



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 02:37 pm BST

PDB ID : 1NVM
Title : Crystal structure of a bifunctional aldolase-dehydrogenase : sequestering a reactive and volatile intermediate
Authors : Manjasetty, A.B.; Powlowski, J.; Vrielink, A.
Deposited on : 2003-02-04
Resolution : 1.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

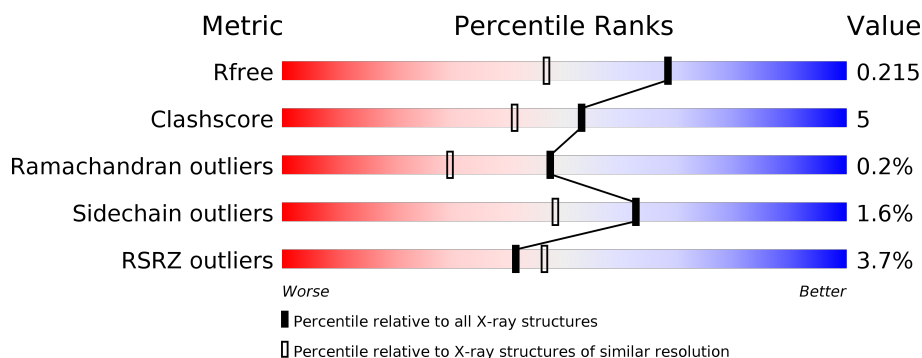
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	345	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>•</div> </div> </div>
1	C	345	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>••</div> </div> </div>
1	E	345	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>••</div> </div> </div>
1	G	345	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>••</div> </div> </div>
2	B	312	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>•</div> </div> </div>
2	D	312	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	312	
2	H	312	

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
6	MPD	B	3528	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22561 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 4-hydroxy-2-oxovalerate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	13	5	0
			2599	1619	470	491	19			
1	C	337	Total	C	N	O	S	5	4	0
			2568	1598	462	489	19			
1	E	338	Total	C	N	O	S	8	6	0
			2579	1606	461	492	20			
1	G	339	Total	C	N	O	S	12	5	0
			2588	1613	467	489	19			

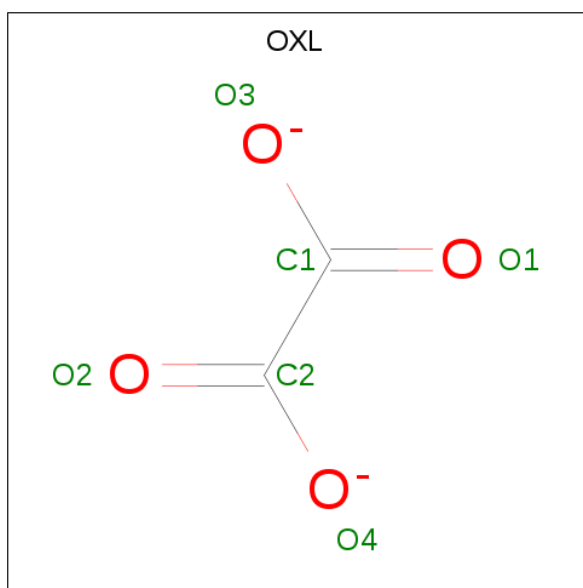
- Molecule 2 is a protein called acetaldehyde dehydrogenase (acylating).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	312	Total	C	N	O	S	19	13	0
			2316	1463	392	442	19			
2	D	308	Total	C	N	O	S	15	10	0
			2280	1441	389	433	17			
2	F	309	Total	C	N	O	S	10	13	0
			2289	1450	387	434	18			
2	H	307	Total	C	N	O	S	20	7	0
			2263	1433	384	430	16			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

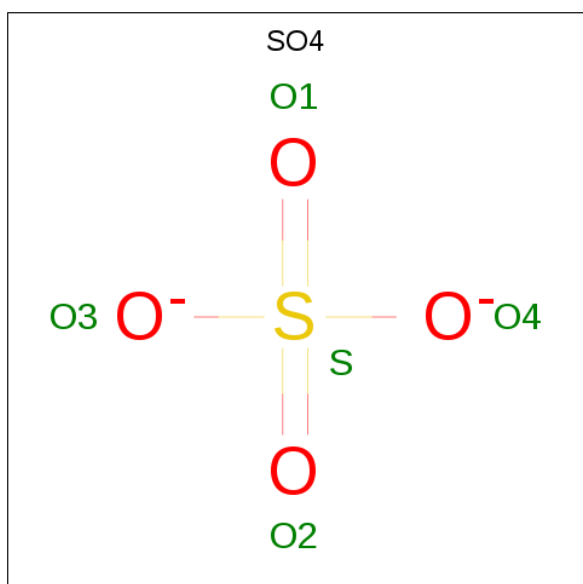
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	E	1	Total	Mn	0	0
			1	1		

- Molecule 4 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



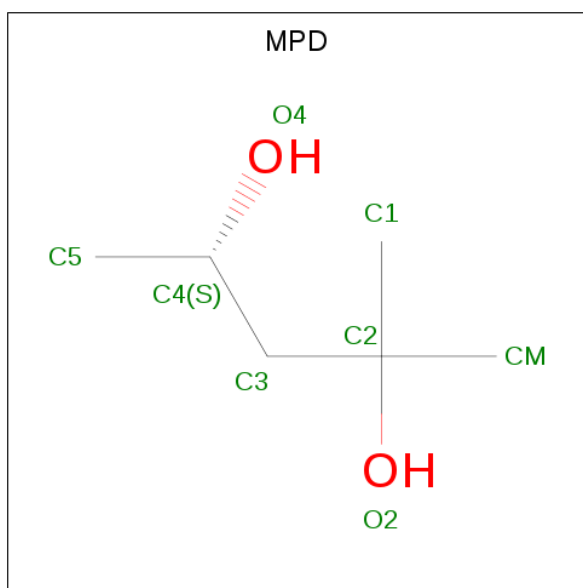
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	2	4		
4	C	1	Total	C	O	0	0
			6	2	4		
4	E	1	Total	C	O	0	0
			6	2	4		
4	G	1	Total	C	O	0	0
			6	2	4		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



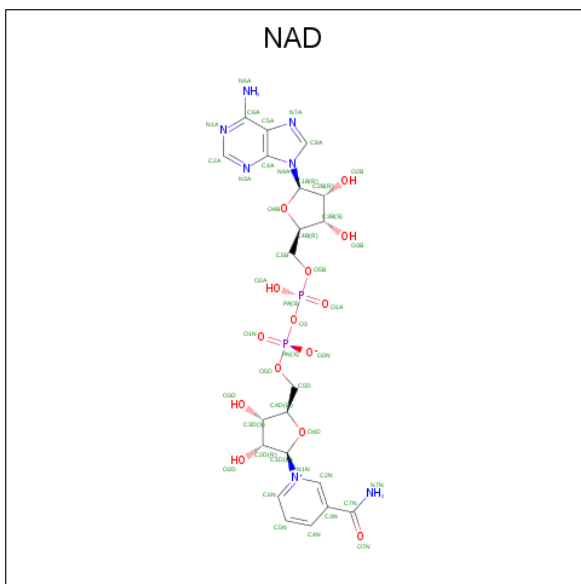
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0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

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	2	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	C	1	Total	C	O	0	0
			8	6	2		
6	C	1	Total	C	O	0	0
			8	6	2		
6	E	1	Total	C	O	4	0
			8	6	2		
6	G	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

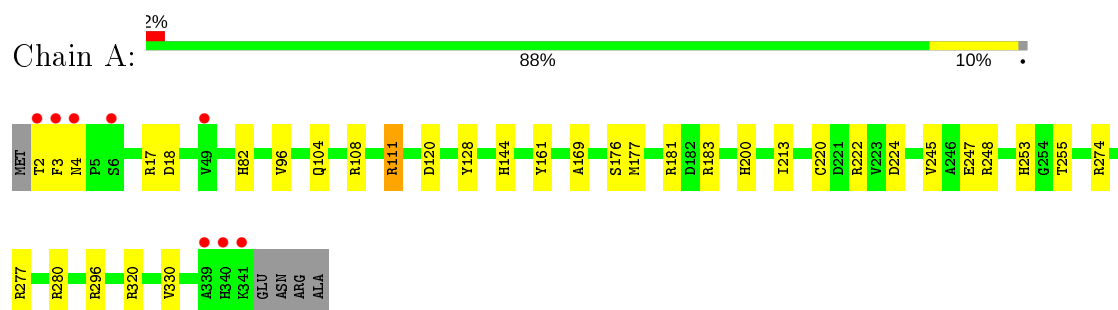
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	414	Total 414	O 414	0	0
8	B	378	Total 378	O 378	0	0
8	C	412	Total 412	O 412	0	0
8	D	293	Total 293	O 293	0	0
8	E	363	Total 363	O 363	0	0
8	F	338	Total 338	O 338	0	0
8	G	340	Total 340	O 340	0	0
8	H	273	Total 273	O 273	0	0

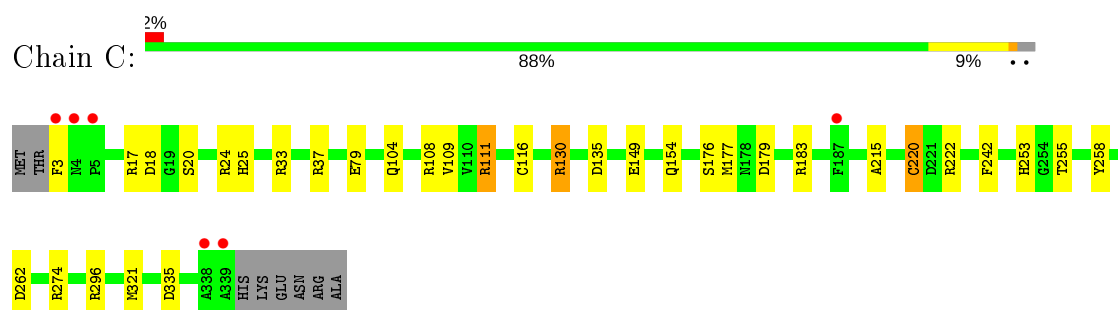
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

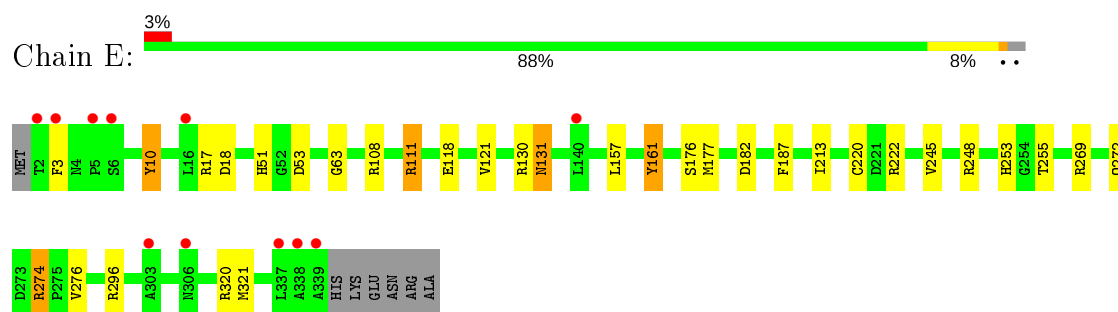
- Molecule 1: 4-hydroxy-2-oxovalerate aldolase



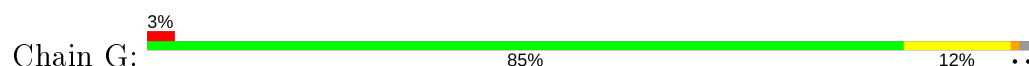
- Molecule 1: 4-hydroxy-2-oxovalerate aldolase

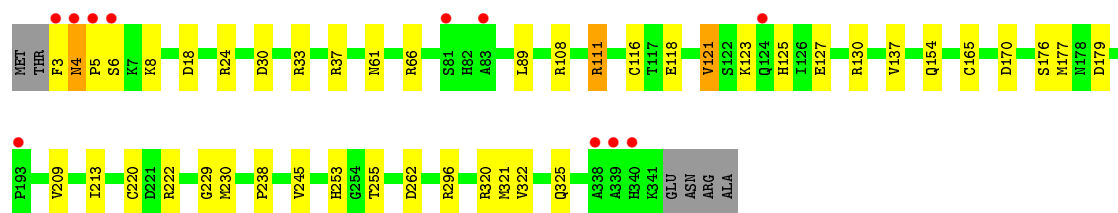


- Molecule 1: 4-hydroxy-2-oxovalerate aldolase

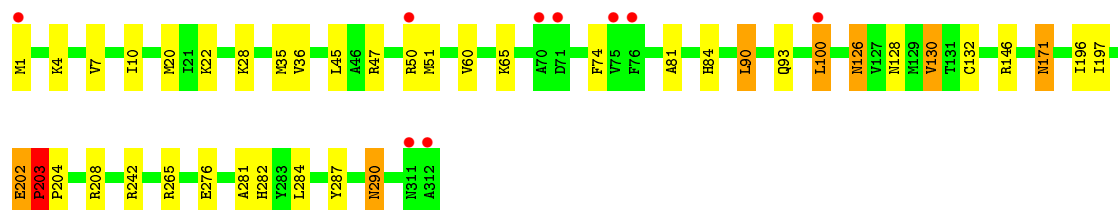
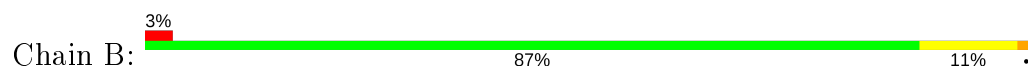


- Molecule 1: 4-hydroxy-2-oxovalerate aldolase

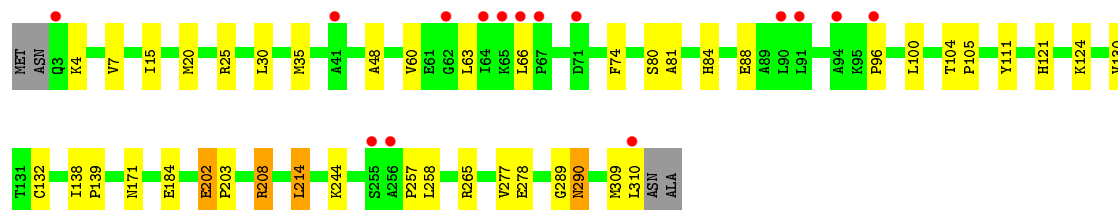
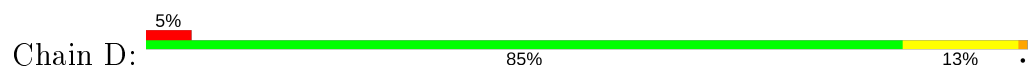




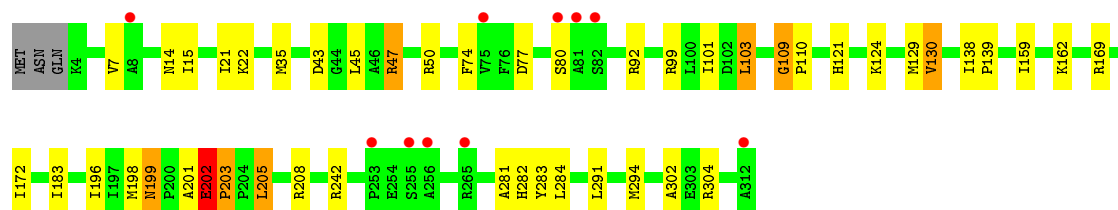
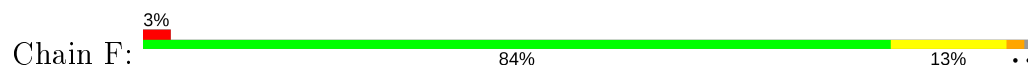
- Molecule 2: acetaldehyde dehydrogenase (acylating)



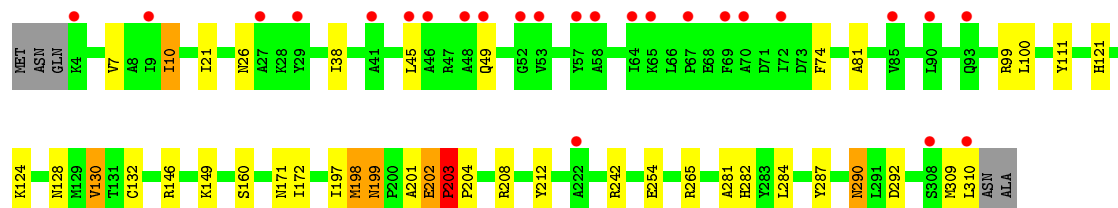
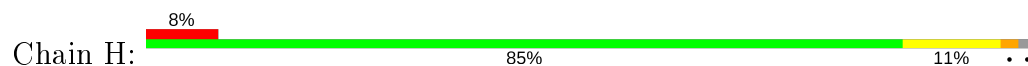
- Molecule 2: acetaldehyde dehydrogenase (acylating)



- Molecule 2: acetaldehyde dehydrogenase (acylating)



- Molecule 2: acetaldehyde dehydrogenase (acylating)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.20 Å 140.00 Å 191.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 19.96 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-1.70) 99.4 (19.96-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.70 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.189 , 0.230 0.179 , 0.215	Depositor DCC
R_{free} test set	15063 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22561	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OXL, MPD, MN, SO4, 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	A	0.61	0/2671	1.30	19/3607 (0.5%)
1	C	0.63	0/2634	1.37	23/3558 (0.6%)
1	E	0.58	0/2653	1.30	22/3585 (0.6%)
1	G	0.58	0/2660	1.27	21/3593 (0.6%)
2	B	0.58	0/2412	1.24	15/3273 (0.5%)
2	D	0.58	1/2366 (0.0%)	1.17	9/3211 (0.3%)
2	F	0.57	0/2395	1.33	26/3251 (0.8%)
2	H	0.54	0/2332	1.21	18/3167 (0.6%)
All	All	0.59	1/20123 (0.0%)	1.28	153/27245 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
2	B	0	2
2	D	0	2
2	F	0	5
2	H	0	3
All	All	0	14

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	278	GLU	CD-OE2	-6.01	1.19	1.25

The worst 5 of 153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	47	ARG	NE-CZ-NH2	-19.91	110.34	120.30
1	C	296	ARG	NE-CZ-NH1	15.73	128.16	120.30
1	C	111	ARG	NE-CZ-NH1	14.31	127.45	120.30
1	E	274	ARG	NE-CZ-NH1	14.06	127.33	120.30
1	C	274	ARG	NE-CZ-NH1	13.90	127.25	120.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	GLN	Sidechain
2	B	202	GLU	Mainchain,Peptide
1	C	258	TYR	Sidechain
2	D	202	GLU	Mainchain,Peptide
2	F	109	GLY	Mainchain

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	2599	0	2570	17	0
1	C	2568	0	2533	14	0
1	E	2579	0	2547	14	0
1	G	2588	0	2555	32	0
2	B	2316	0	2385	39	0
2	D	2280	0	2346	35	0
2	F	2289	0	2348	30	0
2	H	2263	0	2335	27	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	6	0	0	0	0
4	C	6	0	0	0	0
4	E	6	0	0	0	0
4	G	6	0	0	0	0
5	A	10	0	0	0	0
5	C	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	15	0	0	0	0
5	F	10	0	0	0	0
5	G	10	0	0	0	0
6	A	8	0	14	1	0
6	B	8	0	14	14	0
6	C	16	0	28	6	0
6	E	8	0	14	1	0
6	G	8	0	14	5	0
7	B	44	0	26	1	0
7	D	44	0	26	4	0
7	H	44	0	26	5	0
8	A	414	0	0	5	0
8	B	378	0	0	6	0
8	C	412	0	0	3	0
8	D	293	0	0	1	0
8	E	363	0	0	1	0
8	F	338	0	0	3	0
8	G	340	0	0	0	0
8	H	273	0	0	1	0
All	All	22561	0	19781	212	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 5.

The worst 5 of 212 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:E:177[B]:MET:SD	1:G:177[B]:MET:SD	2.60	0.97
1:A:177[B]:MET:SD	1:C:177[B]:MET:SD	2.63	0.97
6:B:3528:MPD:C5	6:B:3528:MPD:HM2	1.96	0.96
1:G:3:PHE:CE1	1:G:4:ASN:O	2.20	0.95
1:G:4:ASN:HD22	1:G:5:PRO:HD2	1.29	0.95

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	343/345 (99%)	331 (96%)	12 (4%)	0	100	100
1	C	339/345 (98%)	330 (97%)	9 (3%)	0	100	100
1	E	342/345 (99%)	335 (98%)	7 (2%)	0	100	100
1	G	342/345 (99%)	334 (98%)	8 (2%)	0	100	100
2	B	323/312 (104%)	315 (98%)	6 (2%)	2 (1%)	25	11
2	D	316/312 (101%)	306 (97%)	9 (3%)	1 (0%)	41	24
2	F	320/312 (103%)	310 (97%)	8 (2%)	2 (1%)	25	11
2	H	312/312 (100%)	302 (97%)	8 (3%)	2 (1%)	25	11
All	All	2637/2628 (100%)	2563 (97%)	67 (2%)	7 (0%)	47	24

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	130[A]	VAL
2	F	130[B]	VAL
2	B	203	PRO
2	H	203	PRO
2	B	130	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	271/270 (100%)	267 (98%)	4 (2%)	65	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	267/270 (99%)	264 (99%)	3 (1%)	73	63
1	E	270/270 (100%)	265 (98%)	5 (2%)	57	41
1	G	270/270 (100%)	262 (97%)	8 (3%)	41	22
2	B	250/237 (106%)	245 (98%)	5 (2%)	55	38
2	D	244/237 (103%)	241 (99%)	3 (1%)	71	59
2	F	247/237 (104%)	243 (98%)	4 (2%)	62	48
2	H	240/237 (101%)	235 (98%)	5 (2%)	53	36
All	All	2059/2028 (102%)	2022 (98%)	37 (2%)	62	43

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	131	ASN
2	F	80	SER
2	H	199	ASN
1	E	220[A]	CYS
1	E	220[B]	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	51	HIS
2	F	86	GLN
2	H	199	ASN
1	E	253	HIS
2	F	199	ASN

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 [i](#)

There are no carbohydrates 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
5	SO4	A	3512	-	4,4,4	0.56	0	6,6,6	0.07	0
5	SO4	E	3517	-	4,4,4	0.62	0	6,6,6	0.38	0
6	MPD	C	3524	-	7,7,7	0.47	0	9,10,10	1.03	1 (11%)
5	SO4	G	3520	-	4,4,4	0.62	0	6,6,6	0.42	0
6	MPD	B	3528	-	7,7,7	0.63	0	9,10,10	1.34	1 (11%)
4	OXL	E	3510	3	0,5,5	0.00	-	0,6,6	0.00	-
5	SO4	F	3519	-	4,4,4	0.61	0	6,6,6	0.29	0
6	MPD	E	3527	-	7,7,7	3.69	1 (14%)	9,10,10	1.87	2 (22%)
5	SO4	A	3513	-	4,4,4	0.61	0	6,6,6	0.07	0
6	MPD	C	3529	-	7,7,7	0.58	0	9,10,10	0.70	0
4	OXL	C	3509	3	0,5,5	0.00	-	0,6,6	0.00	-
6	MPD	A	3525	-	7,7,7	1.16	1 (14%)	9,10,10	1.00	1 (11%)
7	NAD	H	3503	-	42,48,48	1.16	3 (7%)	50,73,73	2.01	13 (26%)
4	OXL	G	3511	3	0,5,5	0.00	-	0,6,6	0.00	-
7	NAD	B	3501	-	42,48,48	1.14	3 (7%)	50,73,73	1.95	9 (18%)
5	SO4	C	3515	-	4,4,4	0.61	0	6,6,6	0.16	0
6	MPD	G	3526	-	7,7,7	0.53	0	9,10,10	0.80	0
5	SO4	C	3516	-	4,4,4	0.60	0	6,6,6	0.11	0
4	OXL	A	3508	3	0,5,5	0.00	-	0,6,6	0.00	-
5	SO4	G	3521	-	4,4,4	0.61	0	6,6,6	0.13	0
5	SO4	F	3523	-	4,4,4	0.70	0	6,6,6	0.54	0
5	SO4	C	3514	-	4,4,4	0.55	0	6,6,6	0.47	0
7	NAD	D	3502	-	42,48,48	1.22	4 (9%)	50,73,73	1.83	9 (18%)
5	SO4	E	3518	-	4,4,4	0.62	0	6,6,6	0.14	0
5	SO4	E	3522	-	4,4,4	0.63	0	6,6,6	0.21	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
6	MPD	B	3528	-	-	1/5/5/5	-
6	MPD	A	3525	-	-	5/5/5/5	-
4	OXL	A	3508	3	-	0/0/4/4	-
6	MPD	C	3529	-	-	1/5/5/5	-
6	MPD	C	3524	-	-	2/5/5/5	-
4	OXL	C	3509	3	-	0/0/4/4	-
7	NAD	D	3502	-	-	5/26/62/62	0/5/5/5
7	NAD	H	3503	-	-	5/26/62/62	0/5/5/5
6	MPD	E	3527	-	-	2/5/5/5	-
4	OXL	G	3511	3	-	0/0/4/4	-
7	NAD	B	3501	-	-	5/26/62/62	0/5/5/5
4	OXL	E	3510	3	-	0/0/4/4	-
6	MPD	G	3526	-	-	1/5/5/5	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	3527	MPD	C3-C2	9.70	1.80	1.53
7	B	3501	NAD	C3N-C7N	4.13	1.56	1.50
7	H	3503	NAD	C3N-C7N	4.06	1.56	1.50
7	D	3502	NAD	C3N-C7N	3.83	1.56	1.50
7	B	3501	NAD	O4B-C1B	3.13	1.45	1.41

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	3503	NAD	C5N-C4N-C3N	-6.83	112.26	120.34
7	B	3501	NAD	C5N-C4N-C3N	-6.74	112.37	120.34
7	B	3501	NAD	C6N-C5N-C4N	6.21	128.47	119.44
7	D	3502	NAD	C6N-C5N-C4N	5.55	127.50	119.44
7	D	3502	NAD	C5N-C4N-C3N	-5.49	113.84	120.34

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	3524	MPD	C2-C3-C4-O4

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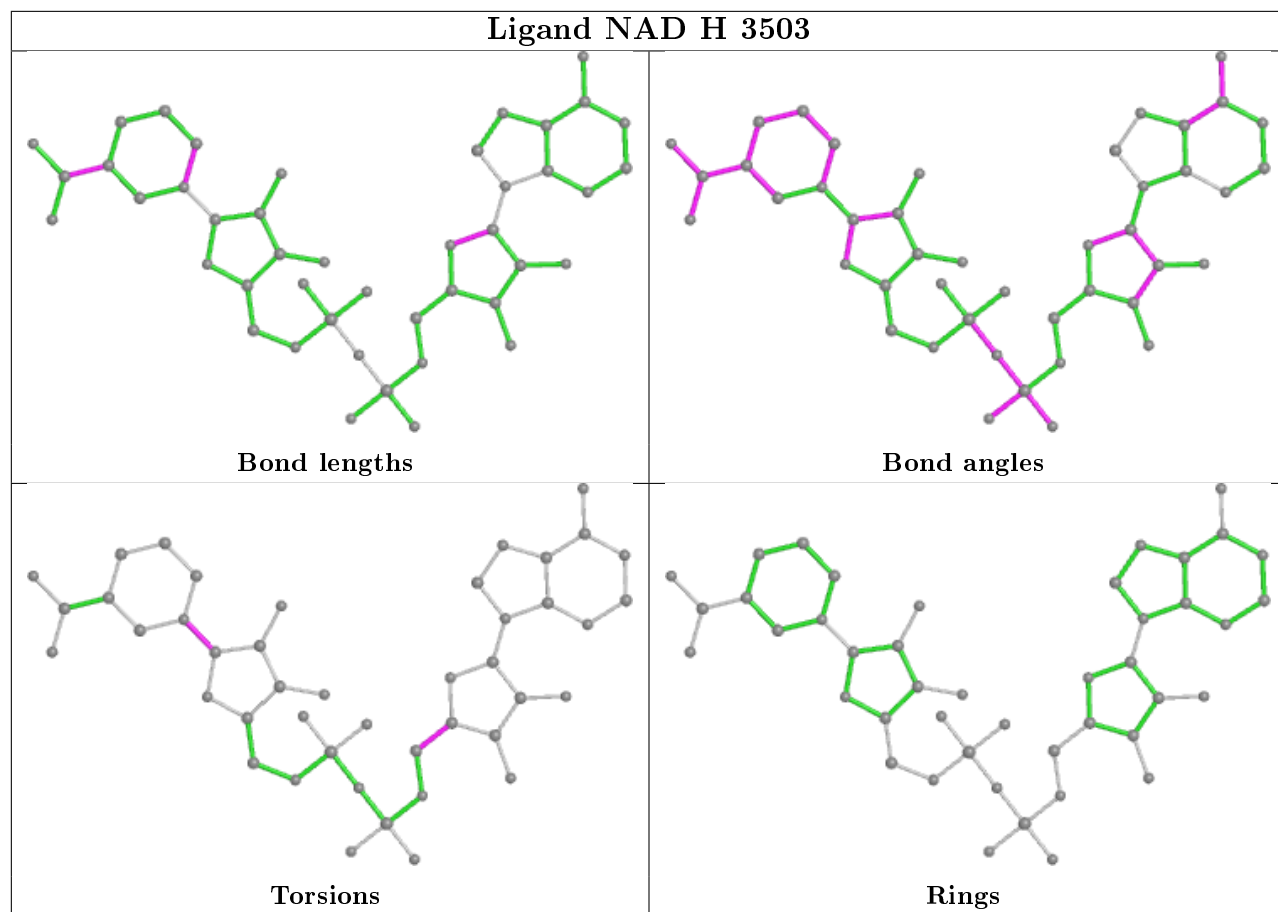
Mol	Chain	Res	Type	Atoms
6	E	3527	MPD	C2-C3-C4-O4
6	A	3525	MPD	C1-C2-C3-C4
6	A	3525	MPD	O2-C2-C3-C4
6	A	3525	MPD	C2-C3-C4-O4

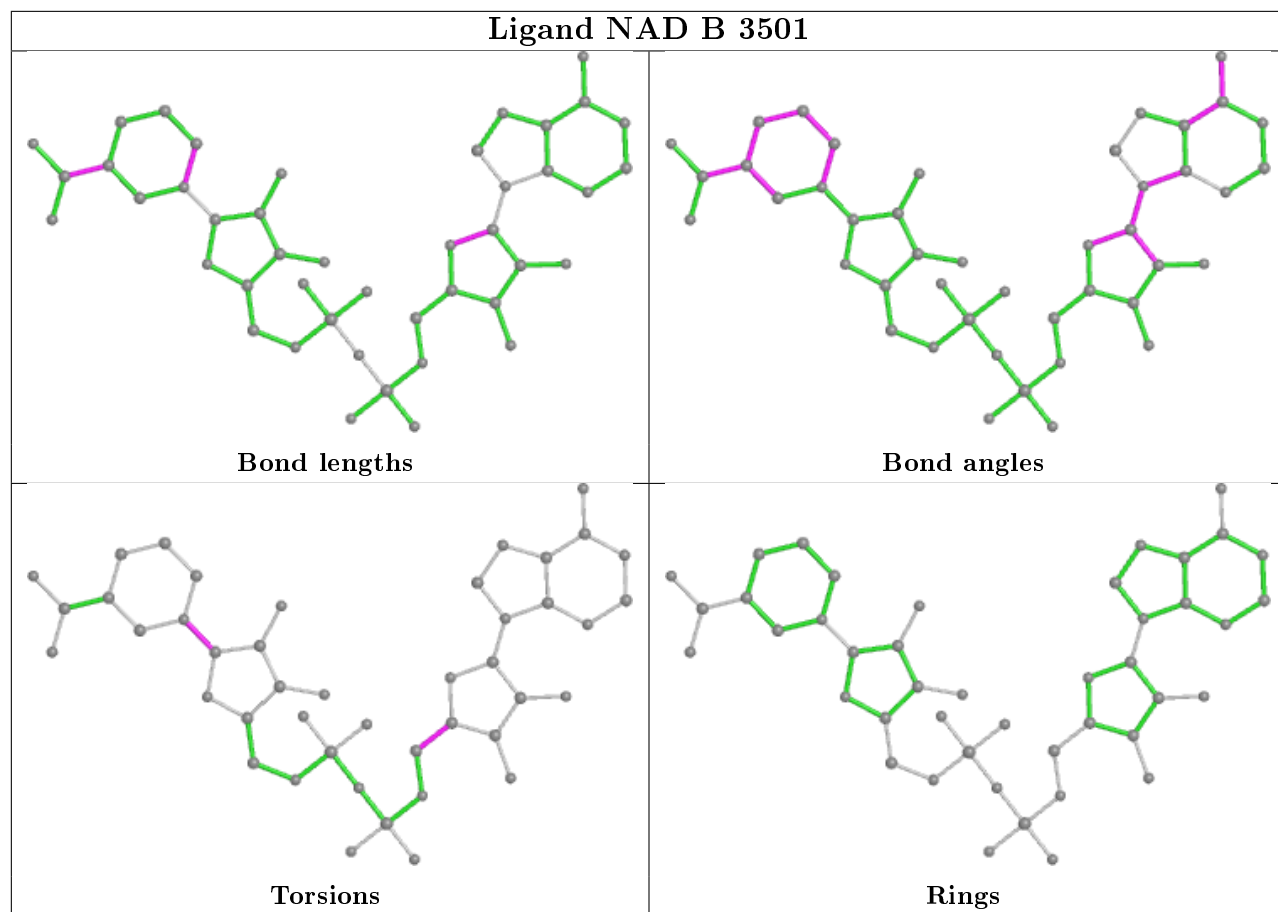
There are no ring outliers.

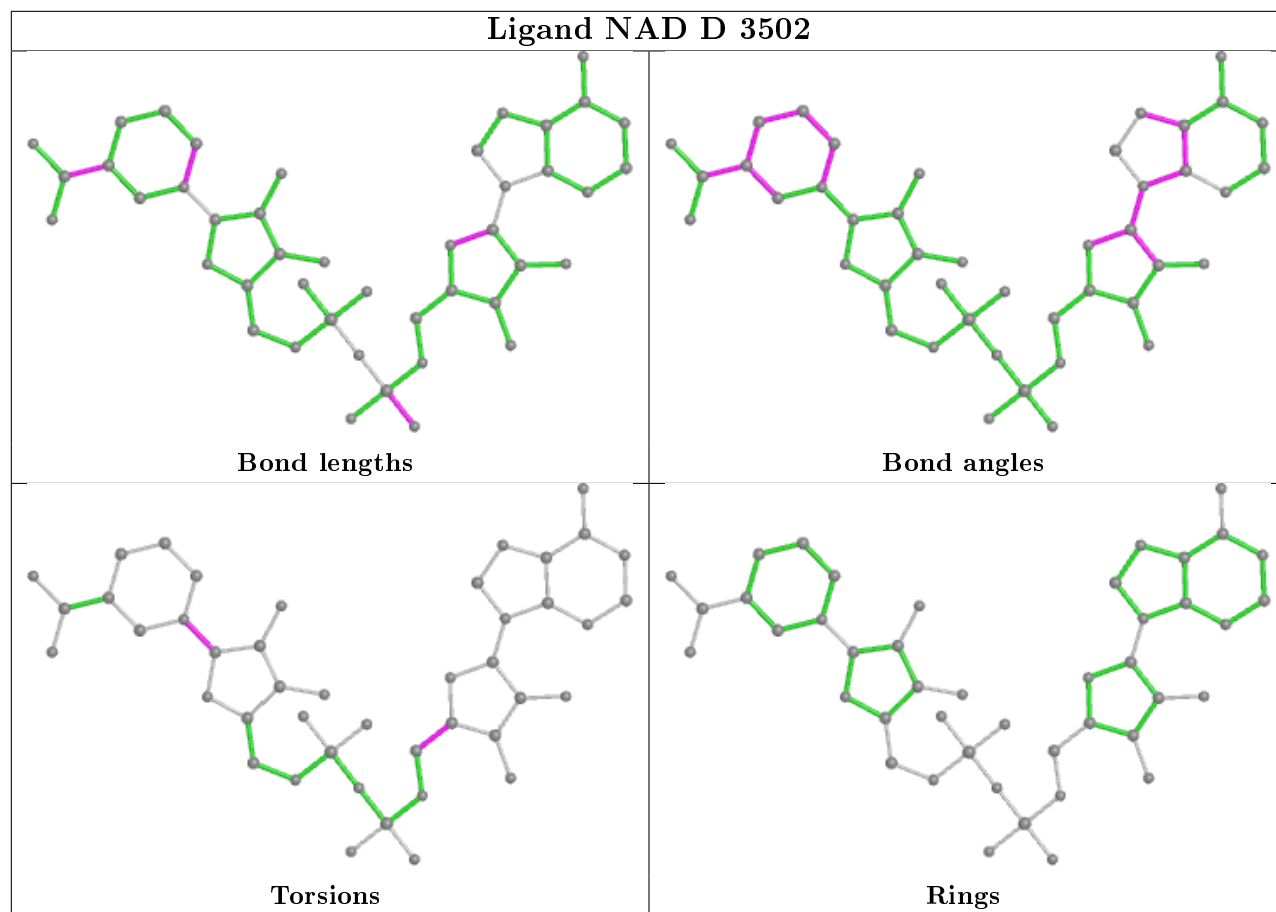
9 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	3524	MPD	5	0
6	B	3528	MPD	14	0
6	E	3527	MPD	1	0
6	C	3529	MPD	1	0
6	A	3525	MPD	1	0
7	H	3503	NAD	5	0
7	B	3501	NAD	1	0
6	G	3526	MPD	5	0
7	D	3502	NAD	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	340/345 (98%)	-0.11	8 (2%) 59 63	16, 21, 32, 52	21 (6%)
1	C	337/345 (97%)	-0.13	6 (1%) 68 72	17, 22, 30, 51	13 (3%)
1	E	338/345 (97%)	0.01	11 (3%) 46 51	18, 24, 35, 51	13 (3%)
1	G	339/345 (98%)	0.10	11 (3%) 47 52	19, 26, 35, 48	20 (5%)
2	B	312/312 (100%)	0.02	9 (2%) 51 56	17, 25, 38, 52	15 (4%)
2	D	308/312 (98%)	0.22	15 (4%) 29 33	18, 28, 43, 59	22 (7%)
2	F	309/312 (99%)	0.02	10 (3%) 47 52	20, 26, 36, 47	15 (4%)
2	H	307/312 (98%)	0.40	25 (8%) 12 14	21, 30, 45, 59	23 (7%)
All	All	2590/2628 (98%)	0.06	95 (3%) 41 46	16, 25, 39, 59	142 (5%)

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	3	PHE	8.2
1	E	3	PHE	8.0
1	E	2	THR	6.5
1	G	339	ALA	6.1
1	C	4	ASN	5.0

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 carbohydrates in this entry.

6.4 Ligands ⓘ

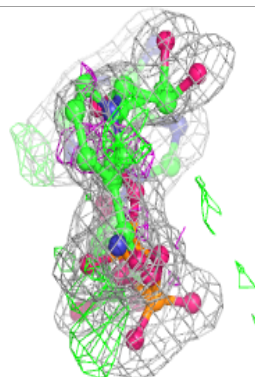
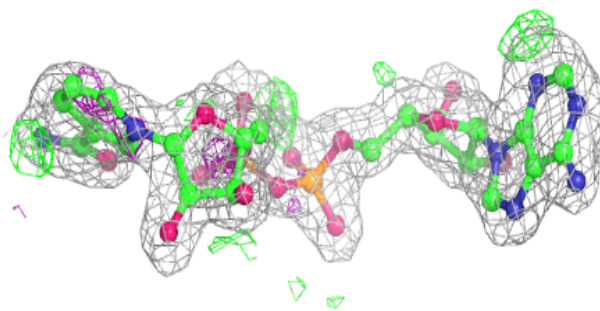
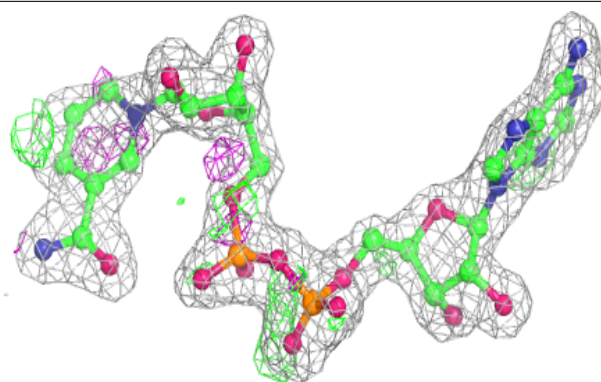
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MPD	C	3529	8/8	0.68	0.21	47,48,49,49	0
6	MPD	C	3524	8/8	0.69	0.27	26,27,27,27	7
6	MPD	B	3528	8/8	0.74	0.39	46,47,48,48	5
6	MPD	G	3526	8/8	0.76	0.18	35,36,37,39	1
5	SO4	E	3518	5/5	0.77	0.20	56,56,56,56	5
5	SO4	F	3523	5/5	0.78	0.27	34,36,38,38	3
5	SO4	E	3522	5/5	0.83	0.18	43,44,44,44	5
5	SO4	F	3519	5/5	0.85	0.17	35,35,36,36	4
4	OXL	A	3508	6/6	0.86	0.18	22,24,28,29	0
6	MPD	E	3527	8/8	0.86	0.13	28,29,41,41	4
4	OXL	C	3509	6/6	0.88	0.18	21,24,26,31	0
5	SO4	A	3513	5/5	0.88	0.13	48,49,49,49	5
4	OXL	E	3510	6/6	0.88	0.21	25,28,30,33	0
4	OXL	G	3511	6/6	0.90	0.22	26,29,31,34	0
6	MPD	A	3525	8/8	0.90	0.11	28,41,41,42	2
5	SO4	G	3521	5/5	0.91	0.13	49,49,49,49	5
5	SO4	C	3516	5/5	0.92	0.13	52,52,52,52	5
5	SO4	C	3515	5/5	0.93	0.14	51,51,51,52	5
7	NAD	H	3503	44/44	0.94	0.13	28,33,37,38	0
5	SO4	G	3520	5/5	0.94	0.12	28,30,30,30	5
7	NAD	D	3502	44/44	0.95	0.11	26,28,33,36	0
7	NAD	B	3501	44/44	0.96	0.09	21,25,28,32	0
5	SO4	A	3512	5/5	0.97	0.18	36,37,38,39	2
5	SO4	E	3517	5/5	0.97	0.21	44,44,45,46	0
5	SO4	C	3514	5/5	0.98	0.20	36,37,37,38	0
3	MN	G	3507	1/1	0.99	0.03	24,24,24,24	0
3	MN	C	3505	1/1	0.99	0.03	20,20,20,20	0
3	MN	A	3504	1/1	1.00	0.02	19,19,19,19	0
3	MN	E	3506	1/1	1.00	0.01	22,22,22,22	0

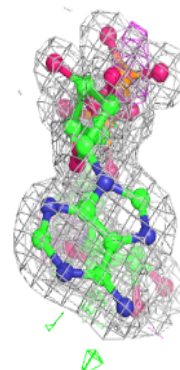
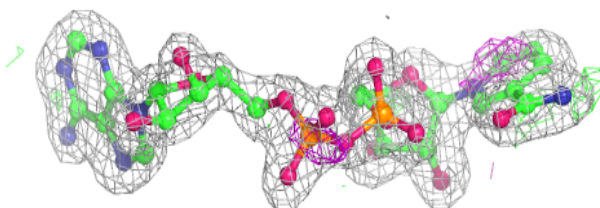
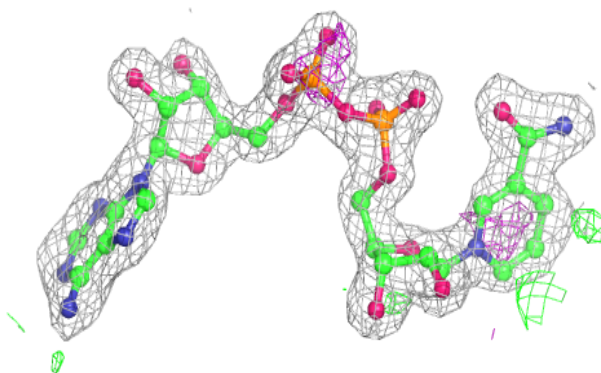
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

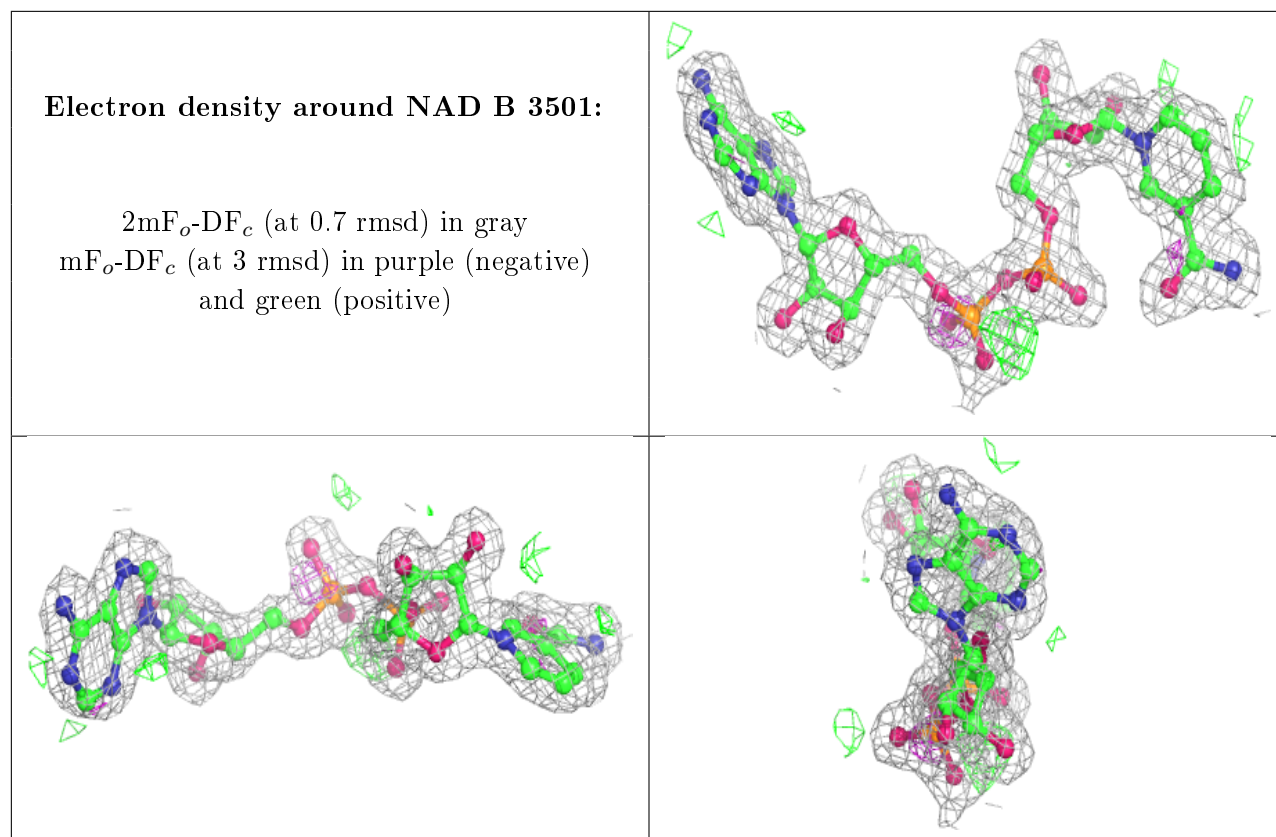
Electron density around NAD H 3503:

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

**Electron density around NAD D 3502:**

$2mF_o-DF_c$ (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.