



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 11:08 pm BST

PDB ID : 3GGG
Title : The crystal structure of A. aeolicus prephenate dehydrogenase in complex with tyrosine and NAD⁺
Authors : Sun, W.; Shahinas, D.; Christendat, D.
Deposited on : 2009-02-27
Resolution : 2.21 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

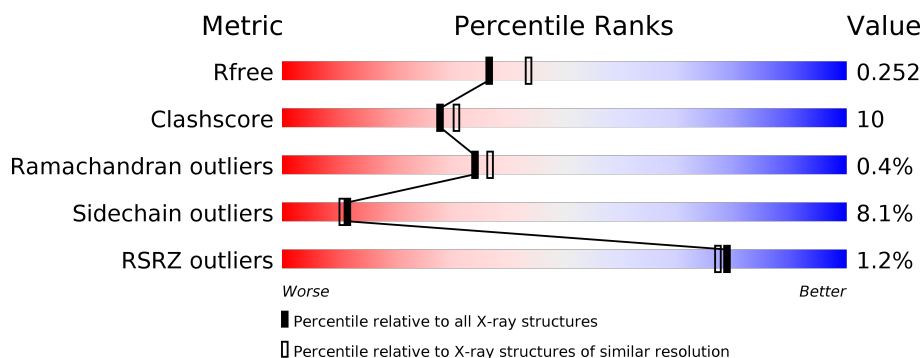
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	314	<div> <div>71%</div> <div>16%</div> <div>• • 9%</div> </div>
1	B	314	<div> <div>72%</div> <div>18%</div> <div>• 8%</div> </div>
1	C	314	<div> <div>%</div> <div>68%</div> <div>18%</div> <div>• 11%</div> </div>
1	D	314	<div> <div>3%</div> <div>71%</div> <div>18%</div> <div>• • 7%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9393 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 Prephenate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	293	Total	C	N	O	S	0	0	0
			2315	1495	382	430	8			
1	A	285	Total	C	N	O	S	0	0	0
			2239	1442	370	419	8			
1	B	290	Total	C	N	O	S	0	0	0
			2293	1481	379	425	8			
1	C	281	Total	C	N	O	S	0	0	0
			2215	1430	363	415	7			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	MET	-	EXPRESSION TAG	UNP O67636
D	-1	GLY	-	EXPRESSION TAG	UNP O67636
D	0	SER	-	EXPRESSION TAG	UNP O67636
D	1	SER	-	EXPRESSION TAG	UNP O67636
D	2	HIS	-	EXPRESSION TAG	UNP O67636
D	3	HIS	-	EXPRESSION TAG	UNP O67636
D	4	HIS	-	EXPRESSION TAG	UNP O67636
D	5	HIS	-	EXPRESSION TAG	UNP O67636
D	6	HIS	-	EXPRESSION TAG	UNP O67636
D	7	HIS	-	EXPRESSION TAG	UNP O67636
D	8	SER	-	EXPRESSION TAG	UNP O67636
D	9	SER	-	EXPRESSION TAG	UNP O67636
D	10	GLY	-	EXPRESSION TAG	UNP O67636
D	11	LEU	-	EXPRESSION TAG	UNP O67636
D	12	VAL	-	EXPRESSION TAG	UNP O67636
D	13	PRO	-	EXPRESSION TAG	UNP O67636
D	14	ARG	-	EXPRESSION TAG	UNP O67636
D	15	GLY	-	EXPRESSION TAG	UNP O67636
D	16	SER	-	EXPRESSION TAG	UNP O67636
D	17	HIS	-	EXPRESSION TAG	UNP O67636
D	18	MET	-	EXPRESSION TAG	UNP O67636

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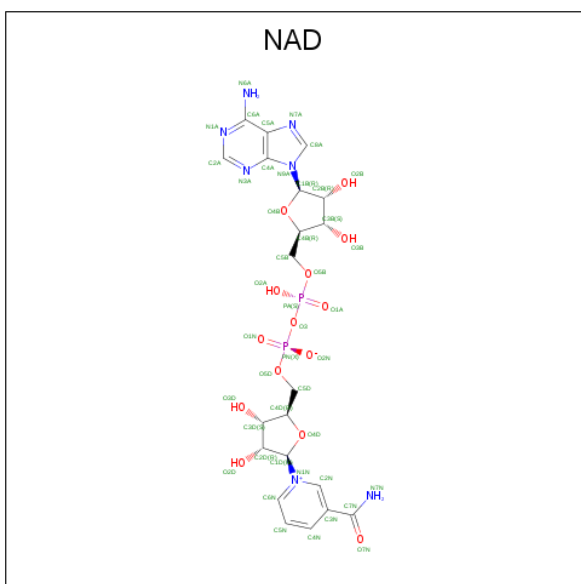
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP O67636
A	-1	GLY	-	EXPRESSION TAG	UNP O67636
A	0	SER	-	EXPRESSION TAG	UNP O67636
A	1	SER	-	EXPRESSION TAG	UNP O67636
A	2	HIS	-	EXPRESSION TAG	UNP O67636
A	3	HIS	-	EXPRESSION TAG	UNP O67636
A	4	HIS	-	EXPRESSION TAG	UNP O67636
A	5	HIS	-	EXPRESSION TAG	UNP O67636
A	6	HIS	-	EXPRESSION TAG	UNP O67636
A	7	HIS	-	EXPRESSION TAG	UNP O67636
A	8	SER	-	EXPRESSION TAG	UNP O67636
A	9	SER	-	EXPRESSION TAG	UNP O67636
A	10	GLY	-	EXPRESSION TAG	UNP O67636
A	11	LEU	-	EXPRESSION TAG	UNP O67636
A	12	VAL	-	EXPRESSION TAG	UNP O67636
A	13	PRO	-	EXPRESSION TAG	UNP O67636
A	14	ARG	-	EXPRESSION TAG	UNP O67636
A	15	GLY	-	EXPRESSION TAG	UNP O67636
A	16	SER	-	EXPRESSION TAG	UNP O67636
A	17	HIS	-	EXPRESSION TAG	UNP O67636
A	18	MET	-	EXPRESSION TAG	UNP O67636
B	-2	MET	-	EXPRESSION TAG	UNP O67636
B	-1	GLY	-	EXPRESSION TAG	UNP O67636
B	0	SER	-	EXPRESSION TAG	UNP O67636
B	1	SER	-	EXPRESSION TAG	UNP O67636
B	2	HIS	-	EXPRESSION TAG	UNP O67636
B	3	HIS	-	EXPRESSION TAG	UNP O67636
B	4	HIS	-	EXPRESSION TAG	UNP O67636
B	5	HIS	-	EXPRESSION TAG	UNP O67636
B	6	HIS	-	EXPRESSION TAG	UNP O67636
B	7	HIS	-	EXPRESSION TAG	UNP O67636
B	8	SER	-	EXPRESSION TAG	UNP O67636
B	9	SER	-	EXPRESSION TAG	UNP O67636
B	10	GLY	-	EXPRESSION TAG	UNP O67636
B	11	LEU	-	EXPRESSION TAG	UNP O67636
B	12	VAL	-	EXPRESSION TAG	UNP O67636
B	13	PRO	-	EXPRESSION TAG	UNP O67636
B	14	ARG	-	EXPRESSION TAG	UNP O67636
B	15	GLY	-	EXPRESSION TAG	UNP O67636
B	16	SER	-	EXPRESSION TAG	UNP O67636
B	17	HIS	-	EXPRESSION TAG	UNP O67636
B	18	MET	-	EXPRESSION TAG	UNP O67636

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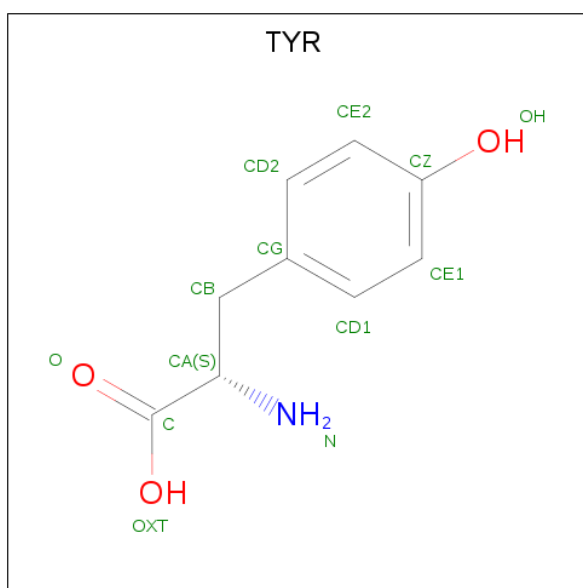
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C	-2	MET	-	EXPRESSION TAG	UNP O67636
C	-1	GLY	-	EXPRESSION TAG	UNP O67636
C	0	SER	-	EXPRESSION TAG	UNP O67636
C	1	SER	-	EXPRESSION TAG	UNP O67636
C	2	HIS	-	EXPRESSION TAG	UNP O67636
C	3	HIS	-	EXPRESSION TAG	UNP O67636
C	4	HIS	-	EXPRESSION TAG	UNP O67636
C	5	HIS	-	EXPRESSION TAG	UNP O67636
C	6	HIS	-	EXPRESSION TAG	UNP O67636
C	7	HIS	-	EXPRESSION TAG	UNP O67636
C	8	SER	-	EXPRESSION TAG	UNP O67636
C	9	SER	-	EXPRESSION TAG	UNP O67636
C	10	GLY	-	EXPRESSION TAG	UNP O67636
C	11	LEU	-	EXPRESSION TAG	UNP O67636
C	12	VAL	-	EXPRESSION TAG	UNP O67636
C	13	PRO	-	EXPRESSION TAG	UNP O67636
C	14	ARG	-	EXPRESSION TAG	UNP O67636
C	15	GLY	-	EXPRESSION TAG	UNP O67636
C	16	SER	-	EXPRESSION TAG	UNP O67636
C	17	HIS	-	EXPRESSION TAG	UNP O67636
C	18	MET	-	EXPRESSION TAG	UNP O67636

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



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

- Molecule 3 is TYROSINE (three-letter code: TYR) (formula: $C_9H_{11}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			12	9	1	2		
3	C	1	Total	C	N	O	0	0
			12	9	1	2		

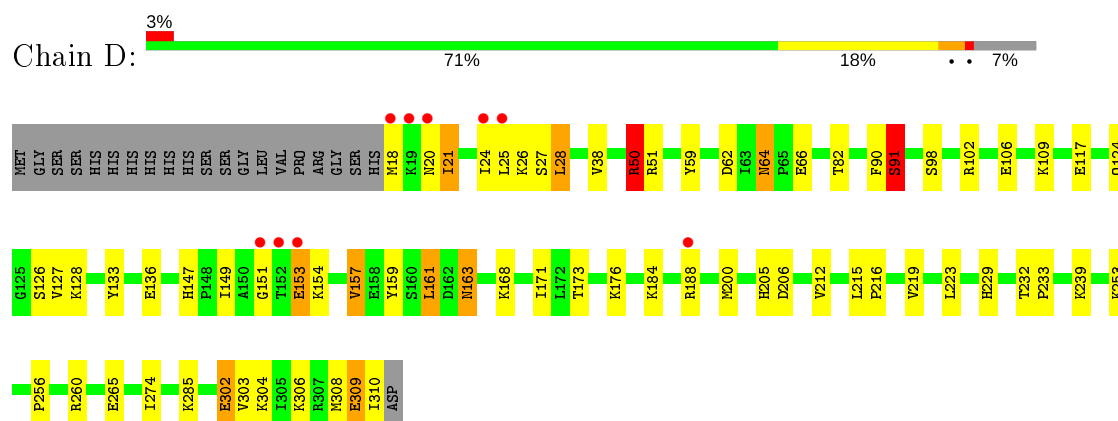
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	27	Total	O	0	0
			27	27		
4	A	29	Total	O	0	0
			29	29		
4	B	35	Total	O	0	0
			35	35		
4	C	40	Total	O	0	0
			40	40		

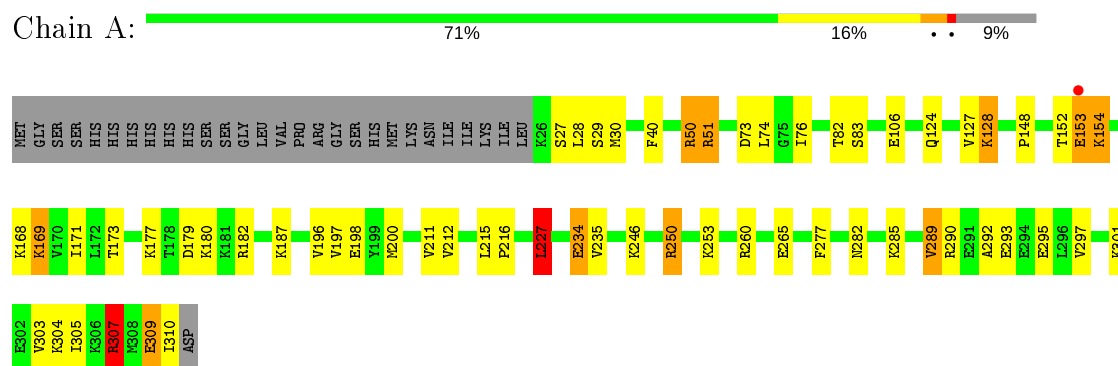
3 Residue-property plots [i](#)

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

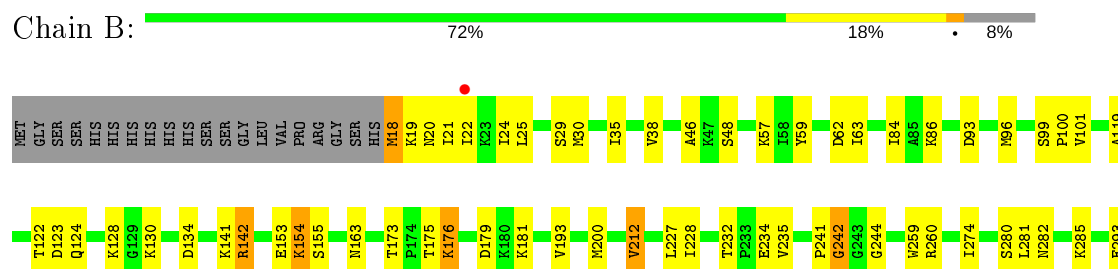
- Molecule 1: Prephenate dehydrogenase

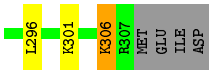


- Molecule 1: Prephenate dehydrogenase

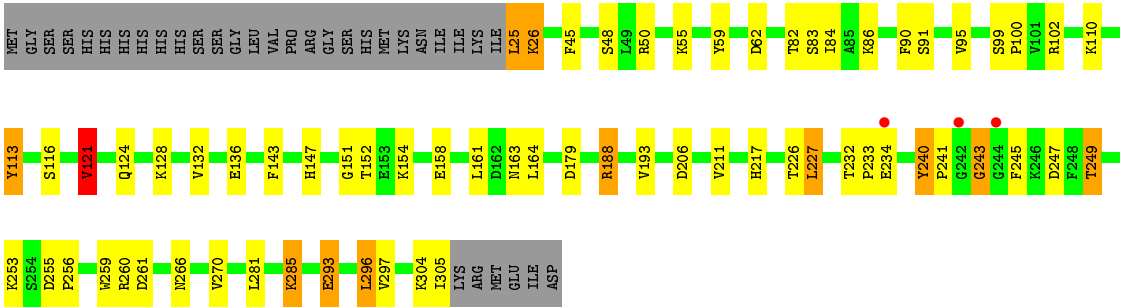


- Molecule 1: Prephenate dehydrogenase





● Molecule 1: Prephenate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.43 Å 93.69 Å 163.66 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.85 – 2.21 46.85 – 2.21	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.85-2.21) 98.9 (46.85-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.93 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.193 , 0.254 0.200 , 0.252	Depositor DCC
R_{free} test set	1913 reflections (3.10%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9393	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.02	3/2282 (0.1%)	0.95	3/3069 (0.1%)
1	B	0.99	0/2336	0.96	6/3141 (0.2%)
1	C	1.03	1/2258 (0.0%)	0.95	4/3040 (0.1%)
1	D	1.00	1/2358 (0.0%)	0.91	2/3171 (0.1%)
All	All	1.01	5/9234 (0.1%)	0.94	15/12421 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	290	ARG	CD-NE	7.54	1.59	1.46
1	C	45	PHE	CE2-CZ	5.55	1.47	1.37
1	A	303	VAL	CB-CG2	-5.38	1.41	1.52
1	A	106	GLU	CG-CD	5.33	1.59	1.51
1	D	302	GLU	CG-CD	5.27	1.59	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	ARG	NE-CZ-NH2	-11.20	114.70	120.30
1	A	307	ARG	NE-CZ-NH2	-8.65	115.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	D	50	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	C	240	TYR	N-CA-C	6.02	127.25	111.00
1	D	161	LEU	CA-CB-CG	5.86	128.78	115.30
1	A	234	GLU	CA-CB-CG	5.73	126.01	113.40
1	B	212	VAL	CG1-CB-CG2	5.61	119.87	110.90
1	B	134	ASP	CB-CG-OD1	5.45	123.21	118.30
1	C	227	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	227	LEU	CA-CB-CG	5.29	127.47	115.30
1	B	260	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	50	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	259	TRP	CA-CB-CG	-5.02	104.17	113.70
1	C	121	VAL	CG1-CB-CG2	5.02	118.93	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	242	GLY	Peptide
1	C	243	GLY	Peptide

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	2239	0	2277	58	0
1	B	2293	0	2366	55	0
1	C	2215	0	2266	54	0
1	D	2315	0	2385	48	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	2	0
2	D	44	0	26	2	0
3	B	12	0	8	0	0
3	C	12	0	8	3	0
4	A	29	0	0	1	0
4	B	35	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	40	0	0	0	0
4	D	27	0	0	5	0
All	All	9393	0	9414	185	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 10.

All (185) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:MET:HE1	1:B:123:ASP:C	1.63	1.18
1:B:96:MET:CE	1:B:123:ASP:HA	1.86	1.06
1:B:96:MET:HE1	1:B:123:ASP:CA	1.88	1.04
1:A:50:ARG:HH11	1:A:50:ARG:HG2	1.24	0.99
1:B:35:ILE:CD1	1:B:46:ALA:HB2	1.96	0.96
1:A:307:ARG:HD3	1:C:249:THR:HG23	1.47	0.95
1:B:96:MET:CE	1:B:123:ASP:CA	2.43	0.93
1:C:152:THR:HG23	1:C:154:LYS:H	1.34	0.93
1:B:21:ILE:HD12	1:B:21:ILE:H	1.35	0.91
1:A:250:ARG:NH1	1:A:253:LYS:HE2	1.87	0.89
1:A:307:ARG:CD	1:C:249:THR:HG23	2.02	0.89
1:A:187:LYS:HG3	1:A:197:VAL:HG21	1.55	0.89
1:A:307:ARG:HD3	1:C:249:THR:CG2	2.02	0.88
1:A:292:ALA:HB1	1:A:295:GLU:HG3	1.53	0.87
1:D:256:PRO:HG2	1:B:301:LYS:HD3	1.56	0.86
1:B:19:LYS:HB2	1:B:19:LYS:NZ	1.90	0.84
1:B:96:MET:HE3	1:B:123:ASP:HA	1.59	0.84
1:D:309:GLU:HB3	4:D:1009:HOH:O	1.77	0.83
1:A:307:ARG:CD	1:C:249:THR:CG2	2.56	0.82
1:B:35:ILE:HD13	1:B:46:ALA:HB2	1.67	0.76
1:D:50:ARG:HG3	1:D:50:ARG:HH11	1.49	0.76
1:A:227:LEU:HD22	1:C:211:VAL:HG12	1.67	0.76
1:B:96:MET:HE1	1:B:124:GLN:N	2.02	0.74
1:A:153:GLU:HG3	1:A:253:LYS:O	1.86	0.73
1:C:240:TYR:N	1:C:241:PRO:HD2	2.06	0.70
1:D:304:LYS:HG2	1:D:308:MET:HE2	1.74	0.70
1:A:292:ALA:HB1	1:A:295:GLU:CG	2.22	0.69
1:B:306:LYS:HA	1:B:306:LYS:HE2	1.73	0.69
1:B:21:ILE:H	1:B:21:ILE:CD1	2.05	0.69
1:B:281:LEU:O	1:B:285:LYS:HG3	1.93	0.69
1:D:147:HIS:ND1	1:D:205:HIS:HE1	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:LYS:HB2	1:B:19:LYS:HZ2	1.57	0.68
1:B:35:ILE:HD11	1:B:46:ALA:HB2	1.78	0.66
1:B:21:ILE:HD12	1:B:21:ILE:N	2.09	0.65
1:C:266:ASN:O	1:C:270:VAL:HG23	1.96	0.65
1:B:20:ASN:HB2	1:B:21:ILE:HD12	1.78	0.64
1:C:147:HIS:NE2	3:C:5959:TYR:OH	2.25	0.64
1:A:285:LYS:O	1:A:289:VAL:HG12	1.98	0.64
1:C:245:PHE:O	1:C:249:THR:HB	1.98	0.63
1:B:19:LYS:HB2	1:B:19:LYS:HZ3	1.64	0.63
1:B:241:PRO:O	1:B:242:GLY:C	2.36	0.63
1:B:119:ALA:O	1:B:142:ARG:HG2	1.98	0.63
1:A:260:ARG:HD3	1:C:293:GLU:HG3	1.80	0.63
2:C:5686:NAD:O7N	3:C:5959:TYR:N	2.32	0.62
1:A:250:ARG:HH12	1:A:253:LYS:HE2	1.64	0.62
1:A:297:VAL:HG23	1:C:260:ARG:HD3	1.81	0.62
1:B:96:MET:HE3	1:B:123:ASP:CA	2.21	0.62
1:C:151:GLY:HA2	1:C:164:LEU:HD11	1.82	0.61
1:D:188:ARG:HH11	1:D:188:ARG:HG3	1.64	0.61
1:B:18:MET:N	1:B:21:ILE:HD13	2.16	0.61
1:D:274:ILE:HG21	1:B:285:LYS:HD2	1.82	0.61
1:D:62:ASP:O	1:D:82:THR:HG22	2.01	0.61
1:A:297:VAL:O	1:A:301:LYS:HG2	2.01	0.60
1:D:153:GLU:HG2	1:D:253:LYS:HB3	1.83	0.60
1:D:163:ASN:H	1:D:163:ASN:HD22	1.48	0.60
1:A:50:ARG:HG2	1:A:50:ARG:NH1	2.05	0.60
1:B:141:LYS:HD2	1:B:179:ASP:HB2	1.84	0.59
1:C:241:PRO:HB3	1:C:245:PHE:HB3	1.84	0.59
1:C:240:TYR:H	1:C:241:PRO:HD2	1.68	0.59
1:A:40:PHE:CE1	1:A:154:LYS:HG3	2.38	0.58
1:D:59:TYR:CD2	1:D:90:PHE:HB3	2.37	0.58
1:D:256:PRO:CG	1:B:301:LYS:HD3	2.32	0.58
1:A:211:VAL:HG12	1:C:227:LEU:HD22	1.86	0.57
1:B:57:LYS:HD2	1:B:59:TYR:OH	2.04	0.57
1:D:38:VAL:HG12	1:D:157:VAL:HG11	1.87	0.56
1:D:304:LYS:HG2	1:D:308:MET:CE	2.35	0.56
1:A:169:LYS:HB2	1:A:169:LYS:HZ3	1.70	0.56
1:D:285:LYS:HD2	1:B:274:ILE:HG21	1.87	0.56
1:A:212:VAL:HG12	1:C:227:LEU:HD13	1.88	0.56
1:D:147:HIS:ND1	1:D:205:HIS:CE1	2.73	0.56
1:D:173:THR:HA	1:D:200:MET:O	2.06	0.56
1:A:152:THR:HG21	1:A:154:LYS:HE2	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:GLU:HB2	4:D:1053:HOH:O	2.05	0.55
1:D:127:VAL:HG21	1:D:265:GLU:HG2	1.89	0.55
1:A:187:LYS:CG	1:A:197:VAL:HG21	2.34	0.54
1:A:124:GLN:HE21	1:A:148:PRO:HG3	1.72	0.54
1:D:215:LEU:HB3	1:D:216:PRO:HD3	1.90	0.54
1:A:153:GLU:CG	1:A:253:LYS:O	2.54	0.53
1:D:98:SER:O	2:D:6686:NAD:H51N	2.09	0.53
1:D:117:GLU:HG2	4:D:1031:HOH:O	2.08	0.53
1:C:102:ARG:HD3	1:C:261:ASP:OD2	2.08	0.53
1:B:99:SER:HB2	1:B:100:PRO:HD2	1.91	0.52
1:B:282:ASN:ND2	4:B:1092:HOH:O	2.38	0.52
1:D:106:GLU:O	1:D:109:LYS:HB2	2.09	0.52
1:A:171:ILE:CG2	1:A:200:MET:HE2	2.40	0.52
1:A:171:ILE:HG21	1:A:200:MET:CE	2.40	0.52
1:D:229:HIS:HE1	1:B:280:SER:OG	1.93	0.52
1:A:307:ARG:HD2	1:C:249:THR:CG2	2.40	0.52
1:D:260:ARG:HG2	1:B:296:LEU:HD23	1.92	0.51
1:D:306:LYS:HD3	1:B:228:ILE:HG12	1.92	0.51
1:C:158:GLU:CD	1:C:158:GLU:H	2.14	0.51
1:A:307:ARG:CG	1:C:249:THR:HG23	2.40	0.51
1:B:99:SER:HB2	1:B:100:PRO:CD	2.40	0.51
1:C:304:LYS:HB2	1:C:305:ILE:HG12	1.92	0.51
1:D:304:LYS:HE2	1:D:308:MET:HE1	1.93	0.51
1:A:127:VAL:HG21	1:A:265:GLU:HG2	1.92	0.51
1:C:232:THR:HB	1:C:233:PRO:HD2	1.93	0.50
1:A:277:PHE:HA	1:C:226:THR:OG1	2.12	0.50
1:B:306:LYS:CE	1:B:306:LYS:HA	2.33	0.49
1:A:74:LEU:HB2	1:A:76:ILE:HG13	1.95	0.49
1:D:205:HIS:HD2	1:D:206:ASP:OD1	1.94	0.49
1:A:260:ARG:HG2	1:C:296:LEU:HD13	1.95	0.48
1:D:153:GLU:HG2	1:D:253:LYS:CB	2.42	0.48
1:A:282:ASN:HD22	1:A:285:LYS:HD3	1.78	0.48
1:A:173:THR:HA	1:A:200:MET:O	2.14	0.48
1:B:21:ILE:HA	1:B:24:ILE:HD12	1.94	0.48
1:A:171:ILE:HG21	1:A:200:MET:HE2	1.96	0.48
1:B:96:MET:HE3	1:B:122:THR:C	2.35	0.47
1:C:152:THR:O	3:C:5959:TYR:N	2.46	0.47
1:B:175:THR:HB	1:B:176:LYS:HZ3	1.79	0.47
1:A:153:GLU:CG	1:A:253:LYS:HB3	2.45	0.47
1:C:281:LEU:O	1:C:285:LYS:HG2	2.14	0.47
1:C:304:LYS:O	1:C:305:ILE:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:CD2	1:C:211:VAL:HG12	2.41	0.47
1:A:309:GLU:O	1:A:310:ILE:HB	2.15	0.47
1:A:293:GLU:OE2	1:C:102:ARG:NH2	2.46	0.46
1:A:51:ARG:HH11	1:A:51:ARG:CG	2.27	0.46
1:B:30:MET:HA	1:B:93:ASP:OD1	2.16	0.46
1:A:307:ARG:HD3	1:C:249:THR:HG22	1.93	0.46
1:A:227:LEU:HD22	1:C:211:VAL:CG1	2.41	0.46
1:C:255:ASP:HA	1:C:256:PRO:HD3	1.85	0.46
1:A:293:GLU:CD	1:C:102:ARG:HH22	2.19	0.45
1:C:132:VAL:O	1:C:136:GLU:HG3	2.16	0.45
1:A:27:SER:O	1:A:28:LEU:C	2.53	0.45
1:D:239:LYS:HB3	1:D:239:LYS:NZ	2.32	0.45
1:A:179:ASP:HB3	1:A:182:ARG:HB2	1.99	0.45
1:A:187:LYS:HE2	1:A:197:VAL:CG2	2.47	0.45
1:C:179:ASP:OD1	1:C:179:ASP:C	2.56	0.45
1:C:25:LEU:HB2	1:C:26:LYS:HD2	1.98	0.45
1:A:153:GLU:HA	1:A:153:GLU:OE1	2.17	0.45
1:D:274:ILE:HG21	1:B:285:LYS:CD	2.47	0.45
1:B:96:MET:HE3	1:B:122:THR:O	2.17	0.44
1:C:110:LYS:HA	1:C:113:TYR:CE1	2.52	0.44
1:D:24:ILE:HG13	1:D:28:LEU:HD22	1.99	0.44
1:A:305:ILE:O	1:A:309:GLU:HG2	2.16	0.44
1:A:51:ARG:HH11	1:A:51:ARG:HG2	1.83	0.44
1:B:18:MET:CE	1:B:22:ILE:CD1	2.96	0.44
1:A:304:LYS:HE2	1:C:253:LYS:O	2.16	0.44
1:D:124:GLN:O	2:D:6686:NAD:H6N	2.17	0.44
1:A:307:ARG:NH2	4:A:1030:HOH:O	2.50	0.44
1:A:215:LEU:HB3	1:A:216:PRO:HD3	1.99	0.43
1:C:188:ARG:O	1:C:188:ARG:HD3	2.17	0.43
1:B:48:SER:HB3	1:B:193:VAL:HB	2.00	0.43
1:D:154:LYS:HE3	1:D:159:TYR:CD2	2.54	0.43
1:D:310:ILE:CD1	4:D:1014:HOH:O	2.66	0.43
1:B:18:MET:O	1:B:22:ILE:HD12	2.17	0.43
1:D:163:ASN:N	1:D:163:ASN:HD22	2.06	0.43
1:D:90:PHE:O	1:D:91:SER:C	2.57	0.43
1:A:198:GLU:OE1	1:C:240:TYR:OH	2.31	0.42
1:D:64:ASN:ND2	1:D:66:GLU:H	2.17	0.42
1:D:310:ILE:HD11	4:D:1014:HOH:O	2.18	0.42
1:B:154:LYS:HD2	1:B:154:LYS:HA	1.78	0.42
1:B:96:MET:HE3	1:B:123:ASP:N	2.33	0.42
1:A:128:LYS:HA	1:A:128:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:VAL:HB	1:C:121:VAL:HB	2.01	0.42
1:D:149:ILE:HD11	1:D:171:ILE:HD12	2.01	0.42
1:B:155:SER:CB	4:B:1023:HOH:O	2.66	0.42
1:C:121:VAL:O	1:C:143:PHE:HA	2.20	0.42
1:A:307:ARG:HG3	1:C:249:THR:HG23	2.02	0.42
1:C:217:HIS:CE1	1:C:259:TRP:CZ2	3.08	0.42
1:D:229:HIS:CE1	1:B:280:SER:OG	2.72	0.42
1:B:86:LYS:HG3	1:B:86:LYS:O	2.20	0.42
1:D:163:ASN:N	1:D:163:ASN:ND2	2.67	0.42
1:A:50:ARG:HA	1:A:50:ARG:HD3	1.56	0.42
1:C:48:SER:HB3	1:C:193:VAL:HB	2.01	0.41
1:B:173:THR:HA	1:B:200:MET:O	2.21	0.41
1:A:50:ARG:HH11	1:A:50:ARG:CG	2.11	0.41
1:C:121:VAL:HG22	1:C:143:PHE:HD1	1.86	0.41
1:C:124:GLN:O	2:C:5686:NAD:H6N	2.21	0.41
1:B:29:SER:O	1:B:93:ASP:OD1	2.39	0.41
1:C:99:SER:HB2	1:C:100:PRO:HD2	2.03	0.41
1:C:243:GLY:O	1:C:247:ASP:OD2	2.39	0.41
1:D:310:ILE:HD13	1:D:310:ILE:HA	1.65	0.41
1:B:232:THR:OG1	1:B:234:GLU:HG2	2.21	0.41
1:B:38:VAL:N	1:B:62:ASP:OD1	2.49	0.41
1:C:206:ASP:HB3	1:C:266:ASN:HD21	1.85	0.41
1:D:21:ILE:HB	1:D:24:ILE:HG22	2.03	0.41
1:B:242:GLY:HA2	1:B:244:GLY:H	1.86	0.40
1:D:133:TYR:HA	1:D:136:GLU:HG2	2.03	0.40
1:C:59:TYR:CD2	1:C:90:PHE:HB3	2.55	0.40
1:C:232:THR:HB	1:C:233:PRO:CD	2.52	0.40
1:D:18:MET:O	1:D:21:ILE:HD13	2.21	0.40
1:D:232:THR:HB	1:D:233:PRO:CD	2.52	0.40
1:C:62:ASP:O	1:C:82:THR:HA	2.21	0.40
1:D:212:VAL:HG12	1:B:227:LEU:HD21	2.02	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	283/314 (90%)	273 (96%)	9 (3%)	1 (0%)	34	37
1	B	288/314 (92%)	274 (95%)	14 (5%)	0	100	100
1	C	279/314 (89%)	265 (95%)	14 (5%)	0	100	100
1	D	291/314 (93%)	272 (94%)	16 (6%)	3 (1%)	15	13
All	All	1141/1256 (91%)	1084 (95%)	53 (5%)	4 (0%)	34	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	151	GLY
1	A	29	SER
1	D	21	ILE
1	D	91	SER

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	245/275 (89%)	223 (91%)	22 (9%)	9	8
1	B	254/275 (92%)	238 (94%)	16 (6%)	18	19
1	C	245/275 (89%)	225 (92%)	20 (8%)	11	10
1	D	256/275 (93%)	233 (91%)	23 (9%)	9	8
All	All	1000/1100 (91%)	919 (92%)	81 (8%)	11	11

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	20	ASN
1	D	25	LEU
1	D	26	LYS
1	D	27	SER

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Mol	Chain	Res	Type
1	D	28	LEU
1	D	50	ARG
1	D	51	ARG
1	D	64	ASN
1	D	91	SER
1	D	102	ARG
1	D	126	SER
1	D	128	LYS
1	D	153	GLU
1	D	157	VAL
1	D	161	LEU
1	D	163	ASN
1	D	168	LYS
1	D	176	LYS
1	D	184	LYS
1	D	219	VAL
1	D	223	LEU
1	D	303	VAL
1	D	309	GLU
1	A	30	MET
1	A	50	ARG
1	A	51	ARG
1	A	73	ASP
1	A	82	THR
1	A	83	SER
1	A	128	LYS
1	A	153	GLU
1	A	154	LYS
1	A	168	LYS
1	A	169	LYS
1	A	177	LYS
1	A	180	LYS
1	A	196	VAL
1	A	227	LEU
1	A	234	GLU
1	A	235	VAL
1	A	246	LYS
1	A	250	ARG
1	A	289	VAL
1	A	307	ARG
1	A	309	GLU
1	B	18	MET

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Mol	Chain	Res	Type
1	B	25	LEU
1	B	63	ILE
1	B	84	ILE
1	B	101	VAL
1	B	128	LYS
1	B	130	LYS
1	B	153	GLU
1	B	154	LYS
1	B	163	ASN
1	B	176	LYS
1	B	181	LYS
1	B	212	VAL
1	B	235	VAL
1	B	293	GLU
1	B	306	LYS
1	C	25	LEU
1	C	26	LYS
1	C	55	LYS
1	C	83	SER
1	C	84	ILE
1	C	86	LYS
1	C	91	SER
1	C	113	TYR
1	C	116	SER
1	C	121	VAL
1	C	128	LYS
1	C	161	LEU
1	C	163	ASN
1	C	188	ARG
1	C	234	GLU
1	C	249	THR
1	C	285	LYS
1	C	293	GLU
1	C	296	LEU
1	C	297	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	20	ASN
1	D	64	ASN
1	D	124	GLN

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Mol	Chain	Res	Type
1	D	163	ASN
1	D	205	HIS
1	D	229	HIS
1	D	282	ASN
1	A	124	GLN
1	A	282	ASN
1	B	137	ASN
1	B	163	ASN
1	B	266	ASN
1	B	269	ASN
1	B	282	ASN
1	C	163	ASN
1	C	229	HIS
1	C	266	ASN
1	C	282	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	C	5686	-	42,48,48	1.78	8 (19%)	50,73,73	2.08	17 (34%)
2	NAD	B	4686	-	42,48,48	1.66	6 (14%)	50,73,73	2.12	10 (20%)
2	NAD	A	3686	-	42,48,48	2.02	7 (16%)	50,73,73	1.72	9 (18%)
2	NAD	D	6686	-	42,48,48	1.96	9 (21%)	50,73,73	2.18	10 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	C	5686	-	-	7/26/62/62	0/5/5/5
2	NAD	B	4686	-	-	7/26/62/62	0/5/5/5
2	NAD	A	3686	-	-	3/26/62/62	0/5/5/5
2	NAD	D	6686	-	-	4/26/62/62	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3686	NAD	O7N-C7N	8.84	1.41	1.24
2	D	6686	NAD	O7N-C7N	8.42	1.40	1.24
2	C	5686	NAD	O7N-C7N	6.93	1.37	1.24
2	B	4686	NAD	O7N-C7N	5.53	1.34	1.24
2	A	3686	NAD	C2A-N3A	4.19	1.38	1.32
2	D	6686	NAD	C2A-N3A	4.05	1.38	1.32
2	B	4686	NAD	C2A-N3A	3.97	1.38	1.32
2	A	3686	NAD	C2D-C1D	-3.49	1.48	1.53
2	C	5686	NAD	C2A-N1A	3.43	1.40	1.33
2	C	5686	NAD	C2A-N3A	3.41	1.37	1.32
2	D	6686	NAD	C7N-N7N	3.30	1.39	1.33
2	B	4686	NAD	C2A-N1A	3.05	1.39	1.33
2	D	6686	NAD	C2A-N1A	3.04	1.39	1.33
2	A	3686	NAD	O4D-C1D	2.94	1.45	1.41
2	A	3686	NAD	C2A-N1A	2.65	1.38	1.33
2	B	4686	NAD	C2N-N1N	2.53	1.38	1.35
2	D	6686	NAD	O4B-C1B	-2.47	1.37	1.41
2	D	6686	NAD	PA-O2A	-2.47	1.43	1.55
2	C	5686	NAD	O3B-C3B	2.44	1.48	1.43
2	B	4686	NAD	C6N-C5N	2.42	1.44	1.38
2	C	5686	NAD	C5B-C4B	2.28	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3686	NAD	PA-O2A	-2.24	1.44	1.55
2	C	5686	NAD	C4A-N3A	-2.22	1.32	1.35
2	C	5686	NAD	C2B-C1B	-2.20	1.50	1.53
2	B	4686	NAD	C2B-C1B	-2.20	1.50	1.53
2	D	6686	NAD	C8A-N7A	2.19	1.38	1.34
2	D	6686	NAD	C6N-N1N	2.14	1.40	1.35
2	A	3686	NAD	PN-O2N	-2.09	1.45	1.55
2	D	6686	NAD	C3N-C7N	2.06	1.53	1.50
2	C	5686	NAD	O4B-C1B	2.04	1.43	1.41

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3686	NAD	N3A-C2A-N1A	-7.53	116.92	128.68
2	B	4686	NAD	O7N-C7N-C3N	-7.41	110.77	119.63
2	D	6686	NAD	C3N-C7N-N7N	7.21	126.41	117.75
2	B	4686	NAD	N3A-C2A-N1A	-6.56	118.42	128.68
2	C	5686	NAD	N3A-C2A-N1A	-6.01	119.29	128.68
2	D	6686	NAD	O7N-C7N-C3N	-5.78	112.72	119.63
2	D	6686	NAD	N3A-C2A-N1A	-5.35	120.32	128.68
2	B	4686	NAD	C3N-C7N-N7N	5.30	124.11	117.75
2	C	5686	NAD	C3N-C7N-N7N	5.02	123.77	117.75
2	C	5686	NAD	O7N-C7N-C3N	-4.30	114.49	119.63
2	A	3686	NAD	PN-O3-PA	-4.22	118.34	132.83
2	D	6686	NAD	C4A-C5A-N7A	-4.01	105.22	109.40
2	D	6686	NAD	O4D-C1D-C2D	-3.98	101.11	106.93
2	C	5686	NAD	C4A-C5A-N7A	-3.80	105.44	109.40
2	B	4686	NAD	C5N-C4N-C3N	-3.77	115.88	120.34
2	C	5686	NAD	PN-O3-PA	-3.69	120.18	132.83
2	D	6686	NAD	PN-O3-PA	-3.61	120.42	132.83
2	C	5686	NAD	C6N-N1N-C2N	-3.57	118.72	121.97
2	B	4686	NAD	C2N-C3N-C4N	3.52	122.25	118.26
2	C	5686	NAD	O5B-PA-O1A	-3.47	95.50	109.07
2	B	4686	NAD	O4D-C1D-C2D	-3.43	101.92	106.93
2	A	3686	NAD	O3D-C3D-C4D	-3.34	101.39	111.05
2	A	3686	NAD	C3N-C7N-N7N	3.19	121.58	117.75
2	B	4686	NAD	PN-O3-PA	-3.15	122.02	132.83
2	D	6686	NAD	C1B-N9A-C4A	-3.11	121.18	126.64
2	C	5686	NAD	C2N-C3N-C4N	3.03	121.70	118.26
2	B	4686	NAD	C1B-N9A-C4A	-2.94	121.47	126.64
2	B	4686	NAD	C6N-N1N-C2N	-2.83	119.40	121.97
2	D	6686	NAD	O2B-C2B-C3B	2.69	120.51	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	6686	NAD	C5A-C6A-N6A	2.65	124.39	120.35
2	A	3686	NAD	C2A-N1A-C6A	2.63	123.25	118.75
2	A	3686	NAD	O3B-C3B-C4B	-2.54	103.71	111.05
2	A	3686	NAD	O2B-C2B-C1B	-2.46	101.77	110.85
2	B	4686	NAD	O2N-PN-O1N	2.41	124.14	112.24
2	C	5686	NAD	C1B-N9A-C4A	-2.40	122.42	126.64
2	C	5686	NAD	C5A-C6A-N6A	2.34	123.91	120.35
2	A	3686	NAD	O7N-C7N-N7N	-2.31	119.30	122.58
2	D	6686	NAD	C6N-N1N-C2N	-2.30	119.88	121.97
2	C	5686	NAD	O4B-C4B-C5B	-2.30	101.81	109.37
2	C	5686	NAD	O3B-C3B-C4B	2.29	117.68	111.05
2	C	5686	NAD	C2D-C3D-C4D	2.29	107.08	102.64
2	C	5686	NAD	C4N-C3N-C7N	-2.27	114.96	121.04
2	C	5686	NAD	C5N-C4N-C3N	-2.20	117.74	120.34
2	C	5686	NAD	O3D-C3D-C2D	-2.20	104.72	111.82
2	A	3686	NAD	O2A-PA-O1A	2.12	122.72	112.24
2	C	5686	NAD	O4D-C1D-C2D	-2.02	103.97	106.93

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	5686	NAD	C5D-O5D-PN-O1N
2	C	5686	NAD	O4D-C1D-N1N-C2N
2	C	5686	NAD	O4D-C1D-N1N-C6N
2	C	5686	NAD	C2D-C1D-N1N-C2N
2	C	5686	NAD	C2D-C1D-N1N-C6N
2	A	3686	NAD	O4D-C1D-N1N-C2N
2	A	3686	NAD	O4D-C1D-N1N-C6N
2	B	4686	NAD	C5D-O5D-PN-O1N
2	B	4686	NAD	O4D-C1D-N1N-C2N
2	B	4686	NAD	O4D-C1D-N1N-C6N
2	B	4686	NAD	C2D-C1D-N1N-C2N
2	B	4686	NAD	C2D-C1D-N1N-C6N
2	D	6686	NAD	O4D-C1D-N1N-C2N
2	D	6686	NAD	C3D-C4D-C5D-O5D
2	D	6686	NAD	O4D-C4D-C5D-O5D
2	C	5686	NAD	C5D-O5D-PN-O3
2	A	3686	NAD	O4B-C4B-C5B-O5B
2	B	4686	NAD	O4B-C4B-C5B-O5B
2	B	4686	NAD	C5D-O5D-PN-O3
2	C	5686	NAD	O4B-C4B-C5B-O5B

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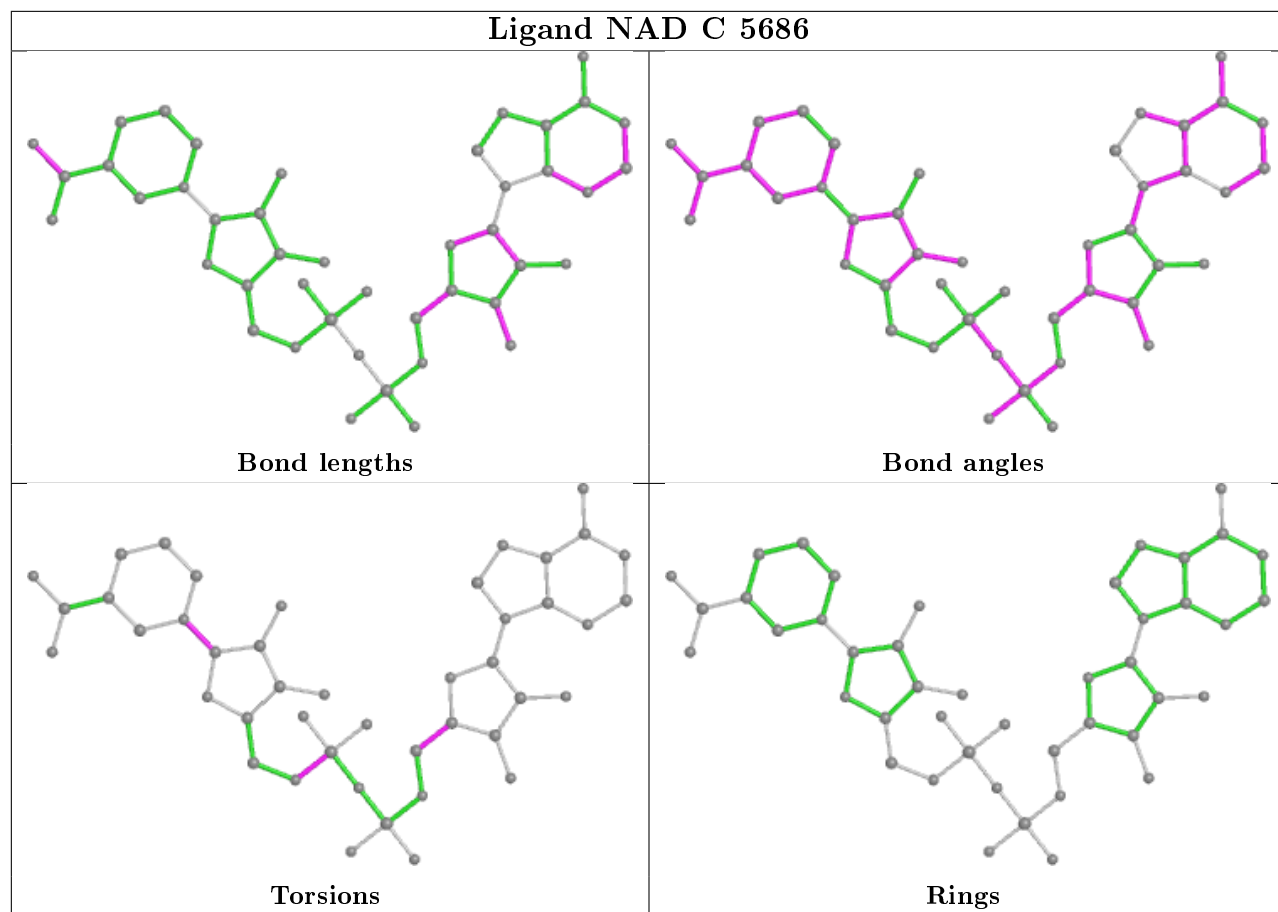
Mol	Chain	Res	Type	Atoms
2	D	6686	NAD	O4B-C4B-C5B-O5B

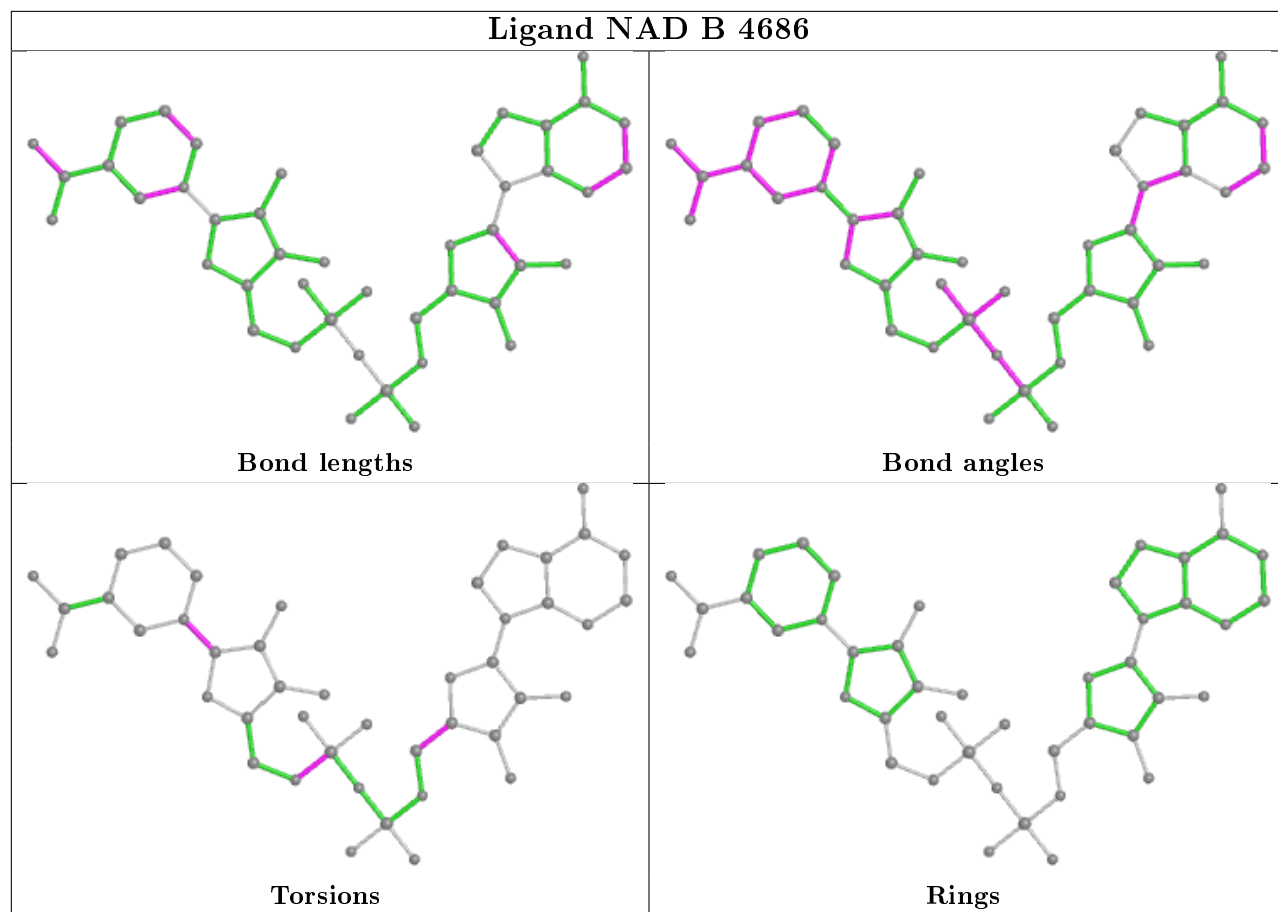
There are no ring outliers.

2 monomers are involved in 4 short contacts:

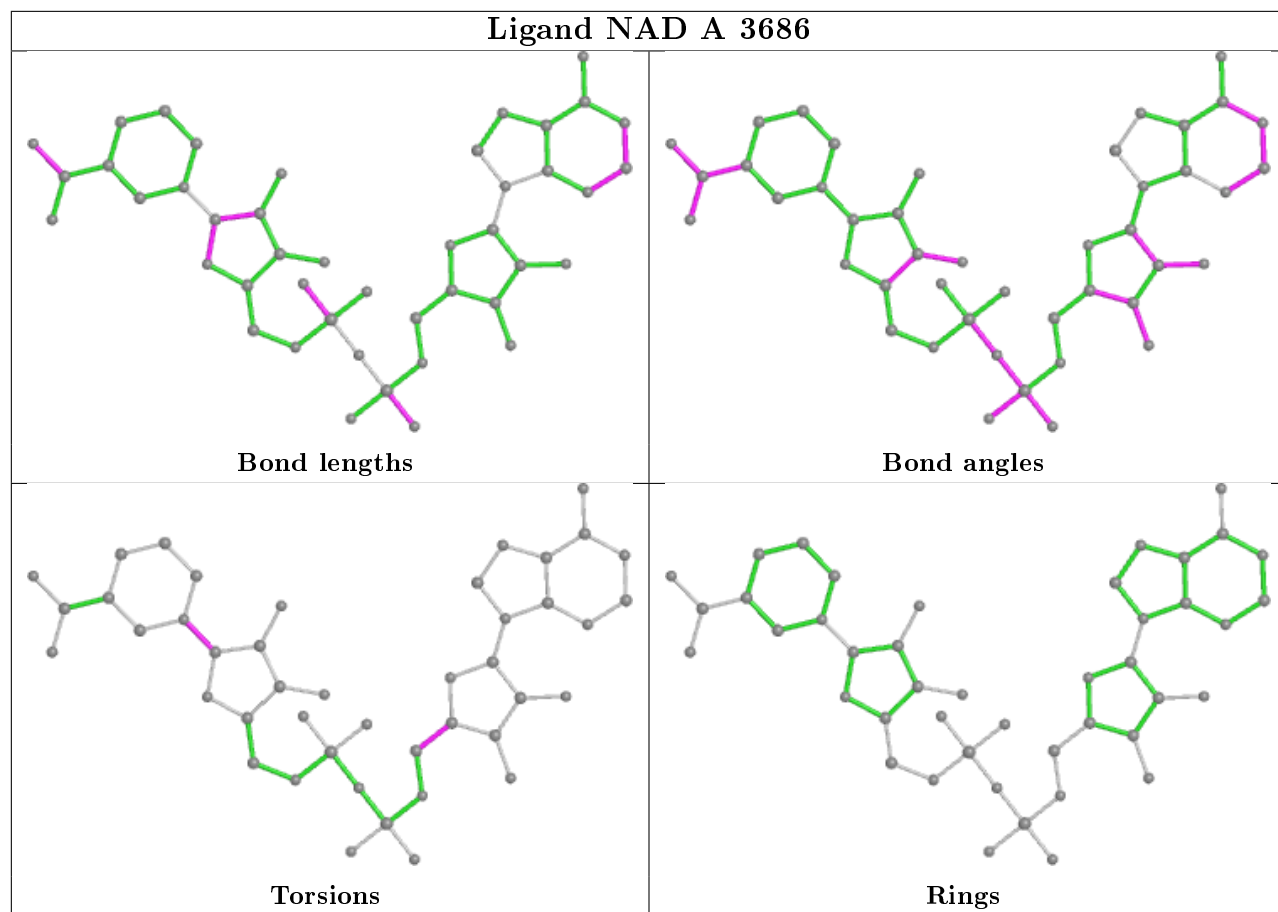
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	5686	NAD	2	0
2	D	6686	NAD	2	0

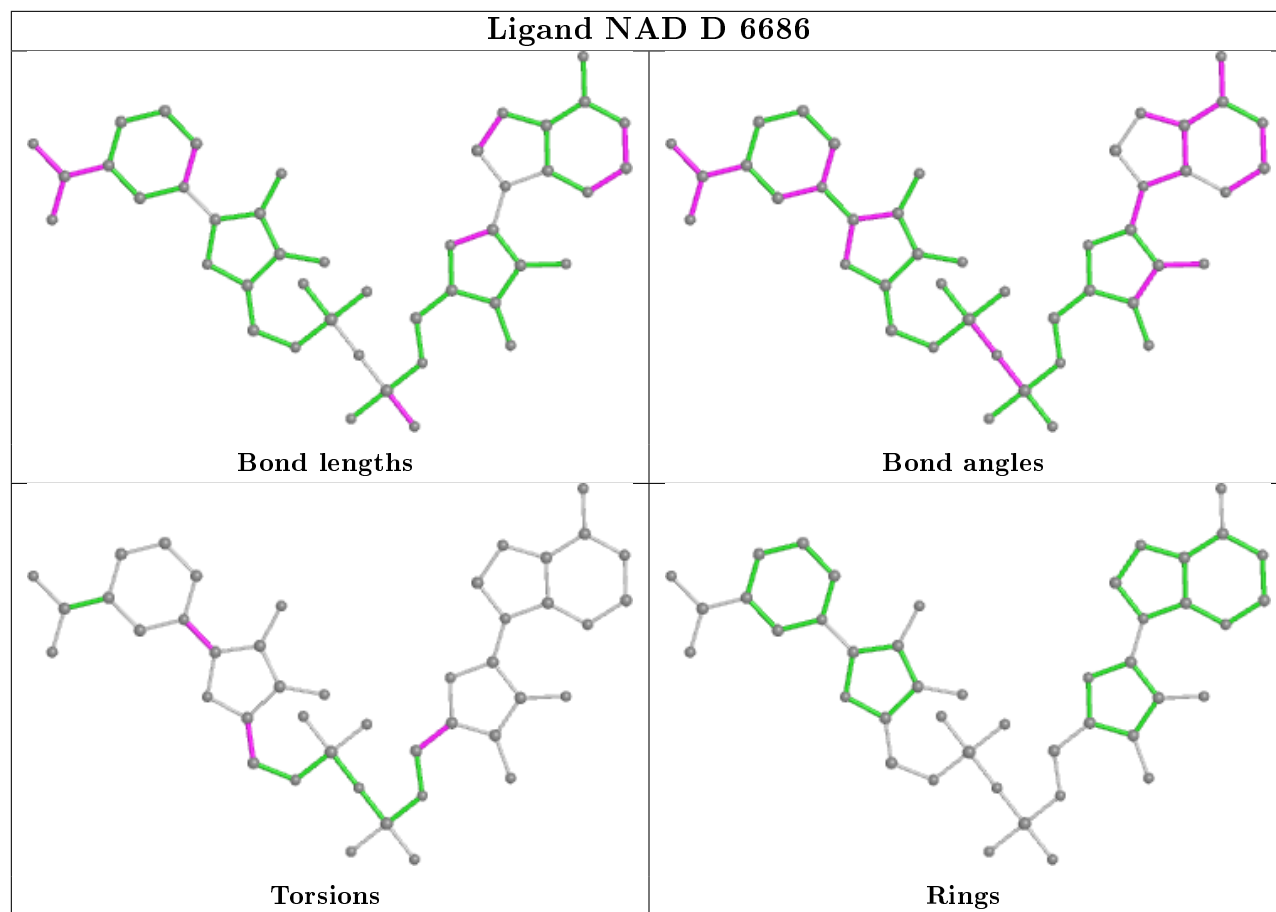
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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





Ligand NAD A 3686





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	285/314 (90%)	-0.38	1 (0%) 92 92	5, 16, 25, 38	0
1	B	290/314 (92%)	-0.41	1 (0%) 94 93	7, 16, 28, 36	0
1	C	281/314 (89%)	-0.44	3 (1%) 80 79	7, 13, 26, 41	0
1	D	293/314 (93%)	-0.28	9 (3%) 49 46	8, 15, 26, 44	0
All	All	1149/1256 (91%)	-0.38	14 (1%) 79 77	5, 15, 27, 44	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	153	GLU	4.2
1	D	152	THR	4.1
1	A	153	GLU	3.1
1	D	151	GLY	3.1
1	D	25	LEU	3.1
1	C	244	GLY	3.0
1	D	24	ILE	2.6
1	D	19	LYS	2.6
1	B	22	ILE	2.4
1	D	18	MET	2.4
1	D	20	ASN	2.1
1	C	242	GLY	2.2
1	D	188	ARG	2.1
1	C	234	GLU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

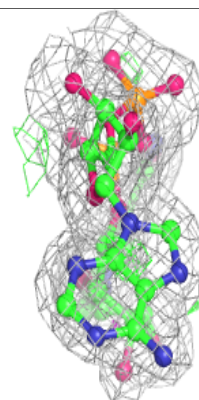
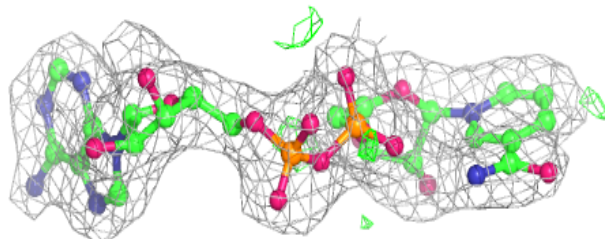
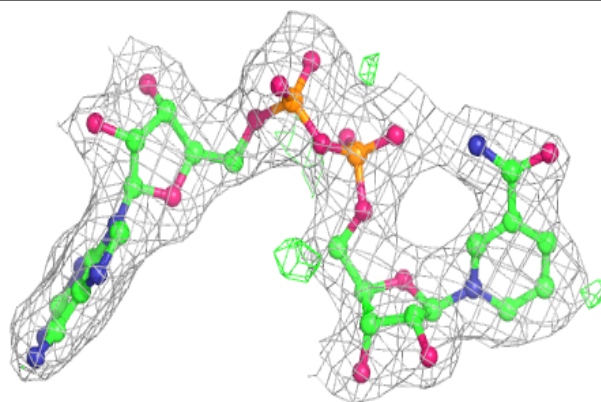
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	TYR	B	6959	12/13	0.90	0.12	26,32,36,36	0
3	TYR	C	5959	12/13	0.91	0.13	28,35,36,38	0
2	NAD	D	6686	44/44	0.96	0.10	31,38,42,44	0
2	NAD	B	4686	44/44	0.98	0.10	20,27,34,35	0
2	NAD	A	3686	44/44	0.98	0.09	25,32,38,43	0
2	NAD	C	5686	44/44	0.98	0.10	18,26,31,33	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.

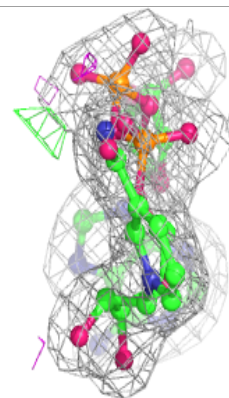
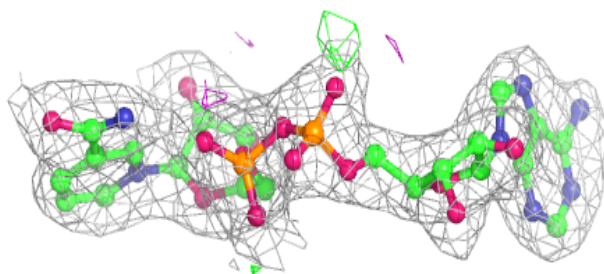
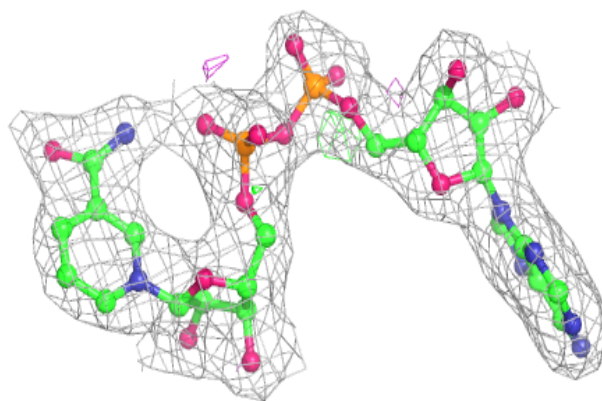
Electron density around NAD D 6686:

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

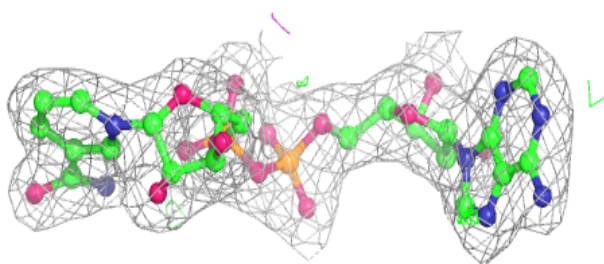
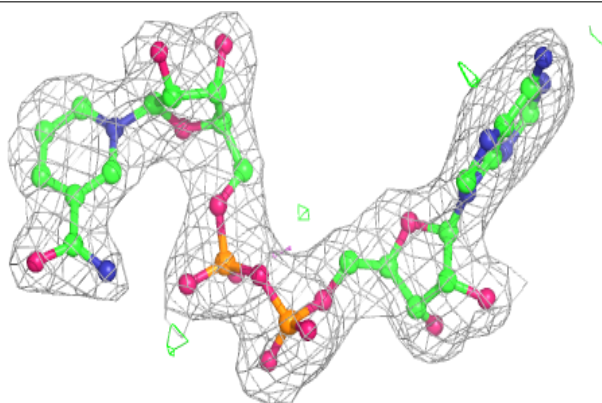


Electron density around NAD B 4686:

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

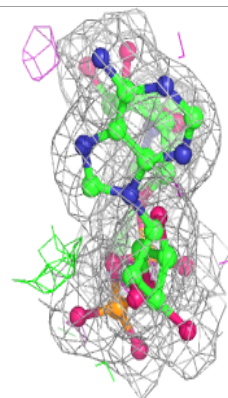
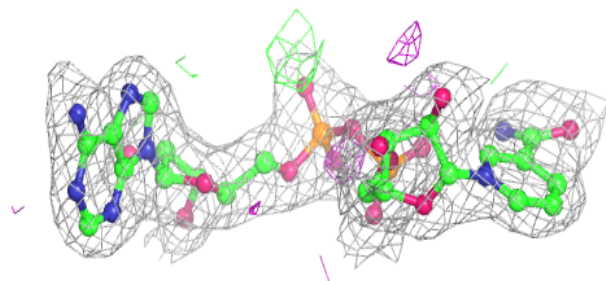
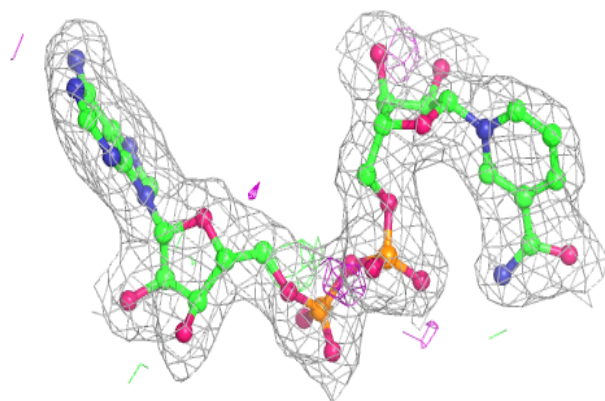
**Electron density around NAD A 3686:**

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



Electron density around NAD C 5686:

$2mF_o-DF_c$ (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.