



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2026 – 01:49 pm BST

PDB ID : 9QYI / pdb_00009qyi
Title : Crystal structure of human S-adenosyl-L-homocysteine hydrolase complex with adenosine
Authors : Malecki, P.H.; Imiolczyk, B.; Gawel, M.; Stepniewska, M.; Brzezinski, K.
Deposited on : 2025-04-18
Resolution : 1.59 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 : 1.8.4, CSD as541be (2020)
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

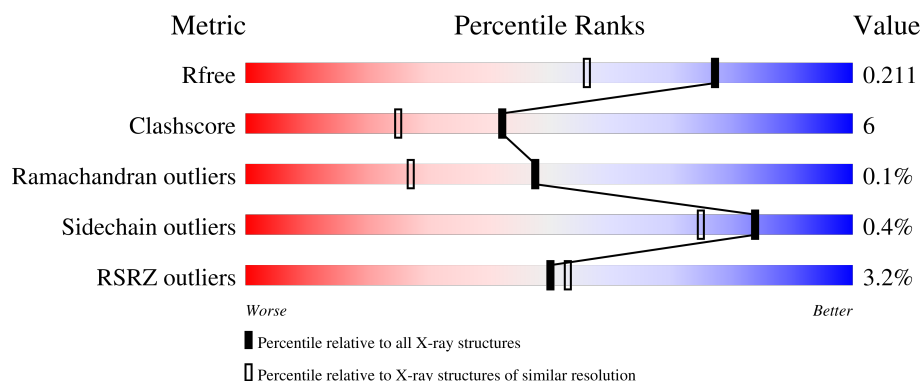
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 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.



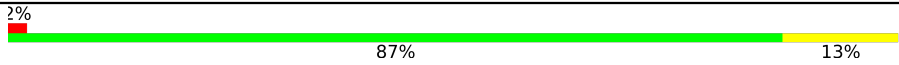

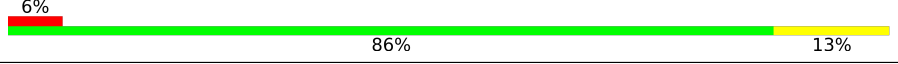
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	431	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 89%; height: 10px; background-color: green;"></div> <div style="width: 10%; height: 10px; background-color: yellow;"></div> <div>89%10%</div> </div>
1	B	431	<div> <div style="width: 90%; height: 10px; background-color: green;"></div> <div style="width: 10%; height: 10px; background-color: yellow;"></div> <div>90%10%</div> </div>
1	C	431	<div> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 87%; height: 10px; background-color: green;"></div> <div style="width: 12%; height: 10px; background-color: yellow;"></div> <div>2%87%12%</div> </div>
1	D	431	<div> <div style="width: 9%; height: 10px; background-color: red;"></div> <div style="width: 84%; height: 10px; background-color: green;"></div> <div style="width: 16%; height: 10px; background-color: yellow;"></div> <div>9%84%16%</div> </div>
1	E	431	<div> <div style="width: 87%; height: 10px; background-color: green;"></div> <div style="width: 13%; height: 10px; background-color: yellow;"></div> <div>87%13%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	431	 2% 87% 13%
1	G	431	 4% 86% 13%
1	H	431	 6% 86% 13%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 30109 atoms, of which 14 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	5	0
			3365	2138	579	622	26			
1	B	430	Total	C	N	O	S	0	3	0
			3349	2125	576	622	26			
1	D	430	Total	C	N	O	S	0	4	0
			3352	2129	574	622	27			
1	E	430	Total	C	N	O	S	0	5	0
			3363	2135	581	621	26			
1	F	430	Total	C	N	O	S	0	2	0
			3338	2118	572	621	27			
1	G	430	Total	C	N	O	S	0	2	0
			3343	2121	575	621	26			
1	C	430	Total	C	N	O	S	0	1	0
			3335	2116	572	621	26			
1	H	430	Total	C	N	O	S	0	0	0
			3330	2112	572	621	25			

There are 8 discrepancies between the modelled and reference sequences:

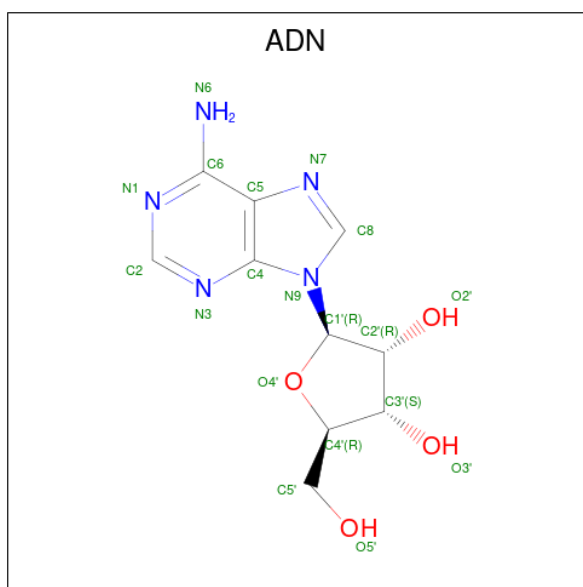
Chain	Residue	Modelled	Actual	Comment	Reference
A	86	ASN	ASP	variant	UNP P23526
B	86	ASN	ASP	variant	UNP P23526
D	86	ASN	ASP	variant	UNP P23526
E	86	ASN	ASP	variant	UNP P23526
F	86	ASN	ASP	variant	UNP P23526
G	86	ASN	ASP	variant	UNP P23526
C	86	ASN	ASP	variant	UNP P23526
H	86	ASN	ASP	variant	UNP P23526

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



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

- Molecule 3 is ADENOSINE (CCD ID: ADN) (formula: C₁₀H₁₃N₅O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	10	5	4		
3	B	1	Total	C	N	O	0	0
			19	10	5	4		
3	D	1	Total	C	N	O	0	0
			19	10	5	4		
3	E	1	Total	C	N	O	0	0
			19	10	5	4		
3	F	1	Total	C	N	O	0	0
			19	10	5	4		
3	G	1	Total	C	N	O	0	0
			19	10	5	4		
3	C	1	Total	C	N	O	0	0
			19	10	5	4		
3	H	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

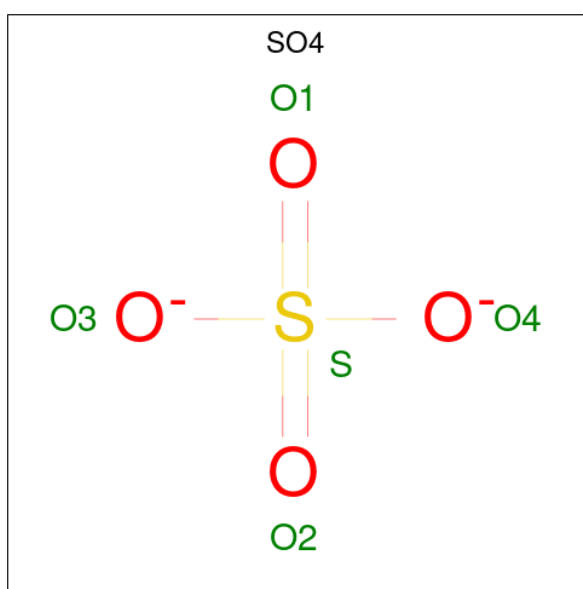
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	B	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		
4	E	1	Total	K	0	0
			1	1		

Continued on next page...

Continued from previous page...

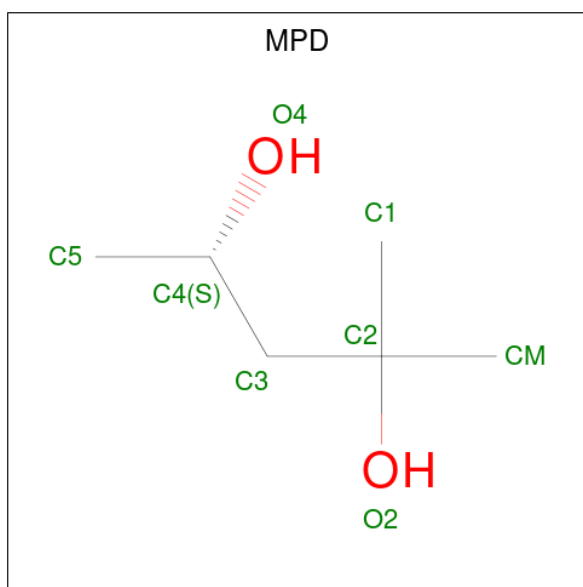
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total K 1 1	0	0
4	G	2	Total K 2 2	0	0
4	C	1	Total K 1 1	0	0
4	H	1	Total K 1 1	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	1	Total	C	H	O	0	0
			22	6	14	2		

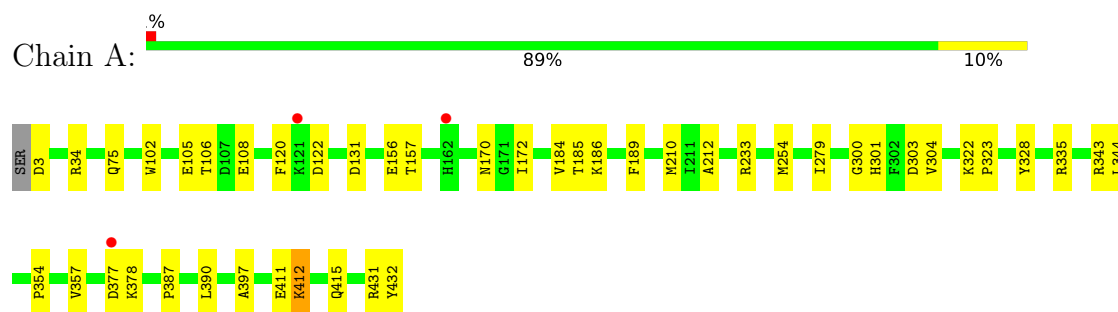
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	374	Total	O	0	7
			380	380		
7	B	391	Total	O	0	12
			404	404		
7	D	318	Total	O	0	17
			335	335		
7	E	351	Total	O	0	6
			356	356		
7	F	352	Total	O	0	4
			355	355		
7	G	319	Total	O	0	5
			324	324		
7	C	315	Total	O	0	10
			325	325		
7	H	293	Total	O	0	7
			300	300		

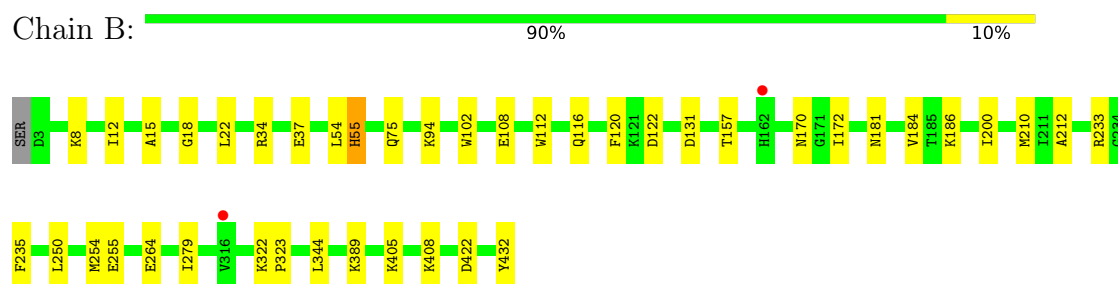
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

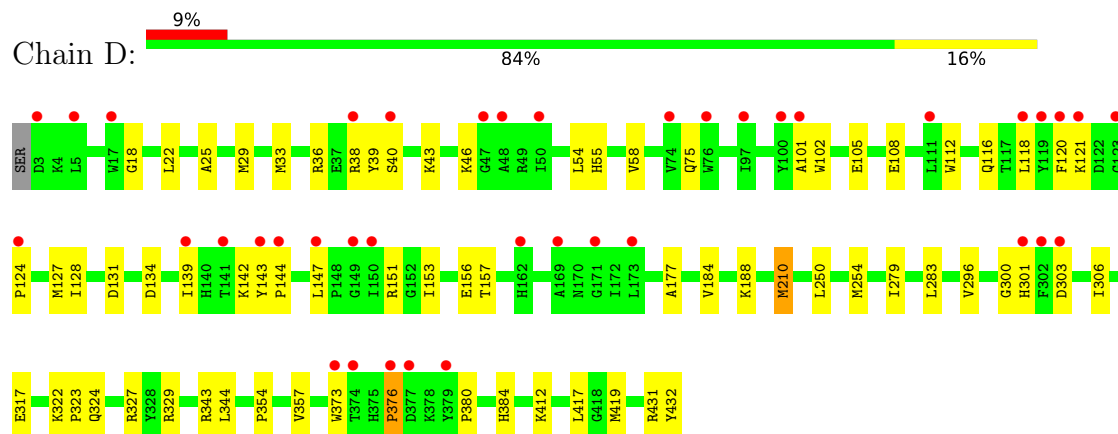
- Molecule 1: Adenosylhomocysteinase



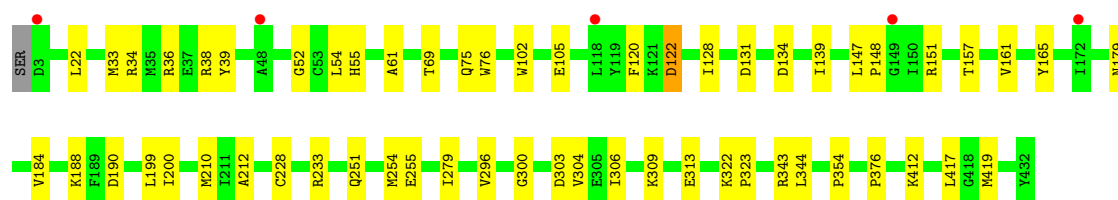
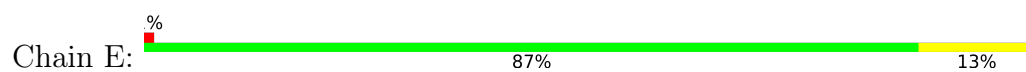
- Molecule 1: Adenosylhomocysteinase



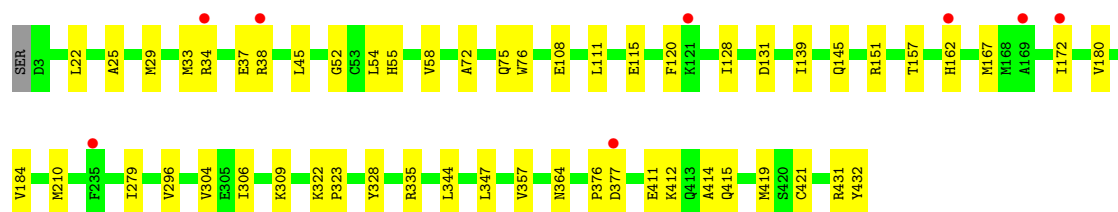
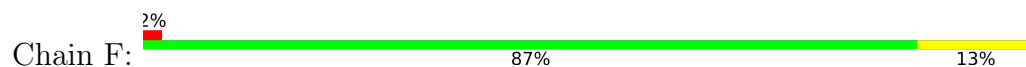
- Molecule 1: Adenosylhomocysteinase



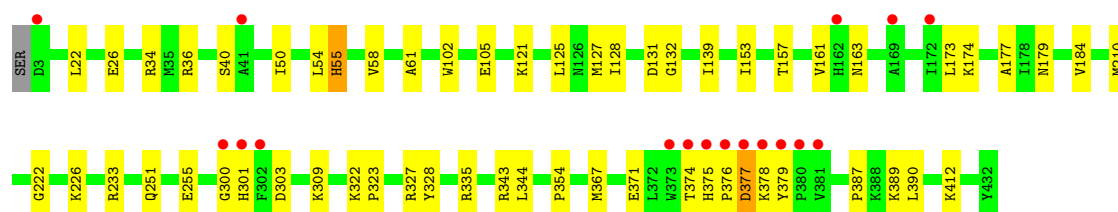
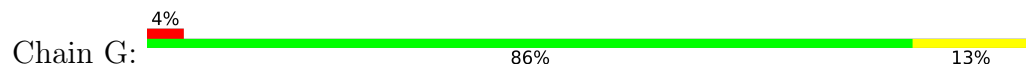
- Molecule 1: Adenosylhomocysteinase



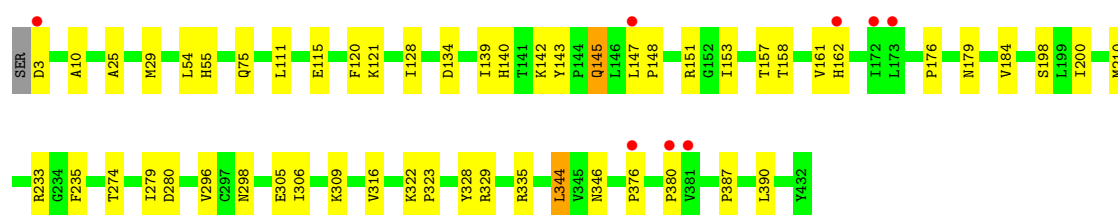
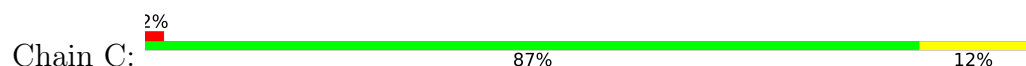
- Molecule 1: Adenosylhomocysteinase



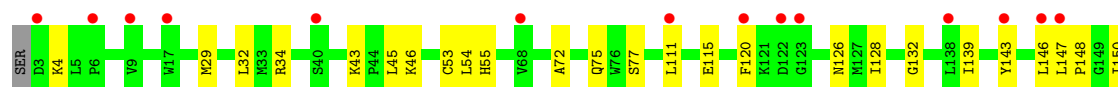
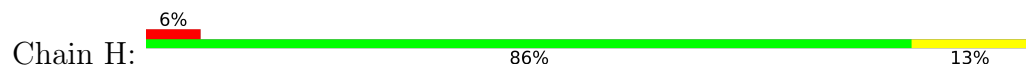
- Molecule 1: Adenosylhomocysteinase

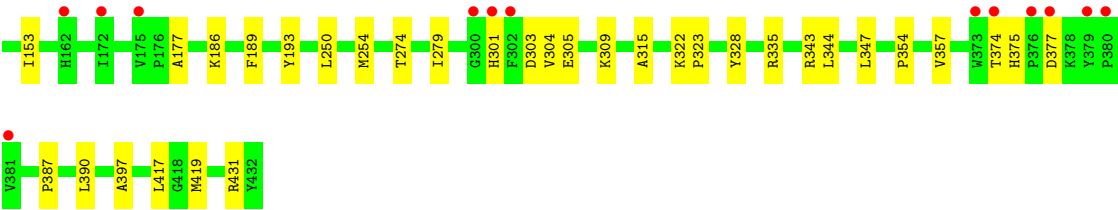


- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.76Å 90.19Å 124.55Å 96.23° 89.57° 105.53°	Depositor
Resolution (Å)	123.78 – 1.59 123.78 – 1.59	Depositor EDS
% Data completeness (in resolution range)	69.1 (123.78-1.59) 69.4 (123.78-1.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 1.58Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419+SVN	Depositor
R, R_{free}	0.177 , 0.214 0.176 , 0.211	Depositor DCC
R_{free} test set	1629 reflections (0.35%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	30109	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAD, K, ADN, MPD

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	0.34	0/3445	0.52	0/4659
1	B	0.34	0/3422	0.53	0/4629
1	C	0.29	0/3402	0.48	0/4603
1	D	0.29	0/3428	0.48	0/4636
1	E	0.33	0/3442	0.51	0/4655
1	F	0.30	0/3408	0.48	0/4611
1	G	0.31	0/3413	0.48	0/4617
1	H	0.28	0/3394	0.46	0/4593
All	All	0.31	0/27354	0.49	0/37003

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3365	0	3397	55	0
1	B	3349	0	3375	33	0
1	C	3335	0	3354	37	0
1	D	3352	0	3384	67	0
1	E	3363	0	3402	48	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3338	0	3359	42	0
1	G	3343	0	3367	46	0
1	H	3330	0	3345	40	0
2	A	44	0	26	2	0
2	B	44	0	26	1	0
2	C	44	0	26	1	0
2	D	44	0	26	1	0
2	E	44	0	26	2	0
2	F	44	0	26	1	0
2	G	44	0	26	1	0
2	H	44	0	26	1	0
3	A	19	0	13	2	0
3	B	19	0	13	1	0
3	C	19	0	13	2	0
3	D	19	0	13	1	0
3	E	19	0	13	1	0
3	F	19	0	13	1	0
3	G	19	0	13	1	0
3	H	19	0	13	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	2	0	0	0	0
4	H	1	0	0	0	0
5	A	5	0	0	0	0
5	D	5	0	0	0	0
5	F	5	0	0	0	0
5	G	5	0	0	0	0
6	H	8	14	14	3	0
7	A	380	0	0	10	0
7	B	404	0	0	6	0
7	C	325	0	0	5	0
7	D	335	0	0	10	0
7	E	356	0	0	7	0
7	F	355	0	0	4	0
7	G	324	0	0	8	0
7	H	300	0	0	2	0
All	All	30095	14	27309	344	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 6.

All (344) 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:143:TYR:HB3	1:H:146:LEU:HD23	1.47	0.94
1:F:210:MET:HE3	1:G:354:PRO:CG	2.07	0.84
1:E:22:LEU:HD21	1:E:61:ALA:HB3	1.61	0.82
1:F:210:MET:HE3	1:G:354:PRO:HG2	1.61	0.80
1:A:34:ARG:HD3	7:A:863:HOH:O	1.80	0.80
1:B:12:ILE:HG13	1:B:94:LYS:HE3	1.62	0.80
1:B:15:ALA:CB	1:B:94:LYS:HG3	2.12	0.80
1:B:15:ALA:HB2	1:B:94:LYS:HG3	1.64	0.80
1:A:411:GLU:HG2	7:A:942:HOH:O	1.84	0.78
1:D:33:MET:HE2	1:D:33:MET:HA	1.65	0.78
1:H:143:TYR:HB3	1:H:146:LEU:CD2	2.14	0.77
1:F:34:ARG:O	1:F:38:ARG:HD2	1.83	0.77
1:E:161[A]:VAL:HG11	1:E:179:ASN:ND2	2.01	0.76
1:D:254[B]:MET:SD	7:E:878:HOH:O	2.44	0.74
1:E:75:GLN:HG3	1:E:120:PHE:CE2	2.22	0.74
7:D:869:HOH:O	1:E:254[B]:MET:SD	2.47	0.73
1:D:75:GLN:HG3	1:D:120:PHE:CE2	2.24	0.72
1:H:387:PRO:HD2	1:H:390:LEU:HD12	1.70	0.72
1:F:344:LEU:HD13	1:F:347:LEU:HB2	1.72	0.71
1:G:387:PRO:HD2	1:G:390:LEU:HD12	1.73	0.70
1:D:38:ARG:HD3	1:D:39:TYR:CZ	2.27	0.69
1:A:172:ILE:HG23	7:A:728:HOH:O	1.92	0.69
1:H:344:LEU:HD13	1:H:347:LEU:HB2	1.75	0.69
1:B:12:ILE:CG1	1:B:94:LYS:HE3	2.22	0.69
1:D:301:HIS:HA	1:D:344:LEU:HD11	1.76	0.68
1:F:128:ILE:HD11	1:F:139:ILE:HD12	1.75	0.68
1:H:279:ILE:HG22	1:H:304:VAL:HB	1.75	0.68
1:A:357:VAL:HG12	1:D:210[A]:MET:HE1	1.74	0.67
1:D:33:MET:HE1	1:D:36:ARG:NE	2.09	0.67
1:D:279:ILE:HD12	1:E:412:LYS:HE2	1.75	0.67
1:E:128:ILE:HD11	1:E:139:ILE:HD12	1.75	0.67
1:A:301:HIS:HA	1:A:344:LEU:HD21	1.76	0.67
1:G:128:ILE:HD11	1:G:139:ILE:HD12	1.76	0.67
1:D:157:THR:HB	7:D:612:HOH:O	1.95	0.66
1:A:354:PRO:HG2	1:D:210[A]:MET:HE2	1.78	0.66
1:G:161:VAL:HG11	1:G:179:ASN:ND2	2.10	0.66
2:G:501:NAD:C4N	3:G:502:ADN:H3'	2.25	0.66
1:A:357:VAL:CG1	1:D:210[A]:MET:HE1	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:GLU:HG3	7:B:803:HOH:O	1.95	0.66
1:G:301:HIS:HA	1:G:344:LEU:HD21	1.77	0.66
1:F:33:MET:O	1:F:37:GLU:HG3	1.97	0.65
1:D:33:MET:HE1	1:D:36:ARG:CZ	2.27	0.65
1:F:162:HIS:HB3	7:F:907:HOH:O	1.98	0.64
1:G:371:GLU:HG3	1:G:379:TYR:CE2	2.33	0.63
1:C:3:ASP:HB3	7:C:793:HOH:O	1.96	0.63
1:A:210:MET:HE2	1:E:254[A]:MET:HE1	1.81	0.63
1:B:12:ILE:HD11	1:B:94:LYS:HG2	1.80	0.63
2:H:501:NAD:C4N	3:H:502:ADN:H3'	2.28	0.63
1:G:22:LEU:HD21	1:G:61:ALA:HB3	1.82	0.62
1:A:378:LYS:HE3	7:A:885:HOH:O	2.00	0.61
1:D:118:LEU:HD22	1:D:139:ILE:HD11	1.81	0.61
1:D:121:LYS:HE3	7:D:829:HOH:O	2.00	0.61
1:D:128:ILE:HB	1:D:153:ILE:HG12	1.81	0.61
1:G:163:ASN:HB2	7:G:858:HOH:O	2.00	0.61
1:A:300:GLY:O	1:A:344:LEU:HD23	2.00	0.61
1:F:210:MET:HE3	1:G:354:PRO:HG3	1.83	0.60
2:D:501:NAD:C4N	3:D:502:ADN:H3'	2.31	0.60
1:F:128:ILE:HD11	1:F:139:ILE:CD1	2.31	0.59
1:A:300:GLY:O	1:A:344:LEU:CD2	2.50	0.59
2:A:501:NAD:C4N	3:A:502:ADN:H3'	2.32	0.59
1:H:322:LYS:HB2	1:H:323:PRO:HD2	1.85	0.59
1:H:374:THR:HG22	1:H:375:HIS:CE1	2.37	0.59
1:A:157:THR:HB	7:A:711:HOH:O	2.01	0.59
1:C:142:LYS:HD2	1:C:143:TYR:CE1	2.37	0.59
1:G:184:VAL:HG22	1:H:431:ARG:CZ	2.32	0.59
2:C:501:NAD:C4N	3:C:502:ADN:H3'	2.33	0.59
1:D:38:ARG:HD3	1:D:39:TYR:CE1	2.38	0.59
1:A:3:ASP:N	7:A:605:HOH:O	2.36	0.59
1:G:378:LYS:HE2	1:G:379:TYR:OH	2.03	0.59
1:D:54:LEU:HD23	1:D:55:HIS:N	2.18	0.59
2:E:501:NAD:C4N	3:E:502:ADN:H3'	2.33	0.59
1:C:128:ILE:HD11	1:C:139:ILE:HD12	1.84	0.59
1:A:34:ARG:HG3	7:A:872:HOH:O	2.03	0.58
1:F:344:LEU:CD1	1:F:347:LEU:HB2	2.33	0.58
1:B:170:ASN:O	1:B:172:ILE:HD13	2.03	0.58
1:E:188:LYS:HD3	7:E:630:HOH:O	2.03	0.58
2:F:501:NAD:C4N	3:F:502:ADN:H3'	2.33	0.58
1:G:121:LYS:HD2	1:G:121:LYS:O	2.04	0.57
1:C:309:LYS:HB2	1:C:309:LYS:HZ3	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:36:ARG:O	1:G:40:SER:HB3	2.05	0.57
1:D:250:LEU:O	1:D:254[B]:MET:HG3	2.05	0.56
6:H:503:MPD:H52	6:H:503:MPD:H13	1.87	0.56
1:H:29:MET:HE2	1:H:32:LEU:HD12	1.88	0.56
1:D:101:ALA:HA	7:D:760[B]:HOH:O	2.06	0.56
1:E:131:ASP:OD1	1:E:157:THR:HG21	2.04	0.56
1:E:33:MET:HE1	1:E:36:ARG:CZ	2.36	0.56
1:A:415:GLN:HG3	7:A:883:HOH:O	2.06	0.55
1:E:128:ILE:HD11	1:E:139:ILE:CD1	2.35	0.55
1:A:170:ASN:HB3	1:A:172:ILE:HD12	1.87	0.55
1:A:254[B]:MET:HE1	1:E:210:MET:HE2	1.88	0.55
1:D:22:LEU:HD23	1:D:58:VAL:HG13	1.89	0.55
1:C:309:LYS:HB2	1:C:309:LYS:NZ	2.21	0.55
1:A:357:VAL:HB	1:D:210[A]:MET:HE1	1.88	0.55
1:B:131:ASP:OD1	1:B:157:THR:HG21	2.05	0.55
1:D:412:LYS:HG2	7:E:644:HOH:O	2.06	0.55
1:G:371:GLU:OE1	1:G:375:HIS:ND1	2.40	0.55
1:C:233:ARG:HD2	7:C:761[B]:HOH:O	2.06	0.55
1:F:279:ILE:HG22	1:F:304:VAL:HB	1.89	0.55
1:D:33:MET:HE2	1:D:33:MET:CA	2.34	0.54
1:E:161[A]:VAL:HG12	1:E:165:TYR:CE2	2.42	0.54
1:C:387:PRO:HD2	1:C:390:LEU:HD12	1.88	0.54
1:C:161:VAL:HG11	1:C:179:ASN:OD1	2.07	0.54
1:A:254[B]:MET:HE1	1:E:210:MET:CE	2.37	0.54
1:H:128:ILE:HB	1:H:153:ILE:HG12	1.89	0.54
1:E:161[A]:VAL:HG11	1:E:179:ASN:CG	2.31	0.54
1:F:322:LYS:HB2	1:F:323:PRO:HD2	1.88	0.54
1:A:387:PRO:HD2	1:A:390:LEU:HD12	1.90	0.54
1:G:125:LEU:HD11	1:G:139:ILE:CD1	2.38	0.54
1:A:210:MET:SD	1:D:357:VAL:HB	2.47	0.54
1:A:354:PRO:CG	1:D:210[A]:MET:HE2	2.38	0.54
1:B:264:GLU:HG3	7:B:740:HOH:O	2.08	0.54
1:A:210:MET:CE	1:E:254[A]:MET:HE1	2.37	0.53
1:F:376:PRO:HA	7:F:797:HOH:O	2.07	0.53
1:G:367:MET:HG2	7:G:887:HOH:O	2.07	0.53
1:G:389:LYS:HB2	7:G:632:HOH:O	2.09	0.53
1:A:131:ASP:OD1	1:A:157:THR:HG21	2.09	0.53
1:G:22:LEU:HD23	1:G:58:VAL:HG13	1.91	0.53
1:A:322:LYS:HB2	1:A:323:PRO:HD2	1.91	0.53
1:G:233:ARG:NH2	7:G:606:HOH:O	2.41	0.53
1:H:344:LEU:CD1	1:H:347:LEU:HB2	2.37	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:THR:HB	1:A:108:GLU:OE1	2.09	0.53
1:C:233:ARG:NH1	7:C:761[B]:HOH:O	2.41	0.53
1:F:108:GLU:CD	1:F:108:GLU:H	2.15	0.52
1:H:43:LYS:HB2	1:H:46:LYS:HE3	1.90	0.52
1:A:357:VAL:CB	1:D:210[A]:MET:HE1	2.39	0.52
1:E:34:ARG:NH2	7:E:605:HOH:O	2.40	0.52
1:F:344:LEU:O	1:F:344:LEU:HD12	2.10	0.52
1:E:417:LEU:HB3	1:E:419:MET:HE3	1.92	0.51
1:E:122:ASP:OD1	1:E:122:ASP:N	2.35	0.51
1:D:134:ASP:HB2	7:D:743:HOH:O	2.09	0.51
1:D:43:LYS:O	1:D:46:LYS:HG2	2.11	0.51
1:B:122:ASP:OD1	1:B:122:ASP:N	2.44	0.51
1:G:327:ARG:HD3	7:G:806:HOH:O	2.10	0.51
1:H:132:GLY:HA3	1:H:301:HIS:NE2	2.26	0.51
1:F:52:GLY:HA3	1:F:76:TRP:CZ3	2.45	0.50
1:E:200:ILE:HG12	7:E:609:HOH:O	2.10	0.50
1:E:151:ARG:HD3	1:E:376:PRO:HG3	1.93	0.50
1:F:184:VAL:HG21	1:F:432:TYR:CE1	2.47	0.50
1:C:128:ILE:HB	1:C:153:ILE:HG12	1.91	0.50
1:A:75:GLN:HG3	1:A:120:PHE:CE2	2.47	0.50
1:D:131:ASP:OD2	1:D:156:GLU:HG2	2.11	0.50
1:D:108:GLU:HB2	7:D:807:HOH:O	2.12	0.50
1:H:75:GLN:HG3	1:H:120:PHE:CE2	2.47	0.50
1:C:210:MET:HB2	1:H:354:PRO:HB2	1.94	0.50
1:D:153:ILE:O	1:D:177:ALA:HA	2.11	0.50
1:E:22:LEU:HD21	1:E:61:ALA:CB	2.36	0.50
1:C:145:GLN:O	1:C:148:PRO:HD2	2.12	0.50
1:C:157:THR:HG22	3:C:502:ADN:O3'	2.11	0.50
1:A:303:ASP:CG	1:A:343[B]:ARG:HD2	2.36	0.49
1:A:34:ARG:HD2	1:A:397:ALA:HB1	1.94	0.49
1:G:132:GLY:HA3	1:G:301:HIS:NE2	2.27	0.49
1:F:131:ASP:OD1	1:F:157:THR:HG21	2.12	0.49
1:A:354:PRO:HB2	1:D:210[A]:MET:HE3	1.95	0.49
1:D:301:HIS:CA	1:D:344:LEU:HD11	2.41	0.49
1:H:147:LEU:HB2	1:H:148:PRO:HD3	1.94	0.49
1:F:111:LEU:O	1:F:115:GLU:HG3	2.13	0.49
1:F:431:ARG:CZ	1:C:184:VAL:HG22	2.43	0.49
1:C:25:ALA:O	1:C:29:MET:HG3	2.13	0.49
1:C:279:ILE:HD12	1:C:280:ASP:OD2	2.13	0.49
1:A:156:GLU:O	1:A:186:LYS:HE3	2.12	0.49
1:B:408:LYS:HE2	7:B:875:HOH:O	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:322:LYS:HB2	1:H:323:PRO:CD	2.42	0.49
1:A:184:VAL:HG21	1:A:432:TYR:CE1	2.47	0.49
1:A:354:PRO:HB2	1:D:210[A]:MET:HB2	1.95	0.49
1:D:250:LEU:O	1:D:254[A]:MET:HG2	2.12	0.49
1:D:322:LYS:HB2	1:D:323:PRO:HD2	1.95	0.49
1:F:296:VAL:HG12	1:F:306:ILE:HD13	1.95	0.49
1:E:38:ARG:HG2	1:E:39:TYR:CE2	2.48	0.49
1:F:167:MET:HA	1:F:172:ILE:HD11	1.95	0.49
1:B:322:LYS:HB2	1:B:323:PRO:HD2	1.95	0.48
1:G:125:LEU:HD11	1:G:139:ILE:HD11	1.94	0.48
1:G:222:GLY:O	1:G:226:LYS:HG3	2.13	0.48
1:H:54:LEU:O	1:H:55:HIS:C	2.56	0.48
1:D:151:ARG:HD3	1:D:376:PRO:HG3	1.96	0.48
1:A:210:MET:HE2	1:E:254[A]:MET:CE	2.43	0.48
1:F:411:GLU:OE2	1:F:415:GLN:NE2	2.46	0.48
1:B:75:GLN:HG3	1:B:120:PHE:CE2	2.48	0.48
1:F:421[A]:CYS:SG	7:F:803:HOH:O	2.61	0.48
1:B:264:GLU:OE1	7:B:601:HOH:O	2.20	0.48
1:F:25:ALA:O	1:F:29:MET:HG3	2.13	0.48
1:H:309:LYS:HB3	1:H:309:LYS:HE3	1.52	0.48
1:D:151:ARG:HD2	1:D:373:TRP:HA	1.95	0.48
1:G:412:LYS:HE2	1:H:279:ILE:HD12	1.93	0.48
1:H:274:THR:HB	1:H:305:GLU:OE1	2.14	0.48
1:G:374:THR:O	1:G:376:PRO:HD3	2.13	0.48
1:D:112:TRP:O	1:D:116:GLN:HG2	2.13	0.47
1:B:108:GLU:HG2	7:B:618[A]:HOH:O	2.14	0.47
1:A:210:MET:HB2	1:D:354:PRO:HB2	1.96	0.47
1:A:377:ASP:HB2	7:A:614:HOH:O	2.12	0.47
1:C:210:MET:SD	1:H:357:VAL:HB	2.54	0.47
1:E:322:LYS:HB2	1:E:323:PRO:CD	2.44	0.47
1:A:102:TRP:O	1:A:105:GLU:HG3	2.14	0.47
1:B:212:ALA:HB2	1:B:235:PHE:O	2.14	0.47
1:G:34:ARG:HG3	7:G:852:HOH:O	2.15	0.46
1:C:298:ASN:O	1:C:344:LEU:HA	2.15	0.46
1:A:233[B]:ARG:HD2	1:E:233[B]:ARG:HH21	1.80	0.46
1:A:354:PRO:HG2	1:D:210[B]:MET:SD	2.55	0.46
1:B:181:ASN:HA	1:B:186:LYS:HD2	1.98	0.46
1:H:315:ALA:HB3	6:H:503:MPD:HM2	1.97	0.46
1:B:389:LYS:HE3	1:B:422:ASP:O	2.15	0.46
1:C:158:THR:HG22	1:C:162:HIS:CE1	2.50	0.46
1:D:322:LYS:HB2	1:D:323:PRO:CD	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:LEU:O	1:E:55:HIS:C	2.58	0.46
1:F:128:ILE:CD1	1:F:139:ILE:HD12	2.44	0.46
1:F:357:VAL:HB	1:G:210:MET:SD	2.56	0.46
1:G:377:ASP:C	1:G:379:TYR:H	2.24	0.46
1:F:45:LEU:HB3	1:F:72:ALA:HB2	1.98	0.46
1:A:157:THR:HG22	3:A:502:ADN:O3'	2.15	0.46
1:D:38:ARG:CD	1:D:39:TYR:CZ	2.98	0.46
1:E:131:ASP:OD1	1:E:157:THR:CG2	2.64	0.46
1:E:279:ILE:HG22	1:E:304:VAL:HB	1.97	0.46
1:F:210:MET:CE	1:G:354:PRO:HG2	2.37	0.46
1:G:309:LYS:HG2	7:G:790:HOH:O	2.15	0.46
1:H:111:LEU:HD22	1:H:115:GLU:CD	2.40	0.46
1:H:250:LEU:O	1:H:254:MET:HG2	2.15	0.46
1:A:303:ASP:CB	1:A:343[B]:ARG:HD2	2.46	0.46
1:A:412:LYS:HG3	1:B:279:ILE:HD11	1.98	0.46
1:D:431:ARG:CZ	1:E:184:VAL:HG22	2.45	0.46
1:H:344:LEU:HD12	1:H:344:LEU:O	2.16	0.46
1:A:210:MET:HE2	1:A:212:ALA:HB3	1.97	0.46
1:B:18:GLY:O	1:B:22:LEU:HD13	2.16	0.46
1:D:317:GLU:HG2	1:D:329:ARG:HB3	1.98	0.46
1:D:327:ARG:HD3	7:D:825:HOH:O	2.16	0.46
1:G:322:LYS:HB2	1:G:323:PRO:HD2	1.98	0.46
1:G:121:LYS:HD2	1:G:121:LYS:C	2.40	0.45
2:B:501:NAD:C4N	3:B:502:ADN:H3'	2.45	0.45
1:D:303:ASP:HB3	1:D:343:ARG:HG3	1.97	0.45
1:C:274:THR:HB	1:C:305:GLU:OE1	2.16	0.45
1:G:153:ILE:O	1:G:177:ALA:HA	2.16	0.45
1:F:377:ASP:OD1	1:F:377:ASP:N	2.50	0.45
1:F:22:LEU:HD23	1:F:58:VAL:HG13	1.98	0.45
1:H:34:ARG:CD	1:H:397:ALA:HB1	2.47	0.45
1:B:250:LEU:O	1:B:254[A]:MET:HG2	2.16	0.45
1:C:111:LEU:O	1:C:115:GLU:HG3	2.17	0.45
1:H:328:TYR:O	1:H:335:ARG:HA	2.16	0.45
1:A:122:ASP:OD1	1:A:122:ASP:N	2.50	0.45
1:D:380:PRO:HD2	1:D:384:HIS:CE1	2.52	0.45
1:G:54:LEU:HG	1:G:131:ASP:HB2	1.99	0.45
1:G:54:LEU:O	1:G:55:HIS:C	2.59	0.45
1:G:301:HIS:CA	1:G:344:LEU:HD21	2.45	0.45
1:E:199:LEU:HD22	1:E:228:CYS:HB3	1.99	0.45
1:A:431:ARG:CZ	1:B:184:VAL:HG22	2.47	0.45
1:B:112:TRP:O	1:B:116:GLN:HG2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:VAL:HG21	1:B:432:TYR:CE1	2.52	0.44
1:E:251:GLN:O	1:E:255:GLU:HG2	2.17	0.44
1:E:309:LYS:HG2	1:E:313:GLU:OE2	2.17	0.44
1:G:300:GLY:C	1:G:344:LEU:HD21	2.42	0.44
1:F:309:LYS:NZ	1:F:309:LYS:HB3	2.32	0.44
1:G:173:LEU:O	1:G:174:LYS:HD3	2.17	0.44
1:D:131:ASP:OD1	1:D:157:THR:HG21	2.17	0.44
1:D:432:TYR:O	1:E:188:LYS:HE2	2.17	0.44
1:G:328:TYR:O	1:G:335:ARG:HA	2.18	0.44
1:E:210:MET:HE2	1:E:212:ALA:HB3	1.99	0.44
1:C:140:HIS:HA	1:C:147:LEU:HD11	2.00	0.44
1:A:328:TYR:O	1:A:335:ARG:HA	2.18	0.44
1:B:233[B]:ARG:NH2	1:B:255:GLU:O	2.51	0.44
1:G:50:ILE:HG12	1:G:127:MET:HB2	2.00	0.44
1:H:53:CYS:HA	1:H:77:SER:O	2.17	0.43
1:F:145:GLN:OE1	1:F:145:GLN:N	2.44	0.43
1:B:210:MET:HB2	1:E:354:PRO:HB2	2.00	0.43
1:C:322:LYS:HB2	1:C:323:PRO:HD2	2.01	0.43
1:A:131:ASP:OD1	1:A:157:THR:CG2	2.66	0.43
1:D:323:PRO:O	1:D:324:GLN:HB2	2.19	0.43
1:E:309:LYS:HB2	1:E:309:LYS:NZ	2.32	0.43
1:C:176:PRO:HB3	1:C:380:PRO:O	2.18	0.43
1:D:25:ALA:O	1:D:29:MET:HG3	2.17	0.43
1:E:300:GLY:O	1:E:344:LEU:CD2	2.66	0.43
1:B:54:LEU:O	1:B:55:HIS:C	2.61	0.43
1:D:210[A]:MET:HE3	1:D:210[A]:MET:HB2	1.66	0.43
1:C:200:ILE:HG21	1:C:235:PHE:CE2	2.53	0.43
1:H:189:PHE:HA	1:H:193:TYR:CD2	2.53	0.43
1:A:279:ILE:HG22	1:A:304:VAL:HB	2.00	0.43
1:C:54:LEU:O	1:C:55:HIS:C	2.61	0.43
1:D:18:GLY:O	1:D:22:LEU:HG	2.18	0.43
1:E:233[B]:ARG:NH2	7:E:612:HOH:O	2.51	0.43
1:F:75:GLN:HG3	1:F:120:PHE:CE2	2.53	0.43
1:C:296:VAL:HG12	1:C:306:ILE:HD13	2.00	0.43
1:A:170:ASN:CB	1:A:172:ILE:HD12	2.49	0.42
1:D:40:SER:O	1:D:43:LYS:HG2	2.19	0.42
1:C:151:ARG:HD3	1:C:376:PRO:HB3	2.00	0.42
1:H:45:LEU:HB3	1:H:72:ALA:HB2	2.01	0.42
1:D:417:LEU:HB3	1:D:419:MET:HE3	2.01	0.42
1:C:121:LYS:O	1:C:121:LYS:HD3	2.19	0.42
1:H:153:ILE:O	1:H:177:ALA:HA	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ASP:HB3	1:A:343[B]:ARG:HD2	2.01	0.42
2:A:501:NAD:C6N	7:A:711:HOH:O	2.68	0.42
1:E:102:TRP:O	1:E:105:GLU:HG3	2.19	0.42
1:G:22:LEU:O	1:G:26:GLU:HG3	2.20	0.42
1:D:188:LYS:HE3	7:D:705:HOH:O	2.19	0.42
1:G:102:TRP:O	1:G:105:GLU:HG3	2.19	0.42
1:C:75:GLN:HG3	1:C:120:PHE:CE2	2.54	0.42
1:B:250:LEU:O	1:B:254[B]:MET:HG3	2.19	0.42
1:H:34:ARG:HD2	1:H:397:ALA:HB1	2.02	0.42
1:H:128:ILE:HD11	1:H:139:ILE:CD1	2.49	0.42
1:E:344:LEU:HD22	2:E:501:NAD:N7N	2.34	0.42
1:H:374:THR:HG22	1:H:375:HIS:ND1	2.34	0.42
1:B:408:LYS:NZ	1:B:422:ASP:OD1	2.53	0.41
1:D:124:PRO:HG3	7:D:908:HOH:O	2.19	0.41
1:F:54:LEU:O	1:F:55:HIS:C	2.63	0.41
1:E:147:LEU:N	1:E:148:PRO:HD2	2.35	0.41
1:A:357:VAL:HB	1:D:210[A]:MET:SD	2.60	0.41
1:D:300:GLY:O	1:D:344:LEU:CD1	2.68	0.41
1:C:134:ASP:HB2	7:C:680:HOH:O	2.20	0.41
1:D:102:TRP:CE2	1:D:105:GLU:HG2	2.56	0.41
1:D:296:VAL:HG12	1:D:306:ILE:HD13	2.02	0.41
1:E:296:VAL:HG12	1:E:306:ILE:HD13	2.03	0.41
1:E:322:LYS:HB2	1:E:323:PRO:HD2	2.02	0.41
1:F:108:GLU:OE1	1:F:108:GLU:N	2.42	0.41
1:B:233[B]:ARG:HD3	7:D:855:HOH:O	2.20	0.41
1:E:303:ASP:HB3	1:E:343[B]:ARG:HG2	2.02	0.41
1:H:417:LEU:HB3	1:H:419:MET:HE3	2.01	0.41
1:F:151:ARG:NH2	7:F:610:HOH:O	2.47	0.41
1:H:126:ASN:HA	1:H:150:ILE:HA	2.03	0.41
1:D:142:LYS:HD3	1:D:143:TYR:CE2	2.56	0.41
1:F:322:LYS:HB2	1:F:323:PRO:CD	2.51	0.41
1:G:157:THR:HA	7:G:712:HOH:O	2.21	0.41
1:A:411:GLU:O	1:A:415:GLN:HG2	2.21	0.41
1:F:414:ALA:HB1	1:F:419:MET:O	2.20	0.41
1:A:300:GLY:O	1:A:344:LEU:HD21	2.20	0.41
1:B:34:ARG:NH1	7:B:628:HOH:O	2.54	0.41
1:D:127:MET:SD	1:D:151:ARG:HB3	2.61	0.41
1:D:144:PRO:HA	1:D:147:LEU:HG	2.03	0.41
1:D:254[B]:MET:HE2	1:D:254[B]:MET:HB3	1.99	0.41
1:C:10:ALA:HA	7:C:803:HOH:O	2.21	0.41
1:H:4:LYS:HG3	7:H:676:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:303:ASP:HB3	1:H:343:ARG:HG2	2.02	0.41
1:B:200:ILE:HG21	1:B:235:PHE:CE2	2.56	0.41
1:F:328:TYR:O	1:F:335:ARG:HA	2.21	0.41
1:F:412:LYS:HD3	1:C:279:ILE:CD1	2.51	0.41
1:C:198:SER:HB2	1:C:346:ASN:HB2	2.03	0.41
1:B:8:LYS:HG2	1:B:102:TRP:CZ3	2.56	0.40
1:E:134:ASP:HB2	7:E:731:HOH:O	2.21	0.40
1:G:251:GLN:O	1:G:255:GLU:HG2	2.21	0.40
1:C:316:VAL:HG22	1:C:329:ARG:O	2.20	0.40
1:D:184:VAL:HG21	1:D:432:TYR:CE1	2.55	0.40
1:E:190:ASP:OD1	1:E:190:ASP:C	2.63	0.40
1:C:200:ILE:HG21	1:C:235:PHE:HE2	1.86	0.40
6:H:503:MPD:H32	7:H:634:HOH:O	2.22	0.40
1:G:303:ASP:HB3	1:G:343[B]:ARG:HG2	2.03	0.40
1:A:185:THR:HA	1:A:189:PHE:CD1	2.56	0.40
1:E:52:GLY:HA3	1:E:76:TRP:CZ3	2.57	0.40
1:F:180:VAL:HG13	1:F:364:ASN:HB3	2.02	0.40
1:C:328:TYR:O	1:C:335:ARG:HA	2.21	0.40
1:H:186:LYS:HD3	1:H:186:LYS:C	2.46	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	433/431 (100%)	423 (98%)	10 (2%)	0	100	100
1	B	431/431 (100%)	421 (98%)	9 (2%)	1 (0%)	43	24
1	C	429/431 (100%)	417 (97%)	12 (3%)	0	100	100
1	D	432/431 (100%)	418 (97%)	13 (3%)	1 (0%)	43	24
1	E	433/431 (100%)	422 (98%)	11 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	430/431 (100%)	420 (98%)	10 (2%)	0	100	100
1	G	430/431 (100%)	417 (97%)	12 (3%)	1 (0%)	43	24
1	H	428/431 (99%)	416 (97%)	12 (3%)	0	100	100
All	All	3446/3448 (100%)	3354 (97%)	89 (3%)	3 (0%)	48	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	55	HIS
1	G	55	HIS
1	D	376	PRO

5.3.2 Protein sidechains ⓘ

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	359/355 (101%)	358 (100%)	1 (0%)	86	78
1	B	357/355 (101%)	355 (99%)	2 (1%)	78	66
1	C	355/355 (100%)	353 (99%)	2 (1%)	78	66
1	D	358/355 (101%)	355 (99%)	3 (1%)	73	59
1	E	359/355 (101%)	357 (99%)	2 (1%)	78	66
1	F	356/355 (100%)	356 (100%)	0	100	100
1	G	356/355 (100%)	355 (100%)	1 (0%)	86	78
1	H	354/355 (100%)	353 (100%)	1 (0%)	86	78
All	All	2854/2840 (100%)	2842 (100%)	12 (0%)	84	75

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	412	LYS
1	B	344	LEU
1	B	405	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	210[A]	MET
1	D	210[B]	MET
1	D	283	LEU
1	E	69	THR
1	E	122	ASP
1	G	377	ASP
1	C	145	GLN
1	C	344	LEU
1	H	377	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	267	GLN
1	A	320	ASN
1	A	415	GLN
1	B	162	HIS
1	D	324	GLN
1	D	429	HIS
1	E	162	HIS
1	E	230	GLN
1	F	267	GLN
1	F	365	GLN
1	F	369	GLN
1	F	403	ASN
1	G	170	ASN
1	G	314	ASN
1	G	324	GLN
1	G	403	ASN
1	C	80	ASN
1	C	162	HIS
1	C	267	GLN
1	C	320	ASN
1	H	163	ASN
1	H	324	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 9 are monoatomic - leaving 21 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	$\# Z > 2$
2	NAD	F	501	-	45,48,48	0.39	0	63,73,73	0.55	0
5	SO4	A	504	-	4,4,4	0.72	0	6,6,6	0.33	0
2	NAD	A	501	-	45,48,48	0.39	0	63,73,73	0.56	0
3	ADN	B	502	-	21,21,21	0.31	0	31,31,31	0.49	0
5	SO4	G	505	-	4,4,4	0.68	0	6,6,6	0.22	0
5	SO4	D	504	-	4,4,4	0.68	0	6,6,6	0.18	0
2	NAD	H	501	-	45,48,48	0.36	0	63,73,73	0.49	0
3	ADN	H	502	-	21,21,21	0.22	0	31,31,31	0.48	0
2	NAD	G	501	-	45,48,48	0.34	0	63,73,73	0.47	0
3	ADN	G	502	-	21,21,21	0.27	0	31,31,31	0.51	0
6	MPD	H	503	-	7,7,7	0.42	0	9,10,10	0.52	0
2	NAD	C	501	-	45,48,48	0.33	0	63,73,73	0.56	1 (1%)
3	ADN	C	502	-	21,21,21	0.26	0	31,31,31	0.56	0
3	ADN	E	502	-	21,21,21	0.24	0	31,31,31	0.55	0
2	NAD	E	501	-	45,48,48	0.43	0	63,73,73	0.51	0
3	ADN	A	502	-	21,21,21	0.28	0	31,31,31	0.55	0
2	NAD	B	501	-	45,48,48	0.37	0	63,73,73	0.61	0
2	NAD	D	501	-	45,48,48	0.37	0	63,73,73	0.53	0
3	ADN	D	502	-	21,21,21	0.27	0	31,31,31	0.50	0
5	SO4	F	504	-	4,4,4	0.66	0	6,6,6	0.12	0
3	ADN	F	502	-	21,21,21	0.29	0	31,31,31	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADN	A	502	-	-	0/6/22/22	0/3/3/3
3	ADN	B	502	-	-	0/6/22/22	0/3/3/3
2	NAD	C	501	-	-	6/30/62/62	0/5/5/5
2	NAD	B	501	-	-	5/30/62/62	0/5/5/5
2	NAD	F	501	-	-	5/30/62/62	0/5/5/5
3	ADN	C	502	-	-	0/6/22/22	0/3/3/3
3	ADN	E	502	-	-	0/6/22/22	0/3/3/3
2	NAD	D	501	-	-	5/30/62/62	0/5/5/5
3	ADN	D	502	-	-	0/6/22/22	0/3/3/3
6	MPD	H	503	-	-	1/5/5/5	-
2	NAD	A	501	-	-	5/30/62/62	0/5/5/5
2	NAD	H	501	-	-	5/30/62/62	0/5/5/5
3	ADN	H	502	-	-	0/6/22/22	0/3/3/3
3	ADN	F	502	-	-	1/6/22/22	0/3/3/3
2	NAD	G	501	-	-	5/30/62/62	0/5/5/5
2	NAD	E	501	-	-	5/30/62/62	0/5/5/5
3	ADN	G	502	-	-	0/6/22/22	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NAD	O5B-PA-O1A	2.11	117.32	109.07

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	O4D-C1D-N1N-C2N
2	A	501	NAD	O4D-C1D-N1N-C6N
2	A	501	NAD	C2D-C1D-N1N-C2N
2	A	501	NAD	C2D-C1D-N1N-C6N
2	B	501	NAD	O4D-C1D-N1N-C2N
2	B	501	NAD	O4D-C1D-N1N-C6N
2	B	501	NAD	C2D-C1D-N1N-C2N
2	B	501	NAD	C2D-C1D-N1N-C6N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	501	NAD	O4D-C1D-N1N-C2N
2	D	501	NAD	O4D-C1D-N1N-C6N
2	D	501	NAD	C2D-C1D-N1N-C2N
2	D	501	NAD	C2D-C1D-N1N-C6N
2	E	501	NAD	O4D-C1D-N1N-C2N
2	E	501	NAD	O4D-C1D-N1N-C6N
2	E	501	NAD	C2D-C1D-N1N-C2N
2	E	501	NAD	C2D-C1D-N1N-C6N
2	F	501	NAD	O4D-C1D-N1N-C2N
2	F	501	NAD	O4D-C1D-N1N-C6N
2	F	501	NAD	C2D-C1D-N1N-C2N
2	F	501	NAD	C2D-C1D-N1N-C6N
2	G	501	NAD	O4D-C1D-N1N-C2N
2	G	501	NAD	O4D-C1D-N1N-C6N
2	G	501	NAD	C2D-C1D-N1N-C2N
2	G	501	NAD	C2D-C1D-N1N-C6N
2	C	501	NAD	O4D-C1D-N1N-C2N
2	C	501	NAD	O4D-C1D-N1N-C6N
2	C	501	NAD	C2D-C1D-N1N-C2N
2	C	501	NAD	C2D-C1D-N1N-C6N
2	H	501	NAD	O4D-C1D-N1N-C2N
2	H	501	NAD	O4D-C1D-N1N-C6N
2	H	501	NAD	C2D-C1D-N1N-C2N
2	H	501	NAD	C2D-C1D-N1N-C6N
2	G	501	NAD	O4B-C4B-C5B-O5B
2	C	501	NAD	O4B-C4B-C5B-O5B
2	B	501	NAD	O4B-C4B-C5B-O5B
2	F	501	NAD	O4B-C4B-C5B-O5B
2	A	501	NAD	O4B-C4B-C5B-O5B
6	H	503	MPD	C2-C3-C4-C5
2	D	501	NAD	O4B-C4B-C5B-O5B
2	E	501	NAD	O4B-C4B-C5B-O5B
2	H	501	NAD	O4B-C4B-C5B-O5B
3	F	502	ADN	C3'-C4'-C5'-O5'
2	C	501	NAD	C2B-C1B-N9A-C8A

There are no ring outliers.

17 monomers are involved in 15 short contacts:

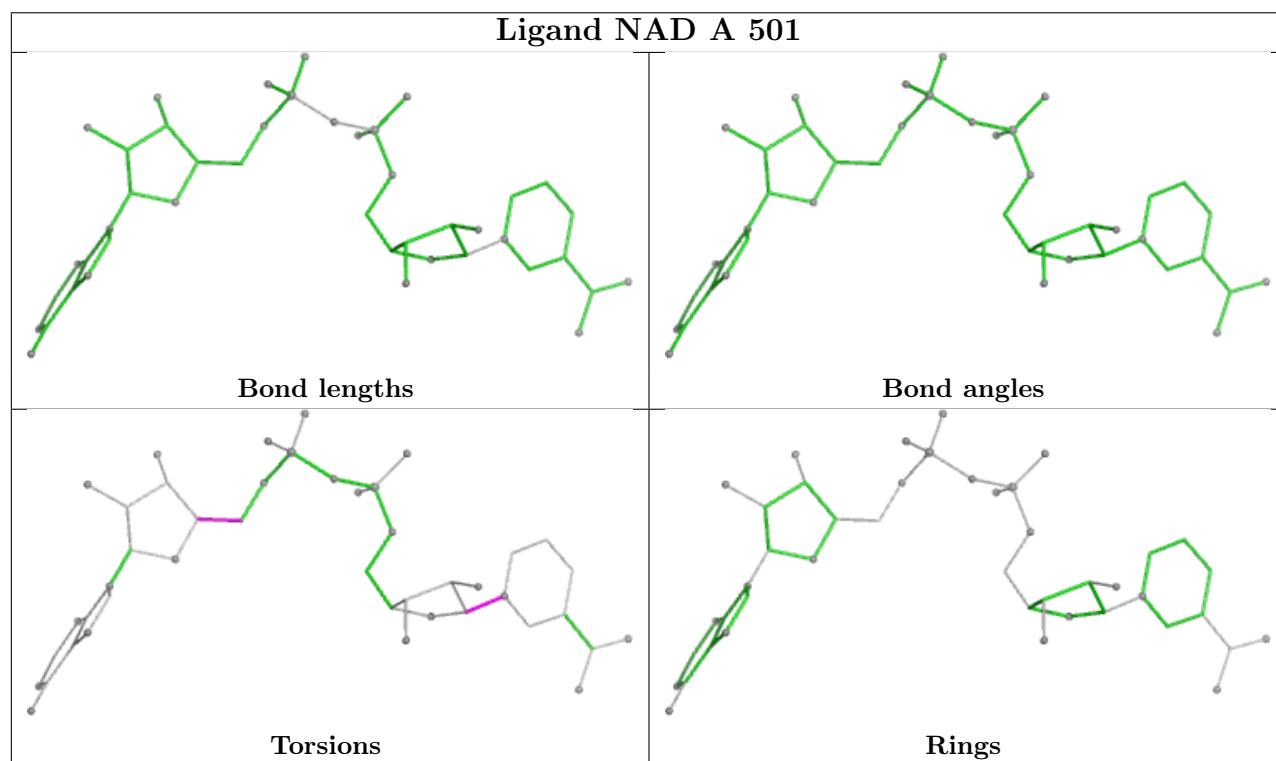
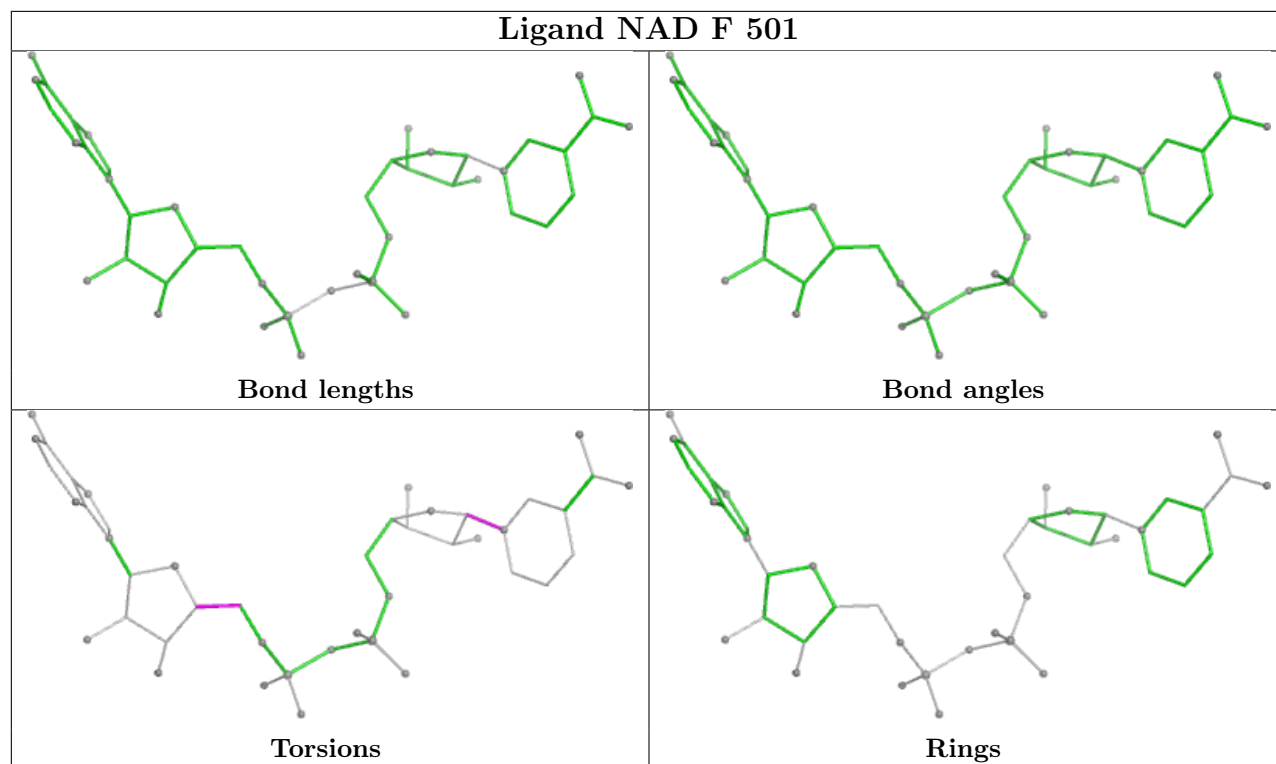
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	NAD	1	0
2	A	501	NAD	2	0

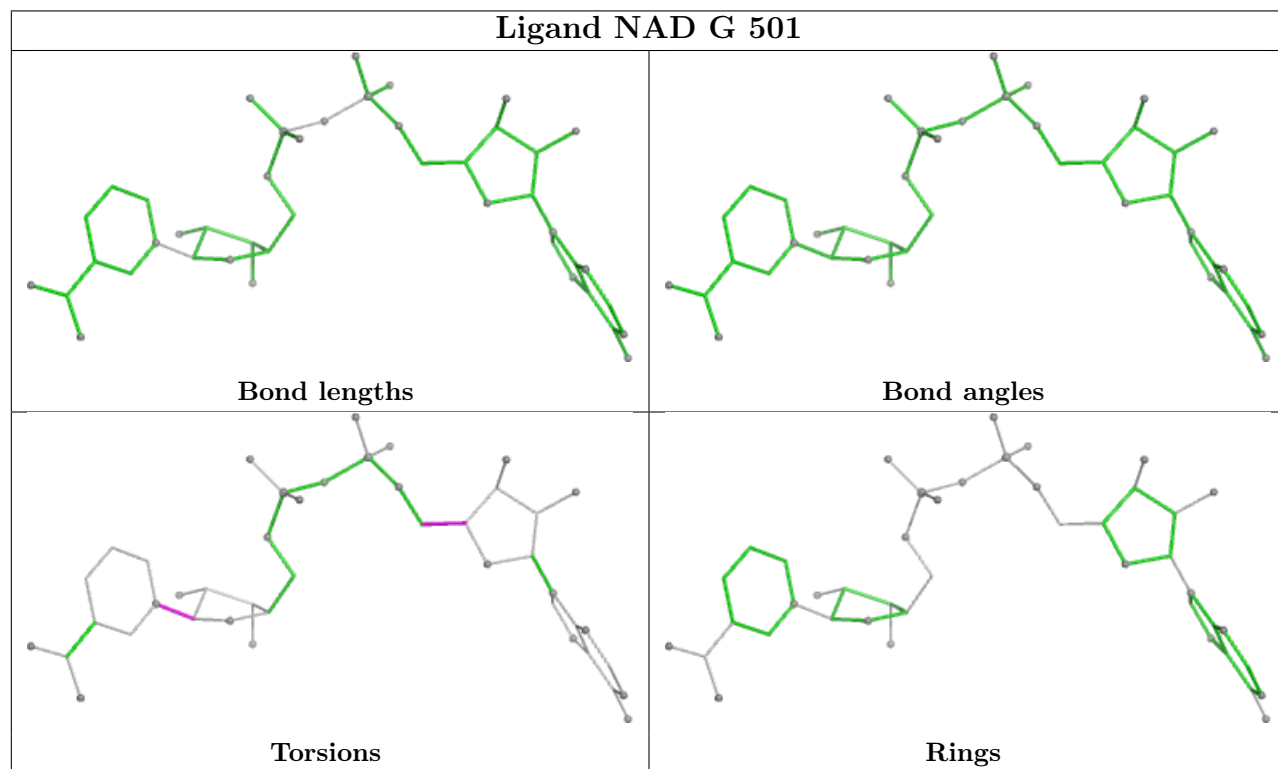
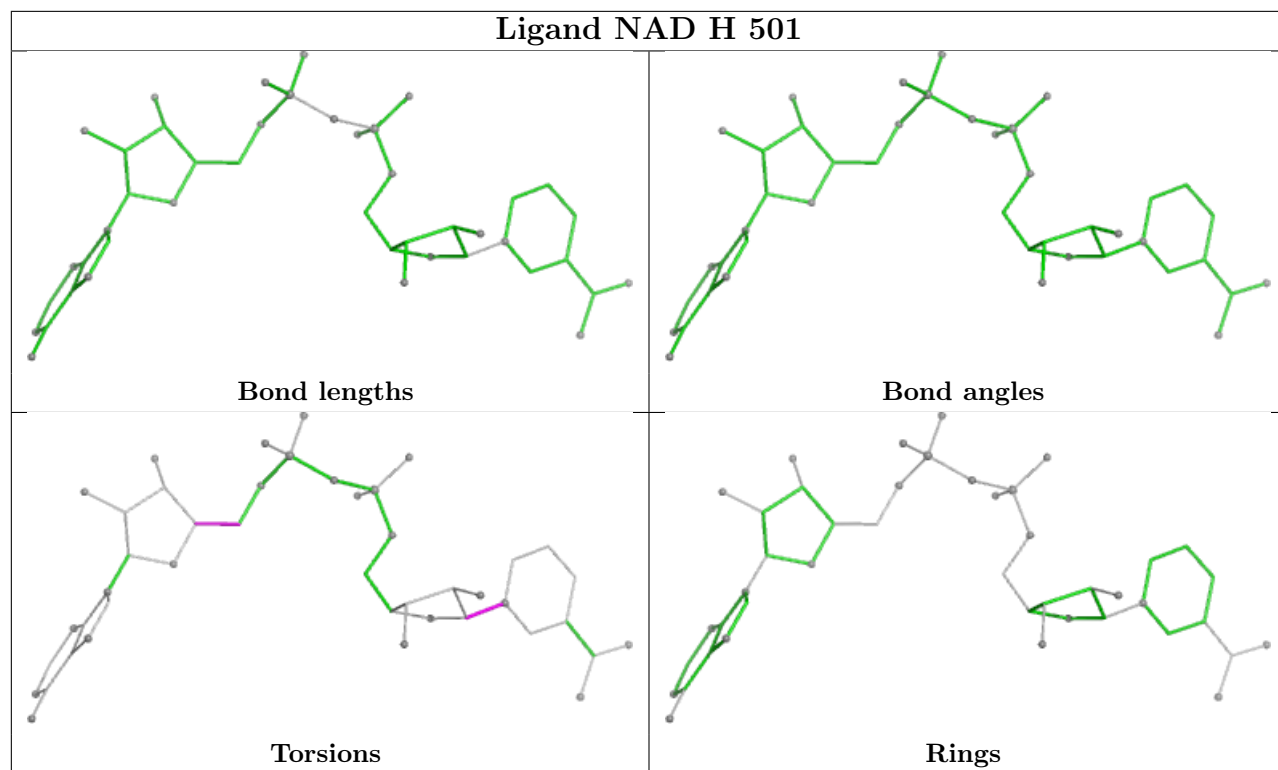
Continued on next page...

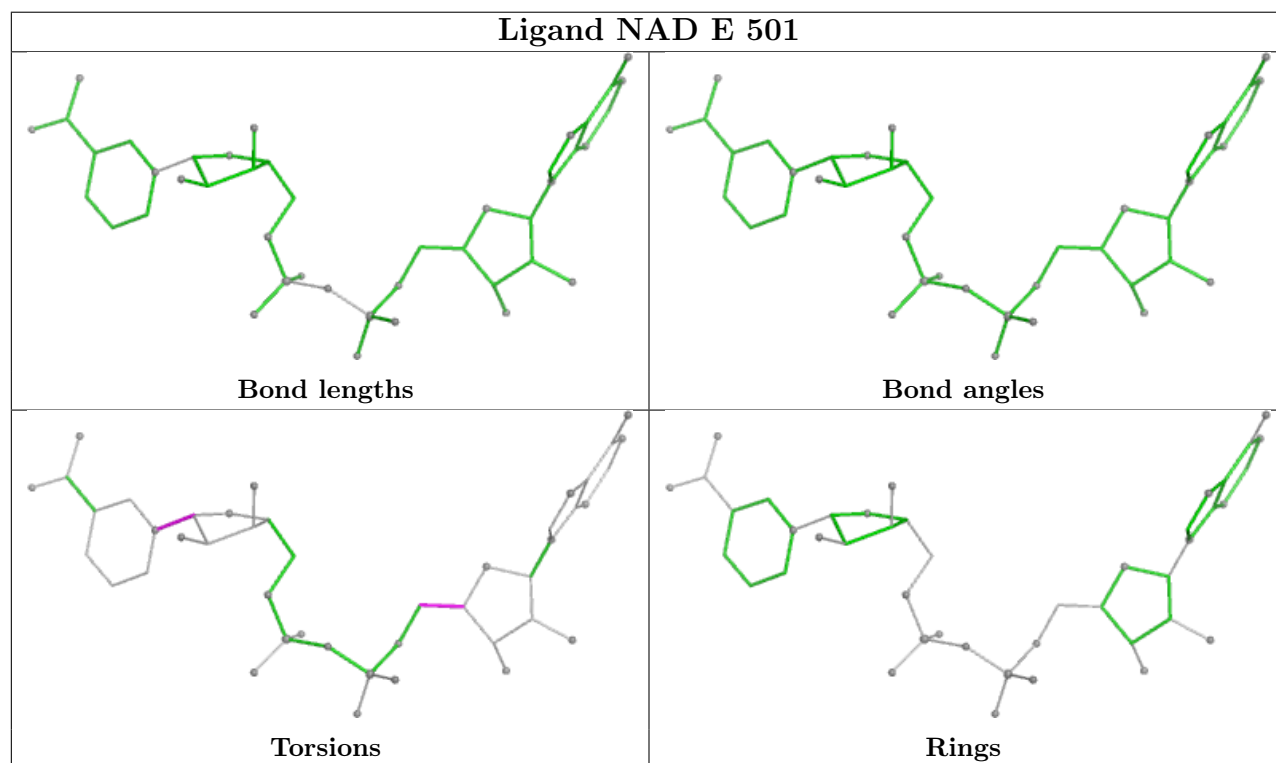
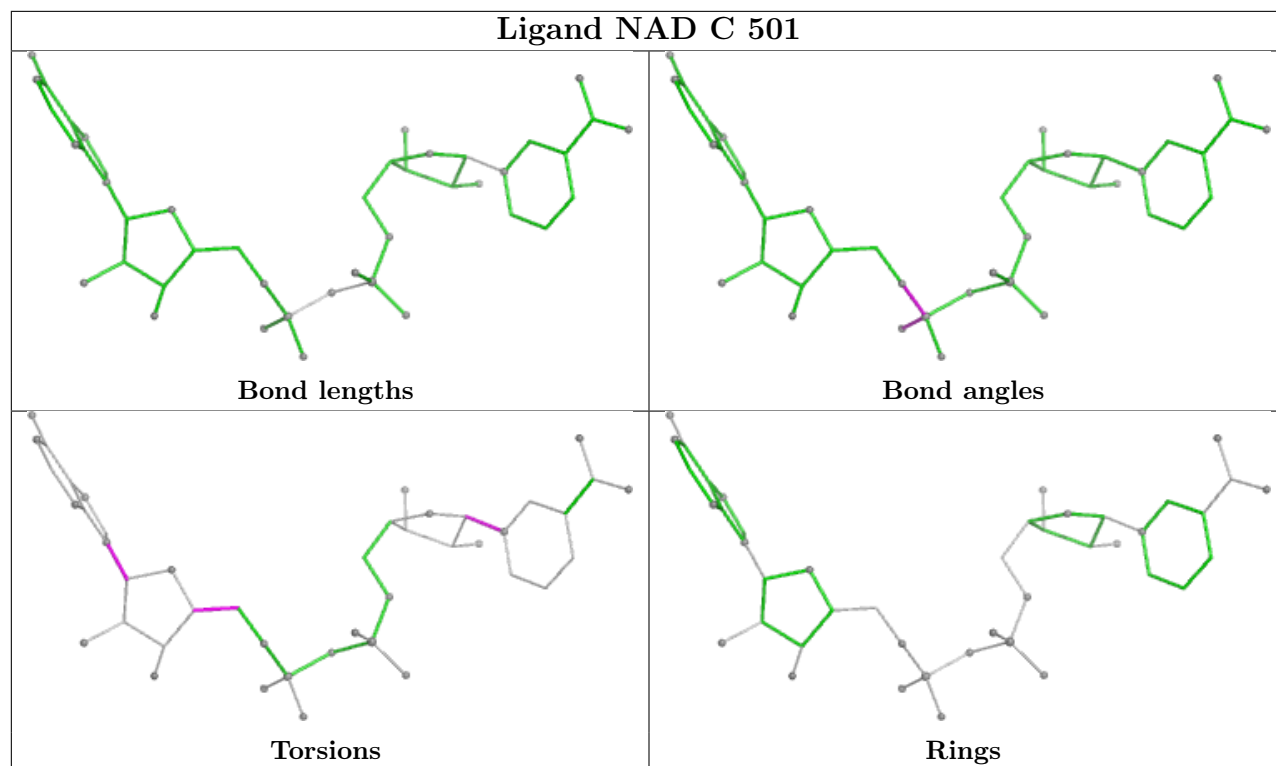
Continued from previous page...

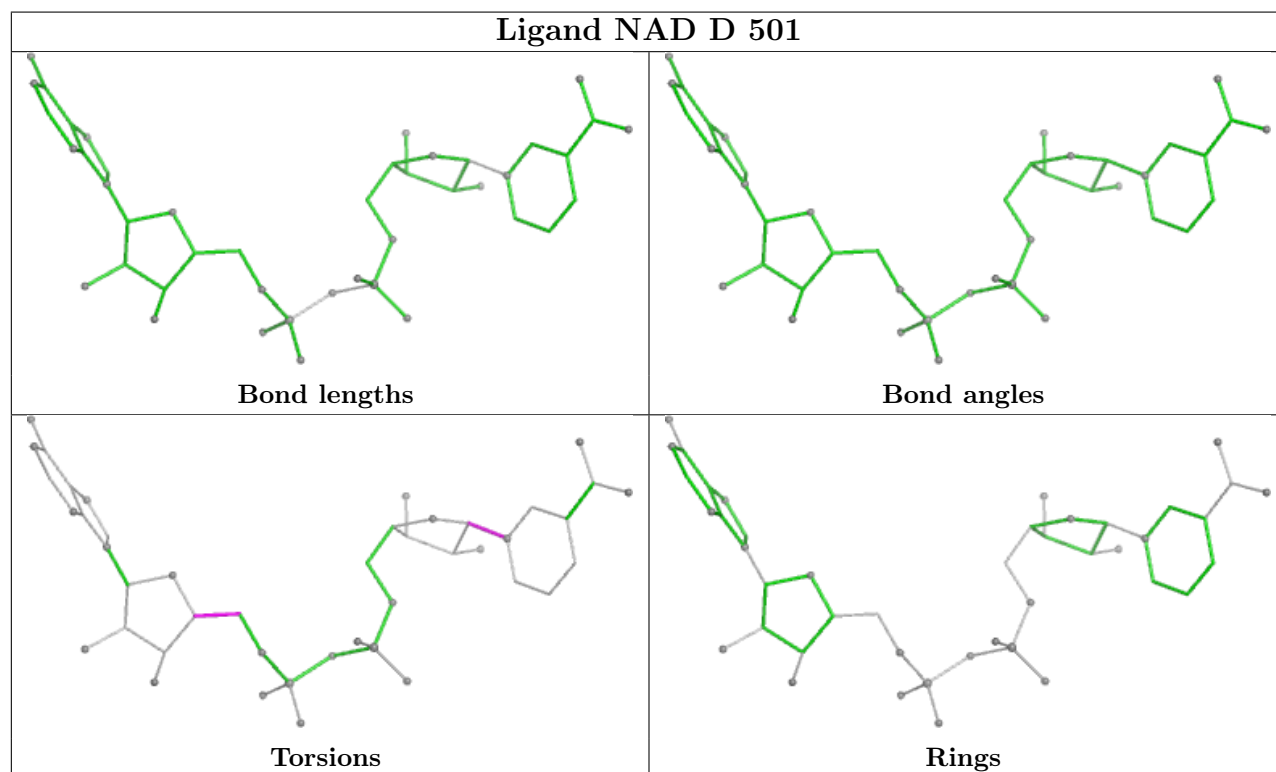
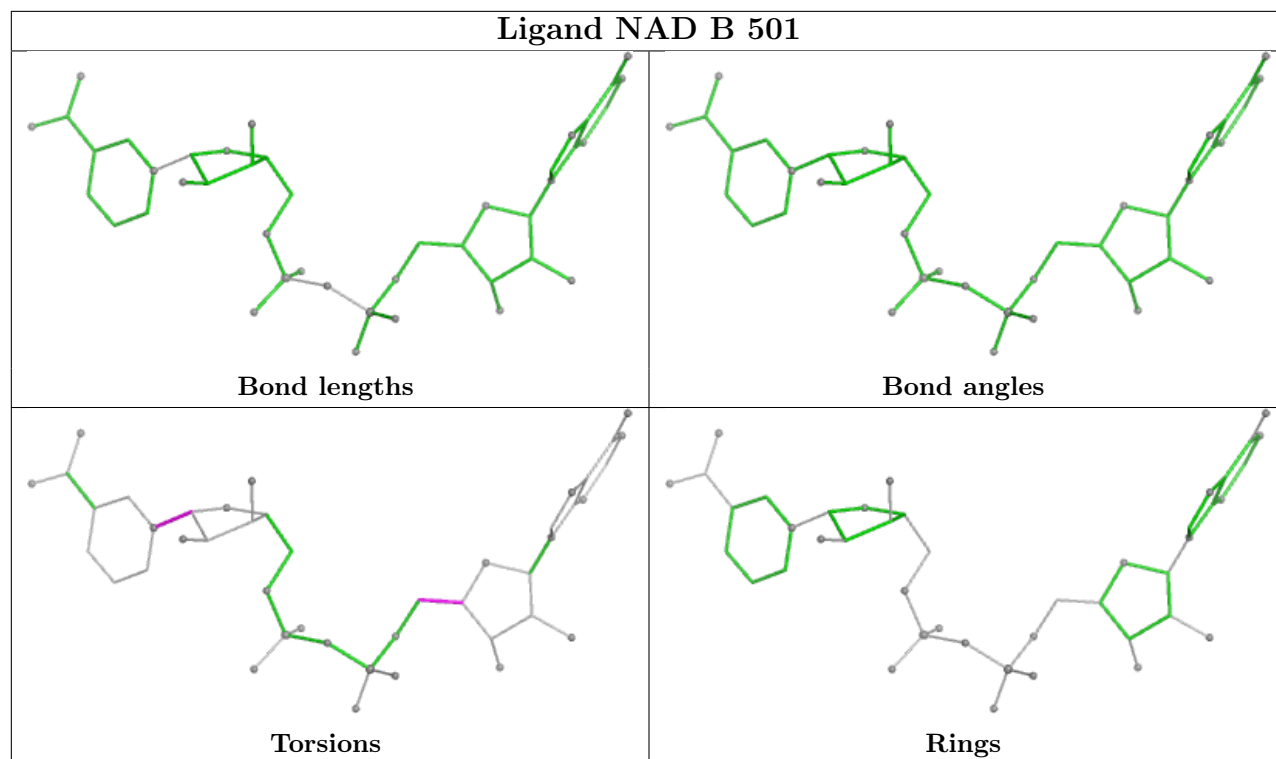
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	ADN	1	0
2	H	501	NAD	1	0
3	H	502	ADN	1	0
2	G	501	NAD	1	0
3	G	502	ADN	1	0
6	H	503	MPD	3	0
2	C	501	NAD	1	0
3	C	502	ADN	2	0
3	E	502	ADN	1	0
2	E	501	NAD	2	0
3	A	502	ADN	2	0
2	B	501	NAD	1	0
2	D	501	NAD	1	0
3	D	502	ADN	1	0
3	F	502	ADN	1	0

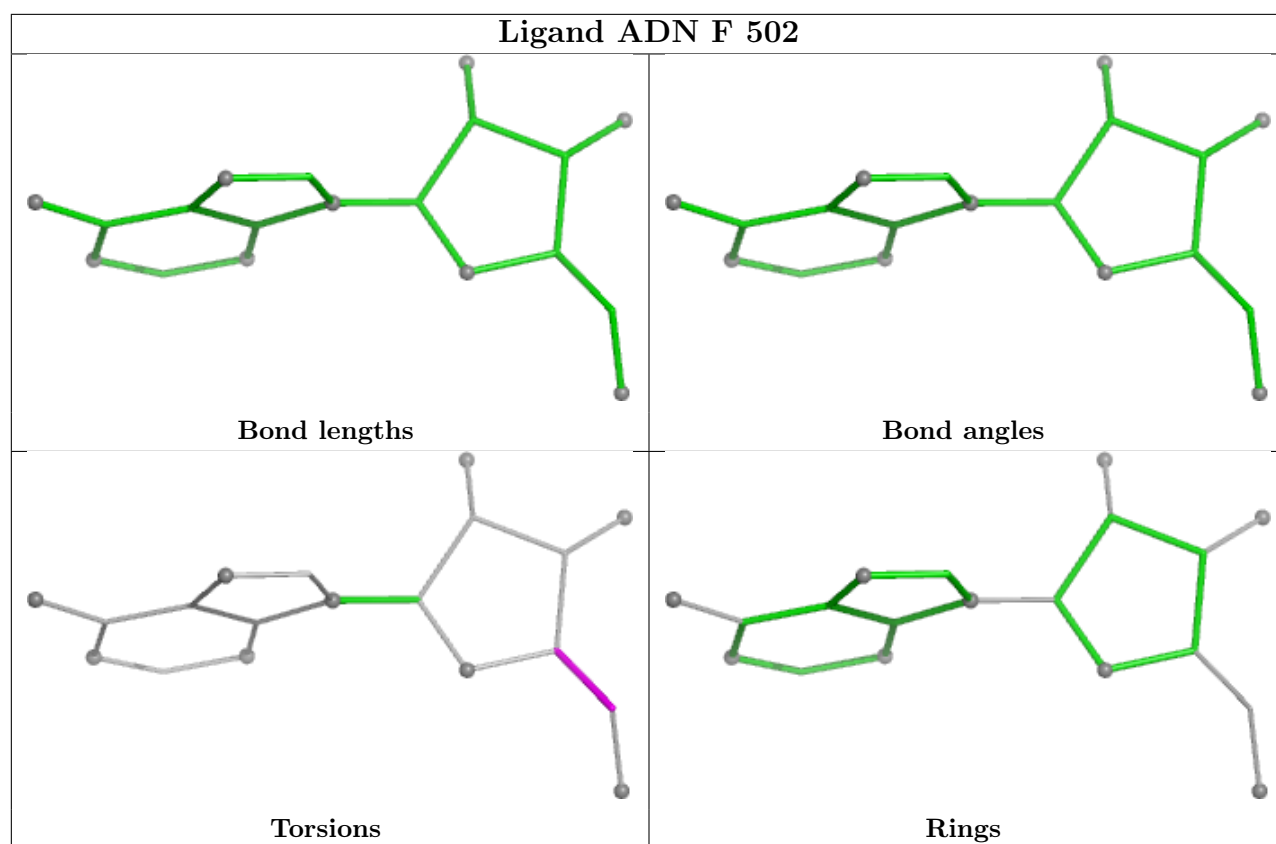
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	430/431 (99%)	-0.11	3 (0%)	84 87	7, 21, 34, 48	5 (1%)
1	B	430/431 (99%)	-0.23	2 (0%)	87 90	7, 19, 32, 52	3 (0%)
1	C	430/431 (99%)	0.14	8 (1%)	66 70	10, 25, 43, 70	1 (0%)
1	D	430/431 (99%)	0.39	39 (9%)	15 15	7, 26, 46, 81	4 (0%)
1	E	430/431 (99%)	0.01	5 (1%)	76 80	8, 23, 39, 80	5 (1%)
1	F	430/431 (99%)	0.03	8 (1%)	66 70	10, 23, 38, 64	2 (0%)
1	G	430/431 (99%)	0.19	17 (3%)	42 44	10, 24, 44, 104	2 (0%)
1	H	430/431 (99%)	0.39	27 (6%)	26 26	13, 26, 51, 76	0
All	All	3440/3448 (99%)	0.10	109 (3%)	50 53	7, 23, 43, 104	22 (0%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	379	TYR	5.9
1	G	376	PRO	5.4
1	D	376	PRO	4.1
1	D	111	LEU	3.7
1	D	301	HIS	3.6
1	D	97	ILE	3.5
1	F	172	ILE	3.5
1	G	377	ASP	3.5
1	E	3	ASP	3.4
1	H	374	THR	3.3
1	F	377	ASP	3.2
1	D	121	LYS	3.1
1	H	381	VAL	3.1
1	H	172	ILE	3.1
1	F	162	HIS	3.1
1	C	172	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	373	TRP	3.0
1	H	147	LEU	3.0
1	D	302	PHE	3.0
1	H	175	VAL	3.0
1	G	301	HIS	2.9
1	G	375	HIS	2.9
1	D	120	PHE	2.8
1	F	169	ALA	2.8
1	D	3	ASP	2.8
1	D	50	ILE	2.7
1	A	121	LYS	2.7
1	G	380	PRO	2.7
1	H	380	PRO	2.7
1	H	146	LEU	2.7
1	D	123	GLY	2.6
1	D	379	TYR	2.6
1	D	74	VAL	2.6
1	H	376	PRO	2.6
1	D	5	LEU	2.6
1	C	380	PRO	2.6
1	G	373	TRP	2.5
1	D	118	LEU	2.5
1	F	38	ARG	2.5
1	D	147	LEU	2.5
1	C	173	LEU	2.5
1	D	377	ASP	2.5
1	D	48	ALA	2.4
1	E	172	ILE	2.4
1	C	147	LEU	2.4
1	A	377	ASP	2.4
1	G	302	PHE	2.4
1	H	3	ASP	2.4
1	G	162	HIS	2.4
1	C	162	HIS	2.4
1	G	169	ALA	2.4
1	H	6	PRO	2.4
1	G	374	THR	2.4
1	H	123	GLY	2.4
1	D	141	THR	2.4
1	G	300	GLY	2.4
1	F	235	PHE	2.4
1	D	169	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	162	HIS	2.3
1	G	381	VAL	2.3
1	D	139	ILE	2.3
1	H	138	LEU	2.3
1	H	143	TYR	2.3
1	H	9	VAL	2.3
1	D	173	LEU	2.3
1	H	379	TYR	2.3
1	A	162	HIS	2.2
1	B	162	HIS	2.2
1	H	300	GLY	2.2
1	F	121	LYS	2.2
1	H	162	HIS	2.2
1	F	34	ARG	2.2
1	H	122	ASP	2.2
1	H	111	LEU	2.2
1	D	100	TYR	2.2
1	D	124	PRO	2.2
1	C	381	VAL	2.2
1	G	378	LYS	2.2
1	H	301	HIS	2.2
1	D	144	PRO	2.1
1	D	171	GLY	2.1
1	E	149	GLY	2.1
1	D	40	SER	2.1
1	D	17	TRP	2.1
1	E	118	LEU	2.1
1	D	374	THR	2.1
1	D	150	ILE	2.1
1	H	17	TRP	2.1
1	H	68	VAL	2.1
1	D	38	ARG	2.1
1	D	76	TRP	2.1
1	H	373	TRP	2.1
1	D	47	GLY	2.1
1	D	303	ASP	2.1
1	C	376	PRO	2.1
1	H	120	PHE	2.0
1	D	101	ALA	2.0
1	G	41	ALA	2.0
1	G	172	ILE	2.0
1	C	3	ASP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	377	ASP	2.0
1	D	149	GLY	2.0
1	E	48	ALA	2.0
1	B	316	VAL	2.0
1	H	302	PHE	2.0
1	H	40	SER	2.0
1	G	3	ASP	2.0
1	D	119	TYR	2.0
1	D	143	TYR	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(\AA^2)	Q<0.9
5	SO4	A	504	5/5	0.76	0.14	22,22,26,33	5
5	SO4	G	505	5/5	0.81	0.13	26,28,32,38	5
5	SO4	F	504	5/5	0.84	0.12	25,27,33,35	5
5	SO4	D	504	5/5	0.85	0.12	22,27,30,34	5
6	MPD	H	503	8/8	0.86	0.10	26,33,39,39	0
4	K	G	504	1/1	0.89	0.13	22,22,22,22	1
3	ADN	B	502	19/19	0.95	0.06	10,15,18,19	0
3	ADN	D	502	19/19	0.95	0.08	16,20,24,30	0
3	ADN	C	502	19/19	0.96	0.06	14,18,24,25	0
3	ADN	H	502	19/19	0.96	0.06	19,22,26,27	0
3	ADN	F	502	19/19	0.96	0.05	13,17,21,22	0
3	ADN	G	502	19/19	0.96	0.06	15,18,25,27	0
2	NAD	C	501	44/44	0.97	0.06	16,18,21,21	0
3	ADN	A	502	19/19	0.97	0.05	13,16,20,20	0

Continued on next page...

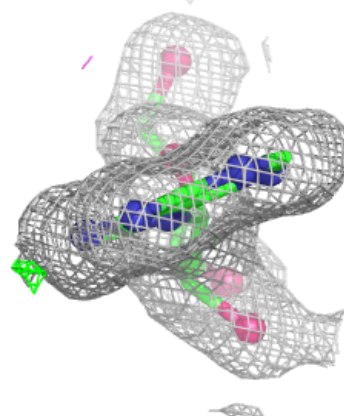
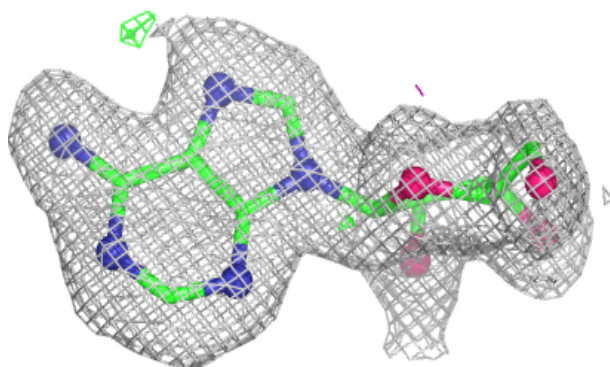
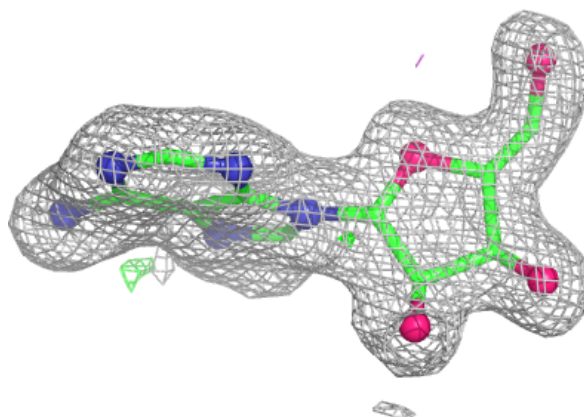
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAD	F	501	44/44	0.97	0.05	14,17,21,22	0
2	NAD	G	501	44/44	0.97	0.05	14,17,21,22	0
3	ADN	E	502	19/19	0.97	0.05	14,16,21,21	0
4	K	H	504	1/1	0.98	0.04	18,18,18,18	1
2	NAD	H	501	44/44	0.98	0.05	15,19,23,24	0
2	NAD	E	501	44/44	0.98	0.04	12,14,18,21	0
2	NAD	A	501	44/44	0.98	0.05	10,14,17,18	0
2	NAD	B	501	44/44	0.98	0.04	9,12,15,16	0
2	NAD	D	501	44/44	0.98	0.05	15,19,21,23	0
4	K	B	503	1/1	0.99	0.02	14,14,14,14	1
4	K	D	503	1/1	0.99	0.03	18,18,18,18	1
4	K	F	503	1/1	0.99	0.02	17,17,17,17	1
4	K	G	503	1/1	0.99	0.07	24,24,24,24	0
4	K	A	503	1/1	0.99	0.03	15,15,15,15	1
4	K	C	503	1/1	0.99	0.02	17,17,17,17	1
4	K	E	503	1/1	1.00	0.02	16,16,16,16	1

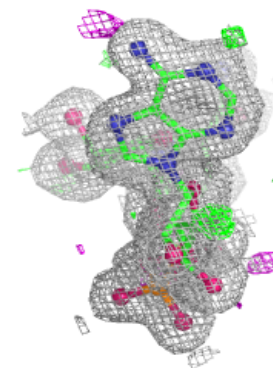
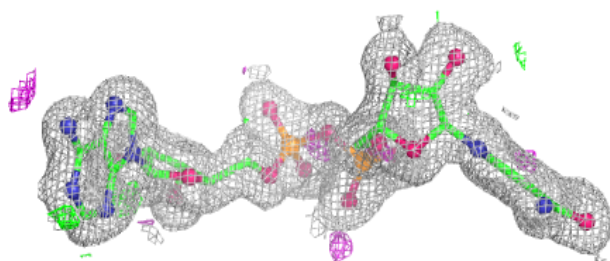
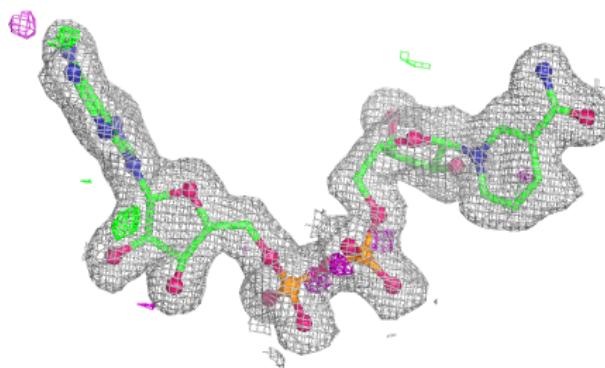
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADN F 502:

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

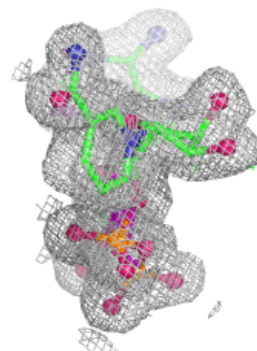
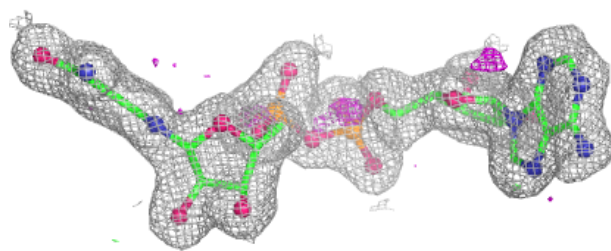
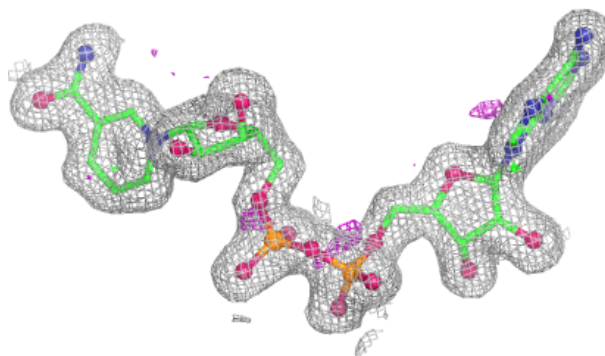
**Electron density around NAD C 501:**

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

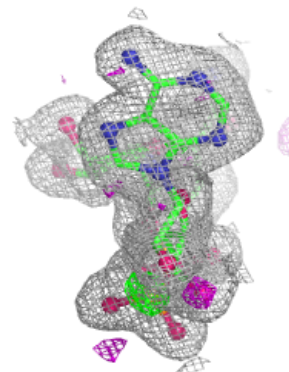
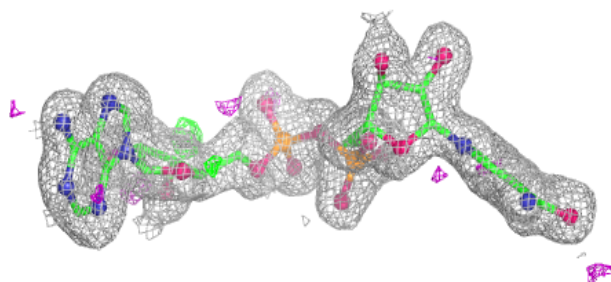
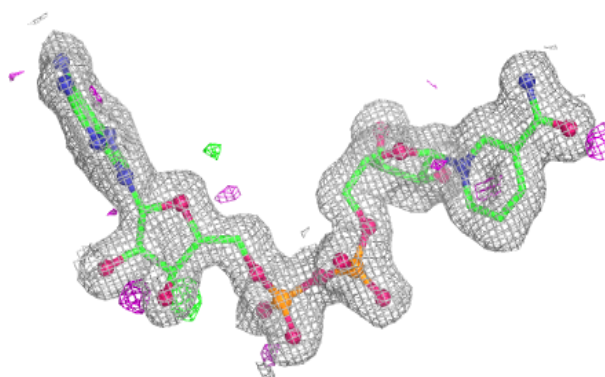


Electron density around NAD F 501:

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

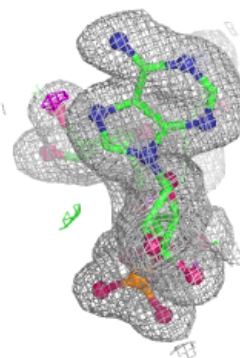
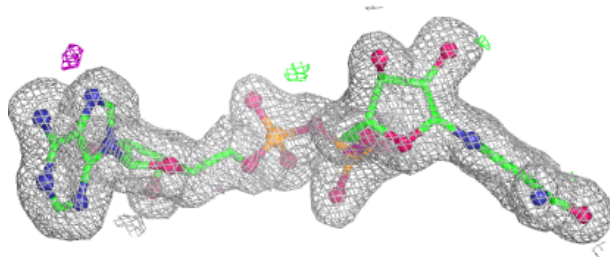
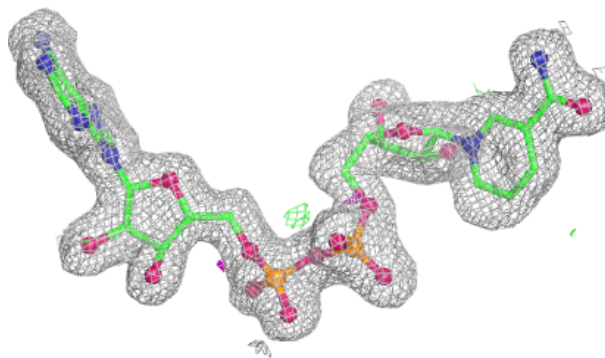
**Electron density around NAD G 501:**

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

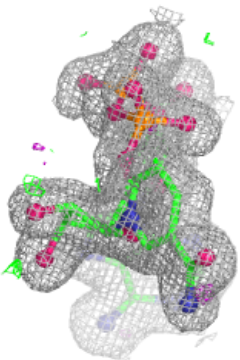
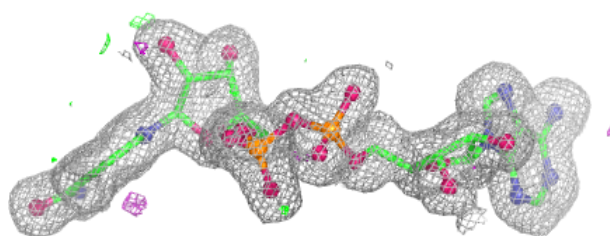
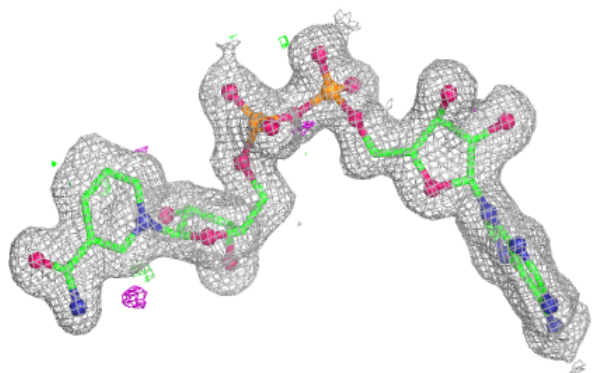


Electron density around NAD H 501:

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

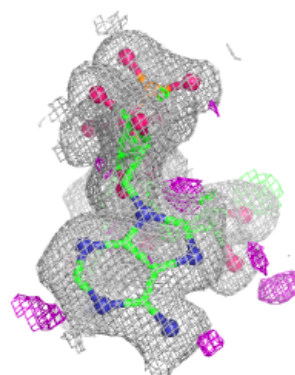
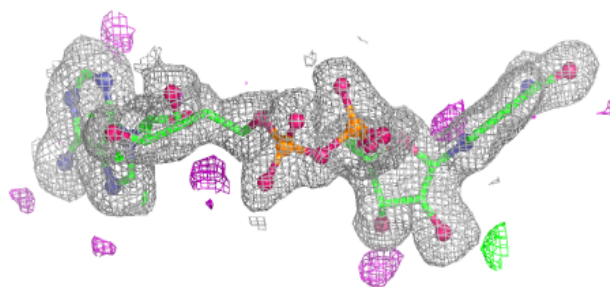
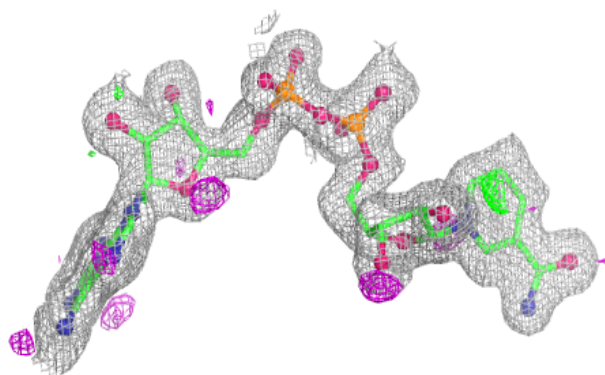
**Electron density around NAD E 501:**

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

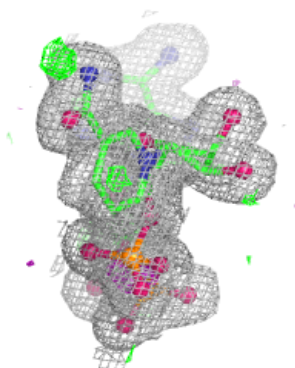
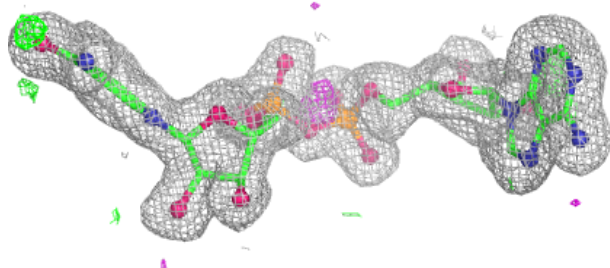
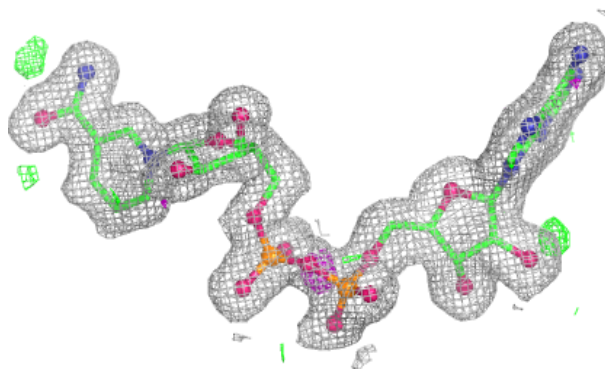


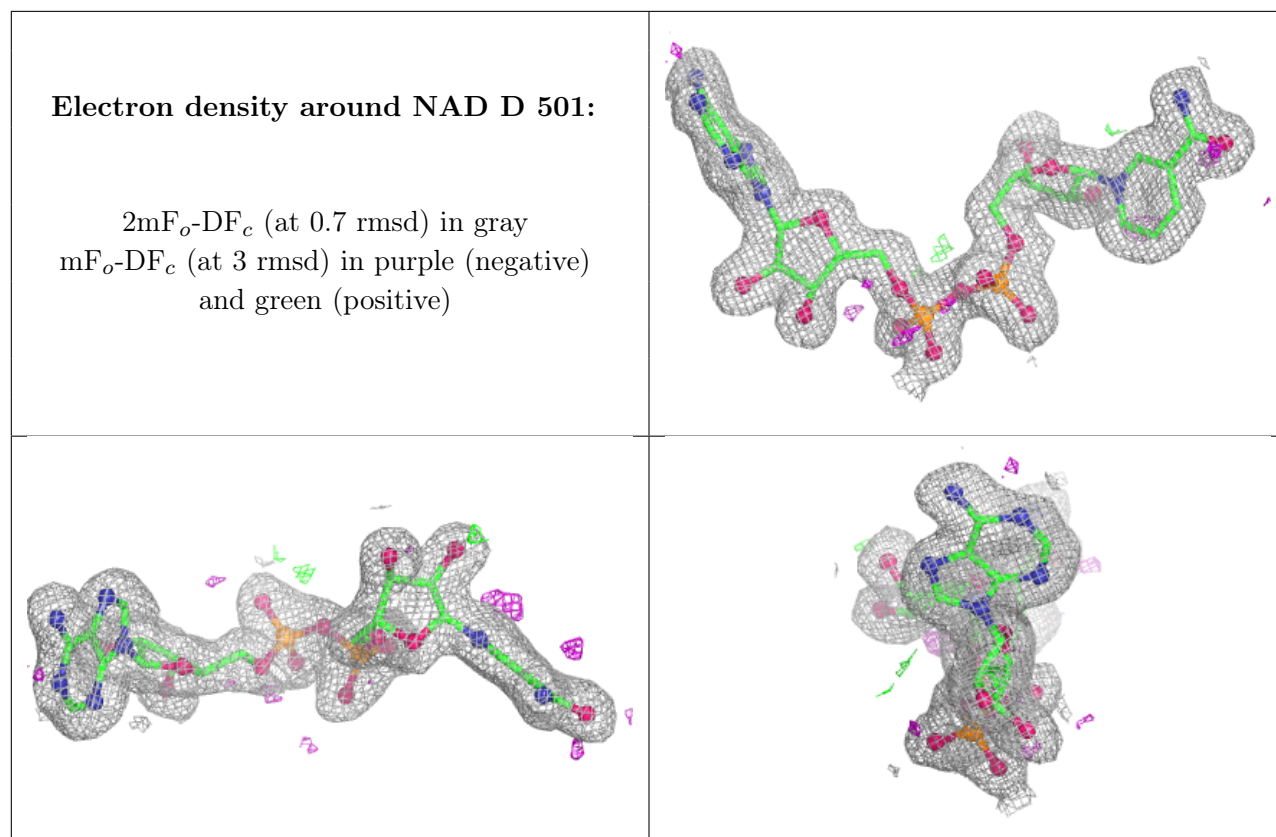
Electron density around NAD A 501:

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

**Electron density around NAD B 501:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.