250:ARG:NH1	2:D:142:TYR:O	2.29	0.66
2:D:1:MET:HG2	2:D:107:ARG:HH22	1.62	0.65
2:C:173:ARG:NH2	2:C:348:LEU:O	2.25	0.64
1:B:557:LEU:HD12	1:B:596:SER:HA	1.80	0.64
3:B:801:NAD:H51N	3:B:801:NAD:H2N	1.80	0.64
1:B:459:ILE:HG21	1:B:489:VAL:HG21	1.82	0.61
1:B:36:GLU:HG3	1:B:40:LYS:HE3	1.83	0.59
1:A:-6:HIS:ND1	4:A:806:SO4:O4	2.34	0.57
1:A:104:PRO:HG3	1:A:216:ALA:HB1	1.87	0.57
2:D:313:ARG:NH1	5:D:601:HOH:O	2.38	0.56
1:B:331:LEU:HB2	1:B:410:GLU:HA	1.88	0.54
1:B:405:VAL:HB	1:B:430:VAL:HG12	1.89	0.54
1:B:418:LEU:HD11	3:B:801:NAD:H61A	1.73	0.54
1:B:462:HIS:HB3	1:B:474:GLU:HB3	1.90	0.54
1:B:355:ASP:OD2	3:B:801:NAD:O2B	2.24	0.53
1:A:-8:HIS:ND1	4:A:806:SO4:O2	2.34	0.53
1:A:36:GLU:HG3	1:A:40:LYS:HE3	1.90	0.53
2:D:299:MET:HE3	2:D:392:GLY:H	1.73	0.53
1:A:459:ILE:HG21	1:A:489:VAL:HG21	1.90	0.52
1:A:331:LEU:HD13	1:A:422:VAL:HG12	1.90	0.52
2:D:172:LEU:HD22	2:D:215:LYS:HG3	1.90	0.52
1:B:414:GLU:OE1	1:B:442:THR:OG1	2.24	0.52
1:B:440:THR:HG21	1:B:443:LEU:HB2	1.92	0.52
2:C:91:PHE:HB2	2:C:390:ILE:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:142:TYR:O	1:A:250:ARG:NH1	2.43	0.52
2:C:295:ASP:HB3	2:C:298:ILE:HG22	1.91	0.52
2:C:302:GLY:N	2:C:303:PRO:HD2	2.24	0.52
2:C:62:VAL:HG21	2:C:130:ASP:HA	1.92	0.51
1:A:439:ASN:O	1:A:439:ASN:ND2	2.43	0.51
2:C:252:HIS:HE1	2:C:332:SER:H	1.59	0.50
2:D:252:HIS:HE1	2:D:332:SER:H	1.58	0.50
1:A:547:PRO:HG2	1:A:550:GLN:HB3	1.94	0.50
2:D:156:ILE:HG12	2:D:298:ILE:HD11	1.94	0.49
2:C:156:ILE:HG12	2:C:298:ILE:HD11	1.94	0.49
1:A:531:GLU:HA	1:A:625:SER:HB3	1.93	0.49
2:D:71:ARG:CZ	2:C:394:MET:HG2	2.42	0.49
1:B:250:ARG:NH1	2:D:145:MET:HG2	2.28	0.49
1:A:410:GLU:OE2	1:A:419:LYS:NZ	2.40	0.49
1:A:470:MET:O	1:A:498:LYS:NZ	2.42	0.48
1:B:477:LYS:HD3	1:B:486:LEU:HD22	1.95	0.48
2:C:99:VAL:HG13	2:C:269:ILE:HD11	1.94	0.48
1:A:162:ILE:HD12	1:A:238:LEU:HD21	1.95	0.48
1:B:-10:HIS:NE2	1:B:43:ASP:OD2	2.37	0.48
1:B:244:SER:HB3	2:D:231:LEU:HD13	1.95	0.48
1:A:388:ALA:O	1:A:392:ARG:HG3	2.13	0.48
2:D:116:ALA:O	2:D:267:VAL:N	2.39	0.48
1:A:370:LYS:HB2	1:A:370:LYS:HE3	1.74	0.48
1:A:414:GLU:OE1	1:A:442:THR:OG1	2.31	0.48
2:D:252:HIS:CE1	2:D:332:SER:H	2.32	0.47
2:D:84:GLY:HA2	2:C:394:MET:HE3	1.96	0.47
1:B:63:THR:HA	1:B:111:GLY:HA3	1.96	0.47
2:C:344:PRO:HG2	2:C:347:LYS:HE3	1.96	0.46
1:A:418:LEU:HD11	3:A:801:NAD:N6A	2.31	0.46
2:C:252:HIS:CE1	2:C:330:PHE:HB3	2.51	0.45
2:C:252:HIS:CE1	2:C:332:SER:H	2.35	0.45
1:A:355:ASP:OD1	3:A:801:NAD:O2B	2.29	0.45
2:D:81:VAL:HG21	2:C:296:PRO:HD3	1.98	0.45
1:A:221:TRP:HA	1:A:226:TYR:CG	2.52	0.45
1:B:396:THR:OG1	1:B:401:ASP:OD2	2.33	0.45
1:B:536:GLU:CD	1:B:547:PRO:HB2	2.42	0.45
1:A:248:ASN:O	1:A:252:GLN:HG2	2.16	0.45
2:D:196:ASP:OD1	2:D:200:LEU:N	2.49	0.45
1:A:141:GLU:HG3	1:A:147:LEU:C	2.41	0.44
1:B:515:ILE:HD11	1:B:551:LEU:HD21	1.99	0.44
2:C:141:ASN:HB3	1:A:246:PRO:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:394:MET:HG2	2:C:71:ARG:CZ	2.47	0.44
1:B:55:VAL:HB	1:B:105:VAL:HG22	2.00	0.44
1:B:392:ARG:HD3	1:B:392:ARG:HA	1.74	0.44
2:D:135:GLY:HA2	2:D:141:ASN:HD22	1.83	0.44
2:D:390:ILE:HD12	2:D:394:MET:HB2	1.98	0.44
1:B:698:VAL:HG13	1:B:714:PRO:HG3	2.00	0.43
1:A:146:LEU:HD22	1:A:291:VAL:HG22	2.00	0.43
1:A:520:ASN:HB3	1:A:581:HIS:CE1	2.54	0.43
1:A:557:LEU:HB2	1:A:596:SER:O	2.18	0.43
1:A:418:LEU:HD11	3:A:801:NAD:H61A	1.83	0.43
2:D:328:GLU:HB3	2:D:355:ILE:HG13	1.99	0.43
2:C:146:PHE:HZ	2:C:228:LEU:HD13	1.83	0.43
1:A:416:GLN:HG3	1:A:448:LEU:HD23	2.01	0.43
1:B:369:GLU:O	1:B:373:ALA:N	2.46	0.43
1:A:536:GLU:CD	1:A:547:PRO:HB2	2.44	0.43
2:C:225:PHE:HA	2:C:230:ALA:HB2	2.01	0.43
2:C:354:ALA:HB1	2:C:359:HIS:HB2	2.00	0.43
1:A:536:GLU:CD	1:A:549:LEU:HB2	2.44	0.43
1:B:250:ARG:HH12	2:D:145:MET:HG2	1.84	0.43
2:C:90:ARG:HH21	2:C:97:GLU:CD	2.27	0.43
1:B:521:GLU:O	1:B:525:MET:HG3	2.19	0.42
2:C:71:ARG:HH22	2:C:81:VAL:HG22	1.84	0.42
2:D:155:LEU:HD13	2:D:248:ILE:HG12	2.01	0.42
1:B:493:THR:HG21	1:B:500:PRO:HB3	2.01	0.42
2:C:136:LEU:HD22	1:A:242:LEU:HD23	2.02	0.42
1:B:345:ALA:O	1:B:389:LEU:HD22	2.20	0.42
2:D:296:PRO:HD3	2:C:81:VAL:HG21	2.02	0.42
2:C:290:ALA:HA	2:C:313:ARG:HH12	1.85	0.42
1:A:65:PHE:HB3	1:A:117:GLY:CA	2.49	0.42
1:A:462:HIS:HB3	1:A:474:GLU:HB3	2.01	0.42
1:A:128:ILE:HG12	1:A:189:GLU:HB2	2.00	0.42
1:A:92:LYS:NZ	1:A:280:SER:O	2.53	0.42
1:B:141:GLU:HG3	1:B:147:LEU:C	2.45	0.41
1:B:327:ARG:HG2	1:B:405:VAL:HG22	2.02	0.41
2:D:110:TRP:CZ2	2:C:288:ALA:HA	2.55	0.41
1:A:55:VAL:HB	1:A:105:VAL:HG22	2.01	0.41
2:D:91:PHE:HB2	2:D:390:ILE:HG23	2.02	0.41
2:D:295:ASP:HB3	2:D:298:ILE:HG22	2.03	0.41
1:A:115:GLY:HA2	1:A:141:GLU:OE1	2.19	0.41
1:A:140:PRO:HA	1:A:173:GLY:HA3	2.02	0.41
2:C:390:ILE:HD12	2:C:394:MET:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ILE:N	1:A:505:ASP:OD2	2.47	0.41
2:C:59:VAL:HG21	2:C:361:LEU:HB3	2.02	0.41
1:B:536:GLU:CD	1:B:549:LEU:HB2	2.46	0.41
1:B:673:PRO:HA	1:B:674:PRO:HD3	1.94	0.41
1:A:415:ASN:HB3	1:A:418:LEU:HB3	2.03	0.40
1:B:518:PHE:HB2	1:B:643:GLU:CD	2.46	0.40
1:A:471:PRO:HG2	1:A:668:MET:HB3	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	725/736 (98%)	700 (97%)	24 (3%)	1 (0%)	48 63
1	B	725/736 (98%)	693 (96%)	31 (4%)	1 (0%)	48 63
2	C	397/403 (98%)	385 (97%)	11 (3%)	1 (0%)	36 49
2	D	397/403 (98%)	387 (98%)	10 (2%)	0	100 100
All	All	2244/2278 (98%)	2165 (96%)	76 (3%)	3 (0%)	48 63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	145	MET
1	A	414	GLU
1	B	332	GLY

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	557/566 (98%)	550 (99%)	7 (1%)	61	78
1	B	556/566 (98%)	552 (99%)	4 (1%)	76	87
2	C	307/310 (99%)	302 (98%)	5 (2%)	55	74
2	D	308/310 (99%)	306 (99%)	2 (1%)	78	88
All	All	1728/1752 (99%)	1710 (99%)	18 (1%)	68	82

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	141	GLU
1	B	356	VAL
1	B	357	SER
1	B	403	LYS
2	D	19	LYS
2	D	369	LEU
2	C	42	ARG
2	C	50	LEU
2	C	81	VAL
2	C	235	ASP
2	C	276	LYS
1	A	27	THR
1	A	79	GLU
1	A	133	LYS
1	A	141	GLU
1	A	426	ILE
1	A	557	LEU
1	A	559	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	252	GLN
1	B	294	GLN
1	B	561	HIS
1	B	681	GLN
2	C	351	ASN

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Mol	Chain	Res	Type
1	A	126	HIS
1	A	136	GLN
1	A	248	ASN
1	A	294	GLN
1	A	681	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

27 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	$\#\|Z\| > 2$
4	SO4	D	502	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	B	805	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	C	504	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	A	805	-	4,4,4	0.24	0	6,6,6	0.08	0
3	NAD	B	801	-	46,48,48	0.65	2 (4%)	64,73,73	0.71	1 (1%)
4	SO4	C	503	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	D	503	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	C	501	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	C	508	-	4,4,4	0.24	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	B	804	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	C	506	-	4,4,4	0.24	0	6,6,6	0.09	0
4	SO4	D	501	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	D	505	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	C	507	-	4,4,4	0.23	0	6,6,6	0.07	0
3	NAD	A	801	-	46,48,48	0.61	1 (2%)	64,73,73	1.02	8 (12%)
4	SO4	C	505	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	D	506	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	A	806	-	4,4,4	0.24	0	6,6,6	0.14	0
4	SO4	C	502	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	B	802	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	A	802	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	D	508	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	B	803	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	A	804	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	D	507	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	A	803	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	D	504	-	4,4,4	0.24	0	6,6,6	0.07	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
3	NAD	A	801	-	-	5/30/62/62	0/5/5/5
3	NAD	B	801	-	-	14/30/62/62	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	NAD	C2N-N1N	2.39	1.37	1.35
3	B	801	NAD	C2N-N1N	2.33	1.37	1.35
3	B	801	NAD	O4D-C1D	2.23	1.43	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	801	NAD	O4B-C1B-N9A	3.00	113.86	108.09
3	B	801	NAD	C6N-N1N-C2N	-2.84	119.46	121.88
3	A	801	NAD	C1B-N9A-C8A	2.51	132.68	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	801	NAD	C6N-N1N-C2N	-2.50	119.75	121.88
3	A	801	NAD	C3B-C2B-C1B	-2.38	96.96	101.46
3	A	801	NAD	O4B-C1B-C2B	-2.37	101.54	106.62
3	A	801	NAD	C4A-N9A-C1B	-2.29	121.27	126.63
3	A	801	NAD	C4B-O4B-C1B	-2.25	104.51	109.47
3	A	801	NAD	O3B-C3B-C2B	-2.11	105.04	111.82

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	801	NAD	C5B-O5B-PA-O1A
3	B	801	NAD	C5B-O5B-PA-O2A
3	B	801	NAD	C5B-O5B-PA-O3
3	B	801	NAD	O4D-C1D-N1N-C2N
3	B	801	NAD	O4D-C1D-N1N-C6N
3	B	801	NAD	C2D-C1D-N1N-C2N
3	B	801	NAD	C2D-C1D-N1N-C6N
3	A	801	NAD	C5B-O5B-PA-O1A
3	A	801	NAD	C5B-O5B-PA-O2A
3	A	801	NAD	C5B-O5B-PA-O3
3	B	801	NAD	C3B-C4B-C5B-O5B
3	B	801	NAD	O4B-C4B-C5B-O5B
3	A	801	NAD	C3B-C4B-C5B-O5B
3	B	801	NAD	PA-O3-PN-O1N
3	B	801	NAD	PA-O3-PN-O5D
3	B	801	NAD	C4D-C5D-O5D-PN
3	A	801	NAD	C4B-C5B-O5B-PA
3	B	801	NAD	C4B-C5B-O5B-PA
3	B	801	NAD	O4D-C4D-C5D-O5D

There are no ring outliers.

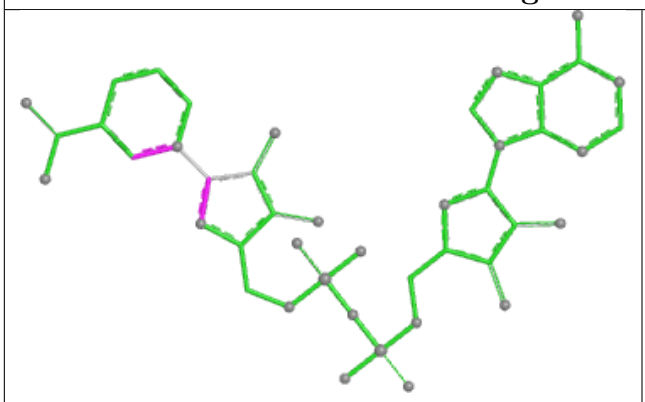
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	NAD	3	0
3	A	801	NAD	3	0
4	A	806	SO4	2	0

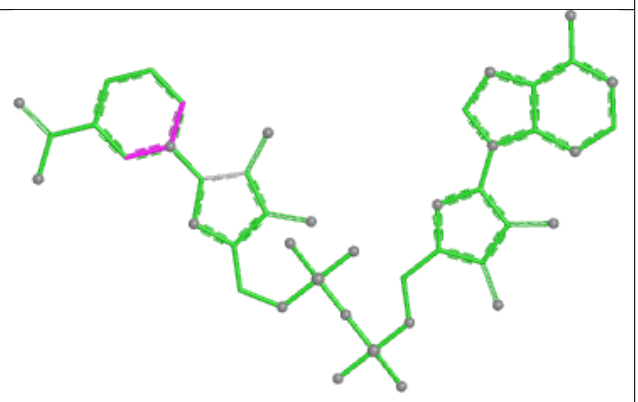
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

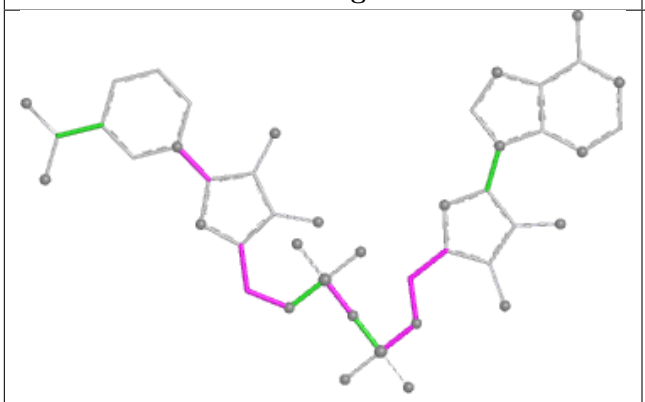
Ligand NAD B 801



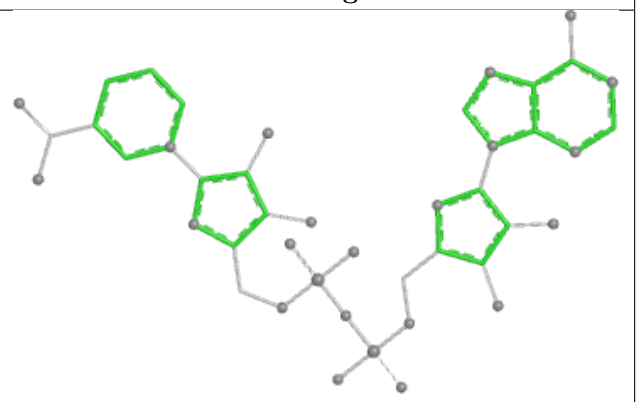
Bond lengths



Bond angles

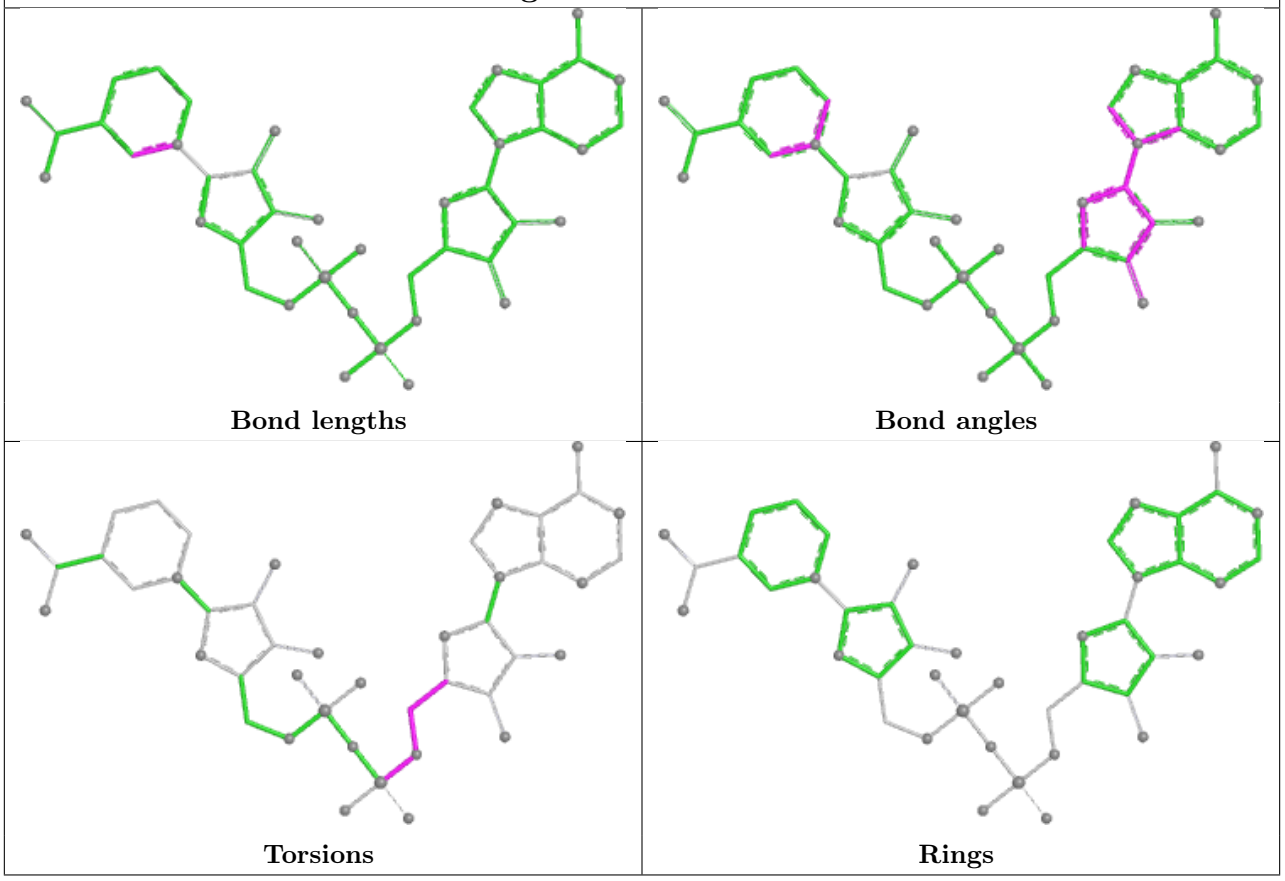


Torsions



Rings

Ligand NAD A 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	729/736 (99%)	0.31	26 (3%)	46	42	53, 89, 154, 198	0
1	B	729/736 (99%)	0.41	43 (5%)	28	24	58, 85, 149, 191	0
2	C	401/403 (99%)	0.17	31 (7%)	19	16	53, 69, 113, 148	0
2	D	401/403 (99%)	0.13	27 (6%)	24	20	51, 64, 105, 149	0
All	All	2260/2278 (99%)	0.29	127 (5%)	30	26	51, 80, 146, 198	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	389	LEU	7.1
1	B	-5	SER	5.9
2	D	298	ILE	5.6
1	A	-7	HIS	5.6
2	C	1	MET	5.2
2	D	389	CYS	5.0
2	C	301	THR	5.0
2	D	135	GLY	4.9
2	C	296	PRO	4.9
2	C	136	LEU	4.8
1	B	571	VAL	4.8
2	D	228	LEU	4.7
2	C	392	GLY	4.6
2	C	228	LEU	4.6
2	D	390	ILE	4.5
2	D	300	LEU	4.4
1	B	393	ILE	4.4
2	C	298	ILE	4.3
1	B	368	SER	4.3
1	A	720	SER	4.2
1	B	358	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
2	D	297	VAL	4.0
2	D	301	THR	4.0
1	B	390	LEU	3.9
1	B	413	PHE	3.9
1	B	559	LEU	3.9
2	D	136	LEU	3.9
1	B	367	TYR	3.8
1	B	388	ALA	3.7
1	B	333	ALA	3.7
1	A	-5	SER	3.6
2	D	2	SER	3.6
2	C	300	LEU	3.6
2	C	390	ILE	3.6
2	C	389	CYS	3.5
2	C	2	SER	3.5
1	B	353	LEU	3.5
2	D	1	MET	3.4
2	C	134	MET	3.4
1	B	371	LEU	3.3
2	C	303	PRO	3.3
1	B	356	VAL	3.3
1	B	395	PRO	3.2
2	C	302	GLY	3.2
1	B	399	ALA	3.2
1	B	579	GLN	3.2
1	A	356	VAL	3.1
1	A	-6	HIS	3.1
2	C	229	ALA	3.0
2	C	299	MET	2.9
1	B	382	THR	2.9
2	D	225	PHE	2.9
2	D	303	PRO	2.9
1	A	413	PHE	2.9
2	C	225	PHE	2.9
2	D	134	MET	2.9
1	A	571	VAL	2.9
2	C	297	VAL	2.9
1	B	362	ALA	2.8
1	B	381	THR	2.8
1	A	599	LEU	2.8
1	B	577	THR	2.8
1	B	342	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	249	ASN	2.7
1	B	-7	HIS	2.7
1	A	395	PRO	2.7
1	A	443	LEU	2.7
1	B	394	THR	2.7
1	B	1	MET	2.6
1	B	376	LEU	2.6
1	B	565	VAL	2.6
2	D	249	ASN	2.6
2	C	135	GLY	2.6
1	A	401	ASP	2.5
2	C	144	VAL	2.5
2	D	233	GLY	2.5
2	C	146	PHE	2.5
1	B	402	PHE	2.5
1	B	418	LEU	2.5
1	A	390	LEU	2.5
1	B	360	ALA	2.5
2	C	304	THR	2.5
2	C	295	ASP	2.4
2	C	224	ALA	2.4
1	A	357	SER	2.4
1	B	359	GLU	2.4
2	D	302	GLY	2.4
1	A	1	MET	2.4
1	B	364	GLY	2.4
1	B	386	SER	2.4
1	B	29	VAL	2.4
1	B	373	ALA	2.3
1	A	361	ALA	2.2
2	D	224	ALA	2.2
2	D	133	ALA	2.2
1	B	576	GLY	2.2
2	D	391	GLY	2.2
2	C	145	MET	2.2
1	A	690	ALA	2.2
2	C	141	ASN	2.2
1	A	577	THR	2.2
1	A	325	ILE	2.2
2	D	231	LEU	2.2
2	C	393	GLY	2.2
1	B	-13	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	361	ALA	2.1
1	A	399	ALA	2.1
2	D	392	GLY	2.1
2	D	295	ASP	2.1
2	C	147	VAL	2.1
2	D	299	MET	2.1
2	D	229	ALA	2.1
1	A	442	THR	2.1
2	D	388	LEU	2.1
1	A	359	GLU	2.1
1	A	249	LEU	2.1
1	B	369	GLU	2.1
1	B	574	ALA	2.1
1	A	575	GLY	2.1
2	C	232	GLY	2.1
1	A	444	PRO	2.1
2	C	391	GLY	2.0
1	B	335	MET	2.0
1	A	360	ALA	2.0
1	B	440	THR	2.0
1	A	328	ILE	2.0
2	D	158	THR	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 oligosaccharides 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
4	SO4	A	806	5/5	0.31	0.14	192,202,238,403	0

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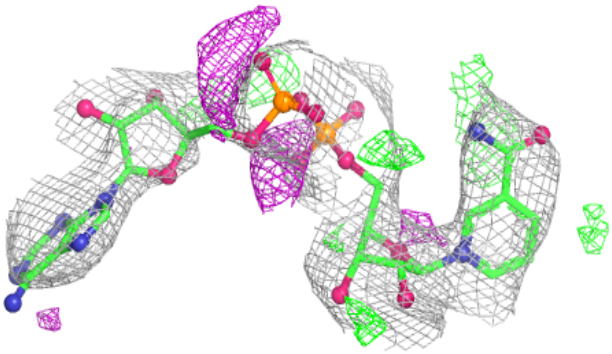
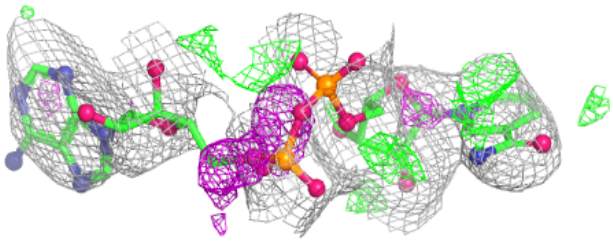
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	C	507	5/5	0.64	0.10	112,114,128,140	0
4	SO4	B	805	5/5	0.66	0.09	125,130,150,152	0
4	SO4	A	804	5/5	0.70	0.09	114,125,137,139	0
4	SO4	A	805	5/5	0.74	0.07	118,129,147,155	0
4	SO4	B	804	5/5	0.74	0.09	98,98,128,129	0
3	NAD	B	801	44/44	0.76	0.15	107,147,161,163	0
4	SO4	C	508	5/5	0.80	0.07	107,112,128,137	0
4	SO4	D	507	5/5	0.82	0.09	82,88,101,106	0
3	NAD	A	801	44/44	0.82	0.15	114,142,157,164	0
4	SO4	C	506	5/5	0.83	0.08	93,96,107,116	0
4	SO4	D	504	5/5	0.87	0.08	94,97,99,103	0
4	SO4	D	508	5/5	0.87	0.19	73,74,78,81	5
4	SO4	B	803	5/5	0.88	0.07	111,115,119,120	0
4	SO4	D	506	5/5	0.89	0.07	82,88,108,111	0
4	SO4	A	803	5/5	0.91	0.06	89,99,104,105	0
4	SO4	C	505	5/5	0.91	0.07	92,95,104,109	0
4	SO4	C	502	5/5	0.91	0.06	86,96,98,99	0
4	SO4	A	802	5/5	0.91	0.07	80,89,95,96	0
4	SO4	D	505	5/5	0.92	0.06	95,96,100,110	0
4	SO4	B	802	5/5	0.93	0.07	89,90,96,97	0
4	SO4	D	501	5/5	0.94	0.09	73,74,81,84	0
4	SO4	D	503	5/5	0.94	0.04	79,83,101,111	0
4	SO4	C	503	5/5	0.94	0.06	77,77,84,93	0
4	SO4	D	502	5/5	0.95	0.06	71,73,86,88	0
4	SO4	C	501	5/5	0.95	0.10	73,75,75,78	5
4	SO4	C	504	5/5	0.95	0.04	87,92,99,104	0

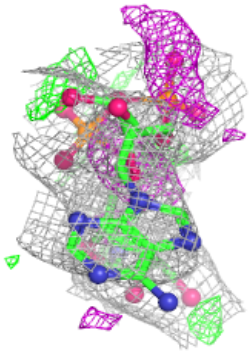
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD B 801:

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

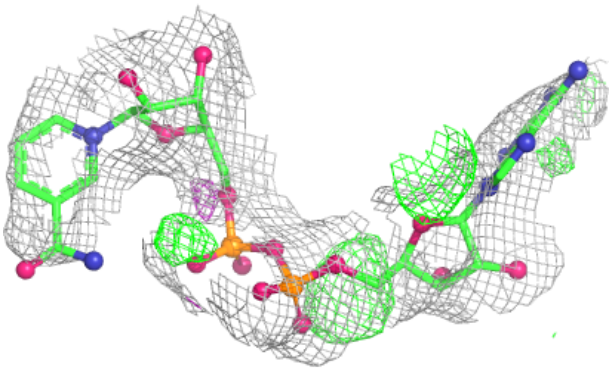


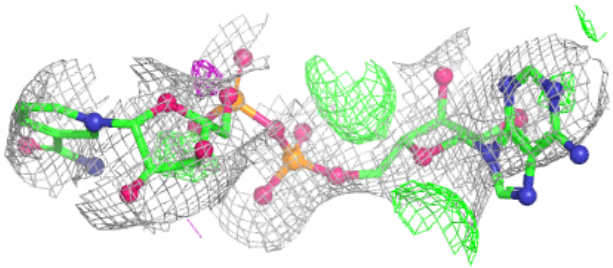


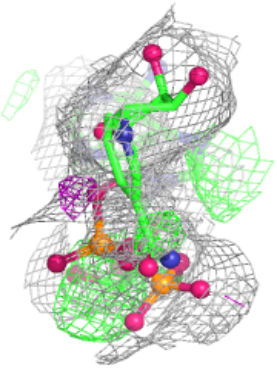


Electron density around NAD A 801:

$2mF_o$-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.