



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 11:51 PM EDT

PDB ID : 1KYQ  
Title : Met8p: A bifunctional NAD-dependent dehydrogenase and ferrochelatase involved in siroheme synthesis.  
Authors : Schubert, H.L.; Raux, E.; Brindley, A.A.; Wilson, K.S.; Hill, C.P.; Warren, M.J.  
Deposited on : 2002-02-05  
Resolution : 2.20 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](mailto: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>.

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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	:	2.36.2
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)	:	2.36.2

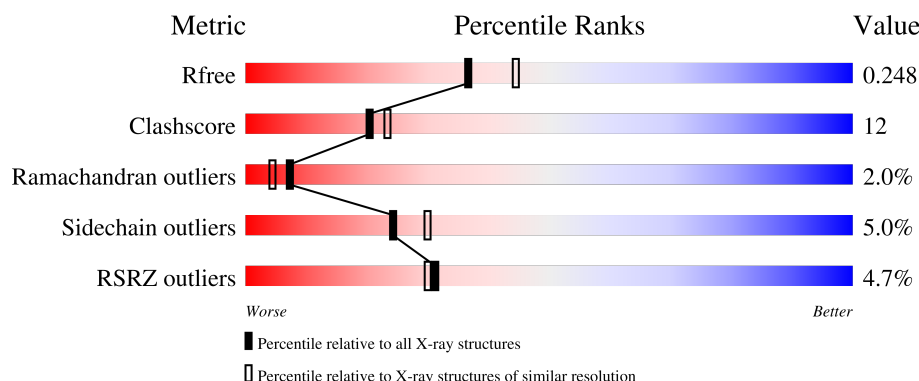
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	274	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>• •</div> </div> </div>
1	B	274	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>6%</div> <div>•</div> </div> </div>
1	C	274	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>• • •</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7289 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 Siroheme biosynthesis protein MET8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	Se	0	6	0
			2178	1392	385	387	8	6			
1	B	273	Total	C	N	O	S	Se	0	2	0
			2247	1430	394	409	8	6			
1	C	262	Total	C	N	O	S	Se	0	3	0
			2154	1375	378	387	8	6			

There are 27 discrepancies between the modelled and reference sequences:

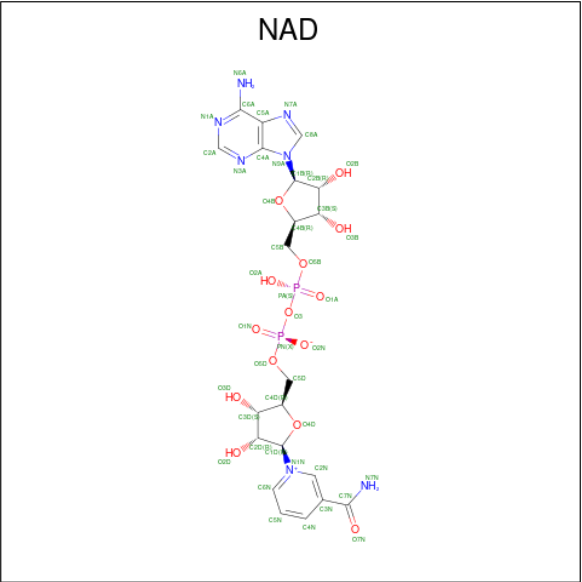
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P15807
A	15	ARG	LYS	SEE REMARK 999	UNP P15807
A	33	MSE	ILE	SEE REMARK 999	UNP P15807
A	61	LYS	GLU	SEE REMARK 999	UNP P15807
A	102	ASN	ASP	SEE REMARK 999	UNP P15807
A	111	MSE	MET	MODIFIED RESIDUE	UNP P15807
A	188	MSE	MET	MODIFIED RESIDUE	UNP P15807
A	221	MSE	MET	MODIFIED RESIDUE	UNP P15807
A	251	MSE	MET	MODIFIED RESIDUE	UNP P15807
B	1	MSE	MET	MODIFIED RESIDUE	UNP P15807
B	15	ARG	LYS	SEE REMARK 999	UNP P15807
B	33	MSE	ILE	SEE REMARK 999	UNP P15807
B	61	LYS	GLU	SEE REMARK 999	UNP P15807
B	102	ASN	ASP	SEE REMARK 999	UNP P15807
B	111	MSE	MET	MODIFIED RESIDUE	UNP P15807
B	188	MSE	MET	MODIFIED RESIDUE	UNP P15807
B	221	MSE	MET	MODIFIED RESIDUE	UNP P15807
B	251	MSE	MET	MODIFIED RESIDUE	UNP P15807
C	1	MSE	MET	MODIFIED RESIDUE	UNP P15807
C	15	ARG	LYS	SEE REMARK 999	UNP P15807
C	33	MSE	ILE	SEE REMARK 999	UNP P15807
C	61	LYS	GLU	SEE REMARK 999	UNP P15807
C	102	ASN	ASP	SEE REMARK 999	UNP P15807

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Chain	Residue	Modelled	Actual	Comment	Reference
C	111	MSE	MET	MODIFIED RESIDUE	UNP P15807
C	188	MSE	MET	MODIFIED RESIDUE	UNP P15807
C	221	MSE	MET	MODIFIED RESIDUE	UNP P15807
C	251	MSE	MET	MODIFIED RESIDUE	UNP P15807

- 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	A	1	Total	C	N	O	P	0	0
			26	10	5	9	2		
2	B	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
2	C	1	Total	C	N	O	P	0	0
			35	15	5	13	2		

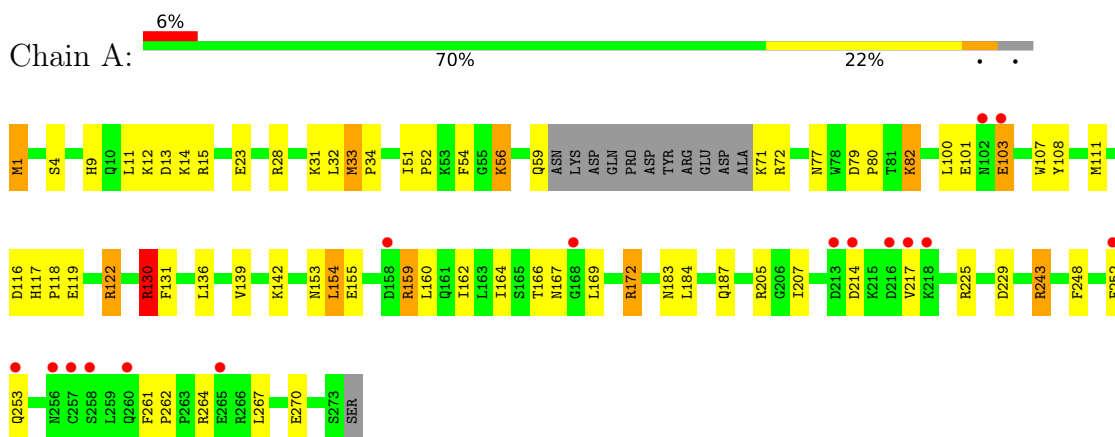
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	174	Total	O	0	0
			174	174		
3	B	229	Total	O	0	0
			229	229		
3	C	211	Total	O	0	0
			211	211		

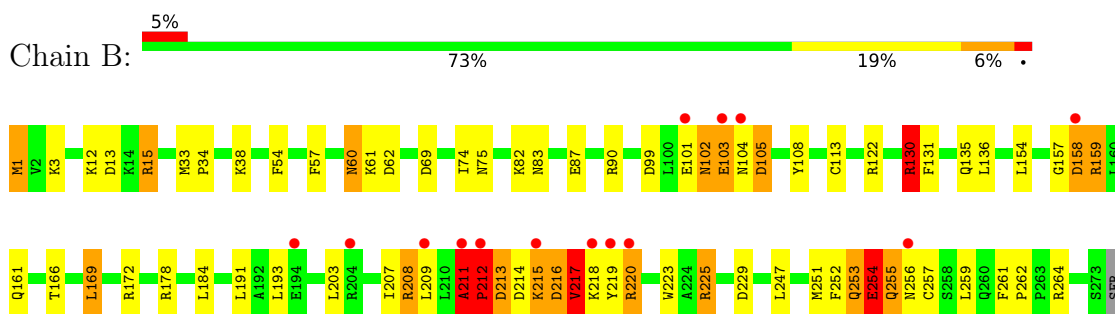
### 3 Residue-property plots [i](#)

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.

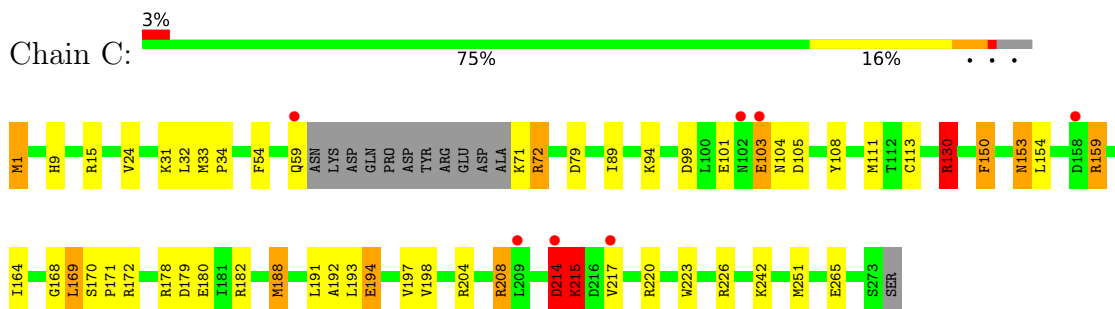
- Molecule 1: Siroheme biosynthesis protein MET8



- Molecule 1: Siroheme biosynthesis protein MET8



- Molecule 1: Siroheme biosynthesis protein MET8



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.99Å 80.86Å 103.97Å 90.00° 121.88° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.81 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.20) 73.8 (29.81-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 1.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.219 , 0.283 0.198 , 0.248	Depositor DCC
$R_{free}$ test set	2818 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 60.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7289	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.55	1/2248 (0.0%)	1.29	20/3019 (0.7%)
1	B	0.47	0/2298	1.44	30/3090 (1.0%)
1	C	0.51	1/2210 (0.0%)	1.25	21/2968 (0.7%)
All	All	0.51	2/6756 (0.0%)	1.33	71/9077 (0.8%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	MSE	SE-CE	16.66	2.93	1.95
1	C	1	MSE	SE-CE	11.85	2.65	1.95

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	ARG	NE-CZ-NH1	-16.57	112.01	120.30
1	A	122[A]	ARG	NE-CZ-NH1	-15.60	112.50	120.30
1	A	122[B]	ARG	NE-CZ-NH1	-15.60	112.50	120.30
1	A	1	MSE	CG-SE-CE	-14.84	66.25	98.90
1	B	220	ARG	NE-CZ-NH2	13.72	127.16	120.30
1	B	130	ARG	CD-NE-CZ	13.07	141.91	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	212	PRO	C-N-CA	12.88	153.89	121.70
1	C	130	ARG	NE-CZ-NH2	-12.72	113.94	120.30
1	B	130	ARG	NE-CZ-NH2	-11.80	114.40	120.30
1	C	1	MSE	CG-SE-CE	-11.65	73.28	98.90
1	B	212	PRO	CB-CA-C	11.62	141.04	112.00
1	B	212	PRO	CA-C-O	11.48	147.76	120.20
1	A	122[A]	ARG	NE-CZ-NH2	10.51	125.55	120.30
1	A	122[B]	ARG	NE-CZ-NH2	10.51	125.55	120.30
1	C	204	ARG	CD-NE-CZ	9.92	137.49	123.60
1	C	130	ARG	CD-NE-CZ	9.50	136.90	123.60
1	B	217	VAL	CA-C-O	8.96	138.91	120.10
1	B	217	VAL	C-N-CA	8.89	143.92	121.70
1	B	122	ARG	NE-CZ-NH1	-8.50	116.05	120.30
1	C	15	ARG	NE-CZ-NH2	-8.49	116.05	120.30
1	A	122[A]	ARG	CB-CG-CD	8.49	133.66	111.60
1	A	122[B]	ARG	CB-CG-CD	8.49	133.66	111.60
1	C	105	ASP	N-CA-CB	-8.27	95.71	110.60
1	B	212	PRO	CA-C-N	-8.19	99.19	117.20
1	A	130[A]	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	A	130[B]	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	B	264	ARG	CD-NE-CZ	7.86	134.61	123.60
1	B	211	ALA	N-CA-CB	7.83	121.06	110.10
1	A	130[A]	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	A	130[B]	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	B	15	ARG	NE-CZ-NH2	7.68	124.14	120.30
1	C	204	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	B	159	ARG	CD-NE-CZ	7.36	133.90	123.60
1	B	130	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	B	211	ALA	CB-CA-C	-7.12	99.42	110.10
1	C	15	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	B	212	PRO	CA-N-CD	-6.94	101.78	111.50
1	B	172	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	C	130	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	1	MSE	CG-SE-CE	-6.58	84.42	98.90
1	B	225	ARG	CD-NE-CZ	6.31	132.43	123.60
1	C	153	ASN	CB-CA-C	-6.20	97.99	110.40
1	C	169	LEU	N-CA-CB	6.07	122.53	110.40
1	B	212	PRO	O-C-N	-6.05	113.03	122.70
1	C	104	ASN	N-CA-CB	-5.96	99.88	110.60
1	C	188	MSE	CA-CB-CG	5.93	123.37	113.30
1	A	15	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	90	ARG	NE-CZ-NH2	-5.84	117.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	LEU	CA-CB-CG	5.83	128.71	115.30
1	C	150	PHE	CA-C-N	5.82	127.84	116.20
1	B	178	ARG	CD-NE-CZ	5.64	131.50	123.60
1	A	264	ARG	CD-NE-CZ	5.59	131.43	123.60
1	B	15	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	C	214	ASP	N-CA-CB	5.58	120.64	110.60
1	C	226	ARG	NE-CZ-NH2	5.57	123.09	120.30
1	A	33	MSE	CA-CB-CG	5.55	122.73	113.30
1	A	243	ARG	CD-NE-CZ	5.52	131.33	123.60
1	C	104	ASN	C-N-CA	5.51	135.49	121.70
1	C	72	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	69	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	72	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	28	ARG	CG-CD-NE	5.20	122.72	111.80
1	A	130[A]	ARG	CD-NE-CZ	5.20	130.88	123.60
1	A	130[B]	ARG	CD-NE-CZ	5.20	130.88	123.60
1	C	104	ASN	CA-C-O	5.18	130.98	120.10
1	B	217	VAL	CA-C-N	-5.13	105.92	117.20
1	B	212	PRO	N-CA-CB	-5.12	96.97	102.60
1	B	169	LEU	N-CA-CB	5.09	120.58	110.40
1	A	1	MSE	CA-CB-CG	5.04	121.86	113.30
1	C	226	ARG	CD-NE-CZ	5.01	130.61	123.60
1	C	103	GLU	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	211	ALA	Mainchain
1	C	153	ASN	Mainchain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2178	0	2198	72	0
1	B	2247	0	2251	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2154	0	2169	39	0
2	A	26	0	12	0	0
2	B	35	0	19	0	0
2	C	35	0	19	2	0
3	A	174	0	0	2	0
3	B	229	0	0	1	0
3	C	211	0	0	2	0
All	All	7289	0	6668	166	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 12.

All (166) 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:1:MSE:CE	1:B:1:MSE:SE	2.23	1.36
1:C:1:MSE:SE	1:C:1:MSE:CE	2.65	0.94
1:B:214:ASP:O	1:B:215:LYS:HB2	1.67	0.91
1:A:167:ASN:HD21	1:B:161:GLN:HE21	0.93	0.90
1:A:167:ASN:ND2	1:B:161:GLN:HE21	1.72	0.87
1:C:214:ASP:O	1:C:215:LYS:HB3	1.77	0.84
1:A:31:LYS:HE2	1:A:153:ASN:HD21	1.43	0.84
1:A:14[A]:LYS:HE2	1:A:108[A]:TYR:CE2	2.15	0.82
1:B:217:VAL:HG22	1:B:220:ARG:HG3	1.60	0.81
1:A:4:SER:H	1:B:161:GLN:HE22	1.28	0.81
1:C:194:GLU:HA	1:C:197:VAL:HB	1.63	0.80
1:C:32:LEU:HD11	1:C:111:MSE:HE1	1.63	0.79
1:A:119:GLU:CD	1:A:122[A]:ARG:HH12	1.86	0.78
1:A:1:MSE:CE	1:A:1:MSE:HG3	2.14	0.78
1:A:11:LEU:HA	1:A:14[A]:LYS:HD2	1.67	0.77
1:A:167:ASN:HD21	1:B:161:GLN:NE2	1.77	0.76
1:A:32:LEU:HD11	1:A:111:MSE:HE1	1.67	0.75
1:B:212:PRO:HB2	1:B:252:PHE:HZ	1.52	0.74
1:B:208:ARG:NE	1:B:220:ARG:HH12	1.85	0.74
1:B:247:LEU:O	1:B:251:MSE:HG3	1.88	0.73
1:B:208:ARG:CZ	1:B:220:ARG:HH12	2.04	0.70
1:A:9:HIS:HD1	1:A:108[B]:TYR:HH	1.34	0.70
1:C:1:MSE:CE	1:C:1:MSE:HG3	2.21	0.69
1:A:31:LYS:HE2	1:A:153:ASN:ND2	2.08	0.67
1:B:212:PRO:HB2	1:B:252:PHE:CZ	2.29	0.67
1:B:217:VAL:CG2	1:B:220:ARG:HE	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MSE:CE	1:A:1:MSE:SE	2.93	0.66
1:B:101:GLU:O	1:B:102:ASN:HB2	1.96	0.66
1:A:14[A]:LYS:HE2	1:A:108[A]:TYR:CD2	2.31	0.66
1:A:119:GLU:OE2	1:A:122[A]:ARG:NH1	2.29	0.64
1:B:101:GLU:O	1:B:102:ASN:CB	2.46	0.62
1:A:1:MSE:CE	1:A:1:MSE:CG	2.78	0.61
1:A:166:THR:HB	1:A:169:LEU:HB2	1.81	0.61
1:C:1:MSE:CE	1:C:1:MSE:CG	2.79	0.61
1:B:1:MSE:CE	1:B:1:MSE:CG	2.79	0.60
1:A:32:LEU:CD1	1:A:111:MSE:HE1	2.31	0.60
1:A:167:ASN:O	1:B:159:ARG:HG2	2.02	0.60
1:B:60:ASN:ND2	1:B:62:ASP:H	1.99	0.60
1:A:100:LEU:HB2	1:A:103:GLU:OE2	2.02	0.59
1:A:139:VAL:HG12	1:A:142:LYS:HG3	1.84	0.59
1:B:217:VAL:HG22	1:B:220:ARG:HE	1.67	0.59
1:C:214:ASP:HA	1:C:217:VAL:HG23	1.85	0.59
1:A:139:VAL:CG1	1:A:142:LYS:HG3	2.33	0.59
1:A:136:LEU:HD21	1:B:108:TYR:OH	2.03	0.58
1:C:99:ASP:OD1	1:C:130:ARG:NH2	2.34	0.58
1:A:262:PRO:HG2	1:A:267:LEU:HD13	1.86	0.57
1:B:213:ASP:O	1:B:217:VAL:HB	2.04	0.57
1:B:253:GLN:O	1:B:255:GLN:N	2.38	0.56
1:A:117[B]:HIS:CE1	1:A:142:LYS:HD3	2.40	0.56
1:A:130[A]:ARG:HH11	1:A:130[A]:ARG:HG3	1.69	0.56
1:B:251:MSE:HE1	1:B:261:PHE:HA	1.87	0.56
1:A:160:LEU:HD23	1:B:166:THR:HG22	1.88	0.56
1:B:214:ASP:O	1:B:215:LYS:CB	2.45	0.55
1:C:108:TYR:HB2	3:C:878:HOH:O	2.06	0.55
1:B:217:VAL:HG22	1:B:220:ARG:CG	2.33	0.54
1:C:24:VAL:HG21	2:C:802:NAD:H4D	1.88	0.54
1:A:79:ASP:HB2	1:A:80:PRO:HD2	1.90	0.54
1:A:117[A]:HIS:HB2	1:A:118:PRO:HD3	1.88	0.54
1:B:261:PHE:HB3	1:B:262:PRO:HD2	1.89	0.54
1:B:217:VAL:CG1	1:B:220:ARG:HH21	2.21	0.54
1:A:51:ILE:HB	1:A:52:PRO:HD3	1.89	0.54
1:A:172:ARG:NH1	1:B:229:ASP:OD1	2.35	0.54
1:A:155:GLU:OE2	1:B:3:LYS:HE2	2.08	0.53
1:B:1:MSE:HE3	1:B:1:MSE:HB2	1.91	0.53
1:A:108[B]:TYR:OH	1:B:136:LEU:HD21	2.09	0.52
1:C:193:LEU:O	1:C:194:GLU:CB	2.53	0.52
1:B:99:ASP:OD1	1:B:130:ARG:NH2	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ARG:HG2	1:C:89:ILE:HG12	1.91	0.52
1:A:79:ASP:HB2	1:A:80:PRO:CD	2.39	0.52
1:A:4:SER:N	1:B:161:GLN:HE22	2.01	0.51
1:A:261:PHE:HB3	1:A:262:PRO:HD2	1.92	0.51
1:B:203:LEU:HG	1:B:207:ILE:HD11	1.91	0.51
1:B:217:VAL:CG1	1:B:220:ARG:HE	2.24	0.51
1:A:12:LYS:O	1:A:13:ASP:HB2	2.11	0.50
1:A:130[A]:ARG:HG3	1:A:130[A]:ARG:NH1	2.27	0.49
1:A:207:ILE:HG23	1:A:248:PHE:CZ	2.47	0.49
1:C:32:LEU:HD11	1:C:111:MSE:CE	2.36	0.49
1:A:9:HIS:ND1	1:A:108[B]:TYR:OH	2.28	0.49
1:B:208:ARG:HA	1:B:211:ALA:HB2	1.95	0.49
1:B:217:VAL:HG22	1:B:220:ARG:NE	2.26	0.49
1:B:103:GLU:OE2	1:B:103:GLU:HA	2.13	0.49
1:A:117[B]:HIS:ND1	1:A:142:LYS:HD3	2.27	0.49
1:B:212:PRO:O	1:B:216:ASP:OD1	2.31	0.48
1:B:219:TYR:CE1	1:B:259:LEU:HD13	2.48	0.48
1:A:243:ARG:HD3	3:A:901:HOH:O	2.14	0.48
1:C:193:LEU:O	1:C:194:GLU:HB3	2.14	0.47
1:A:243:ARG:NH1	1:A:270:GLU:O	2.44	0.47
1:C:31:LYS:HD3	1:C:150:PHE:CD2	2.49	0.47
1:A:103:GLU:OE2	1:A:103:GLU:HA	2.15	0.47
1:A:116:ASP:OD1	1:A:118:PRO:HD2	2.14	0.47
1:B:208:ARG:CD	1:B:220:ARG:HH12	2.27	0.47
1:A:136:LEU:CD2	1:B:108:TYR:OH	2.62	0.46
1:A:159:ARG:CG	1:B:169:LEU:HG	2.45	0.46
1:B:131:PHE:CB	1:B:135:GLN:HE21	2.29	0.46
1:C:170:SER:HB2	1:C:171:PRO:HD2	1.97	0.46
1:A:205:ARG:NH2	1:C:72:ARG:HD2	2.30	0.46
1:C:217:VAL:HG22	1:C:220:ARG:NH1	2.30	0.46
1:C:71:LYS:NZ	1:C:94:LYS:NZ	2.63	0.46
1:A:214:ASP:O	1:A:217:VAL:HG23	2.16	0.46
1:A:11:LEU:HD22	1:A:108[B]:TYR:CD2	2.51	0.46
1:A:56:LYS:HA	1:A:56:LYS:HD2	1.79	0.46
1:A:183[A]:ASN:OD1	1:A:187:GLN:NE2	2.48	0.46
1:C:179:ASP:OD1	1:C:182[B]:ARG:NH1	2.49	0.46
1:A:101:GLU:OE2	1:C:208:ARG:HD3	2.16	0.45
1:B:12:LYS:O	1:B:13:ASP:HB2	2.17	0.45
1:B:217:VAL:HG13	1:B:220:ARG:HE	1.80	0.45
1:A:154:LEU:HD23	1:A:162:ILE:HB	1.98	0.45
1:A:11:LEU:HD22	1:A:108[B]:TYR:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14[A]:LYS:HB3	1:A:108[A]:TYR:CD1	2.52	0.45
1:B:74:ILE:HD13	1:B:87:GLU:HG3	1.98	0.45
1:B:33:MSE:HG3	1:B:54:PHE:CD2	2.51	0.45
1:B:191:LEU:HB2	1:B:193:LEU:HD22	1.99	0.45
1:B:207:ILE:O	1:B:211:ALA:HA	2.17	0.44
1:C:168:GLY:O	1:C:169:LEU:HD23	2.17	0.44
1:B:15:ARG:HD3	1:B:38:LYS:HD3	1.99	0.44
1:B:208:ARG:HG3	1:B:220:ARG:NH1	2.32	0.44
1:C:194:GLU:O	1:C:198:VAL:HG23	2.17	0.44
1:C:223:TRP:HE1	1:C:251:MSE:SE	2.49	0.44
1:B:61:LYS:HG3	3:B:957:HOH:O	2.17	0.44
1:B:253:GLN:HB3	1:B:254:GLU:H	1.67	0.44
1:A:130[B]:ARG:HD2	1:A:131:PHE:CE2	2.52	0.44
1:B:261:PHE:HB3	1:B:262:PRO:CD	2.47	0.44
1:C:59:GLN:HG3	3:C:994:HOH:O	2.17	0.44
1:C:164:ILE:HD13	1:C:178:ARG:HB2	2.00	0.44
1:C:32:LEU:CD1	1:C:111:MSE:HE1	2.42	0.44
1:C:179:ASP:OD1	1:C:182[A]:ARG:NH1	2.50	0.44
1:A:33:MSE:HG3	1:A:54:PHE:CD2	2.52	0.43
1:C:191:LEU:O	1:C:192:ALA:C	2.57	0.43
1:B:211:ALA:O	1:B:212:PRO:C	2.57	0.43
1:B:217:VAL:HG13	1:B:220:ARG:NE	2.34	0.43
1:C:159:ARG:NH1	1:C:194:GLU:OE1	2.52	0.43
1:A:11:LEU:CD2	1:A:108[B]:TYR:CE2	3.02	0.43
1:A:225:ARG:NH1	1:A:229:ASP:OD2	2.52	0.43
1:C:194:GLU:H	1:C:197:VAL:H	1.66	0.42
1:B:104:ASN:OD1	1:B:105:ASP:N	2.51	0.42
1:A:9:HIS:CE1	1:A:108[B]:TYR:HH	2.35	0.42
1:A:33:MSE:N	1:A:34:PRO:CD	2.83	0.42
1:A:100:LEU:HD21	1:A:107:TRP:CZ2	2.55	0.42
1:C:33:MSE:HG3	1:C:54:PHE:CD2	2.55	0.42
1:B:33:MSE:HE2	1:B:33:MSE:HA	2.02	0.42
1:B:57:PHE:CE2	1:B:75:ASN:HB2	2.54	0.42
1:B:208:ARG:O	1:B:211:ALA:CB	2.67	0.42
1:B:256:ASN:O	1:B:257:CYS:C	2.58	0.42
1:C:103:GLU:O	1:C:103:GLU:HG3	2.19	0.42
1:B:217:VAL:HG22	1:B:220:ARG:CD	2.50	0.41
1:A:32:LEU:HD11	1:A:111:MSE:CE	2.44	0.41
1:B:223:TRP:HE1	1:B:251:MSE:SE	2.52	0.41
1:C:188:MSE:HG3	1:C:191:LEU:HD21	2.03	0.41
1:A:164:ILE:N	1:A:164:ILE:HD12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:TYR:O	1:B:223:TRP:N	2.49	0.41
1:C:217:VAL:HG22	1:C:220:ARG:HH12	1.85	0.41
1:A:77:ASN:O	1:A:82:LYS:HD2	2.21	0.41
1:A:184:LEU:HD22	1:B:184:LEU:HD22	2.01	0.41
1:C:214:ASP:O	1:C:215:LYS:CB	2.57	0.41
1:A:159:ARG:HG2	1:B:169:LEU:HG	2.02	0.41
1:A:79:ASP:H	1:A:82:LYS:HG3	1.86	0.41
1:A:243:ARG:HG2	3:A:920:HOH:O	2.20	0.41
1:B:82:LYS:O	1:B:83:ASN:HB2	2.21	0.41
1:C:24:VAL:HG21	2:C:802:NAD:C4D	2.50	0.41
1:A:154:LEU:CD2	1:A:162:ILE:HB	2.51	0.41
1:B:33:MSE:N	1:B:34:PRO:CD	2.84	0.41
1:B:217:VAL:HG13	1:B:220:ARG:HH21	1.86	0.40
1:B:220:ARG:HH11	1:B:220:ARG:HD2	1.51	0.40
1:C:9:HIS:ND1	1:C:108:TYR:OH	2.37	0.40
1:A:14[A]:LYS:HG2	1:A:108[A]:TYR:CZ	2.57	0.40
1:C:33:MSE:N	1:C:34:PRO:CD	2.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	264/274 (96%)	249 (94%)	13 (5%)	2 (1%)	19	19
1	B	273/274 (100%)	242 (89%)	19 (7%)	12 (4%)	2	1
1	C	261/274 (95%)	250 (96%)	9 (3%)	2 (1%)	19	19
All	All	798/822 (97%)	741 (93%)	41 (5%)	16 (2%)	7	4

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	102	ASN
1	B	158	ASP
1	B	212	PRO
1	B	213	ASP
1	B	217	VAL
1	B	254	GLU
1	A	253	GLN
1	B	215	LYS
1	B	218	LYS
1	B	253	GLN
1	B	255	GLN
1	C	215	LYS
1	B	211	ALA
1	C	194	GLU
1	A	252	PHE
1	B	157	GLY

### 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	243/242 (100%)	232 (96%)	11 (4%)	27	34
1	B	249/242 (103%)	236 (95%)	13 (5%)	23	28
1	C	240/242 (99%)	227 (95%)	13 (5%)	22	26
All	All	732/726 (101%)	695 (95%)	37 (5%)	24	29

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	56	LYS
1	A	59	GLN
1	A	71	LYS
1	A	82	LYS
1	A	103	GLU
1	A	130[A]	ARG

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Mol	Chain	Res	Type
1	A	130[B]	ARG
1	A	154	LEU
1	A	159	ARG
1	A	172	ARG
1	B	60	ASN
1	B	103	GLU
1	B	105	ASP
1	B	113	CYS
1	B	130	ARG
1	B	154	LEU
1	B	158	ASP
1	B	208	ARG
1	B	209	LEU
1	B	212	PRO
1	B	216	ASP
1	B	225	ARG
1	B	254	GLU
1	C	79	ASP
1	C	101	GLU
1	C	113	CYS
1	C	130	ARG
1	C	154	LEU
1	C	159	ARG
1	C	172	ARG
1	C	180	GLU
1	C	208	ARG
1	C	214	ASP
1	C	215	LYS
1	C	242	LYS
1	C	265	GLU

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

Mol	Chain	Res	Type
1	A	83	ASN
1	A	135	GLN
1	A	153	ASN
1	A	238	ASN
1	B	60	ASN
1	B	83	ASN
1	B	135	GLN
1	B	161	GLN

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Mol	Chain	Res	Type
1	C	77	ASN
1	C	83	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

3 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	B	801	-	33,38,48	0.75	1 (3%)	37,58,73	1.02	1 (2%)
2	NAD	C	802	-	33,38,48	0.84	0	37,58,73	1.49	5 (13%)
2	NAD	A	800	-	21,28,48	0.72	0	23,42,73	1.00	1 (4%)

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	B	801	-	-	4/18/51/62	0/4/4/5
2	NAD	C	802	-	-	7/18/51/62	0/4/4/5
2	NAD	A	800	-	-	2/9/31/62	0/3/3/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	NAD	PA-O2A	-2.01	1.45	1.55

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	802	NAD	O3D-C3D-C2D	3.96	121.60	112.04
2	C	802	NAD	PN-O3-PA	-3.61	120.43	132.83
2	C	802	NAD	O2D-C2D-C3D	3.44	117.79	111.27
2	C	802	NAD	C5A-C6A-N6A	3.01	124.93	120.35
2	A	800	NAD	C5A-C6A-N6A	2.70	124.45	120.35
2	C	802	NAD	O4D-C4D-C3D	2.52	106.94	104.70
2	B	801	NAD	C5A-C6A-N6A	2.49	124.13	120.35

There are no chirality outliers.

All (13) torsion outliers are listed below:

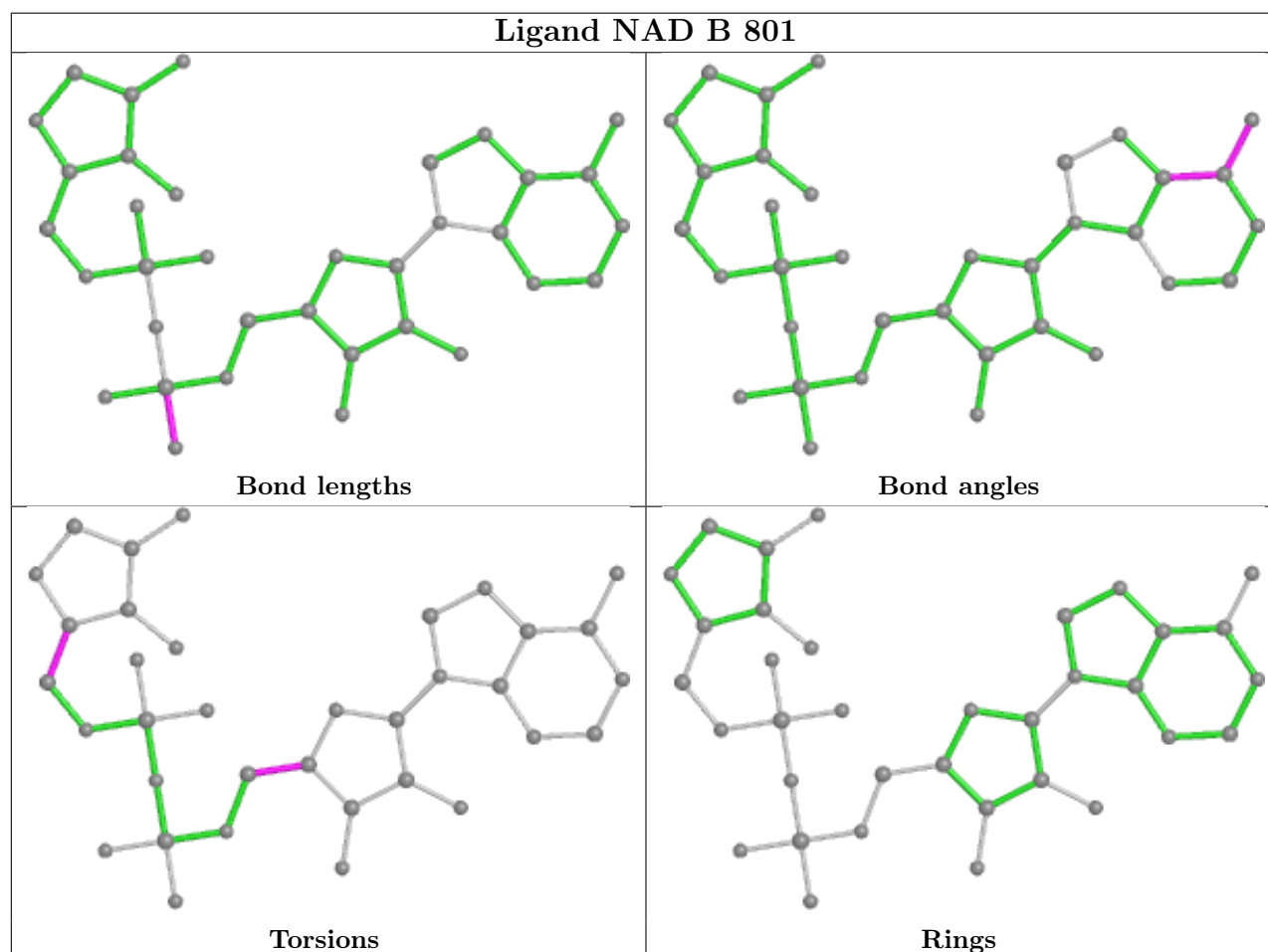
Mol	Chain	Res	Type	Atoms
2	C	802	NAD	O4B-C4B-C5B-O5B
2	C	802	NAD	C5D-O5D-PN-O1N
2	C	802	NAD	C3B-C4B-C5B-O5B
2	B	801	NAD	O4B-C4B-C5B-O5B
2	A	800	NAD	O4B-C4B-C5B-O5B
2	C	802	NAD	C5D-O5D-PN-O3
2	C	802	NAD	O4D-C4D-C5D-O5D
2	C	802	NAD	C5D-O5D-PN-O2N
2	B	801	NAD	C3D-C4D-C5D-O5D
2	B	801	NAD	O4D-C4D-C5D-O5D
2	A	800	NAD	C3B-C4B-C5B-O5B
2	B	801	NAD	C3B-C4B-C5B-O5B
2	C	802	NAD	PA-O3-PN-O2N

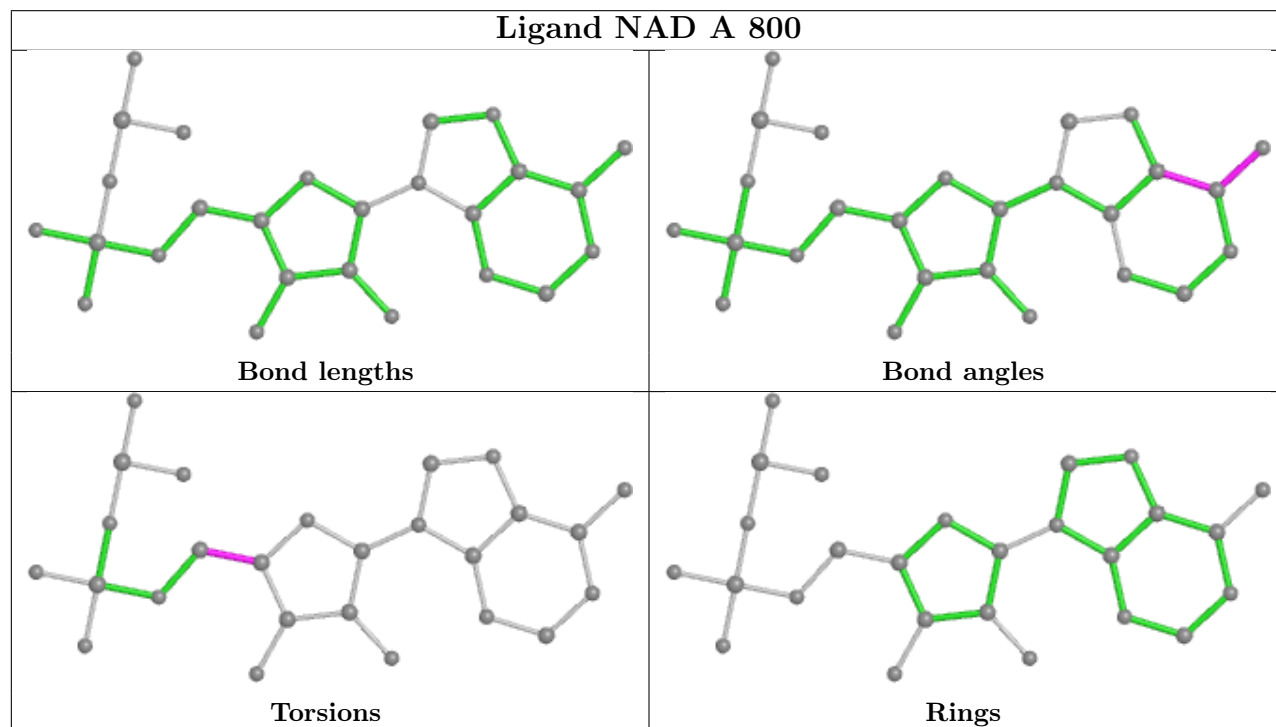
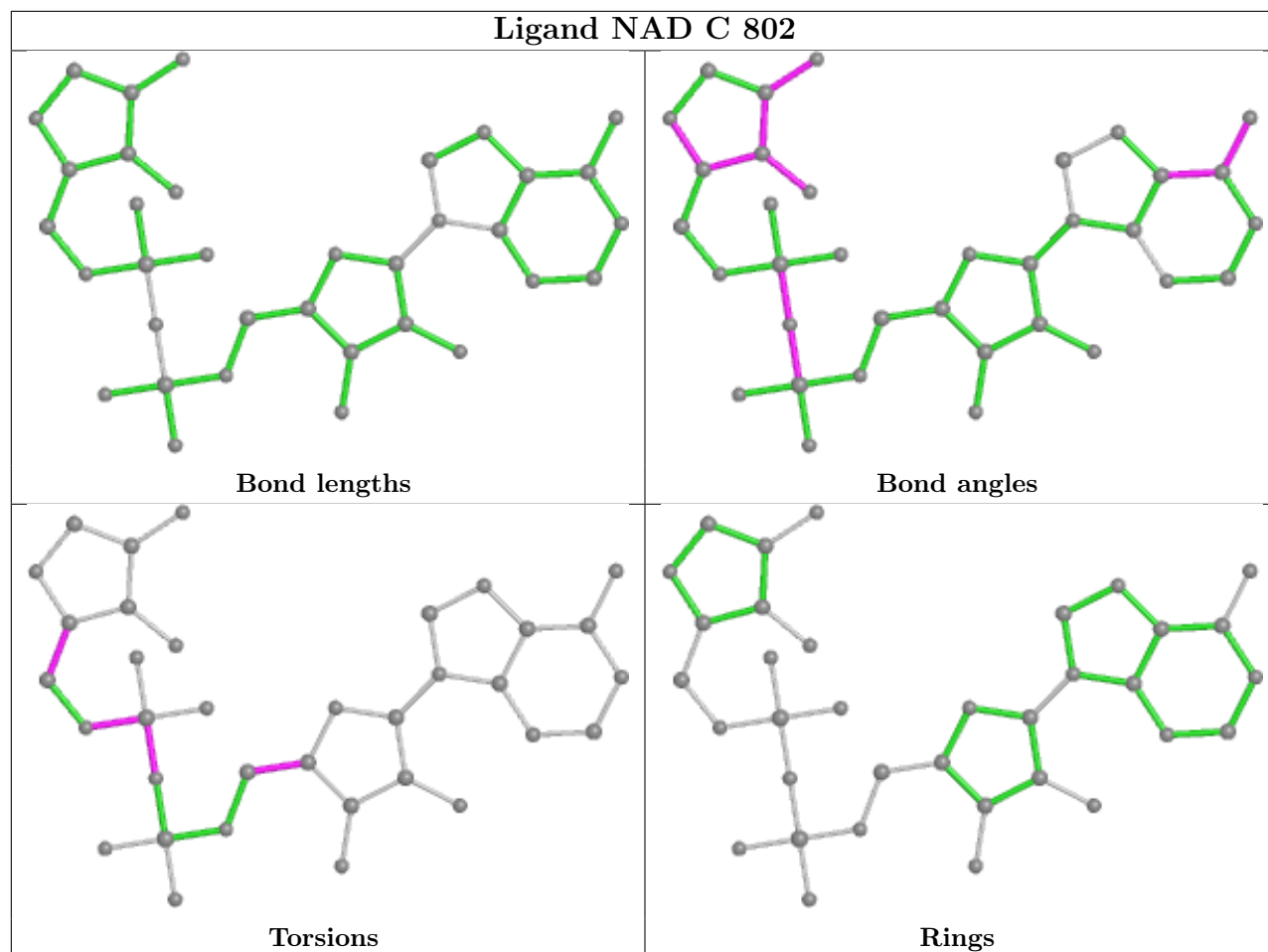
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	802	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.





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	256/274 (93%)	-0.16	16 (6%) 20 19	16, 36, 66, 87	0
1	B	267/274 (97%)	-0.09	14 (5%) 27 26	16, 35, 67, 100	0
1	C	256/274 (93%)	-0.22	7 (2%) 54 52	16, 35, 59, 78	0
All	All	779/822 (94%)	-0.16	37 (4%) 31 30	16, 35, 65, 100	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	LYS	6.6
1	A	217	VAL	6.5
1	B	256	ASN	5.1
1	A	256	ASN	4.8
1	B	101	GLU	4.7
1	B	212	PRO	4.5
1	A	214	ASP	4.1
1	B	218	LYS	4.0
1	C	158	ASP	3.3
1	A	257	CYS	3.2
1	C	214	ASP	3.2
1	A	168	GLY	3.1
1	A	102	ASN	3.0
1	C	59	GLN	2.9
1	A	103	GLU	2.9
1	B	104	ASN	2.9
1	B	211	ALA	2.8
1	A	213	ASP	2.8
1	A	252	PHE	2.7
1	C	102	ASN	2.7
1	B	103	GLU	2.7
1	C	103	GLU	2.7
1	A	260	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	217	VAL	2.5
1	B	194	GLU	2.5
1	B	204	ARG	2.4
1	A	258	SER	2.4
1	C	209	LEU	2.3
1	B	220	ARG	2.3
1	B	158	ASP	2.2
1	A	265	GLU	2.2
1	B	219	TYR	2.2
1	A	253	GLN	2.2
1	A	158	ASP	2.1
1	A	218	LYS	2.0
1	B	209	LEU	2.0
1	A	216	ASP	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

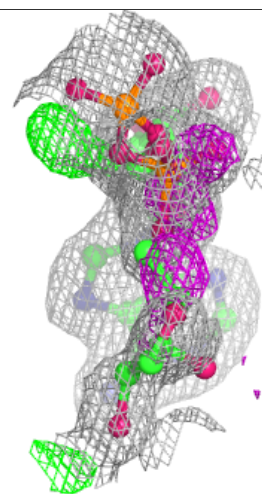
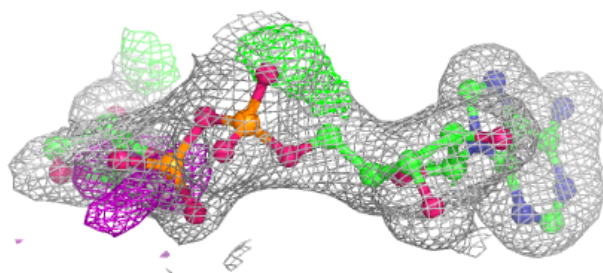
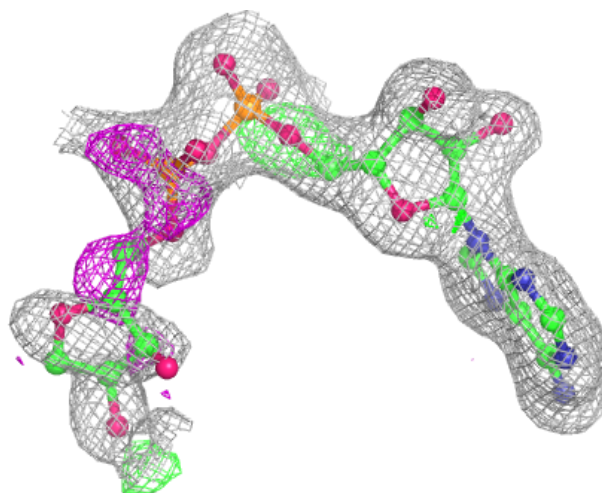
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAD	C	802	35/44	0.89	0.14	23,32,65,65	0
2	NAD	B	801	35/44	0.93	0.11	18,25,49,50	0
2	NAD	A	800	26/44	0.93	0.07	28,33,46,48	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 C 802:**

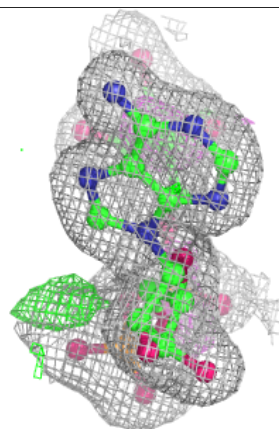
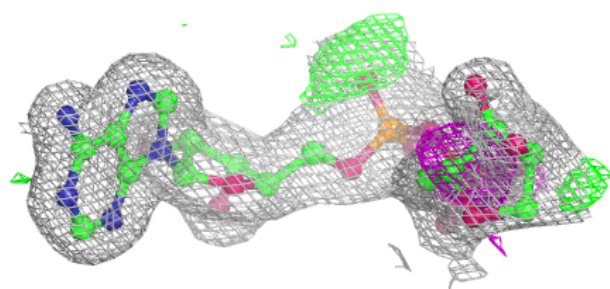
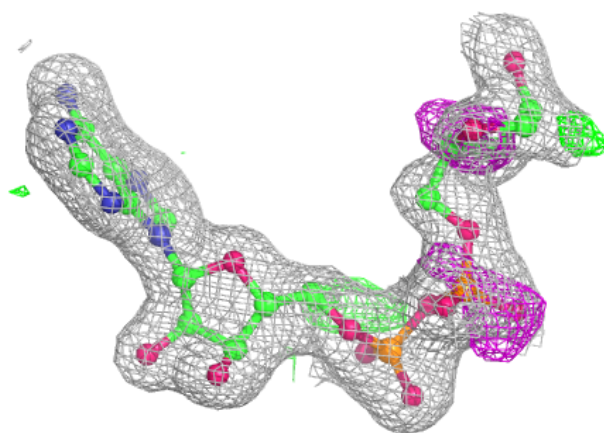
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



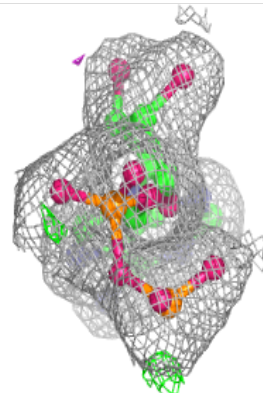
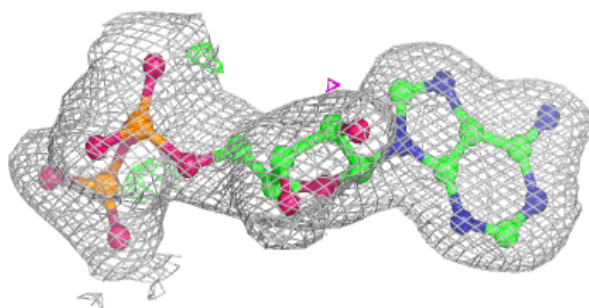
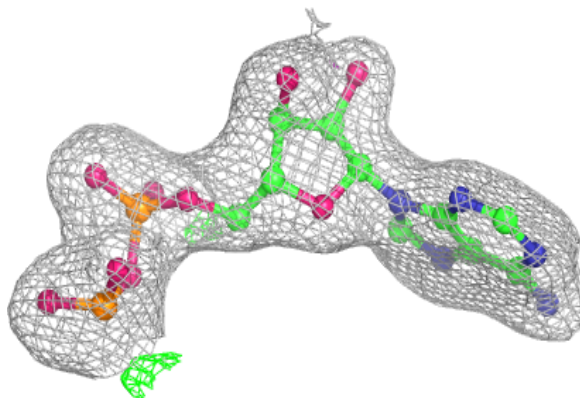


**Electron density around NAD B 801:**

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

**Electron density around NAD A 800:**

$2mF_o-DF_c$  (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.