



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:14 AM EDT

PDB ID : 2ONP / pdb_00002onp
Title : Arg475Gln Mutant of Human Mitochondrial Aldehyde Dehydrogenase, complexed with NAD+
Authors : Larson, H.N.; Hurley, T.D.
Deposited on : 2007-01-24
Resolution : 2.00 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

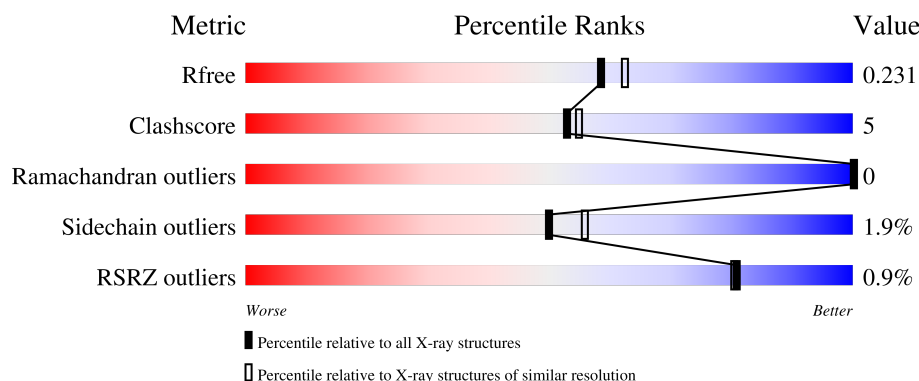
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

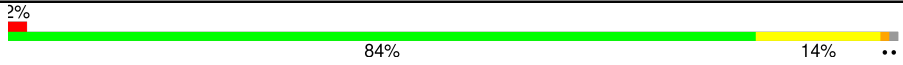
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	500	
1	B	500	
1	C	500	
1	D	500	
1	E	500	

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Mol	Chain	Length	Quality of chain
1	F	500	 88% 10% ..
1	G	500	 86% 12% ..
1	H	500	 84% 14% ..

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
5	EDO	E	6945	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 33651 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	B	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	C	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	D	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	E	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	F	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	G	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	H	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	475	GLN	ARG	engineered mutation	UNP P05091
B	475	GLN	ARG	engineered mutation	UNP P05091
C	475	GLN	ARG	engineered mutation	UNP P05091
D	475	GLN	ARG	engineered mutation	UNP P05091
E	475	GLN	ARG	engineered mutation	UNP P05091
F	475	GLN	ARG	engineered mutation	UNP P05091
G	475	GLN	ARG	engineered mutation	UNP P05091
H	475	GLN	ARG	engineered mutation	UNP P05091

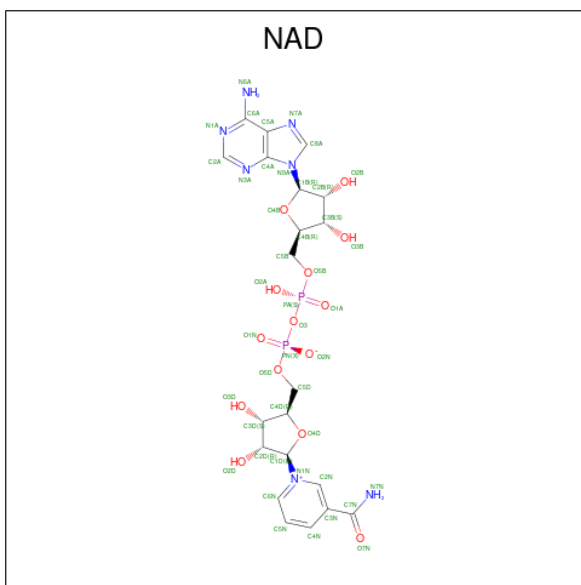
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0
3	E	1	Total Na 1 1	0	0
3	F	1	Total Na 1 1	0	0
3	G	1	Total Na 1 1	0	0
3	H	1	Total Na 1 1	0	0

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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

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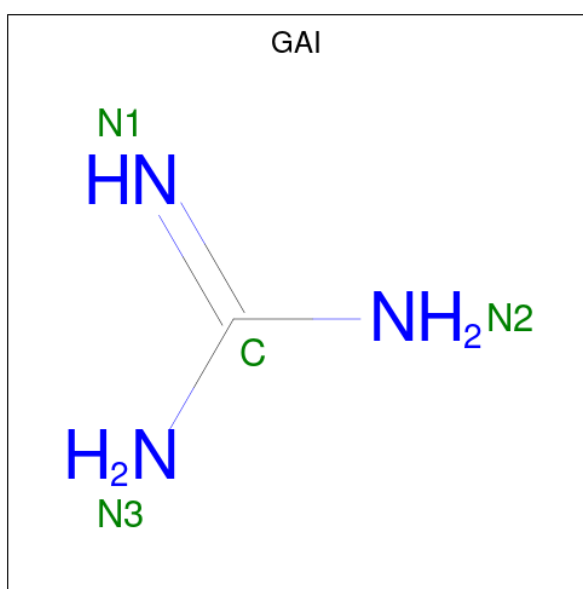
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GUANIDINE (CCD ID: GAI) (formula: CH_5N_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			4	1	3		
6	A	1	Total	C	N	0	0
			4	1	3		
6	A	1	Total	C	N	0	0
			4	1	3		
6	A	1	Total	C	N	0	0
			4	1	3		
6	B	1	Total	C	N	0	0
			4	1	3		
6	B	1	Total	C	N	0	0
			4	1	3		
6	B	1	Total	C	N	0	0
			4	1	3		

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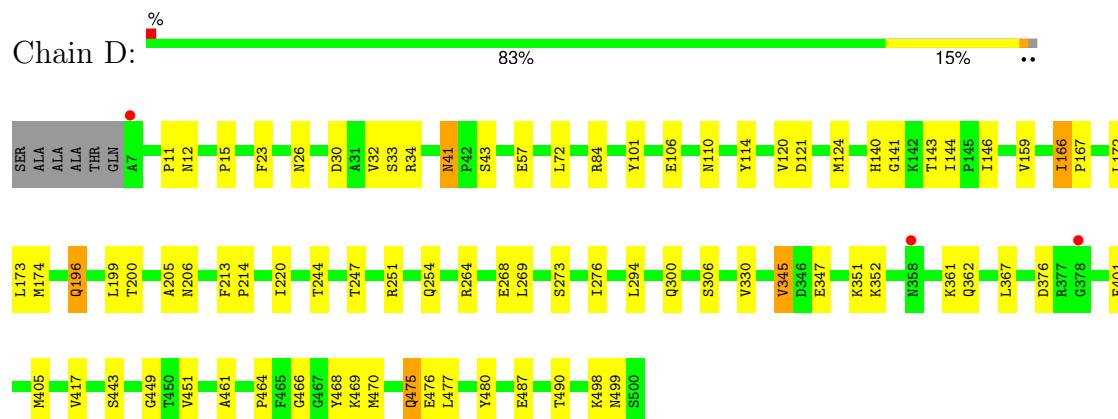
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total 4	C 1	N 3	0	0
6	C	1	Total 4	C 1	N 3	0	0
6	C	1	Total 4	C 1	N 3	0	0
6	C	1	Total 4	C 1	N 3	0	0
6	D	1	Total 4	C 1	N 3	0	0
6	D	1	Total 4	C 1	N 3	0	0
6	D	1	Total 4	C 1	N 3	0	0
6	D	1	Total 4	C 1	N 3	0	0
6	E	1	Total 4	C 1	N 3	0	0
6	E	1	Total 4	C 1	N 3	0	0
6	E	1	Total 4	C 1	N 3	0	0
6	E	1	Total 4	C 1	N 3	0	0
6	E	1	Total 4	C 1	N 3	0	0
6	F	1	Total 4	C 1	N 3	0	0
6	F	1	Total 4	C 1	N 3	0	0
6	F	1	Total 4	C 1	N 3	0	0
6	G	1	Total 4	C 1	N 3	0	0
6	G	1	Total 4	C 1	N 3	0	0
6	G	1	Total 4	C 1	N 3	0	0
6	H	1	Total 4	C 1	N 3	0	0
6	H	1	Total 4	C 1	N 3	0	0
6	H	1	Total 4	C 1	N 3	0	0

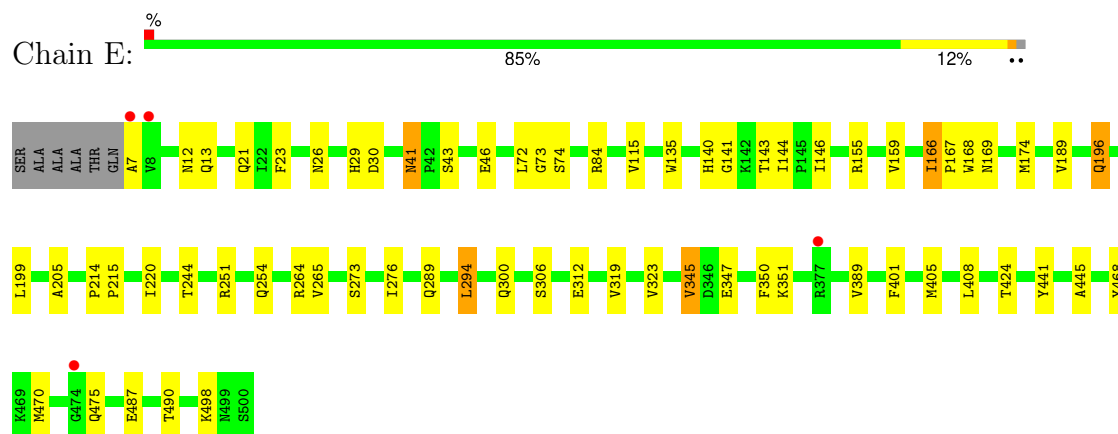
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	292	Total 292	O 292	0	0
7	B	317	Total 317	O 317	0	0
7	C	398	Total 398	O 398	0	0
7	D	333	Total 333	O 333	0	0
7	E	338	Total 338	O 338	0	0
7	F	410	Total 410	O 410	0	0
7	G	292	Total 292	O 292	0	0
7	H	267	Total 267	O 267	0	0

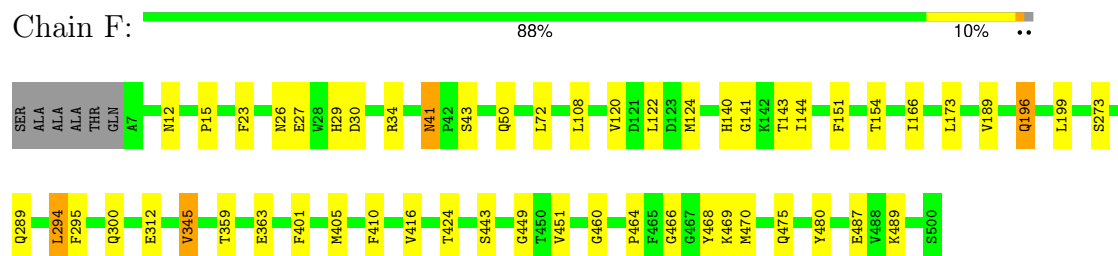
- Molecule 1: Aldehyde dehydrogenase



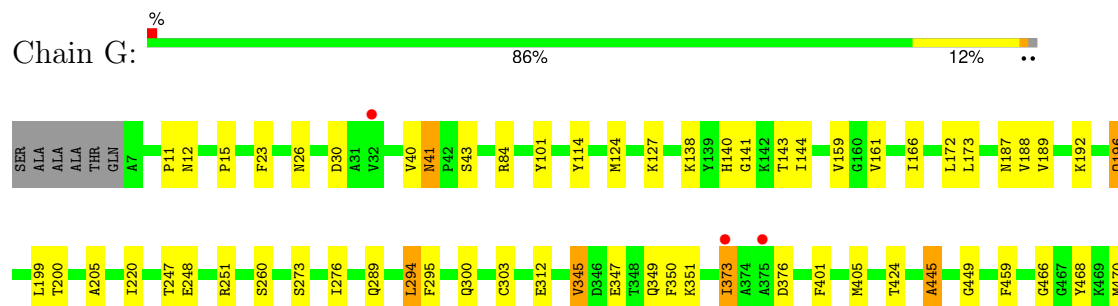
- Molecule 1: Aldehyde dehydrogenase

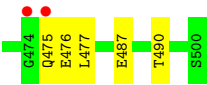


- Molecule 1: Aldehyde dehydrogenase

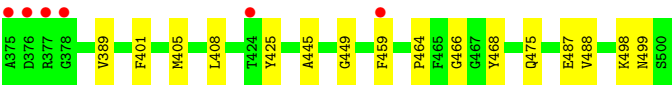
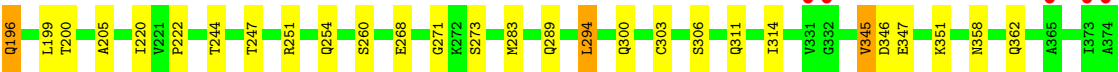
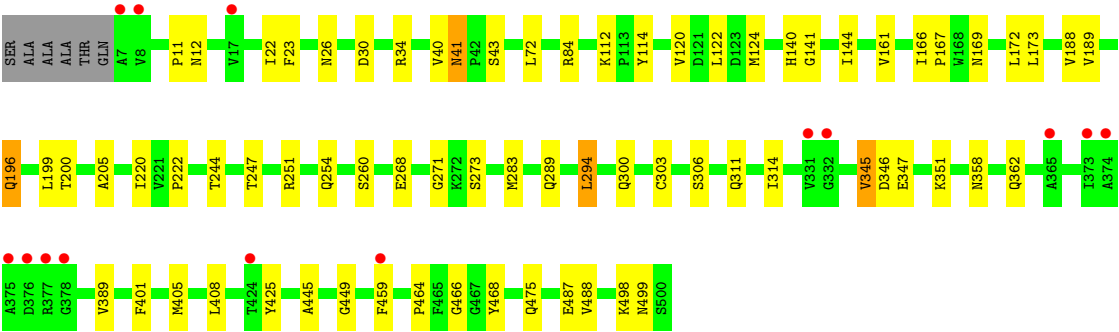
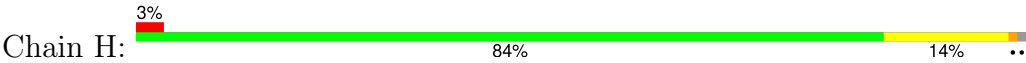


- Molecule 1: Aldehyde dehydrogenase





● Molecule 1: Aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	142.85Å 150.84Å 177.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 2.00 29.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.97-2.00) 97.6 (29.97-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.26	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.00Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.240 0.195 , 0.231	Depositor DCC
R_{free} test set	12705 reflections (4.24%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtrriage
Anisotropy	0.774	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33651	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 67.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0895e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GAI, NA, NAD, MG, EDO

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	0.59	1/3880 (0.0%)	0.96	15/5265 (0.3%)
1	B	0.59	0/3880	0.97	21/5265 (0.4%)
1	C	0.62	1/3880 (0.0%)	0.97	17/5265 (0.3%)
1	D	0.55	0/3880	0.96	14/5265 (0.3%)
1	E	0.55	0/3880	0.96	16/5265 (0.3%)
1	F	0.59	0/3880	0.96	15/5265 (0.3%)
1	G	0.52	0/3880	0.95	16/5265 (0.3%)
1	H	0.51	0/3880	0.94	15/5265 (0.3%)
All	All	0.56	2/31040 (0.0%)	0.96	129/42120 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	124	MET	SD-CE	-6.48	1.63	1.79
1	A	488	VAL	CA-CB	5.83	1.61	1.53

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	LEU	N-CA-C	10.27	122.05	111.07
1	E	144	ILE	N-CA-C	9.58	118.33	107.89
1	F	199	LEU	N-CA-C	9.46	121.19	111.07
1	A	199	LEU	N-CA-C	9.34	122.42	111.02
1	H	199	LEU	N-CA-C	9.26	120.98	111.07
1	D	199	LEU	N-CA-C	9.22	121.02	110.97
1	E	199	LEU	N-CA-C	9.04	120.82	110.97
1	F	144	ILE	N-CA-C	8.79	117.47	107.89
1	C	144	ILE	N-CA-C	8.77	117.45	107.89
1	G	345	VAL	N-CA-C	8.70	119.49	110.62
1	B	144	ILE	N-CA-C	8.38	117.02	107.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	LEU	N-CA-C	8.33	121.11	111.11
1	A	144	ILE	N-CA-C	8.18	116.81	107.89
1	D	144	ILE	N-CA-C	7.98	116.59	107.89
1	B	345	VAL	N-CA-C	7.97	118.75	110.62
1	H	144	ILE	N-CA-C	7.97	116.58	107.89
1	G	166	ILE	N-CA-C	7.94	116.65	107.84
1	G	199	LEU	N-CA-C	7.90	120.66	111.02
1	G	144	ILE	N-CA-C	7.85	116.45	107.89
1	F	345	VAL	N-CA-C	7.75	118.53	110.62
1	E	345	VAL	N-CA-C	7.69	118.47	110.62
1	B	166	ILE	N-CA-C	7.47	116.13	107.84
1	A	345	VAL	N-CA-C	7.32	118.96	110.62
1	F	166	ILE	N-CA-C	7.31	115.95	107.84
1	H	345	VAL	N-CA-C	7.23	118.00	110.62
1	G	189	VAL	N-CA-C	7.09	119.02	108.46
1	H	140	HIS	N-CA-C	7.04	120.42	110.50
1	E	189	VAL	N-CA-C	7.03	118.93	108.46
1	B	140	HIS	N-CA-C	7.02	119.90	110.35
1	D	166	ILE	N-CA-C	7.01	115.62	107.84
1	F	312	GLU	N-CA-C	6.90	119.68	111.33
1	C	345	VAL	N-CA-C	6.88	117.64	110.62
1	A	312	GLU	N-CA-C	6.87	119.64	111.33
1	C	166	ILE	N-CA-C	6.85	115.45	107.84
1	C	312	GLU	N-CA-C	6.85	119.61	111.33
1	D	345	VAL	N-CA-C	6.79	118.36	110.62
1	E	166	ILE	N-CA-C	6.69	115.27	107.84
1	B	189	VAL	N-CA-C	6.68	119.14	108.85
1	F	140	HIS	N-CA-C	6.64	119.86	110.50
1	C	30	ASP	N-CA-C	-6.63	101.60	110.55
1	G	140	HIS	N-CA-C	6.62	119.84	110.50
1	F	295	PHE	N-CA-C	6.58	121.14	113.18
1	E	84	ARG	N-CA-C	-6.44	104.26	111.28
1	A	189	VAL	N-CA-C	6.42	118.02	108.46
1	D	140	HIS	N-CA-C	6.39	119.52	110.50
1	B	312	GLU	N-CA-C	6.38	119.05	111.33
1	C	189	VAL	N-CA-C	6.38	117.96	108.46
1	E	140	HIS	N-CA-C	6.32	119.42	110.50
1	A	40	VAL	N-CA-C	6.26	118.04	108.71
1	C	295	PHE	N-CA-C	6.25	120.64	112.89
1	F	141	GLY	N-CA-C	-6.25	103.03	112.41
1	E	273	SER	N-CA-C	6.25	118.48	109.48
1	F	30	ASP	N-CA-C	-6.22	102.15	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	273	SER	N-CA-C	6.22	118.44	109.48
1	D	141	GLY	N-CA-C	-6.22	103.09	112.41
1	B	141	GLY	N-CA-C	-6.17	103.16	112.41
1	F	189	VAL	N-CA-C	6.15	117.62	108.46
1	C	12	ASN	N-CA-C	-6.11	98.58	108.41
1	C	273	SER	N-CA-C	6.10	118.27	109.48
1	G	312	GLU	N-CA-C	6.08	118.69	111.33
1	F	273	SER	N-CA-C	6.04	118.18	109.48
1	B	445	ALA	N-CA-C	6.04	118.82	111.82
1	A	169	ASN	N-CA-C	6.03	118.64	111.71
1	G	143	THR	N-CA-C	-6.01	98.72	108.52
1	H	141	GLY	N-CA-C	-6.01	103.40	112.41
1	A	12	ASN	N-CA-C	-5.95	98.84	108.41
1	D	30	ASP	N-CA-C	-5.90	102.92	110.53
1	C	140	HIS	N-CA-C	5.86	118.27	110.53
1	G	273	SER	N-CA-C	5.86	117.92	109.48
1	H	189	VAL	N-CA-C	5.84	118.38	108.86
1	D	143	THR	N-CA-C	-5.84	99.01	108.52
1	A	273	SER	N-CA-C	5.82	117.86	109.48
1	E	312	GLU	N-CA-C	5.79	119.16	111.75
1	A	30	ASP	N-CA-C	-5.78	102.75	110.55
1	C	168	TRP	N-CA-C	5.77	120.48	113.38
1	A	140	HIS	N-CA-C	5.75	118.61	110.50
1	B	276	ILE	N-CA-C	5.74	116.38	107.99
1	E	30	ASP	N-CA-C	-5.72	102.05	110.52
1	B	30	ASP	N-CA-C	-5.71	103.16	110.53
1	E	143	THR	N-CA-C	-5.71	99.87	109.07
1	E	168	TRP	N-CA-C	5.71	120.40	113.38
1	H	84	ARG	N-CA-C	-5.63	105.28	111.82
1	G	40	VAL	N-CA-C	5.61	117.67	108.97
1	G	445	ALA	N-CA-C	5.58	118.30	111.82
1	G	84	ARG	N-CA-C	-5.57	105.30	111.71
1	G	276	ILE	N-CA-C	5.57	116.12	107.99
1	A	276	ILE	N-CA-C	5.54	116.08	107.99
1	B	40	VAL	N-CA-C	5.53	117.54	108.97
1	H	30	ASP	N-CA-C	-5.52	103.10	110.55
1	B	12	ASN	N-CA-C	-5.49	99.57	108.41
1	F	12	ASN	N-CA-C	-5.45	99.64	108.41
1	A	141	GLY	N-CA-C	-5.44	104.25	112.41
1	H	40	VAL	N-CA-C	5.44	117.71	109.12
1	H	12	ASN	N-CA-C	-5.43	99.67	108.41
1	C	445	ALA	N-CA-C	5.40	118.08	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	40	VAL	N-CA-C	5.40	117.33	108.97
1	D	84	ARG	N-CA-C	-5.37	105.43	111.28
1	F	469	LYS	CB-CA-C	-5.36	110.37	116.54
1	G	30	ASP	N-CA-C	-5.35	103.32	110.55
1	C	141	GLY	N-CA-C	-5.34	104.41	112.41
1	D	273	SER	N-CA-C	5.33	117.16	109.48
1	F	143	THR	N-CA-C	-5.30	99.88	108.52
1	D	276	ILE	N-CA-C	5.28	116.30	108.23
1	B	383	PRO	N-CA-C	-5.26	102.43	110.95
1	D	469	LYS	CB-CA-C	-5.24	110.51	116.54
1	B	295	PHE	N-CA-C	5.23	119.50	113.18
1	B	122	LEU	CA-CB-CG	-5.22	98.01	116.30
1	B	168	TRP	N-CA-C	5.22	119.80	113.38
1	B	221	VAL	N-CA-C	5.21	113.31	108.15
1	D	121	ASP	N-CA-C	5.16	116.59	111.07
1	C	151	PHE	N-CA-C	-5.16	100.00	108.41
1	H	169	ASN	N-CA-C	5.16	117.80	111.82
1	E	141	GLY	N-CA-C	-5.14	104.70	112.41
1	G	141	GLY	N-CA-C	-5.14	104.70	112.41
1	H	166	ILE	CA-C-N	5.13	126.47	120.98
1	H	166	ILE	C-N-CA	5.13	126.47	120.98
1	B	282	ASP	N-CA-C	-5.12	101.77	109.15
1	C	143	THR	N-CA-C	-5.12	100.18	108.52
1	E	169	ASN	N-CA-C	5.10	117.73	111.82
1	E	276	ILE	N-CA-C	5.09	115.43	107.99
1	E	12	ASN	N-CA-C	-5.09	100.21	108.41
1	G	295	PHE	N-CA-C	5.08	119.32	113.18
1	B	273	SER	N-CA-C	5.07	118.46	109.58
1	D	330	VAL	N-CA-C	5.07	115.63	107.98
1	A	330	VAL	N-CA-C	5.06	115.52	108.84
1	B	469	LYS	CB-CA-C	-5.06	110.73	116.54
1	F	151	PHE	N-CA-C	-5.05	100.29	108.52
1	A	151	PHE	N-CA-C	-5.05	100.18	108.41
1	H	346	ASP	N-CA-C	5.03	115.17	108.38

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	3796	0	3740	47	0
1	B	3796	0	3740	45	0
1	C	3796	0	3740	34	0
1	D	3796	0	3740	49	0
1	E	3796	0	3740	47	0
1	F	3796	0	3740	26	0
1	G	3796	0	3740	41	0
1	H	3796	0	3740	45	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	44	0	26	0	0
4	B	44	0	26	0	0
4	C	44	0	26	0	0
4	D	44	0	26	0	0
4	E	44	0	26	0	0
4	F	44	0	26	0	0
4	G	44	0	26	0	0
4	H	44	0	26	0	0
5	A	20	0	30	5	0
5	B	20	0	30	4	0
5	C	24	0	36	2	0
5	D	12	0	18	1	0
5	E	24	0	36	14	0
5	F	24	0	36	1	0
5	G	16	0	24	3	0
5	H	16	0	24	2	0
6	A	16	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	12	0	15	0	0
6	C	16	0	19	1	0
6	D	16	0	20	0	0
6	E	16	0	18	1	0
6	F	12	0	15	0	0
6	G	12	0	14	0	0
6	H	12	0	14	0	0
7	A	292	0	0	2	0
7	B	317	0	0	3	0
7	C	398	0	0	3	0
7	D	333	0	0	3	0
7	E	338	0	0	4	0
7	F	410	0	0	1	0
7	G	292	0	0	3	0
7	H	267	0	0	4	0
All	All	33651	0	30496	309	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.

All (309) 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:H:196:GLN:HE21	1:H:196:GLN:H	1.02	0.98
1:D:475:GLN:NE2	1:D:480:TYR:HB3	1.84	0.93
1:G:196:GLN:H	1:G:196:GLN:HE21	1.16	0.92
1:D:475:GLN:HE21	1:D:480:TYR:HB3	1.34	0.92
1:F:196:GLN:H	1:F:196:GLN:HE21	1.24	0.84
1:G:294:LEU:HD22	1:G:405:MET:HB2	1.59	0.82
1:C:196:GLN:HE21	1:C:196:GLN:H	1.28	0.81
1:H:311:GLN:HG3	7:H:2748:HOH:O	1.82	0.78
1:D:300:GLN:HE22	1:D:345:VAL:H	1.33	0.76
1:G:347:GLU:HG2	1:G:351:LYS:HE2	1.67	0.76
1:G:300:GLN:HE22	1:G:345:VAL:H	1.34	0.76
1:H:445:ALA:HB2	5:H:6948:EDO:H11	1.68	0.76
1:B:196:GLN:H	1:B:196:GLN:HE21	1.33	0.74
1:C:475:GLN:HE21	1:C:480:TYR:HB3	1.50	0.74
1:H:196:GLN:H	1:H:196:GLN:NE2	1.83	0.73
1:E:347:GLU:HG2	1:E:351:LYS:HE2	1.69	0.73
1:H:294:LEU:HD22	1:H:405:MET:HB2	1.70	0.73
1:H:300:GLN:HE22	1:H:345:VAL:H	1.35	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:300:GLN:HE22	1:E:345:VAL:H	1.37	0.71
1:A:300:GLN:HE22	1:A:345:VAL:H	1.39	0.70
1:C:124:MET:HE3	1:C:173:LEU:HD22	1.73	0.70
1:C:300:GLN:HE22	1:C:345:VAL:H	1.38	0.70
1:F:300:GLN:HE22	1:F:345:VAL:H	1.40	0.68
1:G:445:ALA:HB2	5:G:6947:EDO:H11	1.75	0.68
1:A:124:MET:HE3	1:A:173:LEU:HD22	1.76	0.67
1:H:41:ASN:HD22	1:H:43:SER:H	1.40	0.67
1:B:300:GLN:HE22	1:B:345:VAL:H	1.42	0.67
1:D:196:GLN:H	1:D:196:GLN:HE21	1.43	0.67
1:A:475:GLN:HG3	1:A:480:TYR:HB3	1.76	0.66
1:D:41:ASN:C	1:D:41:ASN:HD22	2.03	0.66
1:A:41:ASN:C	1:A:41:ASN:HD22	2.03	0.66
1:H:196:GLN:HE21	1:H:196:GLN:N	1.84	0.65
1:F:294:LEU:HD22	1:F:405:MET:HB2	1.77	0.65
1:F:41:ASN:C	1:F:41:ASN:HD22	2.04	0.65
1:G:41:ASN:C	1:G:41:ASN:HD22	2.04	0.65
1:F:120:VAL:HG12	1:F:124:MET:HE2	1.79	0.64
1:E:251:ARG:HH21	1:E:470:MET:HE1	1.63	0.64
1:B:41:ASN:C	1:B:41:ASN:HD22	2.06	0.63
1:C:120:VAL:HG12	1:C:124:MET:HE2	1.80	0.63
1:C:294:LEU:HD22	1:C:405:MET:HB2	1.79	0.63
1:D:294:LEU:HD22	1:D:405:MET:HB2	1.80	0.63
1:G:196:GLN:H	1:G:196:GLN:NE2	1.94	0.63
1:H:358:ASN:O	1:H:362:GLN:HG2	1.99	0.62
1:H:41:ASN:ND2	1:H:43:SER:H	1.96	0.62
1:E:441:TYR:CE1	5:E:6945:EDO:H22	2.35	0.62
1:F:124:MET:HE3	1:F:173:LEU:HD22	1.80	0.61
1:B:445:ALA:HB2	5:B:6942:EDO:H11	1.83	0.61
1:E:196:GLN:H	1:E:196:GLN:HE21	1.47	0.61
1:A:196:GLN:H	1:A:196:GLN:HE21	1.48	0.61
1:C:41:ASN:C	1:C:41:ASN:HD22	2.08	0.61
1:E:487:GLU:HG3	1:F:468:TYR:CE1	2.36	0.61
1:H:41:ASN:HD22	1:H:41:ASN:C	2.08	0.61
1:G:251:ARG:NH2	1:H:260:SER:O	2.34	0.60
1:G:172:LEU:HD21	1:G:200:THR:HB	1.82	0.60
1:B:172:LEU:HD21	1:B:200:THR:HB	1.83	0.59
1:F:289:GLN:NE2	7:F:3289:HOH:O	2.33	0.59
1:F:475:GLN:OE1	1:F:480:TYR:HB3	2.03	0.59
1:B:196:GLN:H	1:B:196:GLN:NE2	1.98	0.59
1:A:260:SER:O	1:B:251:ARG:NH2	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:LEU:HD22	1:B:405:MET:HB2	1.84	0.59
1:B:347:GLU:HG3	5:B:6962:EDO:H12	1.84	0.59
1:C:445:ALA:HB2	5:C:6943:EDO:H11	1.85	0.58
1:C:424:THR:CG2	1:C:470:MET:SD	2.92	0.58
1:E:155:ARG:HD2	5:E:6905:EDO:H22	1.85	0.58
1:F:41:ASN:ND2	1:F:43:SER:H	2.01	0.58
1:D:41:ASN:ND2	1:D:43:SER:H	2.02	0.57
1:D:475:GLN:HE21	1:D:480:TYR:CB	2.14	0.57
1:E:74:SER:HA	5:E:6955:EDO:H22	1.85	0.57
1:E:264:ARG:HD2	6:E:6835:GAI:N1	2.20	0.57
1:B:41:ASN:HD22	1:B:43:SER:H	1.53	0.57
1:B:347:GLU:HG2	1:B:351:LYS:HE2	1.87	0.56
1:A:41:ASN:ND2	1:A:43:SER:H	2.03	0.56
1:C:487:GLU:HG3	1:D:468:TYR:CE1	2.41	0.56
1:E:41:ASN:HB2	5:E:6915:EDO:H11	1.87	0.56
1:E:72:LEU:HD21	5:F:6946:EDO:H11	1.86	0.56
1:E:347:GLU:O	1:E:351:LYS:HG2	2.05	0.56
1:H:120:VAL:HG12	1:H:124:MET:HE2	1.88	0.56
1:C:475:GLN:NE2	1:C:480:TYR:HB3	2.18	0.55
1:A:445:ALA:HB2	5:A:6941:EDO:H11	1.88	0.55
1:A:196:GLN:H	1:A:196:GLN:NE2	2.04	0.55
1:G:196:GLN:HE21	1:G:196:GLN:N	1.97	0.55
1:A:475:GLN:HG3	1:A:480:TYR:CB	2.36	0.55
1:H:124:MET:HE3	1:H:173:LEU:HD22	1.89	0.55
1:C:260:SER:O	1:D:251:ARG:NH2	2.40	0.55
1:E:424:THR:CG2	1:E:470:MET:SD	2.95	0.55
1:E:468:TYR:CE1	1:F:487:GLU:HG3	2.42	0.55
1:G:101:TYR:CG	5:G:6927:EDO:H11	2.42	0.55
1:E:46:GLU:HB2	5:E:6915:EDO:H21	1.88	0.54
1:F:196:GLN:H	1:F:196:GLN:NE2	1.99	0.54
1:B:41:ASN:ND2	1:B:43:SER:H	2.05	0.54
1:E:289:GLN:NE2	7:E:3288:HOH:O	2.39	0.54
1:D:172:LEU:HD21	1:D:200:THR:HB	1.89	0.54
1:D:294:LEU:HD12	1:D:306:SER:HA	1.90	0.54
1:G:468:TYR:CE1	1:H:487:GLU:HG3	2.43	0.53
1:A:120:VAL:HG12	1:A:124:MET:HE2	1.89	0.53
1:A:205:ALA:HB2	1:A:220:ILE:HD12	1.90	0.53
1:A:11:PRO:HB3	1:A:114:TYR:CZ	2.43	0.53
1:A:498:LYS:HG2	1:A:499:ASN:N	2.24	0.53
1:D:124:MET:HE3	1:D:173:LEU:HD22	1.90	0.53
1:A:251:ARG:NH2	1:B:260:SER:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:ASN:C	1:E:41:ASN:HD22	2.17	0.53
1:F:424:THR:CG2	1:F:470:MET:SD	2.96	0.53
1:G:475:GLN:HE21	1:H:488:VAL:HG21	1.74	0.53
1:B:11:PRO:HB3	1:B:114:TYR:CZ	2.45	0.52
1:D:120:VAL:HG12	1:D:124:MET:HE2	1.92	0.52
1:A:302:CYS:SG	7:A:3143:HOH:O	2.58	0.52
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.44	0.52
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.43	0.52
1:B:289:GLN:NE2	7:B:3301:HOH:O	2.29	0.52
1:G:349:GLN:HG3	7:G:3432:HOH:O	2.09	0.52
1:B:205:ALA:HB2	1:B:220:ILE:HD12	1.92	0.52
1:G:487:GLU:HG3	1:H:468:TYR:CE1	2.45	0.52
1:A:247:THR:O	1:A:251:ARG:HG3	2.09	0.52
1:H:172:LEU:HD21	1:H:200:THR:HB	1.92	0.52
1:D:347:GLU:O	1:D:351:LYS:HG2	2.10	0.52
1:H:205:ALA:HB2	1:H:220:ILE:HD12	1.92	0.52
1:C:468:TYR:CE1	1:D:487:GLU:HG3	2.45	0.51
1:A:441:TYR:CD1	5:A:6941:EDO:H12	2.45	0.51
1:C:41:ASN:ND2	1:C:43:SER:H	2.09	0.51
1:E:41:ASN:ND2	1:E:43:SER:H	2.08	0.51
1:G:289:GLN:NE2	7:G:3261:HOH:O	2.34	0.51
1:H:449:GLY:HA3	1:H:466:GLY:O	2.10	0.51
1:E:41:ASN:CB	5:E:6915:EDO:H11	2.41	0.51
1:G:260:SER:O	1:H:251:ARG:NH2	2.43	0.51
1:G:41:ASN:ND2	1:G:43:SER:H	2.08	0.51
1:G:124:MET:HE2	1:G:173:LEU:HD21	1.93	0.50
1:D:205:ALA:HB2	1:D:220:ILE:HD12	1.92	0.50
1:G:294:LEU:HD22	1:G:405:MET:CB	2.38	0.50
1:D:196:GLN:H	1:D:196:GLN:NE2	2.08	0.50
1:A:41:ASN:HD22	1:A:43:SER:H	1.60	0.50
1:G:424:THR:CG2	1:G:470:MET:SD	3.00	0.50
1:E:294:LEU:HD22	1:E:405:MET:HB2	1.94	0.49
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.48	0.49
1:F:41:ASN:HD22	1:F:43:SER:H	1.60	0.49
1:B:33:SER:O	1:B:34:ARG:HB2	2.11	0.49
5:E:6945:EDO:H11	1:F:72:LEU:HD21	1.95	0.49
1:D:167:PRO:HD3	1:D:244:THR:HB	1.95	0.49
1:F:15:PRO:HD2	1:F:108:LEU:HD22	1.93	0.49
1:E:350:PHE:CE2	5:E:6965:EDO:H12	2.46	0.49
1:D:41:ASN:HD22	1:D:43:SER:H	1.61	0.48
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.48	0.48
5:C:6943:EDO:H11	1:D:72:LEU:HD21	1.94	0.48
1:G:205:ALA:HB2	1:G:220:ILE:HD12	1.96	0.48
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.48	0.48
1:H:271:GLY:HA2	1:H:425:TYR:CG	2.48	0.48
1:A:172:LEU:HD21	1:A:200:THR:HB	1.96	0.48
1:G:449:GLY:HA3	1:G:466:GLY:O	2.13	0.48
1:B:449:GLY:HA3	1:B:466:GLY:O	2.13	0.48
1:E:115:VAL:HG23	7:E:1458:HOH:O	2.13	0.48
1:E:167:PRO:HD3	1:E:244:THR:HB	1.96	0.48
1:B:475:GLN:OE1	1:B:480:TYR:HB3	2.14	0.48
1:G:161:VAL:HA	1:G:188:VAL:HG23	1.96	0.47
1:C:196:GLN:H	1:C:196:GLN:NE2	2.04	0.47
1:D:294:LEU:HD13	7:D:1077:HOH:O	2.14	0.47
1:E:135:TRP:CE2	1:G:138:LYS:HD3	2.49	0.47
1:A:289:GLN:NE2	7:A:3151:HOH:O	2.37	0.47
1:A:490:THR:OG1	1:B:464:PRO:HG2	2.15	0.47
1:B:441:TYR:CD1	5:B:6942:EDO:H12	2.50	0.47
1:H:167:PRO:HD3	1:H:244:THR:HB	1.96	0.47
1:E:490:THR:OG1	1:F:464:PRO:HG2	2.15	0.47
1:G:11:PRO:HB3	1:G:114:TYR:CZ	2.50	0.47
1:A:449:GLY:HA3	1:A:466:GLY:O	2.14	0.47
1:B:27:GLU:HB2	1:B:29:HIS:CE1	2.49	0.47
1:H:389:VAL:HB	1:H:408:LEU:HG	1.97	0.47
1:E:21:GLN:HB3	1:E:29:HIS:O	2.14	0.47
1:C:490:THR:OG1	1:D:464:PRO:HG2	2.15	0.46
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.50	0.46
1:C:349:GLN:HB3	7:C:2406:HOH:O	2.14	0.46
1:D:268:GLU:HB3	7:D:1339:HOH:O	2.15	0.46
1:E:174:MET:HE2	1:E:174:MET:HA	1.97	0.46
1:H:294:LEU:HD13	7:H:1076:HOH:O	2.15	0.46
1:E:146:ILE:HG13	1:F:460:GLY:HA3	1.97	0.46
1:G:350:PHE:HZ	1:G:373:ILE:CG2	2.28	0.46
1:D:352:LYS:HD3	7:D:1766:HOH:O	2.14	0.46
1:H:112:LYS:HB2	7:H:1922:HOH:O	2.16	0.46
1:D:247:THR:HA	1:D:269:LEU:HD13	1.97	0.46
1:A:46:GLU:HB2	5:A:6911:EDO:H21	1.97	0.46
1:B:59:VAL:O	1:B:63:VAL:HG23	2.15	0.46
1:D:361:LYS:HD3	1:D:367:LEU:HD22	1.98	0.46
1:A:464:PRO:HG2	1:B:490:THR:OG1	2.17	0.45
1:C:464:PRO:HG2	1:D:490:THR:OG1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:MET:HE3	1:C:173:LEU:CD2	2.44	0.45
1:B:161:VAL:HA	1:B:188:VAL:HG23	1.99	0.45
1:E:441:TYR:CD1	5:E:6945:EDO:H12	2.52	0.45
1:C:24:ILE:O	1:C:27:GLU:HG2	2.17	0.45
1:D:294:LEU:HD13	1:D:405:MET:HA	1.99	0.45
1:H:445:ALA:HB2	5:H:6948:EDO:C1	2.43	0.45
1:H:289:GLN:NE2	7:H:3279:HOH:O	2.48	0.45
1:C:268:GLU:HB3	7:C:1687:HOH:O	2.17	0.44
1:B:167:PRO:HD3	1:B:244:THR:HB	1.99	0.44
1:E:445:ALA:HB2	5:E:6945:EDO:H11	2.00	0.44
1:G:303:CYS:SG	1:G:459:PHE:HZ	2.41	0.44
1:A:159:VAL:HG12	1:A:187:ASN:OD1	2.17	0.44
1:B:193:VAL:HG11	1:B:201:ALA:CB	2.47	0.44
1:B:347:GLU:HG3	5:B:6962:EDO:C1	2.47	0.44
1:C:424:THR:HG22	1:C:470:MET:HB2	1.99	0.44
1:E:389:VAL:HB	1:E:408:LEU:HG	2.00	0.44
1:H:11:PRO:HB3	1:H:114:TYR:CZ	2.52	0.44
1:C:120:VAL:O	1:C:124:MET:HG3	2.18	0.44
1:D:461:ALA:HA	1:D:477:LEU:HD22	2.00	0.44
1:D:498:LYS:HG2	1:D:499:ASN:N	2.33	0.44
1:F:196:GLN:HE21	1:F:196:GLN:N	2.04	0.44
1:E:13:GLN:NE2	7:E:3330:HOH:O	2.50	0.44
1:E:254:GLN:NE2	1:E:265:VAL:HG11	2.32	0.44
1:H:294:LEU:HD12	1:H:306:SER:HA	1.99	0.43
1:B:41:ASN:C	1:B:41:ASN:ND2	2.76	0.43
1:C:174:MET:HE3	1:C:174:MET:HA	2.00	0.43
1:G:490:THR:OG1	1:H:464:PRO:HG2	2.19	0.43
1:A:101:TYR:CD2	5:A:6921:EDO:H11	2.52	0.43
1:E:73:GLY:C	5:E:6955:EDO:H12	2.43	0.43
1:C:460:GLY:HA3	1:D:146:ILE:HG13	2.00	0.43
6:C:6834:GAI:N1	1:D:264:ARG:HD2	2.33	0.43
1:E:350:PHE:HE2	5:E:6965:EDO:H12	1.83	0.43
1:G:41:ASN:HD22	1:G:43:SER:H	1.65	0.43
1:A:21:GLN:HB3	1:A:29:HIS:O	2.18	0.43
1:B:283:MET:HE1	1:B:314:ILE:HB	2.01	0.43
1:B:461:ALA:HA	1:B:477:LEU:HD22	2.00	0.43
1:E:196:GLN:H	1:E:196:GLN:NE2	2.15	0.43
1:F:410:PHE:CD1	1:F:416:VAL:HB	2.52	0.43
1:A:120:VAL:O	1:A:124:MET:HG3	2.18	0.43
1:D:33:SER:O	1:D:34:ARG:HB2	2.19	0.43
1:F:154:THR:HA	1:F:489:LYS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ASN:C	1:A:41:ASN:ND2	2.73	0.43
1:A:146:ILE:HG13	1:B:460:GLY:HA3	2.00	0.43
1:B:174:MET:HE2	1:B:174:MET:HA	2.01	0.43
1:H:41:ASN:HD21	1:H:43:SER:HB2	1.84	0.43
1:D:449:GLY:HA3	1:D:466:GLY:O	2.18	0.43
1:C:289:GLN:NE2	7:C:3194:HOH:O	2.40	0.43
1:D:11:PRO:HB3	1:D:114:TYR:CZ	2.53	0.43
1:F:27:GLU:HB2	1:F:29:HIS:CE1	2.54	0.43
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.53	0.42
1:E:74:SER:N	5:E:6955:EDO:H12	2.33	0.42
1:E:498:LYS:HE2	1:E:498:LYS:HB3	1.91	0.42
1:H:498:LYS:HG2	1:H:499:ASN:N	2.34	0.42
1:C:11:PRO:HB3	1:C:114:TYR:CZ	2.54	0.42
1:H:347:GLU:HG2	1:H:351:LYS:HE3	2.01	0.42
1:B:249:ILE:O	1:B:253:ILE:HG12	2.19	0.42
1:D:41:ASN:C	1:D:41:ASN:ND2	2.73	0.42
1:B:27:GLU:HG3	7:B:1707:HOH:O	2.19	0.42
1:C:106:GLU:OE2	1:C:171:PRO:HB2	2.19	0.42
1:G:350:PHE:CZ	1:G:373:ILE:CG2	3.02	0.42
1:H:283:MET:HE1	1:H:314:ILE:HB	2.01	0.42
1:A:443:SER:HA	1:A:451:VAL:HG11	2.01	0.42
1:B:63:VAL:HG11	1:B:235:HIS:CE1	2.54	0.42
1:D:251:ARG:NH1	1:D:470:MET:HE1	2.34	0.42
1:G:12:ASN:O	1:G:15:PRO:HD3	2.18	0.42
1:A:124:MET:HE3	1:A:173:LEU:CD2	2.47	0.42
1:E:214:PRO:HA	1:E:215:PRO:HD3	1.94	0.42
1:E:294:LEU:HD12	1:E:306:SER:HA	2.02	0.42
1:D:166:ILE:HB	1:D:167:PRO:HD2	2.01	0.42
1:H:303:CYS:SG	1:H:459:PHE:HZ	2.43	0.42
1:A:271:GLY:HA2	1:A:425:TYR:CG	2.55	0.41
1:B:172:LEU:CD2	1:B:200:THR:HB	2.50	0.41
1:B:303:CYS:SG	1:B:459:PHE:HZ	2.43	0.41
1:C:154:THR:HA	1:C:489:LYS:O	2.20	0.41
1:D:12:ASN:O	1:D:15:PRO:HD3	2.20	0.41
1:E:166:ILE:HB	1:E:167:PRO:HD2	2.02	0.41
1:H:22:ILE:HG12	1:H:222:PRO:HD2	2.02	0.41
1:C:167:PRO:HD3	1:C:244:THR:HB	2.01	0.41
1:E:205:ALA:HB2	1:E:220:ILE:HD12	2.02	0.41
1:H:161:VAL:HA	1:H:188:VAL:HG23	2.03	0.41
1:A:11:PRO:HB3	1:A:114:TYR:CE1	2.56	0.41
1:A:475:GLN:CG	1:A:480:TYR:HB3	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:CYS:SG	1:C:459:PHE:HZ	2.43	0.41
1:D:32:VAL:HG11	1:D:57:GLU:OE2	2.20	0.41
1:D:498:LYS:HE2	1:D:498:LYS:HB3	1.91	0.41
1:D:106:GLU:O	1:D:110:ASN:HB3	2.21	0.41
1:A:244:THR:HG23	1:A:268:GLU:HG3	2.03	0.41
1:A:319:VAL:O	1:A:323:VAL:HG23	2.20	0.41
1:A:498:LYS:HE2	1:A:498:LYS:HB3	1.86	0.41
1:D:11:PRO:HB3	1:D:114:TYR:CE2	2.55	0.41
1:F:449:GLY:HA3	1:F:466:GLY:O	2.20	0.41
1:G:127:LYS:NZ	7:G:3224:HOH:O	2.51	0.41
1:A:292:PHE:HE1	1:A:457:ASP:HB2	1.85	0.41
1:C:410:PHE:CD1	1:C:416:VAL:HB	2.55	0.41
1:A:107:THR:HG23	1:A:112:LYS:O	2.20	0.41
1:A:294:LEU:HD23	1:A:306:SER:HA	2.02	0.41
1:B:389:VAL:HB	1:B:408:LEU:HG	2.01	0.41
1:D:101:TYR:CB	5:D:6924:EDO:H11	2.50	0.41
1:E:319:VAL:O	1:E:323:VAL:HG23	2.21	0.41
1:F:443:SER:HA	1:F:451:VAL:HG11	2.03	0.41
1:G:159:VAL:HG12	1:G:187:ASN:OD1	2.21	0.41
1:H:247:THR:O	1:H:251:ARG:HG3	2.21	0.41
1:A:254:GLN:HE21	1:A:254:GLN:HB2	1.64	0.41
1:B:294:LEU:HD12	1:B:306:SER:HA	2.02	0.41
1:C:196:GLN:HE21	1:C:196:GLN:N	2.06	0.41
1:D:213:PHE:HA	1:D:214:PRO:HD3	1.95	0.41
1:D:476:GLU:O	1:D:477:LEU:HB2	2.21	0.41
1:E:7:ALA:HA	7:E:2509:HOH:O	2.21	0.41
1:E:347:GLU:CG	1:E:351:LYS:HE2	2.46	0.41
1:G:475:GLN:NE2	1:H:488:VAL:CG2	2.84	0.41
1:A:167:PRO:HD3	1:A:244:THR:HB	2.02	0.40
5:G:6947:EDO:H11	1:H:72:LEU:HD21	2.03	0.40
1:A:12:ASN:O	1:A:15:PRO:HD3	2.21	0.40
1:A:68:ALA:HB1	5:A:6951:EDO:H21	2.03	0.40
1:D:443:SER:HA	1:D:451:VAL:HG11	2.04	0.40
1:F:359:THR:O	1:F:363:GLU:HG2	2.22	0.40
1:G:247:THR:O	1:G:251:ARG:HG3	2.20	0.40
1:G:350:PHE:HZ	1:G:373:ILE:HG21	1.87	0.40
1:G:475:GLN:HE21	1:H:488:VAL:CG2	2.34	0.40
1:E:155:ARG:HH11	5:E:6905:EDO:H22	1.86	0.40
1:B:25:ASN:O	1:B:27:GLU:HG2	2.21	0.40
1:B:107:THR:HG23	1:B:112:LYS:O	2.21	0.40
1:B:159:VAL:HG13	1:B:162:CYS:SG	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:LEU:HD13	7:B:1013:HOH:O	2.21	0.40
1:G:475:GLN:NE2	1:H:488:VAL:HG21	2.37	0.40
1:G:476:GLU:O	1:G:477:LEU:HB2	2.21	0.40
1:H:34:ARG:HD3	1:H:34:ARG:HA	1.89	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	492/500 (98%)	478 (97%)	14 (3%)	0	100	100
1	B	492/500 (98%)	477 (97%)	15 (3%)	0	100	100
1	C	492/500 (98%)	478 (97%)	14 (3%)	0	100	100
1	D	492/500 (98%)	473 (96%)	19 (4%)	0	100	100
1	E	492/500 (98%)	478 (97%)	14 (3%)	0	100	100
1	F	492/500 (98%)	478 (97%)	14 (3%)	0	100	100
1	G	492/500 (98%)	473 (96%)	19 (4%)	0	100	100
1	H	492/500 (98%)	477 (97%)	15 (3%)	0	100	100
All	All	3936/4000 (98%)	3812 (97%)	124 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	399/402 (99%)	393 (98%)	6 (2%)	57	64
1	B	399/402 (99%)	392 (98%)	7 (2%)	51	58
1	C	399/402 (99%)	392 (98%)	7 (2%)	51	58
1	D	399/402 (99%)	388 (97%)	11 (3%)	38	41
1	E	399/402 (99%)	393 (98%)	6 (2%)	57	64
1	F	399/402 (99%)	392 (98%)	7 (2%)	51	58
1	G	399/402 (99%)	391 (98%)	8 (2%)	48	54
1	H	399/402 (99%)	391 (98%)	8 (2%)	48	54
All	All	3192/3216 (99%)	3132 (98%)	60 (2%)	50	56

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	192	LYS
1	A	196	GLN
1	A	264	ARG
1	A	401	PHE
1	A	475	GLN
1	B	41	ASN
1	B	122	LEU
1	B	192	LYS
1	B	196	GLN
1	B	294	LEU
1	B	401	PHE
1	B	498	LYS
1	C	41	ASN
1	C	50	GLN
1	C	174	MET
1	C	196	GLN
1	C	268	GLU
1	C	294	LEU
1	C	401	PHE
1	D	41	ASN
1	D	159	VAL
1	D	174	MET
1	D	196	GLN
1	D	206	ASN

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Mol	Chain	Res	Type
1	D	254	GLN
1	D	362	GLN
1	D	376	ASP
1	D	401	PHE
1	D	417	VAL
1	D	475	GLN
1	E	41	ASN
1	E	159	VAL
1	E	196	GLN
1	E	294	LEU
1	E	401	PHE
1	E	475	GLN
1	F	34	ARG
1	F	41	ASN
1	F	50	GLN
1	F	122	LEU
1	F	196	GLN
1	F	294	LEU
1	F	401	PHE
1	G	41	ASN
1	G	192	LYS
1	G	196	GLN
1	G	248	GLU
1	G	294	LEU
1	G	373	ILE
1	G	376	ASP
1	G	401	PHE
1	H	41	ASN
1	H	122	LEU
1	H	196	GLN
1	H	254	GLN
1	H	268	GLU
1	H	294	LEU
1	H	401	PHE
1	H	475	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	41	ASN
1	A	175	GLN

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Mol	Chain	Res	Type
1	A	196	GLN
1	A	254	GLN
1	A	275	ASN
1	A	300	GLN
1	A	390	GLN
1	A	475	GLN
1	B	21	GLN
1	B	26	ASN
1	B	41	ASN
1	B	50	GLN
1	B	89	ASN
1	B	175	GLN
1	B	196	GLN
1	B	275	ASN
1	B	300	GLN
1	B	349	GLN
1	C	14	GLN
1	C	25	ASN
1	C	41	ASN
1	C	50	GLN
1	C	175	GLN
1	C	196	GLN
1	C	254	GLN
1	C	300	GLN
1	C	390	GLN
1	C	475	GLN
1	D	13	GLN
1	D	41	ASN
1	D	175	GLN
1	D	196	GLN
1	D	254	GLN
1	D	275	ASN
1	D	300	GLN
1	D	447	GLN
1	D	475	GLN
1	E	13	GLN
1	E	25	ASN
1	E	41	ASN
1	E	71	GLN
1	E	175	GLN
1	E	196	GLN
1	E	254	GLN

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Mol	Chain	Res	Type
1	E	275	ASN
1	E	300	GLN
1	E	475	GLN
1	F	13	GLN
1	F	14	GLN
1	F	26	ASN
1	F	29	HIS
1	F	41	ASN
1	F	50	GLN
1	F	175	GLN
1	F	196	GLN
1	F	254	GLN
1	F	275	ASN
1	F	300	GLN
1	F	390	GLN
1	G	13	GLN
1	G	26	ASN
1	G	41	ASN
1	G	175	GLN
1	G	196	GLN
1	G	275	ASN
1	G	300	GLN
1	H	29	HIS
1	H	41	ASN
1	H	175	GLN
1	H	196	GLN
1	H	275	ASN
1	H	300	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

Of 91 ligands modelled in this entry, 16 are monoatomic - leaving 75 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	EDO	C	6923	-	3,3,3	0.32	0	2,2,2	0.49	0
6	GAI	C	6823	-	3,3,3	1.22	1 (33%)	3,3,3	0.99	0
6	GAI	H	6808	-	3,3,3	1.25	1 (33%)	3,3,3	1.17	0
5	EDO	F	6946	-	3,3,3	0.59	0	2,2,2	0.36	0
5	EDO	G	6927	-	3,3,3	0.36	0	2,2,2	0.43	0
5	EDO	F	6906	-	3,3,3	0.58	0	2,2,2	0.29	0
6	GAI	A	6801	-	3,3,3	0.96	0	3,3,3	1.12	0
5	EDO	C	6953	-	3,3,3	0.58	0	2,2,2	0.33	0
6	GAI	A	6811	-	3,3,3	1.20	1 (33%)	3,3,3	1.03	0
4	NAD	F	506	2	46,48,48	2.10	11 (23%)	64,73,73	1.57	12 (18%)
5	EDO	C	6963	-	3,3,3	0.45	0	2,2,2	0.45	0
6	GAI	F	6826	-	3,3,3	1.18	1 (33%)	3,3,3	1.08	0
5	EDO	C	6943	-	3,3,3	0.53	0	2,2,2	0.35	0
4	NAD	D	504	2	46,48,48	2.25	12 (26%)	64,73,73	1.74	15 (23%)
5	EDO	G	6907	-	3,3,3	0.43	0	2,2,2	0.40	0
5	EDO	B	6962	-	3,3,3	0.57	0	2,2,2	0.27	0
6	GAI	F	6816	-	3,3,3	1.11	0	3,3,3	1.00	0
6	GAI	B	6812	-	3,3,3	1.30	1 (33%)	3,3,3	1.03	0
6	GAI	F	6806	-	3,3,3	1.18	0	3,3,3	1.08	0
4	NAD	C	503	2	46,48,48	2.15	10 (21%)	64,73,73	1.61	11 (17%)
5	EDO	C	6903	-	3,3,3	0.44	0	2,2,2	0.31	0
6	GAI	G	6817	-	3,3,3	1.09	0	3,3,3	1.00	0
6	GAI	D	6824	-	3,3,3	1.26	1 (33%)	3,3,3	1.08	0
4	NAD	G	507	2	46,48,48	1.88	8 (17%)	64,73,73	1.53	12 (18%)
6	GAI	E	6815	-	3,3,3	1.33	1 (33%)	3,3,3	1.06	0
5	EDO	H	6908	-	3,3,3	0.53	0	2,2,2	0.44	0
6	GAI	G	6807	-	3,3,3	1.15	0	3,3,3	1.20	0
5	EDO	A	6951	-	3,3,3	0.54	0	2,2,2	0.32	0
5	EDO	H	6918	-	3,3,3	0.52	0	2,2,2	0.31	0
5	EDO	D	6914	-	3,3,3	0.53	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GAI	D	6804	-	3,3,3	1.46	1 (33%)	3,3,3	0.99	0
5	EDO	A	6911	-	3,3,3	0.57	0	2,2,2	0.28	0
6	GAI	C	6834	-	3,3,3	1.48	1 (33%)	3,3,3	1.11	0
5	EDO	G	6947	-	3,3,3	0.59	0	2,2,2	0.30	0
6	GAI	A	6821	-	3,3,3	1.35	1 (33%)	3,3,3	1.08	0
6	GAI	B	6831	-	3,3,3	1.51	1 (33%)	3,3,3	1.10	0
6	GAI	D	6833	-	3,3,3	1.21	1 (33%)	3,3,3	1.07	0
5	EDO	A	6921	-	3,3,3	0.40	0	2,2,2	0.40	0
6	GAI	C	6813	-	3,3,3	1.24	1 (33%)	3,3,3	1.06	0
5	EDO	D	6904	-	3,3,3	0.50	0	2,2,2	0.40	0
5	EDO	E	6955	-	3,3,3	0.50	0	2,2,2	0.33	0
6	GAI	A	6832	-	3,3,3	1.10	0	3,3,3	1.01	0
4	NAD	E	505	2	46,48,48	2.06	8 (17%)	64,73,73	1.65	16 (25%)
5	EDO	A	6941	-	3,3,3	0.60	0	2,2,2	0.29	0
5	EDO	B	6902	-	3,3,3	0.51	0	2,2,2	0.34	0
5	EDO	E	6925	-	3,3,3	0.36	0	2,2,2	0.46	0
5	EDO	F	6966	-	3,3,3	0.69	0	2,2,2	0.37	0
5	EDO	H	6928	-	3,3,3	0.33	0	2,2,2	0.49	0
5	EDO	B	6952	-	3,3,3	0.53	0	2,2,2	0.32	0
5	EDO	F	6916	-	3,3,3	0.41	0	2,2,2	0.43	0
5	EDO	E	6945	-	3,3,3	0.76	0	2,2,2	0.11	0
6	GAI	C	6803	-	3,3,3	0.88	0	3,3,3	1.08	0
5	EDO	C	6913	-	3,3,3	0.49	0	2,2,2	0.40	0
5	EDO	D	6924	-	3,3,3	0.41	0	2,2,2	0.41	0
5	EDO	E	6915	-	3,3,3	0.42	0	2,2,2	0.31	0
6	GAI	E	6835	-	3,3,3	1.01	0	3,3,3	1.22	0
4	NAD	H	508	2	46,48,48	2.16	9 (19%)	64,73,73	1.64	13 (20%)
5	EDO	F	6926	-	3,3,3	0.52	0	2,2,2	0.36	0
6	GAI	D	6814	-	3,3,3	1.41	1 (33%)	3,3,3	1.08	0
6	GAI	E	6836	-	3,3,3	1.04	0	3,3,3	1.18	0
6	GAI	E	6805	-	3,3,3	1.15	0	3,3,3	1.25	0
4	NAD	A	501	2	46,48,48	2.40	10 (21%)	64,73,73	1.54	11 (17%)
5	EDO	E	6905	-	3,3,3	0.41	0	2,2,2	0.48	0
5	EDO	E	6965	-	3,3,3	0.48	0	2,2,2	0.39	0
5	EDO	F	6956	-	3,3,3	0.48	0	2,2,2	0.37	0
5	EDO	G	6917	-	3,3,3	0.47	0	2,2,2	0.37	0
4	NAD	B	502	2	46,48,48	2.23	10 (21%)	64,73,73	1.44	9 (14%)
5	EDO	B	6912	-	3,3,3	0.52	0	2,2,2	0.34	0
6	GAI	H	6818	-	3,3,3	1.21	1 (33%)	3,3,3	1.00	0
6	GAI	B	6802	-	3,3,3	1.22	1 (33%)	3,3,3	1.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GAI	G	6838	-	3,3,3	1.24	1 (33%)	3,3,3	0.93	0
5	EDO	A	6901	-	3,3,3	0.54	0	2,2,2	0.37	0
5	EDO	H	6948	-	3,3,3	0.44	0	2,2,2	0.35	0
6	GAI	H	6837	-	3,3,3	1.04	0	3,3,3	1.04	0
5	EDO	B	6942	-	3,3,3	0.47	0	2,2,2	0.41	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
5	EDO	C	6923	-	-	0/1/1/1	-
5	EDO	F	6946	-	-	1/1/1/1	-
5	EDO	G	6927	-	-	0/1/1/1	-
5	EDO	F	6906	-	-	0/1/1/1	-
5	EDO	C	6953	-	-	0/1/1/1	-
4	NAD	F	506	2	-	3/30/62/62	0/5/5/5
5	EDO	C	6963	-	-	0/1/1/1	-
5	EDO	C	6943	-	-	0/1/1/1	-
4	NAD	D	504	2	-	8/30/62/62	0/5/5/5
5	EDO	G	6907	-	-	0/1/1/1	-
5	EDO	B	6962	-	-	1/1/1/1	-
4	NAD	C	503	2	-	3/30/62/62	0/5/5/5
5	EDO	C	6903	-	-	0/1/1/1	-
4	NAD	G	507	2	-	1/30/62/62	0/5/5/5
5	EDO	H	6908	-	-	0/1/1/1	-
5	EDO	A	6951	-	-	0/1/1/1	-
5	EDO	H	6918	-	-	0/1/1/1	-
5	EDO	D	6914	-	-	0/1/1/1	-
5	EDO	A	6911	-	-	0/1/1/1	-
5	EDO	G	6947	-	-	0/1/1/1	-
5	EDO	A	6921	-	-	0/1/1/1	-
5	EDO	D	6904	-	-	1/1/1/1	-
5	EDO	E	6955	-	-	0/1/1/1	-
4	NAD	E	505	2	-	6/30/62/62	0/5/5/5
5	EDO	A	6941	-	-	0/1/1/1	-
5	EDO	B	6902	-	-	0/1/1/1	-
5	EDO	E	6925	-	-	0/1/1/1	-
5	EDO	F	6966	-	-	0/1/1/1	-
5	EDO	H	6928	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	6952	-	-	0/1/1/1	-
5	EDO	F	6916	-	-	0/1/1/1	-
5	EDO	E	6945	-	-	1/1/1/1	-
5	EDO	C	6913	-	-	0/1/1/1	-
5	EDO	D	6924	-	-	0/1/1/1	-
5	EDO	E	6915	-	-	0/1/1/1	-
4	NAD	H	508	2	-	6/30/62/62	0/5/5/5
5	EDO	F	6926	-	-	1/1/1/1	-
4	NAD	A	501	2	-	9/30/62/62	0/5/5/5
5	EDO	E	6905	-	-	0/1/1/1	-
5	EDO	E	6965	-	-	0/1/1/1	-
5	EDO	F	6956	-	-	1/1/1/1	-
5	EDO	G	6917	-	-	0/1/1/1	-
4	NAD	B	502	2	-	3/30/62/62	0/5/5/5
5	EDO	B	6912	-	-	1/1/1/1	-
5	EDO	A	6901	-	-	1/1/1/1	-
5	EDO	H	6948	-	-	0/1/1/1	-
5	EDO	B	6942	-	-	0/1/1/1	-

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	NAD	C3N-C7N	-10.94	1.34	1.50
4	D	504	NAD	C3N-C7N	-9.72	1.36	1.50
4	E	505	NAD	C3N-C7N	-9.66	1.36	1.50
4	C	503	NAD	C3N-C7N	-9.31	1.36	1.50
4	B	502	NAD	C3N-C7N	-9.30	1.36	1.50
4	H	508	NAD	C3N-C7N	-9.27	1.36	1.50
4	F	506	NAD	C3N-C7N	-9.24	1.36	1.50
4	G	507	NAD	C3N-C7N	-7.87	1.38	1.50
4	A	501	NAD	PN-O3	5.92	1.65	1.59
4	B	502	NAD	PN-O3	5.88	1.65	1.59
4	C	503	NAD	PN-O3	5.59	1.65	1.59
4	D	504	NAD	C8A-N7A	5.32	1.41	1.31
4	H	508	NAD	PN-O3	5.31	1.65	1.59
4	G	507	NAD	C8A-N7A	4.56	1.40	1.31
4	D	504	NAD	PN-O3	4.48	1.64	1.59
4	B	502	NAD	C8A-N7A	4.31	1.40	1.31
4	B	502	NAD	C2A-N3A	4.23	1.41	1.33
4	A	501	NAD	C8A-N7A	4.22	1.39	1.31
4	C	503	NAD	C8A-N7A	4.00	1.39	1.31
4	E	505	NAD	C8A-N7A	3.88	1.39	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	506	NAD	C8A-N7A	3.87	1.39	1.31
4	E	505	NAD	C2A-N3A	3.77	1.40	1.33
4	C	503	NAD	C2A-N3A	3.73	1.40	1.33
4	A	501	NAD	O4D-C1D	3.71	1.45	1.40
4	F	506	NAD	PA-O3	-3.68	1.55	1.59
4	H	508	NAD	C8A-N7A	3.64	1.38	1.31
4	H	508	NAD	C2A-N3A	3.59	1.40	1.33
4	F	506	NAD	C2A-N3A	3.52	1.40	1.33
4	E	505	NAD	C4N-C3N	-3.52	1.34	1.39
4	C	503	NAD	C2A-N1A	3.44	1.40	1.33
4	G	507	NAD	C2A-N1A	3.42	1.40	1.33
4	F	506	NAD	C4N-C3N	-3.39	1.34	1.39
4	H	508	NAD	C5N-C4N	-3.36	1.33	1.38
4	D	504	NAD	C5N-C4N	-3.34	1.33	1.38
4	G	507	NAD	PN-O3	3.32	1.63	1.59
4	F	506	NAD	PN-O3	3.27	1.63	1.59
4	D	504	NAD	C2N-C3N	-3.25	1.33	1.39
4	B	502	NAD	C2A-N1A	3.24	1.39	1.33
4	A	501	NAD	C2N-C3N	-3.24	1.33	1.39
4	D	504	NAD	C2A-N1A	3.22	1.39	1.33
4	A	501	NAD	C2A-N1A	3.15	1.39	1.33
4	F	506	NAD	C2A-N1A	3.06	1.39	1.33
4	H	508	NAD	C2A-N1A	3.06	1.39	1.33
4	G	507	NAD	C2A-N3A	3.01	1.39	1.33
4	H	508	NAD	O4D-C1D	2.96	1.44	1.40
4	B	502	NAD	C4N-C3N	-2.81	1.35	1.39
4	E	505	NAD	C2A-N1A	2.78	1.38	1.33
4	A	501	NAD	C2A-N3A	2.77	1.38	1.33
4	D	504	NAD	C2N-N1N	-2.70	1.32	1.35
4	B	502	NAD	C4A-N3A	2.68	1.39	1.34
4	A	501	NAD	PA-O3	2.68	1.62	1.59
4	D	504	NAD	C4N-C3N	-2.63	1.35	1.39
4	E	505	NAD	C2N-C3N	-2.62	1.34	1.39
6	B	6831	GAI	C-N1	2.60	1.37	1.30
4	B	502	NAD	C5N-C4N	-2.55	1.34	1.38
4	C	503	NAD	C4N-C3N	-2.55	1.35	1.39
6	C	6834	GAI	C-N1	2.52	1.37	1.30
4	D	504	NAD	O4D-C1D	2.48	1.44	1.40
6	D	6804	GAI	C-N1	2.45	1.36	1.30
4	G	507	NAD	C4A-N3A	2.45	1.39	1.34
4	G	507	NAD	C4N-C3N	-2.43	1.35	1.39
4	A	501	NAD	C5N-C4N	-2.40	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	508	NAD	C4N-C3N	-2.40	1.35	1.39
4	B	502	NAD	PA-O3	2.37	1.62	1.59
4	C	503	NAD	O4D-C1D	2.36	1.44	1.40
6	D	6814	GAI	C-N1	2.36	1.36	1.30
4	E	505	NAD	C5N-C4N	-2.36	1.34	1.38
4	F	506	NAD	C2N-C3N	-2.35	1.35	1.39
4	E	505	NAD	O4D-C1D	2.35	1.44	1.40
6	A	6821	GAI	C-N1	2.30	1.36	1.30
4	F	506	NAD	PN-O2N	-2.29	1.44	1.55
4	A	501	NAD	C4N-C3N	-2.29	1.35	1.39
6	E	6815	GAI	C-N1	2.27	1.36	1.30
4	H	508	NAD	C2N-C3N	-2.27	1.35	1.39
4	F	506	NAD	O4D-C1D	2.27	1.43	1.40
4	G	507	NAD	C5N-C4N	-2.27	1.35	1.38
4	D	504	NAD	C5A-N7A	-2.26	1.35	1.39
4	C	503	NAD	PN-O2N	-2.23	1.45	1.55
6	D	6824	GAI	C-N1	2.18	1.36	1.30
6	B	6812	GAI	C-N1	2.16	1.36	1.30
6	C	6813	GAI	C-N1	2.11	1.36	1.30
4	D	504	NAD	C8A-N9A	2.11	1.41	1.37
6	G	6838	GAI	C-N1	2.10	1.36	1.30
4	F	506	NAD	C6A-N1A	2.09	1.41	1.35
4	C	503	NAD	PN-O5D	2.09	1.67	1.59
6	D	6833	GAI	C-N1	2.09	1.35	1.30
6	H	6818	GAI	C-N1	2.09	1.35	1.30
4	C	503	NAD	PA-O3	-2.08	1.57	1.59
6	A	6811	GAI	C-N1	2.08	1.35	1.30
4	D	504	NAD	PA-O2A	-2.07	1.45	1.55
6	C	6823	GAI	C-N1	2.06	1.35	1.30
6	B	6802	GAI	C-N1	2.05	1.35	1.30
6	H	6808	GAI	C-N1	2.03	1.35	1.30
6	F	6826	GAI	C-N1	2.02	1.35	1.30
4	B	502	NAD	O4D-C1D	2.01	1.43	1.40

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	504	NAD	C5A-C4A-N9A	5.52	111.83	105.81
4	E	505	NAD	C5A-C4A-N9A	4.97	111.22	105.81
4	H	508	NAD	N3A-C2A-N1A	-4.88	121.19	128.58
4	A	501	NAD	C5A-C4A-N9A	4.47	110.68	105.81
4	C	503	NAD	O7N-C7N-N7N	-4.42	116.23	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	NAD	N3A-C2A-N1A	-4.37	121.97	128.58
4	G	507	NAD	C5A-C4A-N9A	4.20	110.39	105.81
4	F	506	NAD	O7N-C7N-C3N	4.18	124.70	119.60
4	D	504	NAD	O2A-PA-O3	4.15	118.49	107.27
4	F	506	NAD	N3A-C2A-N1A	-4.14	122.32	128.58
4	C	503	NAD	C5A-C4A-N9A	4.05	110.22	105.81
4	G	507	NAD	O7N-C7N-N7N	-4.03	116.79	122.62
4	E	505	NAD	O7N-C7N-N7N	-4.01	116.83	122.62
4	B	502	NAD	O4D-C4D-C3D	-3.96	97.30	105.15
4	E	505	NAD	N3A-C2A-N1A	-3.84	122.76	128.58
4	H	508	NAD	C6N-C5N-C4N	-3.75	114.05	119.45
4	C	503	NAD	O4B-C1B-C2B	-3.70	98.70	106.62
4	E	505	NAD	C5N-C4N-C3N	3.66	123.97	120.36
4	G	507	NAD	C5N-C4N-C3N	3.63	123.93	120.36
4	D	504	NAD	C5N-C4N-C3N	3.59	123.89	120.36
4	A	501	NAD	O7N-C7N-C3N	-3.58	115.22	119.60
4	C	503	NAD	O7N-C7N-C3N	3.57	123.96	119.60
4	D	504	NAD	C4A-N9A-C8A	-3.55	102.01	105.74
4	H	508	NAD	O7N-C7N-N7N	-3.54	117.50	122.62
4	D	504	NAD	O7N-C7N-N7N	-3.50	117.56	122.62
4	F	506	NAD	C5A-C4A-N9A	3.38	109.50	105.81
4	B	502	NAD	C5A-C4A-N9A	3.33	109.44	105.81
4	F	506	NAD	O7N-C7N-N7N	-3.33	117.81	122.62
4	C	503	NAD	O4D-C4D-C3D	-3.27	98.66	105.15
4	F	506	NAD	O4D-C4D-C3D	-3.24	98.71	105.15
4	D	504	NAD	C6N-C5N-C4N	-3.23	114.80	119.45
4	C	503	NAD	C2B-C3B-C4B	-3.20	96.42	102.61
4	H	508	NAD	C5N-C4N-C3N	3.20	123.51	120.36
4	B	502	NAD	C3N-C7N-N7N	3.18	121.66	117.74
4	B	502	NAD	N3A-C2A-N1A	-3.17	123.78	128.58
4	C	503	NAD	C6N-C5N-C4N	-3.16	114.89	119.45
4	E	505	NAD	C2D-C3D-C4D	-3.13	96.57	102.61
4	B	502	NAD	O7N-C7N-N7N	-3.07	118.18	122.62
4	E	505	NAD	O4D-C4D-C3D	-3.05	99.10	105.15
4	G	507	NAD	N3A-C2A-N1A	-3.04	123.98	128.58
4	A	501	NAD	C4D-O4D-C1D	-3.01	107.17	109.92
4	H	508	NAD	C5A-C4A-N9A	3.00	109.08	105.81
4	D	504	NAD	N3A-C2A-N1A	-2.95	124.11	128.58
4	F	506	NAD	C5N-C4N-C3N	2.94	123.26	120.36
4	A	501	NAD	C5N-C4N-C3N	2.90	123.22	120.36
4	G	507	NAD	C4A-N9A-C8A	-2.88	102.72	105.74
4	C	503	NAD	N3A-C2A-N1A	-2.85	124.27	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	504	NAD	C6A-C5A-C4A	2.84	121.05	117.18
4	A	501	NAD	O7N-C7N-N7N	2.82	126.70	122.62
4	E	505	NAD	O7N-C7N-C3N	2.82	123.05	119.60
4	E	505	NAD	O4B-C1B-N9A	2.74	113.35	108.09
4	G	507	NAD	C3N-C7N-N7N	2.73	121.11	117.74
4	F	506	NAD	C4D-O4D-C1D	2.72	112.42	109.92
4	F	506	NAD	C6N-C5N-C4N	-2.68	115.58	119.45
4	D	504	NAD	N3A-C4A-N9A	-2.68	122.61	127.17
4	E	505	NAD	C4A-N9A-C8A	-2.65	102.95	105.74
4	B	502	NAD	C5A-C4A-N3A	-2.65	123.07	126.72
4	H	508	NAD	O4D-C4D-C3D	-2.64	99.91	105.15
4	H	508	NAD	C6A-C5A-C4A	2.60	120.73	117.18
4	F	506	NAD	C2B-C3B-C4B	-2.60	97.58	102.61
4	A	501	NAD	C6N-C5N-C4N	-2.60	115.71	119.45
4	B	502	NAD	C5N-C4N-C3N	2.59	122.91	120.36
4	G	507	NAD	C6A-C5A-C4A	2.58	120.70	117.18
4	C	503	NAD	C5N-C4N-C3N	2.57	122.89	120.36
4	H	508	NAD	C2B-C3B-C4B	-2.55	97.68	102.61
4	C	503	NAD	C6A-C5A-C4A	2.51	120.61	117.18
4	H	508	NAD	O7N-C7N-C3N	2.50	122.65	119.60
4	G	507	NAD	O4B-C1B-C2B	-2.49	101.28	106.62
4	E	505	NAD	C6N-C5N-C4N	-2.43	115.95	119.45
4	B	502	NAD	C6A-C5A-C4A	2.41	120.47	117.18
4	H	508	NAD	C5N-C6N-N1N	2.38	123.63	120.38
4	F	506	NAD	O3-PN-O1N	2.32	117.69	110.70
4	G	507	NAD	C2B-C3B-C4B	-2.32	98.13	102.61
4	D	504	NAD	O4B-C1B-N9A	2.32	112.54	108.09
4	E	505	NAD	C6A-C5A-C4A	2.31	120.34	117.18
4	D	504	NAD	O4D-C4D-C3D	-2.29	100.61	105.15
4	E	505	NAD	C2B-C3B-C4B	-2.28	98.20	102.61
4	A	501	NAD	C4A-N9A-C8A	-2.28	103.35	105.74
4	D	504	NAD	C4D-O4D-C1D	-2.28	107.84	109.92
4	A	501	NAD	C6A-C5A-C4A	2.27	120.28	117.18
4	F	506	NAD	O4B-C1B-C2B	-2.26	101.79	106.62
4	H	508	NAD	C6A-C5A-N7A	-2.25	127.76	132.09
4	F	506	NAD	C6A-C5A-C4A	2.22	120.21	117.18
4	E	505	NAD	C1B-N9A-C8A	2.18	131.94	127.09
4	B	502	NAD	O4B-C4B-C3B	2.18	109.48	105.15
4	H	508	NAD	C5A-C4A-N3A	-2.16	123.74	126.72
4	A	501	NAD	C2B-C3B-C4B	-2.15	98.45	102.61
4	D	504	NAD	O7N-C7N-C3N	2.15	122.23	119.60
4	A	501	NAD	C5A-C4A-N3A	-2.14	123.77	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503	NAD	C2N-C3N-C4N	2.11	120.71	118.26
4	H	508	NAD	C2N-C3N-C4N	2.10	120.70	118.26
4	E	505	NAD	O2A-PA-O3	2.09	112.93	107.27
4	G	507	NAD	C5A-C4A-N3A	-2.09	123.83	126.72
4	E	505	NAD	C2B-C1B-N9A	-2.08	108.13	113.30
4	G	507	NAD	O7N-C7N-C3N	2.05	122.10	119.60
4	D	504	NAD	C2B-C3B-C4B	-2.05	98.65	102.61
4	G	507	NAD	O5D-C5D-C4D	2.04	115.96	108.99
4	E	505	NAD	C5A-C4A-N3A	-2.03	123.92	126.72
4	D	504	NAD	C6A-C5A-N7A	-2.03	128.18	132.09

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	508	NAD	C4N-C3N-C7N-N7N
4	H	508	NAD	C4N-C3N-C7N-O7N
4	A	501	NAD	C2N-C3N-C7N-O7N
4	H	508	NAD	C2N-C3N-C7N-O7N
4	H	508	NAD	C2N-C3N-C7N-N7N
4	C	503	NAD	C2B-C1B-N9A-C8A
4	D	504	NAD	PN-O3-PA-O1A
4	A	501	NAD	C4N-C3N-C7N-O7N
4	F	506	NAD	C2B-C1B-N9A-C8A
4	A	501	NAD	C4N-C3N-C7N-N7N
4	A	501	NAD	C2B-C1B-N9A-C8A
4	B	502	NAD	C2B-C1B-N9A-C8A
4	D	504	NAD	C2B-C1B-N9A-C8A
4	E	505	NAD	C2B-C1B-N9A-C8A
4	G	507	NAD	C2B-C1B-N9A-C8A
4	H	508	NAD	C2B-C1B-N9A-C8A
4	E	505	NAD	PN-O3-PA-O1A
4	A	501	NAD	C2N-C3N-C7N-N7N
4	A	501	NAD	C5B-O5B-PA-O2A
4	A	501	NAD	C5B-O5B-PA-O3
4	D	504	NAD	C5B-O5B-PA-O2A
4	D	504	NAD	C4N-C3N-C7N-N7N
4	E	505	NAD	C4N-C3N-C7N-N7N
4	B	502	NAD	PN-O3-PA-O1A
4	B	502	NAD	O4B-C1B-N9A-C8A
4	C	503	NAD	O4B-C1B-N9A-C8A
5	B	6962	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	E	505	NAD	C4N-C3N-C7N-O7N
4	E	505	NAD	O4B-C1B-N9A-C8A
5	A	6901	EDO	O1-C1-C2-O2
5	F	6946	EDO	O1-C1-C2-O2
4	D	504	NAD	PN-O3-PA-O2A
4	E	505	NAD	PN-O3-PA-O2A
4	D	504	NAD	O4B-C1B-N9A-C8A
4	F	506	NAD	O4B-C1B-N9A-C8A
4	A	501	NAD	C2B-C1B-N9A-C4A
4	C	503	NAD	C2B-C1B-N9A-C4A
4	F	506	NAD	C2B-C1B-N9A-C4A
5	D	6904	EDO	O1-C1-C2-O2
5	E	6945	EDO	O1-C1-C2-O2
5	F	6926	EDO	O1-C1-C2-O2
5	F	6956	EDO	O1-C1-C2-O2
4	A	501	NAD	O4B-C1B-N9A-C8A
4	H	508	NAD	O4B-C1B-N9A-C8A
4	D	504	NAD	C4N-C3N-C7N-O7N
4	D	504	NAD	C2N-C3N-C7N-N7N
5	B	6912	EDO	O1-C1-C2-O2

There are no ring outliers.

19 monomers are involved in 34 short contacts:

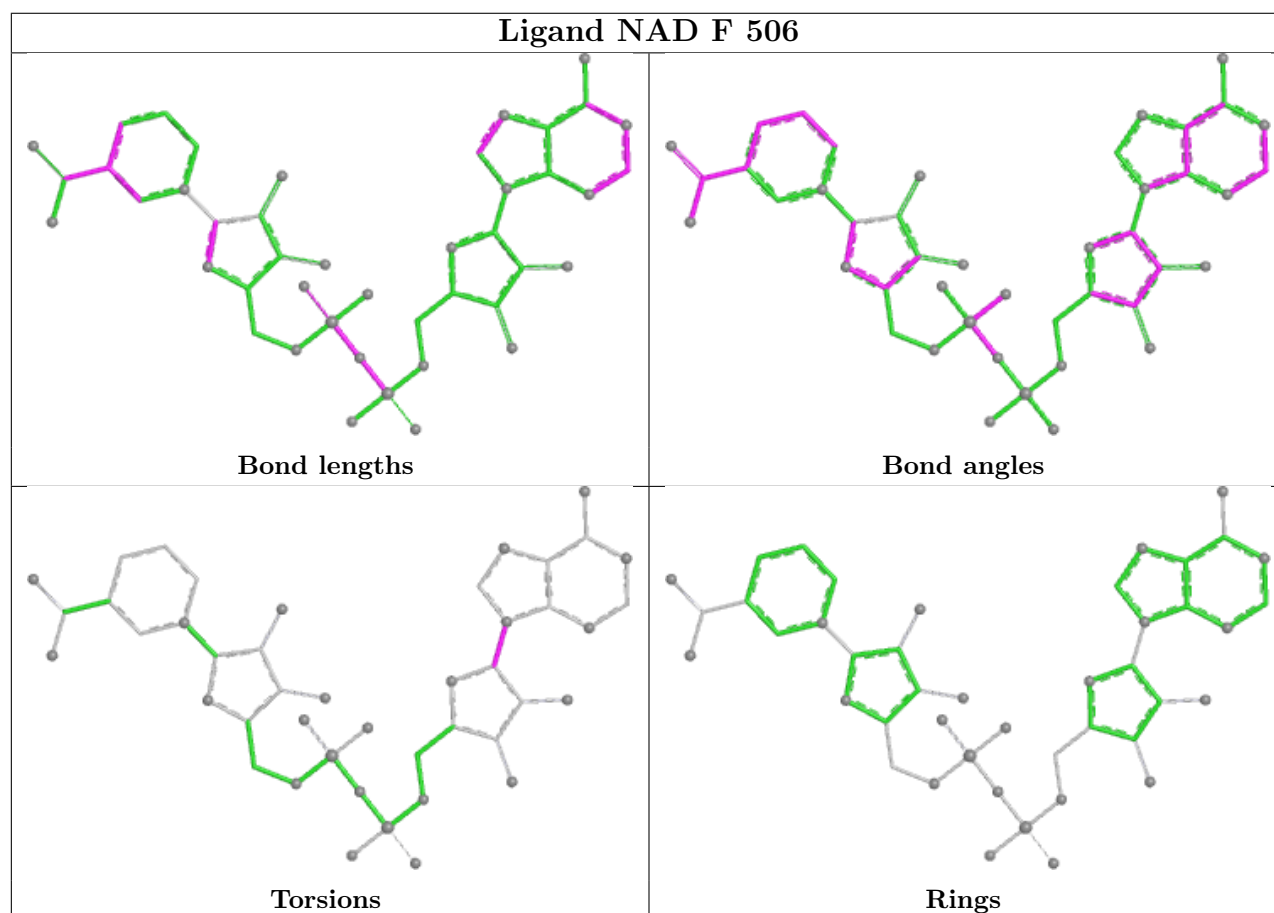
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	6946	EDO	1	0
5	G	6927	EDO	1	0
5	C	6943	EDO	2	0
5	B	6962	EDO	2	0
5	A	6951	EDO	1	0
5	A	6911	EDO	1	0
6	C	6834	GAI	1	0
5	G	6947	EDO	2	0
5	A	6921	EDO	1	0
5	E	6955	EDO	3	0
5	A	6941	EDO	2	0
5	E	6945	EDO	4	0
5	D	6924	EDO	1	0
5	E	6915	EDO	3	0
6	E	6835	GAI	1	0
5	E	6905	EDO	2	0
5	E	6965	EDO	2	0

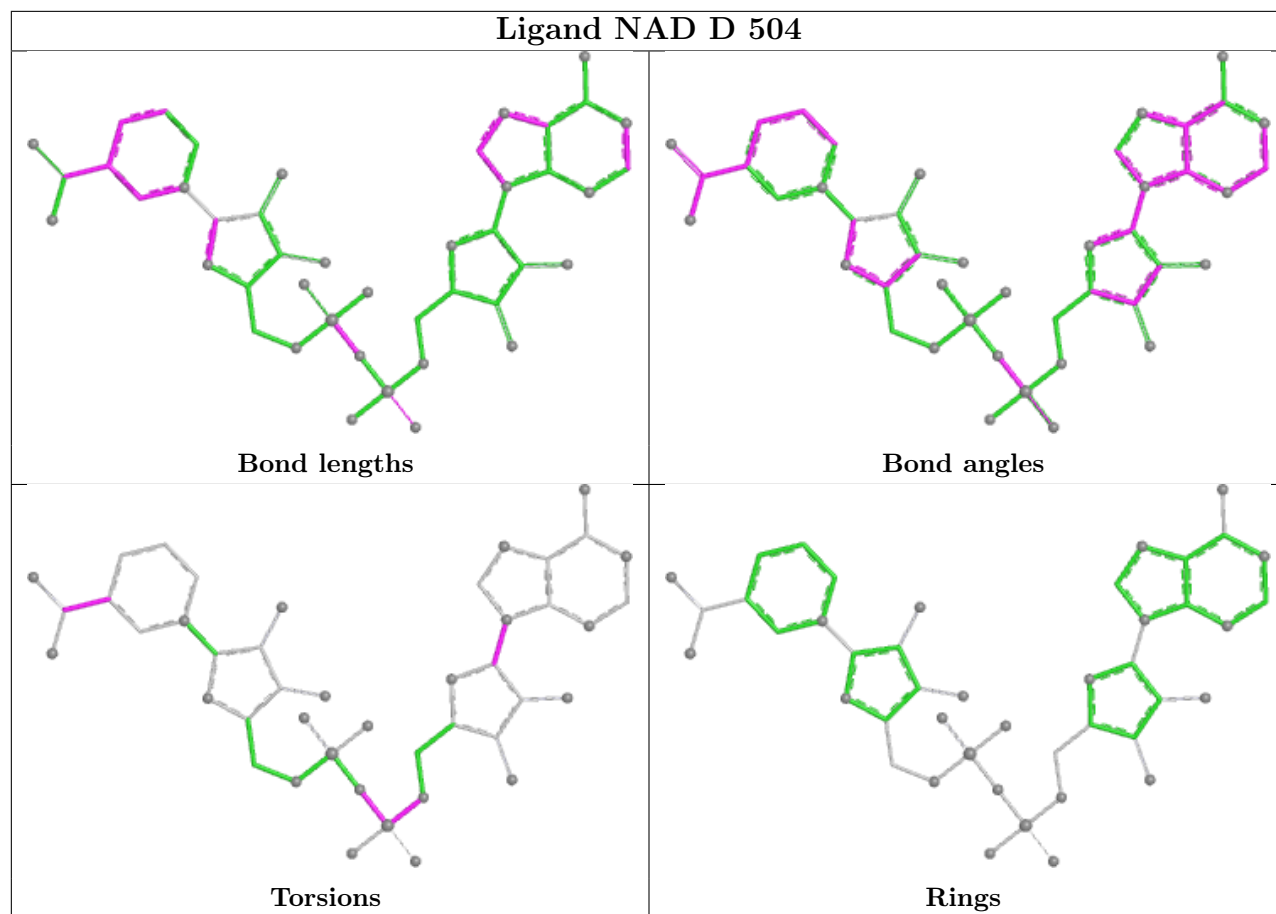
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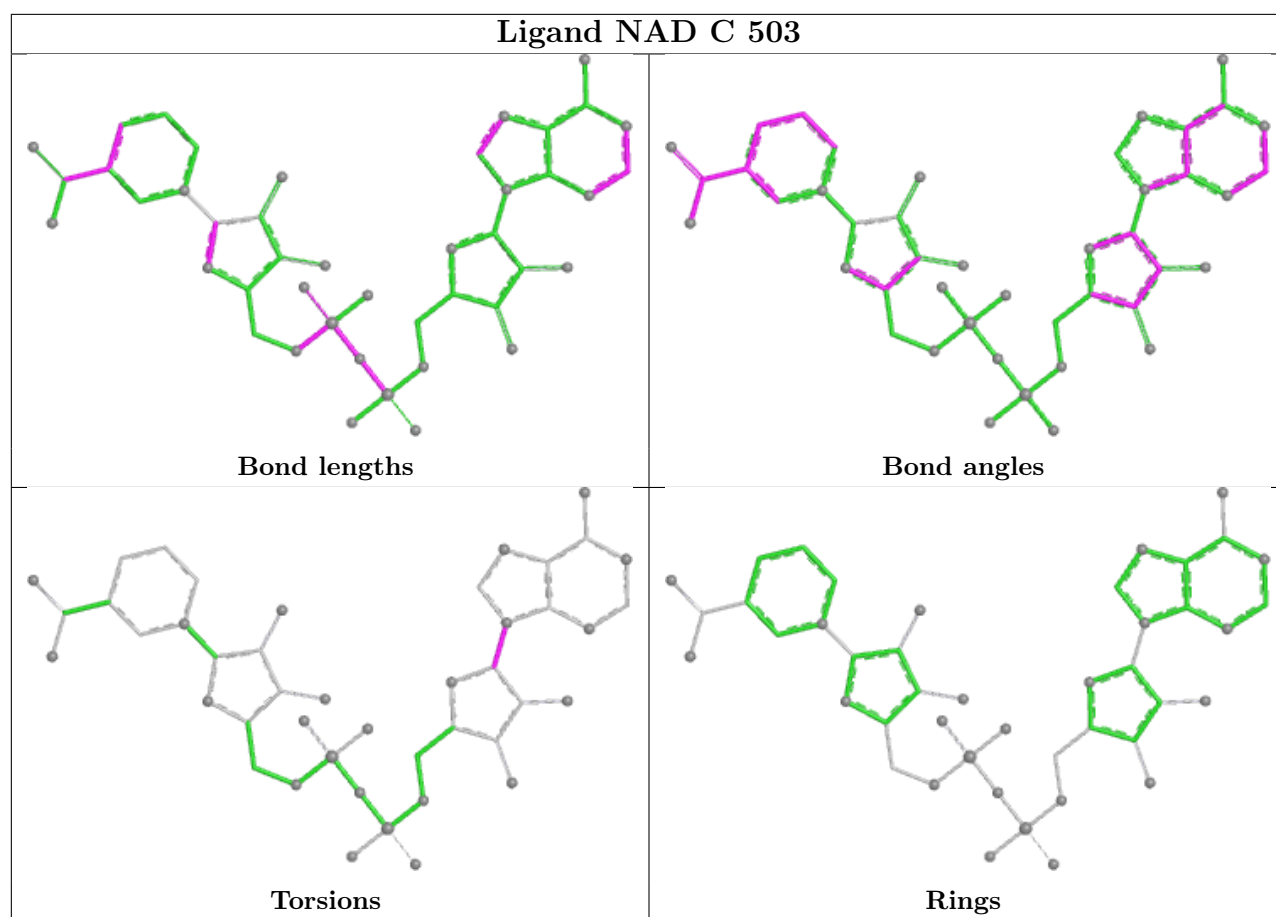
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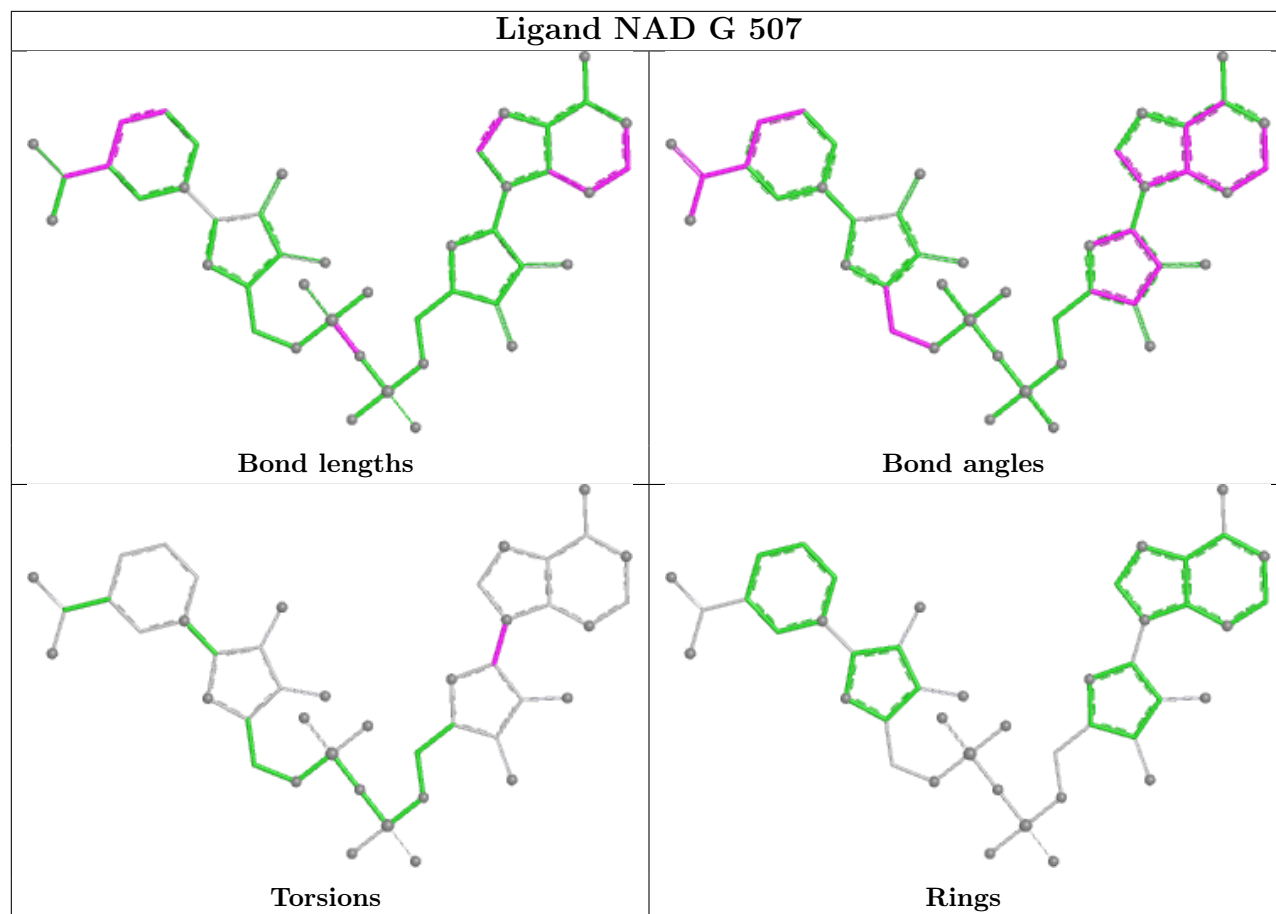
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	6948	EDO	2	0
5	B	6942	EDO	2	0

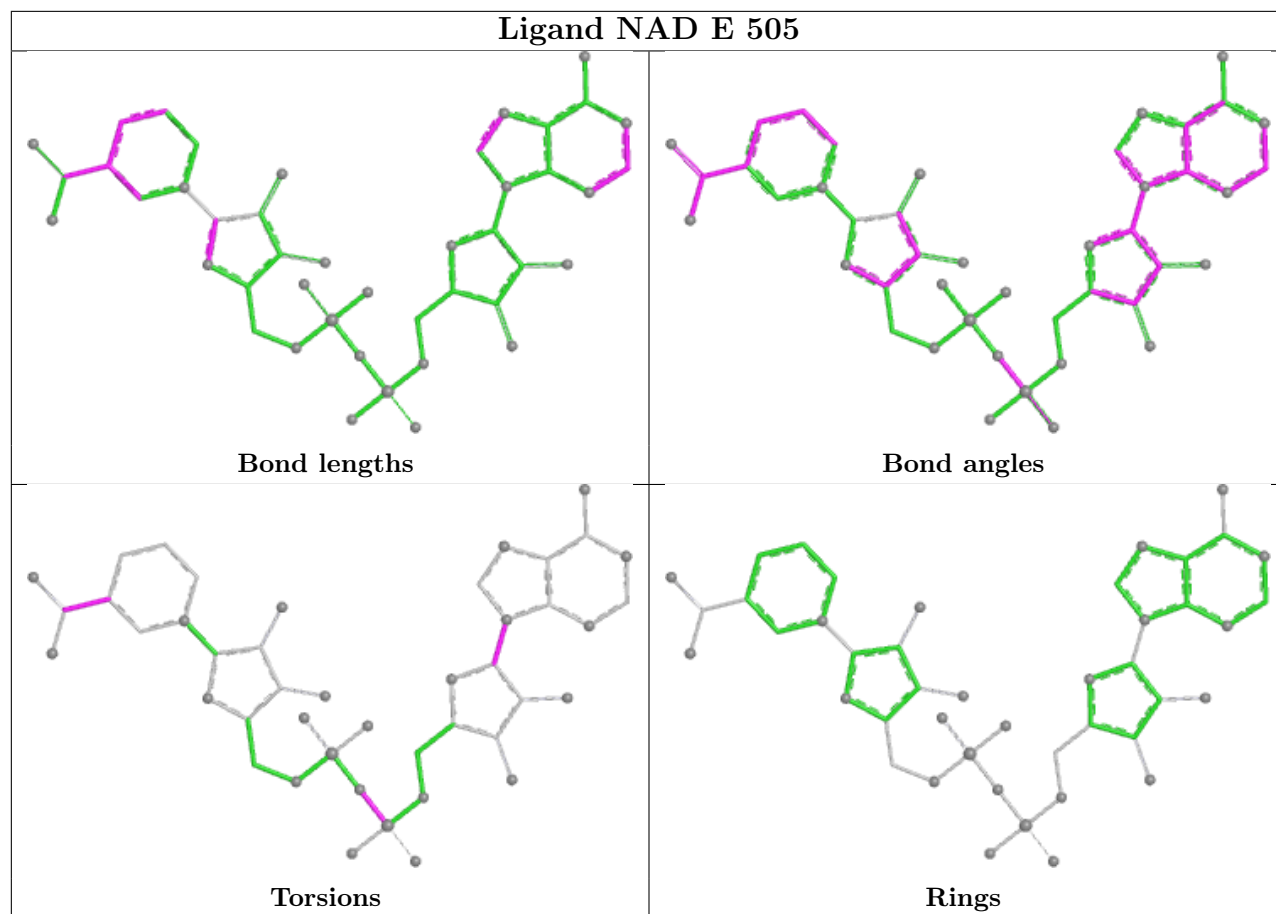
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

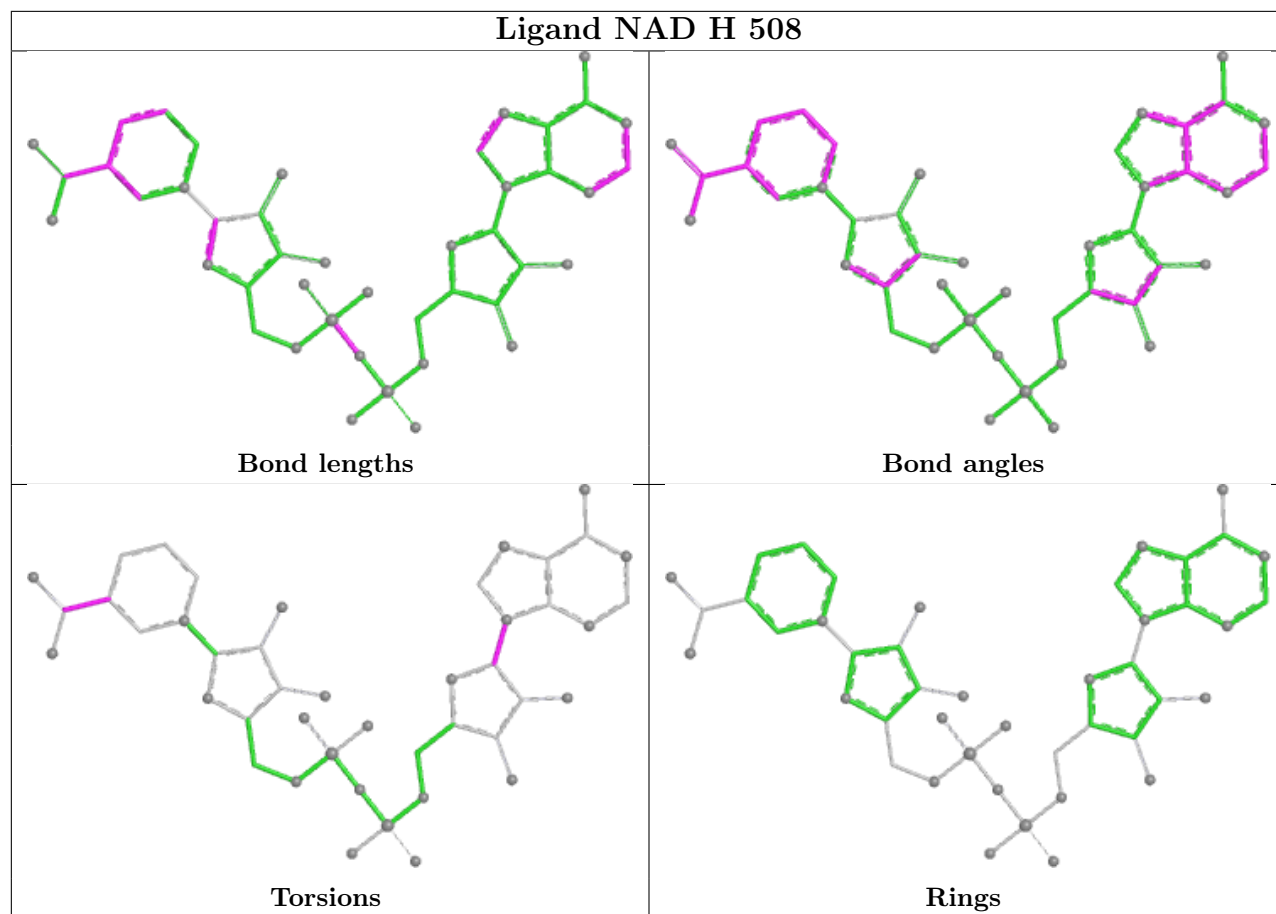


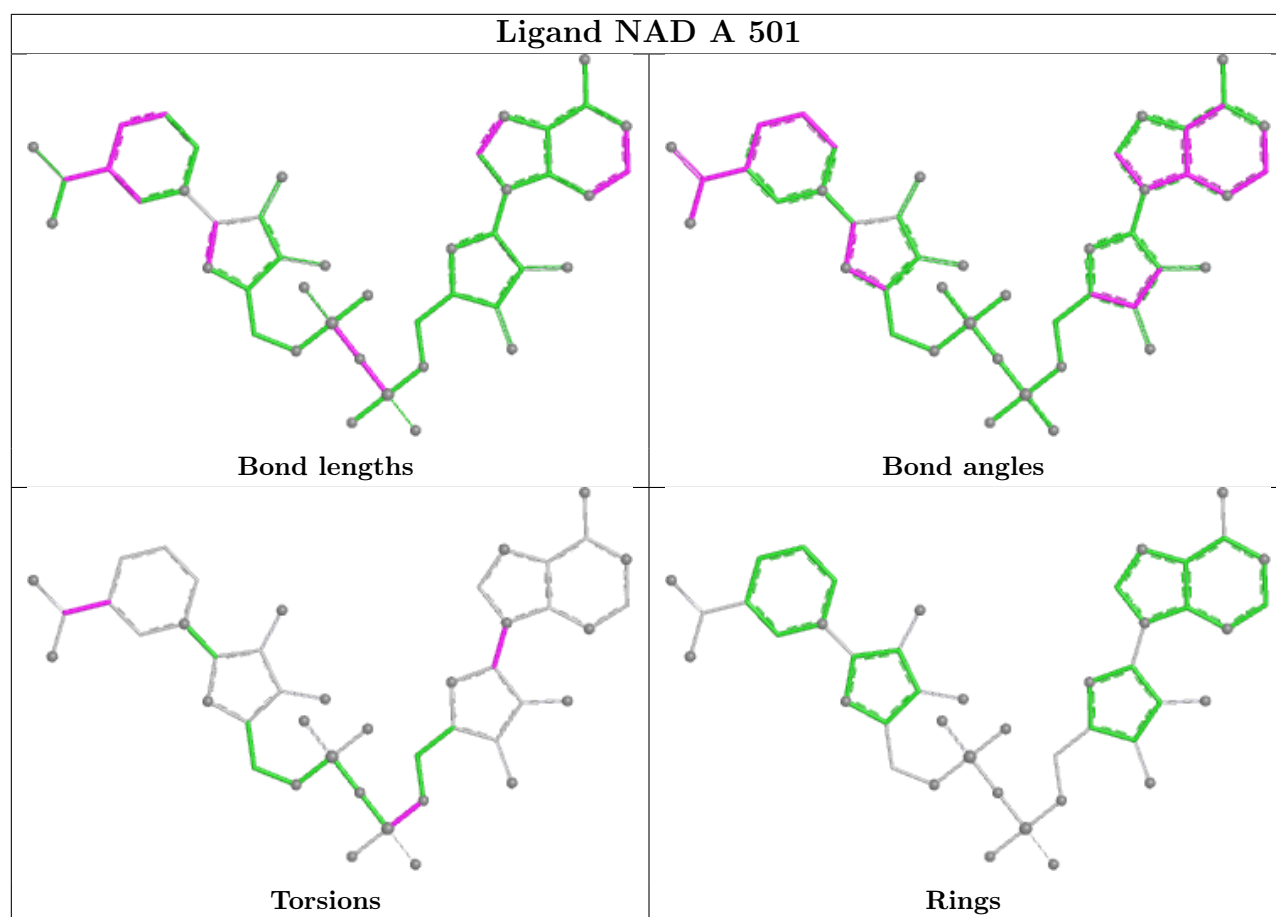


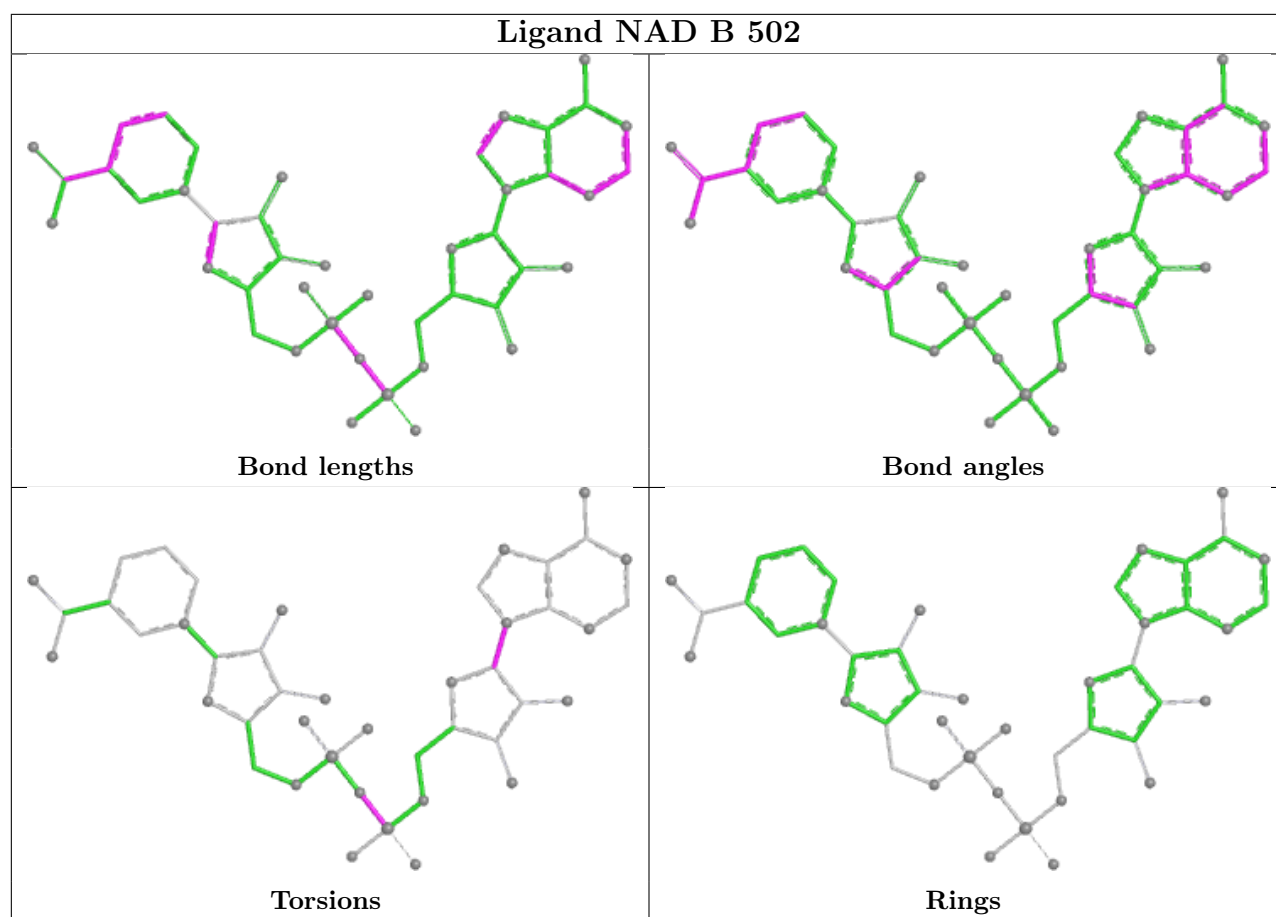












5.7 Other polymers [i](#)

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	494/500 (98%)	0.32	8 (1%) 70 70	17, 32, 47, 62	0
1	B	494/500 (98%)	0.06	2 (0%) 88 88	16, 28, 42, 61	0
1	C	494/500 (98%)	-0.40	1 (0%) 91 90	15, 22, 33, 54	0
1	D	494/500 (98%)	0.15	3 (0%) 85 85	15, 30, 45, 60	0
1	E	494/500 (98%)	-0.11	4 (0%) 82 82	18, 28, 42, 59	0
1	F	494/500 (98%)	-0.46	0 100 100	16, 22, 33, 55	0
1	G	494/500 (98%)	0.10	5 (1%) 79 79	21, 31, 45, 61	0
1	H	494/500 (98%)	0.45	14 (2%) 55 54	20, 35, 52, 72	0
All	All	3952/4000 (98%)	0.01	37 (0%) 81 80	15, 28, 45, 72	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	7	ALA	5.0
1	G	373	ILE	3.5
1	H	7	ALA	3.5
1	A	474	GLY	3.4
1	D	7	ALA	3.2
1	A	7	ALA	3.0
1	H	374	ALA	2.8
1	H	378	GLY	2.7
1	E	377	ARG	2.7
1	H	376	ASP	2.7
1	D	378	GLY	2.6
1	H	424	THR	2.6
1	G	475	GLN	2.5
1	G	474	GLY	2.5
1	H	375	ALA	2.4
1	A	459	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	17	VAL	2.2
1	B	257	ALA	2.2
1	G	375	ALA	2.2
1	H	459	PHE	2.2
1	C	474	GLY	2.2
1	A	367	LEU	2.2
1	H	373	ILE	2.2
1	E	8	VAL	2.2
1	H	365	ALA	2.2
1	H	331	VAL	2.1
1	A	371	GLY	2.1
1	A	465	PHE	2.1
1	H	332	GLY	2.1
1	D	358	ASN	2.1
1	A	378	GLY	2.1
1	E	474	GLY	2.1
1	H	8	VAL	2.1
1	G	32	VAL	2.0
1	H	377	ARG	2.0
1	A	42	PRO	2.0
1	B	474	GLY	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($\text{\AA}^2$)	Q<0.9
3	NA	H	708	1/1	0.54	0.19	55,55,55,55	0
5	EDO	E	6965	4/4	0.64	0.13	69,70,70,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	B	6952	4/4	0.68	0.20	60,60,61,61	0
5	EDO	A	6951	4/4	0.69	0.18	54,55,56,56	0
5	EDO	E	6925	4/4	0.70	0.15	48,49,49,49	0
5	EDO	D	6914	4/4	0.70	0.21	59,59,61,61	0
5	EDO	G	6927	4/4	0.70	0.15	54,54,54,54	0
5	EDO	H	6928	4/4	0.70	0.19	66,66,66,68	0
5	EDO	C	6923	4/4	0.72	0.16	51,52,52,54	0
5	EDO	B	6962	4/4	0.72	0.26	71,71,72,72	0
6	GAI	D	6824	4/4	0.74	0.13	65,66,66,67	0
5	EDO	A	6921	4/4	0.75	0.13	53,53,54,54	0
2	MG	G	607	1/1	0.76	0.24	59,59,59,59	0
6	GAI	A	6811	4/4	0.78	0.16	56,57,57,58	0
2	MG	H	608	1/1	0.78	0.19	59,59,59,59	0
2	MG	D	604	1/1	0.79	0.18	52,52,52,52	0
6	GAI	D	6833	4/4	0.79	0.13	54,55,55,55	0
6	GAI	A	6821	4/4	0.80	0.14	55,56,56,56	0
6	GAI	H	6837	4/4	0.80	0.14	51,52,53,53	0
6	GAI	C	6813	4/4	0.81	0.15	53,53,54,56	0
5	EDO	H	6918	4/4	0.81	0.20	60,61,61,61	0
5	EDO	D	6924	4/4	0.81	0.14	56,57,57,58	0
6	GAI	B	6831	4/4	0.81	0.13	59,59,59,60	0
5	EDO	A	6911	4/4	0.82	0.13	56,57,58,59	0
5	EDO	F	6956	4/4	0.82	0.15	49,51,52,52	0
3	NA	G	707	1/1	0.83	0.10	35,35,35,35	0
5	EDO	F	6926	4/4	0.84	0.12	46,47,47,50	0
5	EDO	E	6955	4/4	0.84	0.17	52,53,55,55	0
5	EDO	E	6945	4/4	0.84	0.17	34,40,40,41	0
5	EDO	H	6908	4/4	0.84	0.12	36,37,38,38	0
6	GAI	F	6826	4/4	0.84	0.14	44,44,44,45	0
6	GAI	H	6818	4/4	0.84	0.20	57,57,57,57	0
6	GAI	B	6812	4/4	0.84	0.14	51,52,53,53	0
6	GAI	G	6838	4/4	0.85	0.12	47,47,49,50	0
5	EDO	G	6907	4/4	0.86	0.13	38,40,40,41	0
2	MG	E	605	1/1	0.86	0.13	50,50,50,50	0
6	GAI	F	6816	4/4	0.86	0.14	50,50,50,51	0
5	EDO	E	6915	4/4	0.86	0.12	42,44,45,47	0
6	GAI	G	6817	4/4	0.86	0.16	52,52,52,53	0
5	EDO	C	6953	4/4	0.86	0.17	54,54,55,56	0
5	EDO	B	6912	4/4	0.86	0.12	46,46,47,48	0
6	GAI	C	6834	4/4	0.86	0.10	42,42,43,45	0
5	EDO	A	6941	4/4	0.87	0.14	38,43,44,44	0
4	NAD	A	501	44/44	0.87	0.10	32,44,50,50	0

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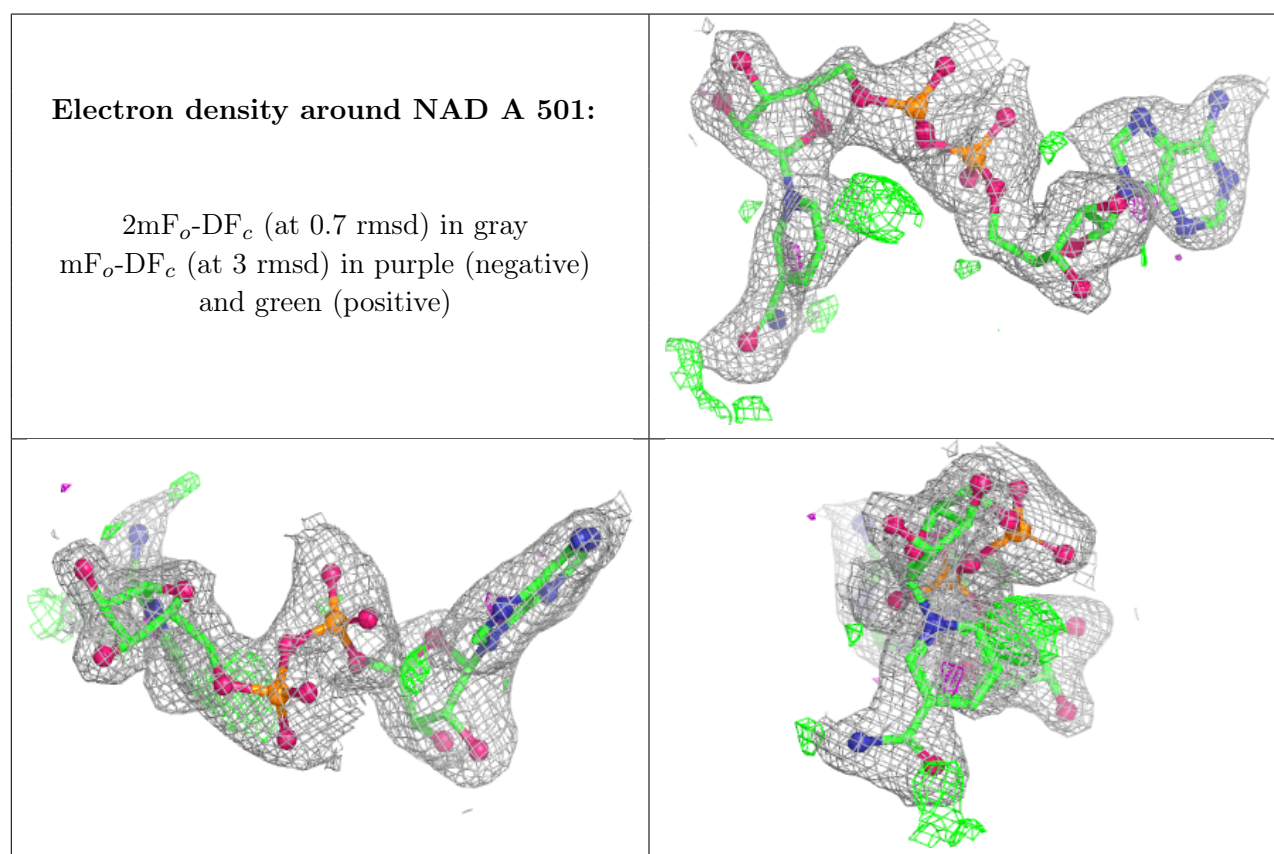
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GAI	C	6823	4/4	0.87	0.10	35,35,36,36	0
5	EDO	E	6905	4/4	0.88	0.11	37,39,40,40	0
5	EDO	F	6966	4/4	0.88	0.14	47,49,49,51	0
5	EDO	B	6902	4/4	0.89	0.10	38,42,42,42	0
6	GAI	D	6814	4/4	0.89	0.12	43,44,45,45	0
2	MG	A	601	1/1	0.89	0.12	49,49,49,49	0
4	NAD	H	508	44/44	0.89	0.10	35,46,50,51	0
3	NA	D	704	1/1	0.89	0.08	41,41,41,41	0
6	GAI	F	6806	4/4	0.90	0.11	31,32,32,33	0
5	EDO	F	6906	4/4	0.90	0.10	37,38,38,40	0
6	GAI	A	6832	4/4	0.90	0.11	48,48,48,50	0
5	EDO	G	6917	4/4	0.90	0.10	50,51,52,53	0
5	EDO	C	6903	4/4	0.90	0.12	37,38,39,39	0
5	EDO	G	6947	4/4	0.90	0.12	34,42,42,43	0
6	GAI	E	6835	4/4	0.90	0.08	37,38,38,40	0
3	NA	E	705	1/1	0.91	0.07	40,40,40,40	0
4	NAD	B	502	44/44	0.91	0.08	35,41,44,47	0
6	GAI	E	6836	4/4	0.91	0.08	37,39,40,41	0
5	EDO	F	6946	4/4	0.91	0.15	29,37,39,39	0
6	GAI	C	6803	4/4	0.91	0.13	32,34,34,36	0
4	NAD	G	507	44/44	0.91	0.09	30,40,44,45	0
6	GAI	G	6807	4/4	0.91	0.12	41,41,42,43	0
2	MG	C	603	1/1	0.91	0.08	41,41,41,41	0
5	EDO	H	6948	4/4	0.91	0.11	45,47,47,49	0
5	EDO	A	6901	4/4	0.91	0.10	33,36,36,36	0
2	MG	B	602	1/1	0.91	0.14	47,47,47,47	0
3	NA	A	701	1/1	0.92	0.07	40,40,40,40	0
6	GAI	E	6815	4/4	0.92	0.09	45,46,46,46	0
5	EDO	D	6904	4/4	0.92	0.09	30,35,35,35	0
4	NAD	E	505	44/44	0.93	0.08	23,33,41,42	0
3	NA	C	703	1/1	0.93	0.09	24,24,24,24	0
5	EDO	C	6943	4/4	0.93	0.16	30,36,37,37	0
4	NAD	D	504	44/44	0.93	0.09	24,36,42,43	0
5	EDO	C	6963	4/4	0.93	0.08	35,35,36,38	0
3	NA	B	702	1/1	0.94	0.06	34,34,34,34	0
5	EDO	F	6916	4/4	0.94	0.08	31,33,33,35	0
6	GAI	A	6801	4/4	0.94	0.08	35,36,37,37	0
6	GAI	B	6802	4/4	0.94	0.09	37,38,39,39	0
6	GAI	E	6805	4/4	0.95	0.07	27,27,28,29	0
6	GAI	H	6808	4/4	0.95	0.11	30,32,32,32	0
2	MG	F	606	1/1	0.95	0.08	41,41,41,41	0
5	EDO	B	6942	4/4	0.95	0.10	36,39,40,40	0

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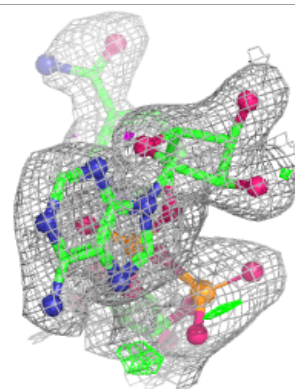
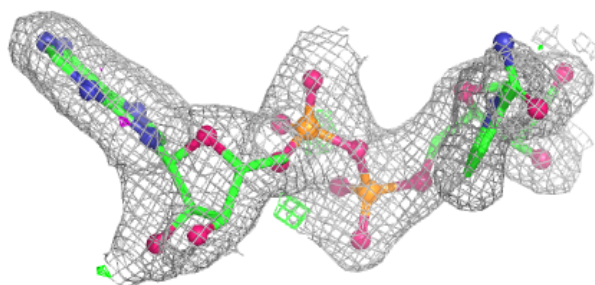
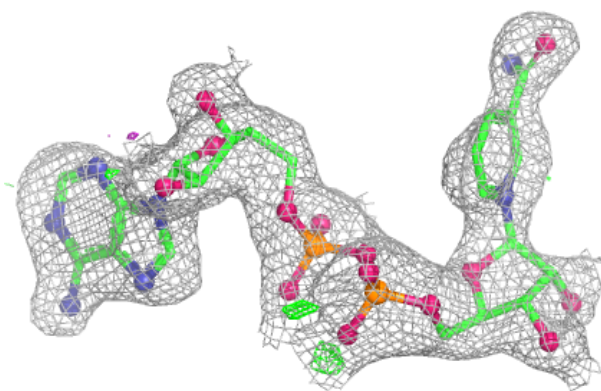
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	C	6913	4/4	0.96	0.08	27,29,30,31	0
6	GAI	D	6804	4/4	0.96	0.06	25,26,27,29	0
4	NAD	C	503	44/44	0.96	0.06	16,26,30,32	0
4	NAD	F	506	44/44	0.97	0.06	16,25,30,31	0
3	NA	F	706	1/1	0.97	0.05	26,26,26,26	0

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.

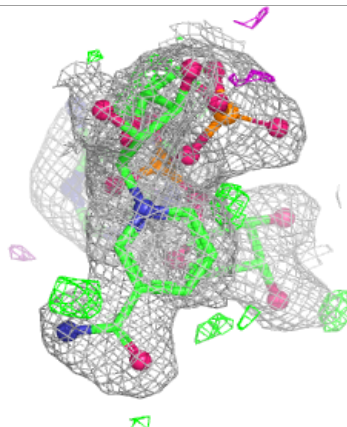
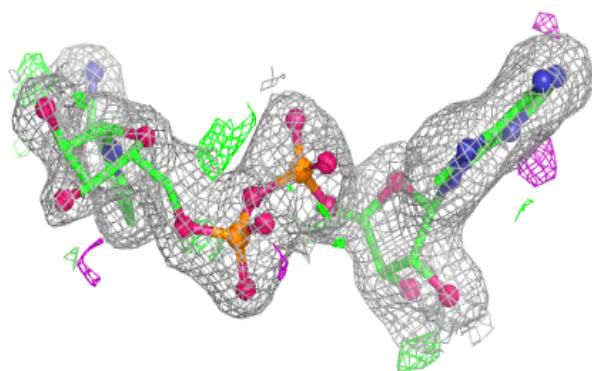
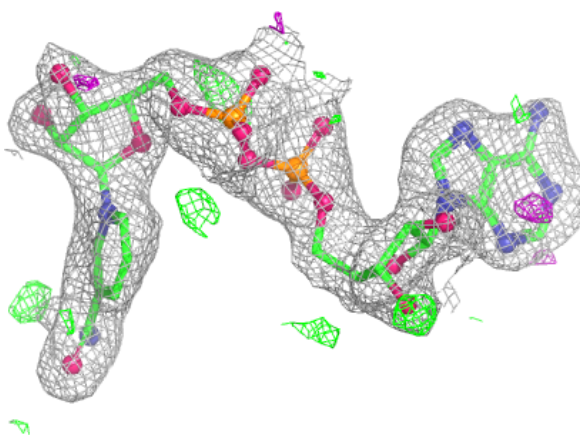


Electron density around NAD H 508:

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

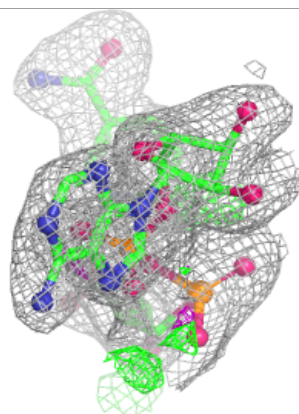
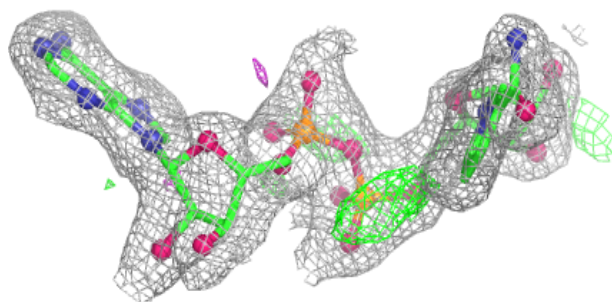
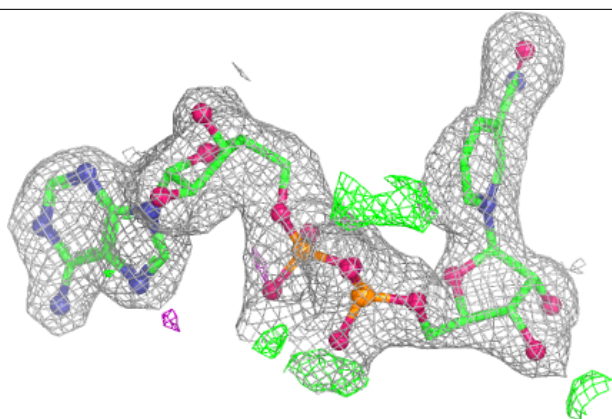
**Electron density around NAD B 502:**

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

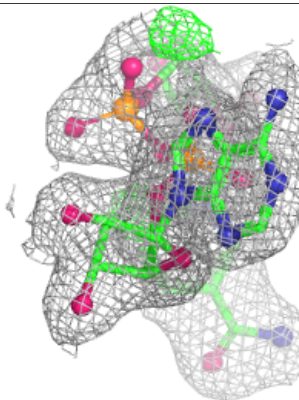
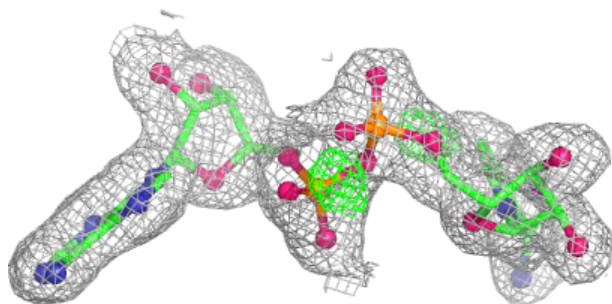
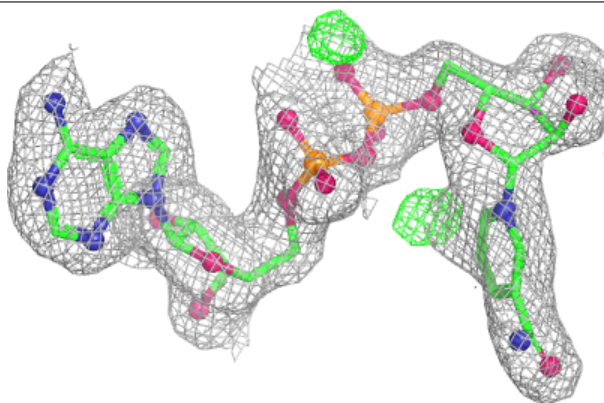


Electron density around NAD G 507:

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

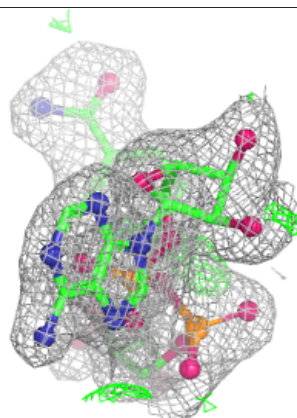
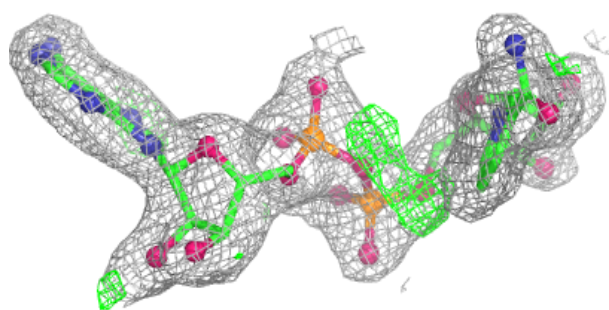
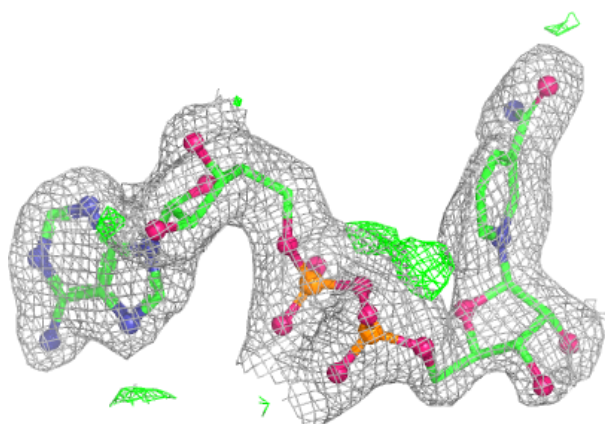
**Electron density around NAD E 505:**

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

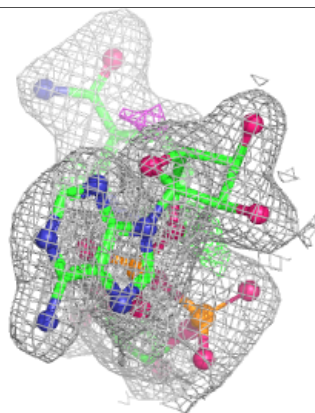
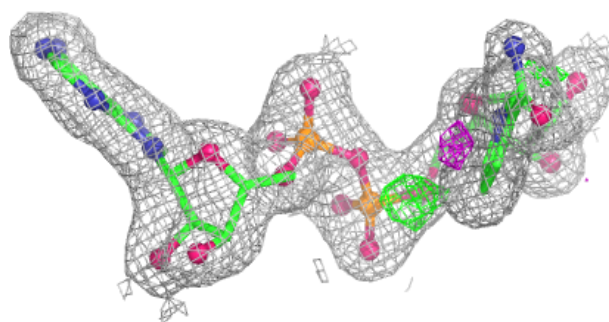
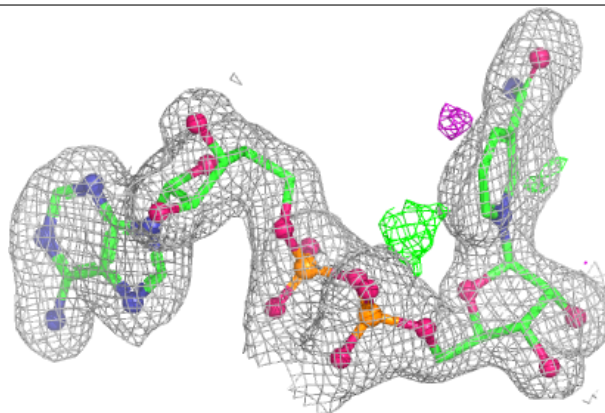


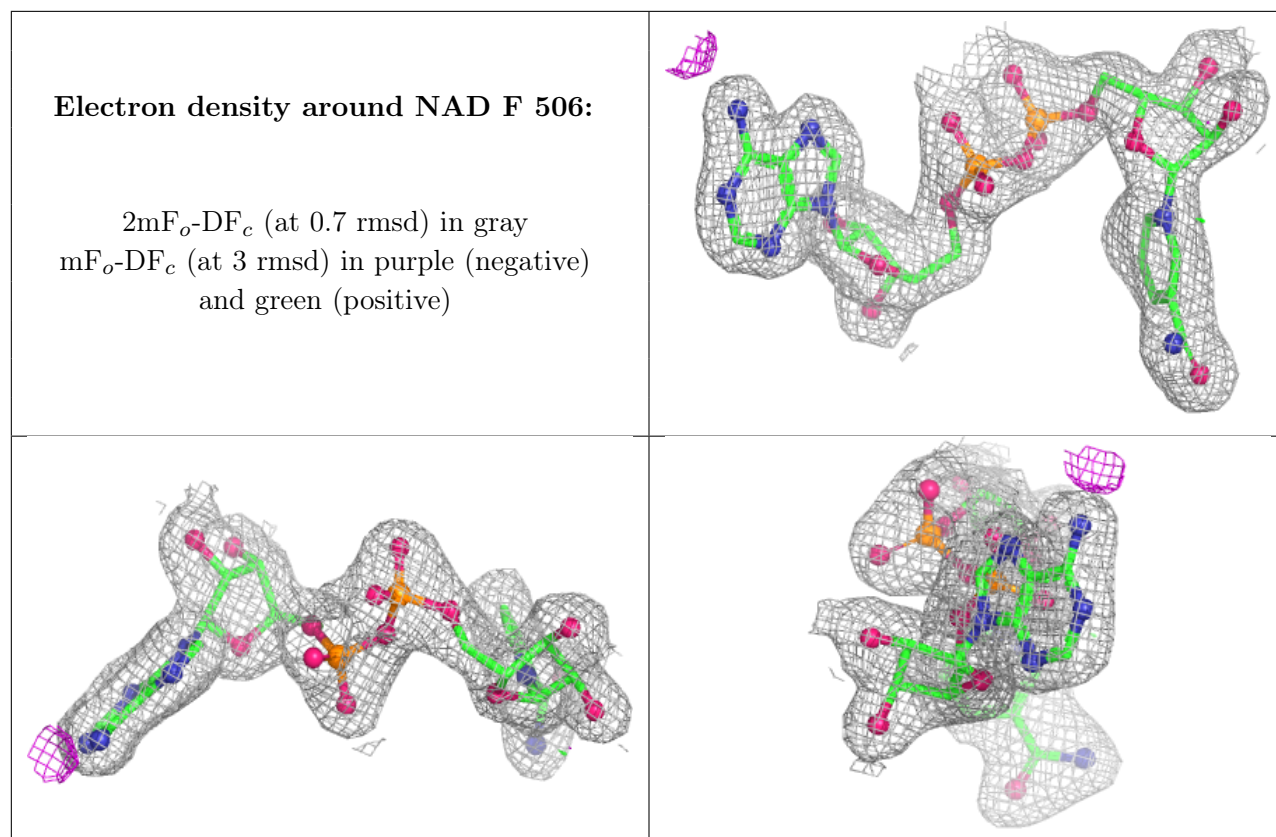
Electron density around NAD D 504:

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

**Electron density around NAD C 503:**

$2mF_o-DF_c$ (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.