



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:45 AM UTC

PDB ID : 1DIR / pdb_00001dir
Title : CRYSTAL STRUCTURE OF A MONOCLINIC FORM OF DIHYDROPTERIDINE REDUCTASE FROM RAT LIVER
Authors : Varughese, K.I.; Su, Y.; Skinner, M.M.; Matthews, D.A.; Whitely, J.M.; Xuong, N.H.
Deposited on : 1994-04-18
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

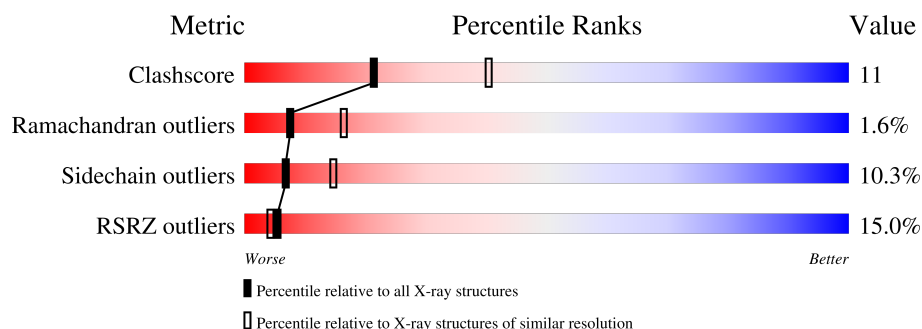
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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.

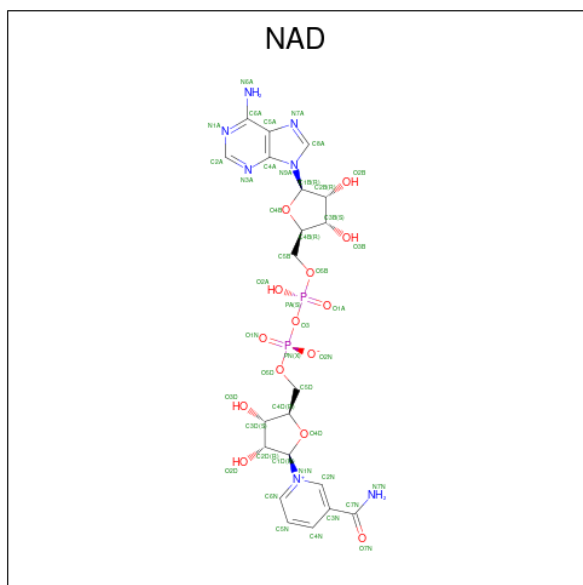
Mol	Chain	Length	Quality of chain
1	A	241	
1	B	241	
1	C	241	
1	D	241	

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 DIHYDROPTERIDINE REDUCTASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	236	Total 2160	C 1111	H 398	N 306	O 334	S 11	0	0	0
1	B	236	Total 2160	C 1111	H 398	N 306	O 334	S 11	0	0	0
1	C	236	Total 2160	C 1111	H 398	N 306	O 334	S 11	0	0	0
1	D	236	Total 2160	C 1111	H 398	N 306	O 334	S 11	0	0	0

- 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 52	C 21	H 8	N 7	O 14	P 2	0	0	
2	B	1	Total 52	C 21	H 8	N 7	O 14	P 2	0	0	

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	P	0	0
			52	21	8	7	14	2		
2	D	1	Total	C	H	N	O	P	0	0
			52	21	8	7	14	2		

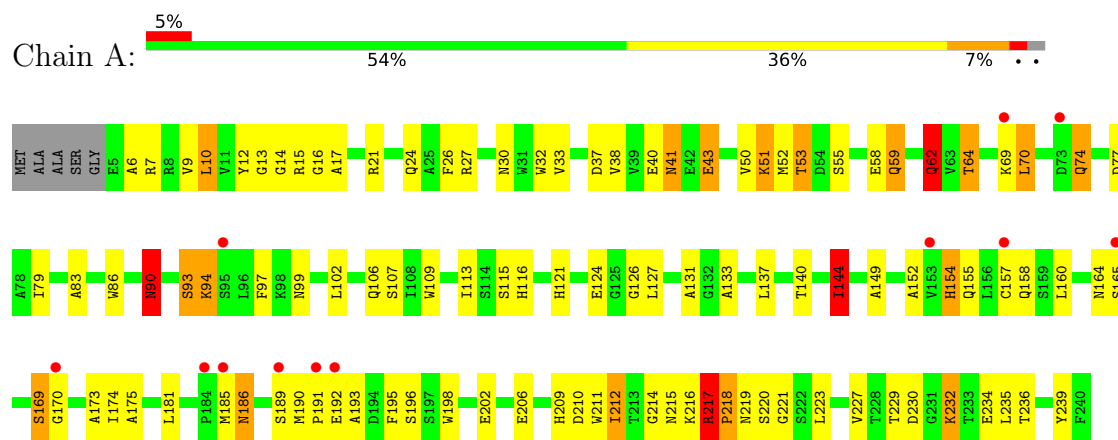
- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	38	Total	H	O	0	0
			114	76	38		
3	B	36	Total	H	O	0	0
			108	72	36		
3	C	39	Total	H	O	0	0
			117	78	39		
3	D	35	Total	H	O	0	0
			105	70	35		

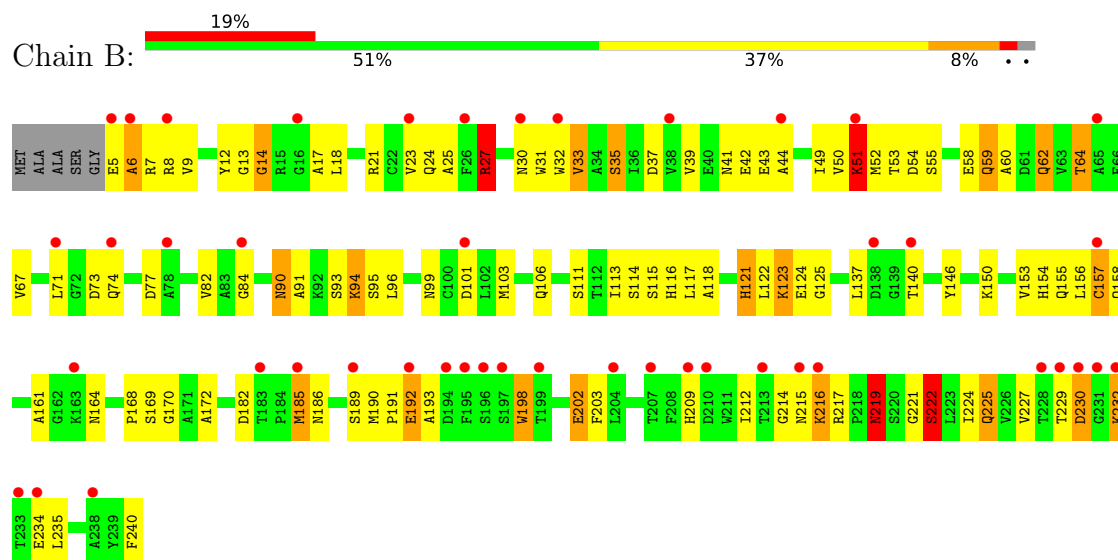
3 Residue-property plots

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.

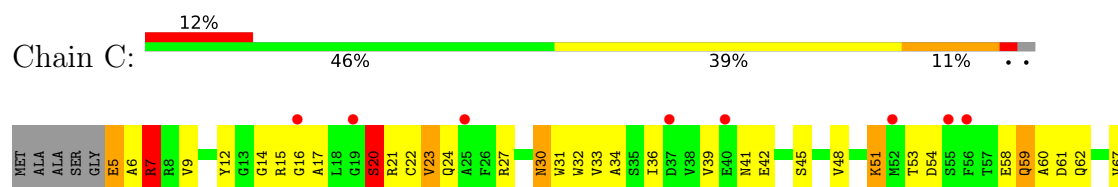
• Molecule 1: DIHYDROPTERIDINE REDUCTASE

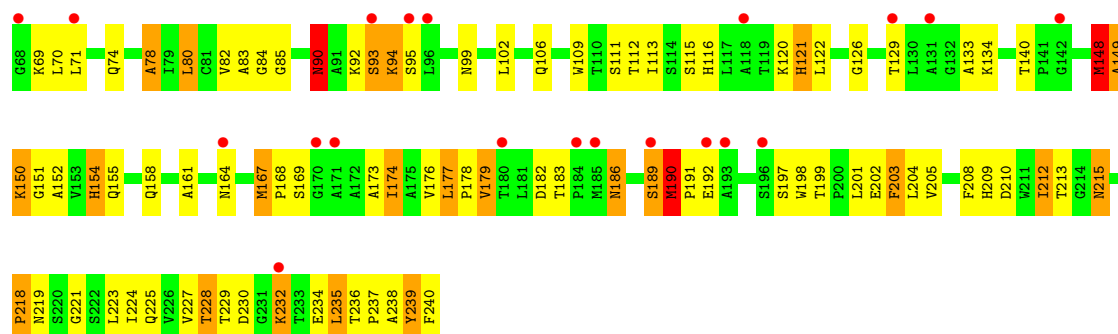


• Molecule 1: DIHYDROPTERIDINE REDUCTASE

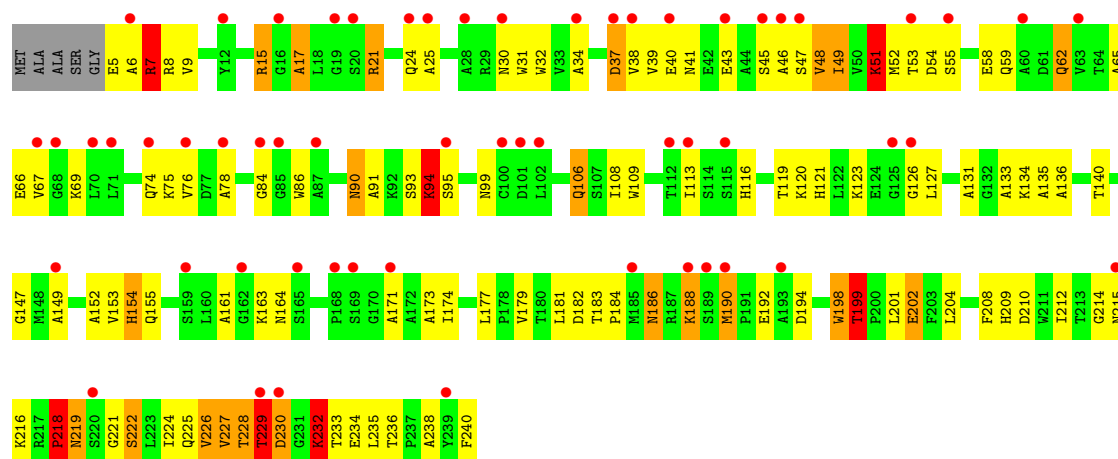


• Molecule 1: DIHYDROPTERIDINE REDUCTASE





● Molecule 1: DIHYDROPTERIDINE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	222.20Å 46.50Å 94.30Å 90.00° 101.10° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60 8.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.60) 92.3 (8.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.54Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.168 , (Not available) 0.292 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 51.0	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	0.81	EDS
Total number of atoms	9292	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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: 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	1.31	9/1797 (0.5%)	2.31	96/2436 (3.9%)
1	B	1.33	9/1797 (0.5%)	2.33	105/2436 (4.3%)
1	C	1.33	15/1797 (0.8%)	2.29	95/2436 (3.9%)
1	D	1.27	8/1797 (0.4%)	2.22	86/2436 (3.5%)
All	All	1.31	41/7188 (0.6%)	2.29	382/9744 (3.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
All	All	0	3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	HIS	CD2-NE2	-8.71	1.28	1.37
1	B	116	HIS	CD2-NE2	-7.41	1.29	1.37
1	B	154	HIS	CD2-NE2	-7.32	1.29	1.37
1	A	121	HIS	CD2-NE2	-7.01	1.30	1.37
1	D	121	HIS	CD2-NE2	-6.83	1.30	1.37
1	A	9	VAL	CA-CB	6.77	1.62	1.54
1	D	140	THR	CA-CB	6.75	1.60	1.53
1	B	209	HIS	CD2-NE2	-6.62	1.30	1.37
1	A	154	HIS	CD2-NE2	-6.61	1.30	1.37
1	D	116	HIS	CD2-NE2	-6.46	1.30	1.37
1	A	209	HIS	CD2-NE2	-6.45	1.30	1.37
1	B	121	HIS	CD2-NE2	-6.26	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	229	THR	CA-CB	-6.19	1.43	1.53
1	D	209	HIS	CD2-NE2	-6.16	1.31	1.37
1	D	183	THR	CA-CB	6.04	1.62	1.53
1	C	209	HIS	CD2-NE2	-6.00	1.31	1.37
1	B	202	GLU	CA-CB	-5.94	1.43	1.53
1	C	116	HIS	CD2-NE2	-5.90	1.31	1.37
1	C	121	HIS	CD2-NE2	-5.90	1.31	1.37
1	C	111	SER	CA-CB	-5.88	1.44	1.53
1	D	116	HIS	CG-ND1	-5.87	1.31	1.38
1	B	23	VAL	CA-CB	5.85	1.61	1.54
1	C	60	ALA	CA-CB	-5.79	1.43	1.53
1	C	224	ILE	CA-CB	5.78	1.60	1.54
1	A	116	HIS	CG-ND1	-5.78	1.31	1.38
1	C	228	THR	CA-CB	-5.74	1.45	1.53
1	A	212	ILE	CA-CB	5.72	1.61	1.54
1	C	154	HIS	CD2-NE2	-5.67	1.31	1.37
1	D	121	HIS	CG-ND1	-5.64	1.32	1.38
1	C	129	THR	CA-CB	5.59	1.62	1.53
1	D	154	HIS	CD2-NE2	-5.49	1.31	1.37
1	C	235	LEU	CA-CB	-5.46	1.46	1.53
1	C	203	PHE	CA-CB	-5.36	1.44	1.53
1	A	140	THR	CA-CB	5.36	1.61	1.53
1	C	179	VAL	CA-CB	-5.34	1.47	1.54
1	C	164	ASN	CA-CB	5.25	1.61	1.53
1	B	209	HIS	CG-ND1	-5.24	1.32	1.38
1	C	183	THR	CA-CB	5.20	1.61	1.54
1	C	109	TRP	CG-CD2	-5.18	1.34	1.43
1	A	154	HIS	CG-ND1	-5.02	1.32	1.38
1	B	121	HIS	CG-ND1	-5.01	1.32	1.38

All (382) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ASN	OD1-CG-ND2	-13.19	109.41	122.60
1	A	90	ASN	OD1-CG-ND2	-11.99	110.61	122.60
1	C	182	ASP	CA-CB-CG	11.88	124.48	112.60
1	C	20	SER	CA-CB-OG	-11.31	88.47	111.10
1	B	225	GLN	OE1-CD-NE2	-11.21	111.39	122.60
1	B	62	GLN	OE1-CD-NE2	-10.79	111.81	122.60
1	A	164	ASN	OD1-CG-ND2	-10.76	111.84	122.60
1	C	41	ASN	OD1-CG-ND2	-10.58	112.02	122.60
1	C	164	ASN	OD1-CG-ND2	-10.45	112.15	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	GLN	OE1-CD-NE2	-9.98	112.62	122.60
1	D	62	GLN	OE1-CD-NE2	-9.89	112.70	122.60
1	B	90	ASN	OD1-CG-ND2	-9.89	112.71	122.60
1	D	219	ASN	OD1-CG-ND2	-9.89	112.71	122.60
1	C	82	VAL	CA-C-O	9.84	129.65	119.91
1	D	186	ASN	OD1-CG-ND2	-9.83	112.77	122.60
1	B	155	GLN	OE1-CD-NE2	-9.82	112.78	122.60
1	C	190	MET	CA-C-N	9.81	129.54	119.64
1	C	190	MET	C-N-CA	9.81	129.54	119.64
1	A	230	ASP	CA-CB-CG	9.60	122.20	112.60
1	B	219	ASN	OD1-CG-ND2	-9.60	113.00	122.60
1	A	30	ASN	OD1-CG-ND2	-9.59	113.01	122.60
1	A	90	ASN	CB-CG-ND2	9.50	130.65	116.40
1	C	90	ASN	OD1-CG-ND2	-9.31	113.29	122.60
1	B	30	ASN	N-CA-C	9.22	124.04	112.24
1	A	62	GLN	OE1-CD-NE2	-9.12	113.48	122.60
1	B	6	ALA	N-CA-C	8.95	129.86	110.80
1	A	158	GLN	OE1-CD-NE2	-8.94	113.66	122.60
1	B	41	ASN	OD1-CG-ND2	-8.89	113.71	122.60
1	B	74	GLN	OE1-CD-NE2	-8.88	113.72	122.60
1	B	99	ASN	OD1-CG-ND2	-8.78	113.82	122.60
1	C	240	PHE	CA-CB-CG	8.76	122.56	113.80
1	A	37	ASP	O-C-N	-8.76	113.93	123.04
1	C	186	ASN	OD1-CG-ND2	-8.75	113.85	122.60
1	C	155	GLN	OE1-CD-NE2	-8.57	114.03	122.60
1	A	126	GLY	O-C-N	-8.48	116.10	122.71
1	A	24	GLN	N-CA-C	8.34	121.12	111.11
1	C	22	CYS	CA-C-O	-8.33	112.08	120.82
1	A	154	HIS	CB-CG-CD2	-8.26	120.46	131.20
1	B	209	HIS	CA-CB-CG	-8.25	105.55	113.80
1	C	24	GLN	N-CA-C	8.24	119.95	110.97
1	A	99	ASN	OD1-CG-ND2	-8.22	114.38	122.60
1	C	150	LYS	O-C-N	-8.20	113.51	122.03
1	B	198	TRP	O-C-N	-8.18	113.68	123.16
1	A	77	ASP	N-CA-C	8.14	120.24	111.36
1	C	62	GLN	OE1-CD-NE2	-8.06	114.54	122.60
1	B	35	SER	N-CA-C	8.06	122.25	107.99
1	B	31	TRP	CG-CD2-CE3	8.02	141.92	133.90
1	B	229	THR	O-C-N	-7.95	113.97	123.27
1	D	91	ALA	N-CA-C	7.94	122.66	112.34
1	A	41	ASN	CB-CG-ND2	7.88	128.22	116.40
1	B	93	SER	N-CA-C	7.87	121.60	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	23	VAL	O-C-N	-7.82	114.29	121.87
1	B	106	GLN	OE1-CD-NE2	-7.81	114.79	122.60
1	A	219	ASN	OD1-CG-ND2	-7.80	114.80	122.60
1	B	8	ARG	CA-CB-CG	-7.74	98.61	114.10
1	C	59	GLN	OE1-CD-NE2	-7.74	114.86	122.60
1	B	209	HIS	CB-CG-CD2	-7.73	121.15	131.20
1	B	42	GLU	N-CA-C	7.72	121.64	111.75
1	A	210	ASP	CA-CB-CG	7.70	120.30	112.60
1	B	8	ARG	N-CA-C	7.67	120.99	108.26
1	A	215	ASN	OD1-CG-ND2	-7.63	114.97	122.60
1	B	222	SER	N-CA-C	7.62	121.31	109.96
1	A	59	GLN	OE1-CD-NE2	-7.59	115.01	122.60
1	A	17	ALA	O-C-N	-7.52	114.27	122.09
1	B	157	CYS	CB-CA-C	-7.47	99.04	110.92
1	D	34	ALA	O-C-N	-7.46	114.84	123.27
1	B	30	ASN	OD1-CG-ND2	-7.44	115.16	122.60
1	D	202	GLU	CB-CG-CD	7.42	125.21	112.60
1	B	164	ASN	N-CA-C	7.41	121.62	111.54
1	C	219	ASN	N-CA-C	7.38	120.52	110.55
1	B	33	VAL	CB-CA-C	-7.34	99.76	110.63
1	D	90	ASN	OD1-CG-ND2	-7.33	115.27	122.60
1	D	48	VAL	O-C-N	-7.31	114.61	122.95
1	A	155	GLN	OE1-CD-NE2	-7.18	115.42	122.60
1	B	227	VAL	N-CA-CB	-7.17	102.43	111.46
1	C	78	ALA	N-CA-C	7.14	120.20	108.99
1	B	155	GLN	CG-CD-NE2	7.12	127.08	116.40
1	C	112	THR	O-C-N	-7.12	114.03	122.15
1	A	181	LEU	O-C-N	-7.10	114.92	123.16
1	C	225	GLN	OE1-CD-NE2	-7.09	115.51	122.60
1	A	32	TRP	CG-CD2-CE3	7.08	140.99	133.90
1	A	53	THR	CA-CB-OG1	-7.07	98.99	109.60
1	D	126	GLY	O-C-N	-7.05	116.75	122.81
1	B	73	ASP	CA-CB-CG	7.03	119.63	112.60
1	A	93	SER	N-CA-C	7.02	120.14	110.24
1	D	155	GLN	OE1-CD-NE2	-7.01	115.59	122.60
1	B	121	HIS	CA-CB-CG	-7.01	106.79	113.80
1	C	54	ASP	CA-CB-CG	7.00	119.60	112.60
1	D	227	VAL	CA-C-O	6.94	127.28	120.27
1	C	148	MET	CB-CA-C	-6.92	95.49	109.55
1	C	116	HIS	CA-CB-CG	-6.89	106.91	113.80
1	A	9	VAL	N-CA-C	6.89	117.81	107.75
1	C	164	ASN	CA-CB-CG	6.87	119.47	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	179	VAL	O-C-N	-6.85	114.01	122.57
1	D	210	ASP	CA-CB-CG	6.83	119.43	112.60
1	B	158	GLN	OE1-CD-NE2	-6.83	115.77	122.60
1	C	61	ASP	CA-CB-CG	6.81	119.41	112.60
1	D	74	GLN	OE1-CD-NE2	-6.80	115.80	122.60
1	A	215	ASN	N-CA-C	6.79	118.92	109.15
1	B	154	HIS	CB-CG-CD2	-6.79	122.38	131.20
1	D	66	GLU	O-C-N	-6.78	114.97	122.03
1	B	5	GLU	CA-CB-CG	6.73	127.56	114.10
1	D	230	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	165	SER	N-CA-C	6.69	119.58	111.82
1	B	225	GLN	CG-CD-NE2	6.65	126.38	116.40
1	D	182	ASP	CA-CB-CG	6.62	119.22	112.60
1	D	120	LYS	N-CA-C	6.61	118.57	111.36
1	D	41	ASN	OD1-CG-ND2	-6.59	116.00	122.60
1	A	137	LEU	N-CA-C	-6.58	104.73	112.89
1	D	21	ARG	O-C-N	-6.57	115.15	122.12
1	D	153	VAL	N-CA-C	6.57	117.32	110.62
1	B	6	ALA	O-C-N	-6.57	113.86	122.59
1	B	186	ASN	CA-CB-CG	6.56	119.16	112.60
1	A	14	GLY	O-C-N	-6.51	115.48	122.19
1	B	190	MET	CA-C-N	6.51	126.74	119.32
1	B	190	MET	C-N-CA	6.51	126.74	119.32
1	A	193	ALA	N-CA-C	6.50	120.13	110.52
1	B	114	SER	CB-CA-C	-6.49	100.02	110.79
1	A	217	ARG	N-CA-C	6.46	117.94	109.93
1	D	164	ASN	OD1-CG-ND2	-6.45	116.15	122.60
1	C	41	ASN	CB-CG-ND2	6.45	126.07	116.40
1	C	82	VAL	N-CA-CB	-6.43	103.73	112.28
1	B	23	VAL	N-CA-C	-6.42	104.49	110.53
1	B	59	GLN	OE1-CD-NE2	-6.41	116.19	122.60
1	D	194	ASP	CA-CB-CG	6.41	119.01	112.60
1	C	234	GLU	N-CA-C	6.39	119.82	109.40
1	D	37	ASP	CA-CB-CG	6.38	118.98	112.60
1	B	94	LYS	CA-C-O	6.36	128.06	121.07
1	A	50	VAL	N-CA-CB	-6.36	104.02	111.39
1	A	115	SER	CB-CA-C	-6.34	100.26	110.79
1	B	24	GLN	N-CA-C	6.34	118.72	111.11
1	C	158	GLN	OE1-CD-NE2	-6.30	116.30	122.60
1	D	43	GLU	N-CA-C	6.30	120.82	113.20
1	C	99	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	D	74	GLN	N-CA-C	6.29	118.96	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	PHE	CA-CB-CG	6.28	120.08	113.80
1	D	62	GLN	CG-CD-NE2	6.27	125.80	116.40
1	A	26	PHE	CA-CB-CG	6.25	120.05	113.80
1	B	62	GLN	CG-CD-NE2	6.24	125.77	116.40
1	C	140	THR	CA-C-N	6.22	125.84	119.56
1	C	140	THR	C-N-CA	6.22	125.84	119.56
1	A	232	LYS	N-CA-C	6.18	118.26	108.67
1	B	232	LYS	CA-CB-CG	6.18	126.47	114.10
1	D	234	GLU	N-CA-C	6.18	119.31	109.24
1	D	153	VAL	O-C-N	-6.17	115.89	121.87
1	B	27	ARG	CA-CB-CG	-6.16	101.78	114.10
1	B	74	GLN	CG-CD-NE2	6.15	125.63	116.40
1	A	106	GLN	OE1-CD-NE2	-6.15	116.45	122.60
1	D	49	ILE	N-CA-C	6.15	116.47	107.37
1	A	62	GLN	CG-CD-NE2	6.14	125.61	116.40
1	A	164	ASN	CB-CG-ND2	6.14	125.61	116.40
1	C	183	THR	N-CA-CB	6.11	117.52	111.10
1	D	17	ALA	O-C-N	-6.11	114.46	122.59
1	A	152	ALA	O-C-N	-6.10	115.65	122.12
1	A	154	HIS	CB-CG-ND1	6.10	131.85	122.70
1	B	123	LYS	N-CA-C	6.10	118.17	110.24
1	D	49	ILE	N-CA-CB	-6.10	103.99	111.67
1	D	229	THR	CA-C-O	6.09	127.02	120.32
1	A	37	ASP	CA-CB-CG	6.08	118.68	112.60
1	B	146	TYR	N-CA-C	6.08	117.57	111.07
1	D	17	ALA	CA-C-O	-6.07	111.83	120.51
1	A	196	SER	N-CA-C	6.06	120.28	113.01
1	B	18	LEU	N-CA-C	6.06	118.68	111.71
1	D	154	HIS	CB-CG-CD2	-6.04	123.35	131.20
1	C	24	GLN	CB-CA-C	-6.04	101.66	110.96
1	D	55	SER	N-CA-C	6.04	118.46	109.59
1	A	12	TYR	O-C-N	-6.02	115.99	123.04
1	C	152	ALA	O-C-N	-6.02	115.87	122.07
1	B	230	ASP	CA-CB-CG	6.00	118.60	112.60
1	B	37	ASP	N-CA-C	5.99	117.35	108.60
1	C	22	CYS	O-C-N	-5.99	115.90	122.07
1	A	14	GLY	N-CA-C	5.99	121.23	113.27
1	D	95	SER	CA-CB-OG	-5.99	99.12	111.10
1	C	7	ARG	N-CA-C	-5.98	105.89	113.43
1	C	230	ASP	CA-CB-CG	5.98	118.58	112.60
1	B	51	LYS	N-CA-C	5.98	118.40	109.25
1	A	10	LEU	O-C-N	-5.97	116.42	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	67	VAL	CA-C-O	5.96	127.14	120.64
1	C	90	ASN	CB-CG-ND2	5.96	125.34	116.40
1	D	25	ALA	N-CA-C	5.95	117.57	111.14
1	B	7	ARG	N-CA-C	5.95	120.23	113.15
1	D	152	ALA	CA-C-N	5.95	128.60	120.46
1	D	152	ALA	C-N-CA	5.95	128.60	120.46
1	B	82	VAL	CA-C-O	5.94	125.37	119.97
1	C	102	LEU	O-C-N	-5.91	115.98	122.07
1	C	203	PHE	O-C-N	-5.87	115.06	122.27
1	B	9	VAL	N-CA-C	5.85	117.11	108.45
1	A	154	HIS	O-C-N	-5.84	115.92	122.12
1	C	129	THR	O-C-N	-5.84	116.40	123.29
1	B	106	GLN	CA-C-O	-5.83	113.76	120.24
1	A	223	LEU	O-C-N	-5.83	116.58	123.22
1	C	85	GLY	CA-C-O	-5.83	117.38	122.16
1	D	199	THR	O-C-N	-5.82	115.30	121.30
1	C	209	HIS	CB-CG-CD2	-5.81	123.64	131.20
1	A	33	VAL	N-CA-C	5.81	116.23	107.75
1	D	51	LYS	CG-CD-CE	5.81	124.66	111.30
1	A	160	LEU	O-C-N	-5.80	115.97	122.12
1	B	101	ASP	CA-CB-CG	5.79	118.39	112.60
1	C	228	THR	CA-CB-OG1	-5.79	100.92	109.60
1	B	14	GLY	N-CA-C	5.78	119.88	112.83
1	D	31	TRP	O-C-N	-5.78	116.04	122.86
1	B	33	VAL	N-CA-CB	5.76	119.36	111.41
1	B	103	MET	O-C-N	-5.76	116.01	122.12
1	C	202	GLU	O-C-N	-5.75	115.49	122.22
1	A	190	MET	CA-C-N	5.74	125.60	119.28
1	A	190	MET	C-N-CA	5.74	125.60	119.28
1	C	115	SER	CA-CB-OG	-5.71	99.68	111.10
1	D	113	ILE	O-C-N	-5.71	116.32	121.91
1	B	52	MET	CA-C-O	5.70	127.19	120.58
1	B	150	LYS	CA-C-N	5.70	126.31	119.98
1	B	150	LYS	C-N-CA	5.70	126.31	119.98
1	D	94	LYS	CA-C-O	5.70	127.43	120.31
1	B	137	LEU	N-CA-C	-5.68	106.32	113.20
1	A	170	GLY	O-C-N	-5.68	115.47	122.23
1	B	234	GLU	CA-CB-CG	-5.68	102.74	114.10
1	B	90	ASN	CB-CG-ND2	5.68	124.92	116.40
1	B	124	GLU	CA-C-O	-5.68	115.37	121.56
1	C	150	LYS	N-CA-C	5.67	117.15	110.97
1	C	167	MET	CA-C-O	-5.67	114.42	119.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	24	GLN	OE1-CD-NE2	-5.66	116.94	122.60
1	A	131	ALA	CA-C-O	5.64	126.41	120.54
1	C	212	ILE	CA-CB-CG2	-5.63	100.92	110.50
1	C	17	ALA	N-CA-C	5.63	117.11	110.97
1	C	149	ALA	CA-C-O	-5.63	114.89	120.80
1	B	23	VAL	CG1-CB-CG2	-5.63	98.42	110.80
1	D	149	ALA	N-CA-C	5.62	117.08	111.07
1	C	70	LEU	N-CA-C	5.62	118.13	111.33
1	A	116	HIS	N-CA-C	5.62	117.20	111.14
1	A	192	GLU	CB-CG-CD	5.59	122.11	112.60
1	B	14	GLY	O-C-N	-5.59	116.75	122.17
1	B	59	GLN	CG-CD-NE2	5.59	124.78	116.40
1	C	126	GLY	N-CA-C	5.58	121.67	112.30
1	B	153	VAL	CB-CA-C	-5.58	104.61	112.14
1	B	227	VAL	O-C-N	-5.57	116.58	123.10
1	C	154	HIS	CB-CG-CD2	-5.57	123.97	131.20
1	B	116	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	D	171	ALA	N-CA-C	5.55	117.49	110.33
1	A	144	ILE	CA-C-N	5.53	126.08	119.94
1	A	144	ILE	C-N-CA	5.53	126.08	119.94
1	C	215	ASN	CA-CB-CG	5.53	118.13	112.60
1	A	121	HIS	CB-CG-CD2	-5.53	124.02	131.20
1	C	201	LEU	N-CA-C	5.53	118.02	111.33
1	B	41	ASN	CB-CG-ND2	5.52	124.68	116.40
1	C	93	SER	N-CA-C	5.52	118.32	110.10
1	A	186	ASN	OD1-CG-ND2	-5.51	117.09	122.60
1	D	30	ASN	OD1-CG-ND2	-5.51	117.09	122.60
1	A	209	HIS	CB-CG-CD2	-5.50	124.04	131.20
1	D	227	VAL	CA-CB-CG1	-5.50	101.05	110.40
1	C	205	VAL	O-C-N	-5.50	116.28	121.94
1	B	203	PHE	N-CA-C	-5.49	105.45	111.82
1	B	164	ASN	CA-CB-CG	-5.49	107.11	112.60
1	D	9	VAL	N-CA-C	5.49	115.79	108.27
1	B	95	SER	N-CA-C	5.47	119.80	113.18
1	D	131	ALA	N-CA-C	5.46	117.60	107.99
1	A	169	SER	CA-C-O	-5.45	115.50	120.95
1	C	14	GLY	N-CA-C	5.45	120.45	114.40
1	D	90	ASN	CB-CG-ND2	5.45	124.58	116.40
1	C	190	MET	N-CA-C	5.45	121.85	109.81
1	D	121	HIS	CB-CG-CD2	-5.44	124.12	131.20
1	B	31	TRP	CE2-CD2-CG	-5.44	100.68	107.20
1	C	30	ASN	OD1-CG-ND2	-5.43	117.17	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	232	LYS	CA-CB-CG	5.43	124.96	114.10
1	A	154	HIS	CB-CA-C	-5.43	101.78	110.79
1	C	80	LEU	CB-CA-C	-5.42	101.17	110.22
1	C	239	TYR	O-C-N	-5.42	116.88	123.27
1	A	94	LYS	CA-C-O	5.40	126.14	120.42
1	B	64	THR	CA-C-O	5.39	126.02	119.49
1	D	32	TRP	N-CA-C	-5.39	101.00	109.25
1	B	224	ILE	CB-CA-C	-5.39	104.41	111.25
1	D	109	TRP	CG-CD1-NE1	-5.39	103.20	110.20
1	C	237	PRO	N-CA-C	5.38	119.32	111.03
1	B	95	SER	CA-CB-OG	-5.38	100.34	111.10
1	A	195	PHE	O-C-N	-5.37	115.34	122.33
1	C	169	SER	N-CA-C	5.37	118.10	110.10
1	B	25	ALA	N-CA-C	5.37	118.99	112.23
1	D	106	GLN	N-CA-C	5.36	118.28	111.69
1	A	140	THR	O-C-N	-5.35	115.16	121.32
1	A	74	GLN	CG-CD-NE2	5.35	124.42	116.40
1	C	174	ILE	O-C-N	-5.34	117.69	123.14
1	A	40	GLU	N-CA-C	5.34	118.38	110.48
1	A	218	PRO	N-CA-C	5.34	119.08	111.13
1	C	164	ASN	CB-CG-ND2	5.33	124.40	116.40
1	B	24	GLN	OE1-CD-NE2	-5.33	117.27	122.60
1	B	153	VAL	O-C-N	-5.33	116.70	121.87
1	C	199	THR	CA-C-N	5.33	125.58	119.83
1	C	199	THR	C-N-CA	5.33	125.58	119.83
1	D	74	GLN	CG-CD-NE2	5.33	124.39	116.40
1	C	215	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	A	113	ILE	CA-C-O	-5.32	115.88	121.41
1	D	147	GLY	O-C-N	-5.32	117.03	122.19
1	B	12	TYR	O-C-N	-5.31	116.49	123.02
1	B	13	GLY	CA-C-N	5.31	125.98	120.03
1	B	13	GLY	C-N-CA	5.31	125.98	120.03
1	B	140	THR	CA-C-N	5.30	125.37	119.32
1	B	140	THR	C-N-CA	5.30	125.37	119.32
1	B	156	LEU	CA-C-O	-5.30	115.22	120.90
1	A	77	ASP	CB-CA-C	-5.30	101.84	110.85
1	B	219	ASN	CB-CG-ND2	5.30	124.35	116.40
1	A	15	ARG	O-C-N	-5.29	115.57	122.39
1	D	238	ALA	O-C-N	-5.29	117.05	123.03
1	D	190	MET	N-CA-C	5.29	118.25	109.79
1	C	199	THR	CA-CB-OG1	-5.28	101.67	109.60
1	B	217	ARG	NE-CZ-NH2	-5.28	114.45	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	62	GLN	CA-C-O	-5.28	115.46	121.00
1	D	173	ALA	N-CA-C	-5.27	99.69	108.34
1	C	150	LYS	CA-C-N	5.27	131.73	121.41
1	C	150	LYS	C-N-CA	5.27	131.73	121.41
1	D	7	ARG	N-CA-C	5.27	121.25	114.56
1	A	216	LYS	N-CA-C	5.26	119.00	112.58
1	C	227	VAL	O-C-N	-5.26	117.61	123.03
1	C	167	MET	CA-C-N	5.26	125.18	119.76
1	C	167	MET	C-N-CA	5.26	125.18	119.76
1	D	198	TRP	CG-CD2-CE3	5.25	139.15	133.90
1	D	215	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	C	74	GLN	OE1-CD-NE2	-5.23	117.37	122.60
1	A	227	VAL	N-CA-C	5.23	115.38	107.75
1	C	120	LYS	CA-CB-CG	5.23	124.55	114.10
1	B	111	SER	O-C-N	-5.22	116.25	122.20
1	B	172	ALA	N-CA-C	5.22	117.33	109.23
1	B	44	ALA	O-C-N	-5.22	117.06	122.96
1	C	109	TRP	CA-C-N	5.22	127.28	120.28
1	C	109	TRP	C-N-CA	5.22	127.28	120.28
1	C	106	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	A	32	TRP	CB-CG-CD1	-5.21	119.08	126.90
1	C	80	LEU	N-CA-CB	5.21	118.92	110.17
1	A	235	LEU	CD1-CG-CD2	-5.20	99.35	110.80
1	D	86	TRP	CG-CD2-CE3	5.19	139.09	133.90
1	A	86	TRP	CE2-CD2-CG	-5.19	100.97	107.20
1	A	64	THR	O-C-N	-5.18	116.24	122.15
1	D	228	THR	CA-C-N	-5.18	115.80	123.05
1	D	228	THR	C-N-CA	-5.18	115.80	123.05
1	C	115	SER	CB-CA-C	-5.18	102.68	110.92
1	A	140	THR	CA-C-N	5.18	124.98	119.28
1	A	140	THR	C-N-CA	5.18	124.98	119.28
1	C	199	THR	CA-CB-CG2	5.17	119.29	110.50
1	B	54	ASP	CA-C-O	5.17	124.83	119.14
1	D	153	VAL	CA-C-O	5.17	126.32	120.95
1	A	109	TRP	CG-CD2-CE3	5.16	139.06	133.90
1	D	219	ASN	CB-CG-ND2	5.16	124.14	116.40
1	B	234	GLU	N-CA-C	5.16	117.48	108.76
1	D	140	THR	O-C-N	-5.16	116.20	121.31
1	D	190	MET	CA-C-N	5.15	124.76	119.56
1	D	190	MET	C-N-CA	5.15	124.76	119.56
1	A	219	ASN	N-CA-C	5.14	117.34	110.35
1	A	99	ASN	N-CA-C	5.14	118.33	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ALA	O-C-N	-5.13	117.37	123.22
1	D	226	VAL	O-C-N	5.13	128.93	122.66
1	D	6	ALA	O-C-N	-5.13	117.57	123.42
1	A	6	ALA	N-CA-C	5.13	116.63	108.79
1	A	53	THR	O-C-N	-5.12	117.54	123.33
1	C	155	GLN	CG-CD-NE2	5.12	124.09	116.40
1	A	13	GLY	CA-C-N	5.12	126.58	120.13
1	A	13	GLY	C-N-CA	5.12	126.58	120.13
1	D	54	ASP	CB-CA-C	-5.12	101.33	110.70
1	C	34	ALA	CB-CA-C	-5.12	102.45	110.79
1	D	47	SER	CA-CB-OG	-5.11	100.87	111.10
1	A	173	ALA	O-C-N	-5.11	117.25	123.13
1	B	74	GLN	CA-C-O	5.11	126.41	120.49
1	B	90	ASN	CA-CB-CG	5.10	117.70	112.60
1	C	111	SER	CB-CA-C	-5.10	102.18	110.85
1	D	136	ALA	O-C-N	-5.09	115.82	122.39
1	B	93	SER	CA-C-O	5.09	127.11	121.56
1	B	30	ASN	CA-CB-CG	-5.08	107.52	112.60
1	D	228	THR	CB-CA-C	-5.08	102.64	110.78
1	D	8	ARG	CA-C-O	-5.08	115.16	120.80
1	D	227	VAL	N-CA-C	5.08	115.28	107.77
1	D	106	GLN	CA-CB-CG	-5.08	103.95	114.10
1	A	52	MET	CB-CA-C	-5.06	102.67	110.26
1	A	121	HIS	CA-CB-CG	-5.06	108.74	113.80
1	B	32	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	C	225	GLN	CG-CD-NE2	5.05	123.98	116.40
1	C	236	THR	O-C-N	-5.05	116.89	121.39
1	C	218	PRO	CA-C-O	-5.05	114.47	121.90
1	B	49	ILE	N-CA-C	5.05	115.03	107.51
1	D	116	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	C	90	ASN	CA-CB-CG	5.03	117.63	112.60
1	C	85	GLY	O-C-N	-5.03	118.28	123.06
1	A	133	ALA	O-C-N	-5.02	117.76	123.48
1	D	99	ASN	CA-CB-CG	-5.01	107.59	112.60
1	A	38	VAL	N-CA-C	5.01	119.24	112.98
1	A	40	GLU	CA-C-N	-5.01	115.57	123.13
1	A	40	GLU	C-N-CA	-5.01	115.57	123.13

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	TYR	Sidechain
1	C	148	MET	Mainchain
1	C	190	MET	Peptide

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	1762	398	1760	28	1
1	B	1762	398	1760	30	13
1	C	1762	398	1760	53	14
1	D	1762	398	1760	49	2
2	A	44	8	26	4	0
2	B	44	8	26	5	0
2	C	44	8	26	2	0
2	D	44	8	26	5	0
3	A	38	76	0	2	0
3	B	36	72	0	4	6
3	C	39	78	0	17	2
3	D	35	70	0	7	2
All	All	7372	1920	7144	157	20

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 11.

All (157) 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:A:186:ASN:HD21	2:A:241:NAD:H72N	1.12	0.93
1:D:51:LYS:HE3	1:D:58:GLU:HG2	1.62	0.80
1:C:92:LYS:HG2	1:D:119:THR:HB	1.64	0.79
1:C:151:GLY:N	3:C:975:HOH:O	2.16	0.78
1:C:235:LEU:HD21	3:C:992:HOH:O	1.90	0.71
1:D:69:LYS:HG3	3:D:970:HOH:O	1.91	0.71
1:B:84:GLY:H	2:B:241:NAD:H52A	1.57	0.69
1:D:15:ARG:HH11	1:D:15:ARG:HA	1.58	0.67
1:D:76:VAL:O	1:D:123:LYS:HG3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ARG:HG2	3:C:965:HOH:O	1.94	0.67
1:A:10:LEU:HB2	1:A:79:ILE:HG12	1.75	0.66
1:B:84:GLY:HA3	2:B:241:NAD:O3D	1.95	0.65
1:B:202:GLU:HG3	3:B:970:HOH:O	1.95	0.65
1:C:94:LYS:HD3	1:C:94:LYS:H	1.61	0.65
1:B:182:ASP:HB2	1:B:198:TRP:HB3	1.79	0.64
1:A:174:ILE:HD13	1:A:218:PRO:HG2	1.80	0.64
1:C:71:LEU:HB2	3:C:976:HOH:O	1.98	0.64
1:D:186:ASN:HD21	2:D:241:NAD:H72N	1.45	0.64
1:C:174:ILE:HD13	1:C:218:PRO:HG2	1.79	0.63
1:D:174:ILE:HD13	3:D:959:HOH:O	2.00	0.62
1:D:51:LYS:H	1:D:62:GLN:NE2	1.98	0.61
1:D:134:LYS:HD3	1:D:179:VAL:HG22	1.80	0.61
1:C:208:PHE:O	1:C:212:ILE:HG13	2.00	0.61
1:A:21:ARG:NH2	1:A:202:GLU:HG3	2.17	0.60
1:C:229:THR:O	1:C:232:LYS:HD3	2.03	0.58
1:D:51:LYS:H	1:D:62:GLN:HE22	1.50	0.58
1:C:32:TRP:CH2	1:C:71:LEU:HD21	2.38	0.58
1:B:27:ARG:HD3	1:B:43:GLU:O	2.04	0.57
1:A:189:SER:O	1:A:191:PRO:HD3	2.04	0.57
1:C:167:MET:HE2	1:C:173:ALA:HB2	1.85	0.57
1:C:6:ALA:HB2	1:C:212:ILE:HG22	1.85	0.57
1:A:55:SER:HB3	1:A:58:GLU:HB2	1.87	0.57
1:A:41:ASN:HA	3:A:990:HOH:O	2.05	0.56
1:C:7:ARG:O	1:C:31:TRP:HB3	2.07	0.55
1:A:7:ARG:HG2	3:A:987:HOH:O	2.07	0.55
1:D:78:ALA:HA	1:D:127:LEU:O	2.06	0.55
1:C:51:LYS:HG3	1:C:51:LYS:O	2.06	0.55
1:D:84:GLY:HA3	2:D:241:NAD:O3D	2.06	0.55
1:D:106:GLN:HG2	2:D:241:NAD:C8A	2.37	0.55
1:D:21:ARG:NH2	1:D:202:GLU:HG3	2.23	0.54
1:C:148:MET:C	3:C:975:HOH:O	2.50	0.54
1:D:65:ALA:O	1:D:69:LYS:HG2	2.07	0.53
1:A:174:ILE:HD11	1:A:218:PRO:O	2.09	0.53
1:C:150:LYS:N	3:C:975:HOH:O	2.41	0.53
1:D:15:ARG:O	1:D:15:ARG:HD3	2.08	0.53
1:C:83:ALA:HA	2:C:241:NAD:H52A	1.89	0.53
1:A:157:CYS:SG	1:A:221:GLY:HA2	2.48	0.53
1:D:48:VAL:HA	3:D:988:HOH:O	2.09	0.52
1:B:189:SER:O	1:B:191:PRO:HD3	2.10	0.52
1:D:133:ALA:H	1:D:177:LEU:HG	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ALA:HB2	1:C:221:GLY:HA3	1.90	0.52
1:B:51:LYS:O	1:B:51:LYS:HG3	2.10	0.50
1:C:149:ALA:C	3:C:975:HOH:O	2.55	0.50
1:B:115:SER:O	1:B:118:ALA:HB3	2.11	0.50
1:C:148:MET:HE1	1:D:108:ILE:HG23	1.94	0.50
1:D:133:ALA:H	1:D:154:HIS:HE1	1.58	0.50
1:A:21:ARG:HH22	1:A:202:GLU:HG3	1.76	0.50
1:B:91:ALA:HA	1:B:96:LEU:HD13	1.94	0.49
1:D:21:ARG:NH1	3:D:974:HOH:O	2.45	0.49
1:B:51:LYS:HE3	1:B:53:THR:HB	1.94	0.49
1:B:185:MET:HB2	3:B:968:HOH:O	2.12	0.49
1:B:6:ALA:HB2	1:B:212:ILE:HG22	1.94	0.49
1:D:184:PRO:O	1:D:188:LYS:HD2	2.12	0.49
1:C:121:HIS:CG	3:C:976:HOH:O	2.64	0.49
1:B:27:ARG:HH11	1:B:27:ARG:HA	1.78	0.49
1:C:92:LYS:HG2	1:D:119:THR:CB	2.38	0.49
1:C:192:GLU:HB2	3:C:956:HOH:O	2.12	0.49
1:D:53:THR:CG2	1:D:59:GLN:HB2	2.43	0.49
1:A:186:ASN:ND2	2:A:241:NAD:H72N	1.94	0.49
1:C:71:LEU:HD12	3:C:976:HOH:O	2.12	0.48
1:B:60:ALA:HB1	3:B:957:HOH:O	2.13	0.48
1:C:197:SER:HA	1:C:228:THR:O	2.14	0.48
1:D:229:THR:O	1:D:232:LYS:HD3	2.13	0.48
1:A:16:GLY:HA3	2:A:241:NAD:O5B	2.13	0.48
1:A:90:ASN:HA	1:A:144:ILE:HG12	1.95	0.48
1:B:59:GLN:HE22	2:B:241:NAD:H62A	1.62	0.48
1:B:51:LYS:NZ	1:B:51:LYS:HB2	2.30	0.47
1:C:161:ALA:HB2	1:C:221:GLY:CA	2.44	0.47
1:C:6:ALA:HB2	1:C:212:ILE:CG2	2.45	0.47
1:D:218:PRO:HB2	3:D:959:HOH:O	2.14	0.47
1:C:5:GLU:CG	1:C:213:THR:HA	2.44	0.47
1:C:23:VAL:HG22	1:C:33:VAL:HG11	1.96	0.47
1:C:12:TYR:OH	1:C:113:ILE:HD12	2.15	0.47
1:A:186:ASN:HB3	1:A:198:TRP:CH2	2.50	0.46
1:B:215:ASN:OD1	1:B:216:LYS:HD3	2.14	0.46
1:C:133:ALA:H	1:C:154:HIS:HE1	1.61	0.46
1:D:199:THR:HG23	1:D:233:THR:HG21	1.96	0.46
1:D:208:PHE:O	1:D:212:ILE:HG13	2.15	0.46
1:B:219:ASN:O	1:B:222:SER:HB2	2.15	0.46
1:D:161:ALA:HB2	1:D:221:GLY:CA	2.46	0.46
1:A:124:GLU:HG3	1:A:169:SER:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:LEU:HB2	2:D:241:NAD:O7N	2.16	0.46
1:D:226:VAL:HG22	1:D:235:LEU:CD2	2.45	0.46
1:D:190:MET:HB2	1:D:198:TRP:HH2	1.81	0.46
1:C:5:GLU:HG2	1:C:213:THR:HA	1.97	0.45
1:C:191:PRO:HG2	3:C:956:HOH:O	2.16	0.45
1:B:161:ALA:HB2	1:B:221:GLY:CA	2.46	0.45
2:B:241:NAD:H2N	2:B:241:NAD:O5D	2.15	0.45
1:A:51:LYS:H	1:A:62:GLN:HE22	1.62	0.45
1:C:122:LEU:HB3	1:C:168:PRO:HG3	1.99	0.45
1:C:33:VAL:HB	3:C:965:HOH:O	2.17	0.45
1:C:189:SER:C	3:C:985:HOH:O	2.59	0.45
1:D:38:VAL:HG11	1:D:52:MET:SD	2.57	0.45
1:C:51:LYS:HE2	1:C:58:GLU:OE2	2.16	0.45
1:C:204:LEU:HD23	1:C:204:LEU:HA	1.83	0.44
1:A:83:ALA:HA	2:A:241:NAD:H52A	1.99	0.44
1:A:107:SER:HB2	1:A:149:ALA:HB1	2.00	0.44
1:D:161:ALA:HB2	1:D:221:GLY:HA3	1.99	0.44
1:C:223:LEU:HB2	1:C:238:ALA:HB3	1.99	0.44
1:B:122:LEU:HD23	1:B:168:PRO:HG2	2.00	0.43
1:D:53:THR:HG22	1:D:59:GLN:HB2	1.99	0.43
1:D:181:LEU:HD21	1:D:204:LEU:HD11	2.01	0.43
1:D:186:ASN:HB3	1:D:198:TRP:CZ3	2.54	0.43
1:B:60:ALA:C	3:B:957:HOH:O	2.61	0.43
1:C:16:GLY:O	1:C:20:SER:HB2	2.18	0.43
1:C:121:HIS:CE1	3:C:976:HOH:O	2.71	0.43
1:C:176:VAL:O	1:C:178:PRO:HD3	2.18	0.43
1:D:69:LYS:HD3	1:D:69:LYS:HA	1.74	0.43
1:D:228:THR:HA	1:D:233:THR:HA	2.00	0.43
1:D:219:ASN:O	1:D:222:SER:HB2	2.18	0.43
1:C:36:ILE:HG23	1:C:48:VAL:HB	2.01	0.43
1:A:198:TRP:CD1	1:A:198:TRP:N	2.83	0.43
1:C:94:LYS:HB2	1:C:94:LYS:HE2	1.86	0.43
1:A:53:THR:HG22	1:A:59:GLN:HB2	2.01	0.43
1:D:133:ALA:N	1:D:177:LEU:HG	2.34	0.42
1:B:50:VAL:HG21	2:B:241:NAD:H2A	2.01	0.42
1:C:203:PHE:HE1	3:C:992:HOH:O	2.02	0.42
1:B:64:THR:HA	1:B:117:LEU:HD21	2.01	0.42
1:C:154:HIS:HD2	3:C:970:HOH:O	2.01	0.42
1:D:37:ASP:O	1:D:49:ILE:HA	2.18	0.42
1:D:21:ARG:HH22	1:D:202:GLU:HG3	1.83	0.42
1:D:224:ILE:CG2	1:D:235:LEU:HD22	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:LYS:O	1:A:70:LEU:C	2.63	0.42
1:C:210:ASP:HB3	1:C:215:ASN:O	2.20	0.41
1:C:9:VAL:HG22	1:C:78:ALA:HB3	2.02	0.41
1:D:7:ARG:HD2	3:D:957:HOH:O	2.19	0.41
1:D:75:LYS:HE3	3:D:991:HOH:O	2.19	0.41
1:A:27:ARG:HG3	1:A:43:GLU:O	2.20	0.41
1:B:225:GLN:O	1:B:235:LEU:HA	2.21	0.41
1:A:27:ARG:HA	1:A:27:ARG:HD2	1.81	0.41
1:B:77:ASP:HA	1:B:123:LYS:HD2	2.02	0.41
1:C:84:GLY:HA3	2:C:241:NAD:O3D	2.20	0.41
1:B:71:LEU:HD12	1:B:121:HIS:ND1	2.35	0.41
1:C:134:LYS:HA	1:C:177:LEU:HD23	2.02	0.41
1:A:211:TRP:HA	1:A:217:ARG:HB2	2.02	0.41
1:D:106:GLN:HG2	2:D:241:NAD:H8A	2.02	0.41
1:A:97:PHE:HE1	1:B:113:ILE:HA	1.86	0.41
1:B:14:GLY:HA3	1:B:35:SER:OG	2.20	0.41
1:C:186:ASN:HB3	1:C:198:TRP:CZ3	2.56	0.41
1:D:94:LYS:N	1:D:94:LYS:HD3	2.36	0.41
1:A:212:ILE:HD13	1:A:212:ILE:HG21	1.78	0.41
1:B:125:GLY:HA2	1:B:170:GLY:O	2.20	0.41
1:C:150:LYS:C	3:C:975:HOH:O	2.61	0.40
1:D:134:LYS:HG2	1:D:225:GLN:HG2	2.03	0.40
1:A:21:ARG:HH22	1:A:202:GLU:CG	2.34	0.40
1:B:55:SER:HB3	1:B:58:GLU:HB3	2.03	0.40
1:C:23:VAL:HG22	1:C:33:VAL:CG1	2.50	0.40

All (20) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ARG:HH12	3:C:991:HOH:O[4_546]	0.64	0.96
1:C:95:SER:CB	3:B:971:HOH:O[4_546]	1.43	0.77
1:B:230:ASP:OD1	1:C:93:SER:OG[4_556]	1.53	0.67
1:B:21:ARG:NH1	3:C:991:HOH:O[4_546]	1.61	0.59
1:B:230:ASP:OD2	1:C:95:SER:OG[4_556]	1.66	0.54
1:B:193:ALA:O	1:C:92:LYS:HZ3[4_556]	1.07	0.53
1:C:95:SER:OG	3:B:971:HOH:O[4_546]	1.67	0.53
1:B:192:GLU:CG	1:D:75:LYS:NZ[4_556]	1.69	0.51
1:C:95:SER:OG	3:B:971:HOH:H2[4_546]	1.10	0.50
1:B:192:GLU:CG	1:D:75:LYS:HZ1[4_556]	1.21	0.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ASP:OD1	1:C:93:SER:CB[4_556]	1.86	0.34
1:A:21:ARG:HH21	1:C:239:TYR:HH[4_555]	1.30	0.30
1:C:90:ASN:ND2	3:B:959:HOH:O[4_546]	1.91	0.29
1:B:193:ALA:O	1:C:92:LYS:NZ[4_556]	2.02	0.18
1:B:230:ASP:OD1	1:C:93:SER:HG[4_556]	1.43	0.17
1:B:192:GLU:OE1	3:D:991:HOH:H1[4_556]	1.46	0.14
1:C:95:SER:CB	3:B:971:HOH:H1[4_546]	1.47	0.13
1:B:230:ASP:OD2	1:C:95:SER:HG[4_556]	1.56	0.04
1:B:192:GLU:OE1	3:D:991:HOH:O[4_556]	2.18	0.02
1:C:95:SER:CB	3:B:971:HOH:H2[4_546]	1.59	0.01

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	234/241 (97%)	215 (92%)	17 (7%)	2 (1%)	14	30
1	B	234/241 (97%)	224 (96%)	7 (3%)	3 (1%)	9	21
1	C	234/241 (97%)	221 (94%)	10 (4%)	3 (1%)	9	21
1	D	234/241 (97%)	211 (90%)	16 (7%)	7 (3%)	3	6
All	All	936/964 (97%)	871 (93%)	50 (5%)	15 (2%)	7	16

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	ALA
1	B	214	GLY
1	B	219	ASN
1	D	93	SER
1	D	214	GLY
1	D	17	ALA
1	D	46	ALA

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Mol	Chain	Res	Type
1	D	135	ALA
1	D	218	PRO
1	A	144	ILE
1	C	177	LEU
1	D	201	LEU
1	A	214	GLY
1	C	190	MET
1	C	179	VAL

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	185/187 (99%)	165 (89%)	20 (11%)	6	13
1	B	185/187 (99%)	170 (92%)	15 (8%)	11	24
1	C	185/187 (99%)	166 (90%)	19 (10%)	7	15
1	D	185/187 (99%)	163 (88%)	22 (12%)	5	10
All	All	740/748 (99%)	664 (90%)	76 (10%)	7	15

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	51	LYS
1	A	62	GLN
1	A	64	THR
1	A	70	LEU
1	A	74	GLN
1	A	90	ASN
1	A	93	SER
1	A	94	LYS
1	A	102	LEU
1	A	127	LEU
1	A	154	HIS
1	A	185	MET

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Mol	Chain	Res	Type
1	A	206	GLU
1	A	217	ARG
1	A	220	SER
1	A	229	THR
1	A	232	LYS
1	A	234	GLU
1	A	236	THR
1	B	27	ARG
1	B	33	VAL
1	B	39	VAL
1	B	51	LYS
1	B	62	GLN
1	B	67	VAL
1	B	90	ASN
1	B	94	LYS
1	B	157	CYS
1	B	169	SER
1	B	185	MET
1	B	192	GLU
1	B	216	LYS
1	B	222	SER
1	B	232	LYS
1	C	5	GLU
1	C	7	ARG
1	C	15	ARG
1	C	20	SER
1	C	21	ARG
1	C	30	ASN
1	C	39	VAL
1	C	42	GLU
1	C	45	SER
1	C	51	LYS
1	C	53	THR
1	C	59	GLN
1	C	67	VAL
1	C	69	LYS
1	C	80	LEU
1	C	90	ASN
1	C	94	LYS
1	C	189	SER
1	C	232	LYS
1	D	5	GLU

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Mol	Chain	Res	Type
1	D	7	ARG
1	D	15	ARG
1	D	39	VAL
1	D	40	GLU
1	D	45	SER
1	D	51	LYS
1	D	90	ASN
1	D	94	LYS
1	D	163	LYS
1	D	188	LYS
1	D	192	GLU
1	D	199	THR
1	D	216	LYS
1	D	218	PRO
1	D	222	SER
1	D	227	VAL
1	D	229	THR
1	D	230	ASP
1	D	232	LYS
1	D	236	THR
1	D	240	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	62	GLN
1	A	74	GLN
1	A	90	ASN
1	A	99	ASN
1	A	155	GLN
1	A	186	ASN
1	B	59	GLN
1	B	62	GLN
1	B	90	ASN
1	B	99	ASN
1	B	158	GLN
1	B	186	ASN
1	B	209	HIS
1	C	59	GLN
1	C	62	GLN
1	C	90	ASN

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Mol	Chain	Res	Type
1	C	99	ASN
1	C	154	HIS
1	C	155	GLN
1	C	158	GLN
1	C	186	ASN
1	C	209	HIS
1	D	30	ASN
1	D	59	GLN
1	D	62	GLN
1	D	90	ASN
1	D	106	GLN
1	D	154	HIS
1	D	186	ASN

5.3.3 RNA [i](#)

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](#)

4 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	D	241	-	46,48,48	2.86	13 (28%)	64,73,73	1.80	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	B	241	-	46,48,48	2.84	12 (26%)	64,73,73	1.78	12 (18%)
2	NAD	A	241	-	46,48,48	2.72	13 (28%)	64,73,73	1.55	9 (14%)
2	NAD	C	241	-	46,48,48	2.68	12 (26%)	64,73,73	1.55	8 (12%)

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	D	241	-	-	5/30/62/62	0/5/5/5
2	NAD	B	241	-	-	10/30/62/62	0/5/5/5
2	NAD	A	241	-	-	6/30/62/62	0/5/5/5
2	NAD	C	241	-	-	8/30/62/62	0/5/5/5

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	241	NAD	O7N-C7N	8.24	1.39	1.24
2	B	241	NAD	O7N-C7N	8.23	1.39	1.24
2	C	241	NAD	O7N-C7N	8.23	1.39	1.24
2	D	241	NAD	PN-O3	8.06	1.68	1.59
2	B	241	NAD	PN-O3	8.01	1.68	1.59
2	D	241	NAD	PA-O3	7.87	1.68	1.59
2	C	241	NAD	PA-O3	7.74	1.67	1.59
2	A	241	NAD	C3N-C7N	-7.55	1.39	1.50
2	D	241	NAD	O7N-C7N	6.99	1.37	1.24
2	B	241	NAD	PA-O3	6.90	1.66	1.59
2	A	241	NAD	PA-O3	6.72	1.66	1.59
2	D	241	NAD	C3N-C7N	-6.07	1.41	1.50
2	B	241	NAD	C3N-C7N	-6.02	1.41	1.50
2	C	241	NAD	C3N-C7N	-5.82	1.41	1.50
2	C	241	NAD	PN-O3	5.80	1.65	1.59
2	B	241	NAD	C8A-N7A	5.75	1.42	1.31
2	A	241	NAD	C8A-N7A	5.66	1.42	1.31
2	A	241	NAD	PN-O3	5.58	1.65	1.59
2	D	241	NAD	C5A-C4A	-5.23	1.29	1.39
2	C	241	NAD	C5A-C4A	-5.17	1.29	1.39
2	D	241	NAD	C8A-N7A	4.93	1.41	1.31
2	D	241	NAD	O4D-C1D	4.73	1.47	1.40
2	C	241	NAD	C8A-N7A	4.55	1.40	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	241	NAD	C2A-N1A	4.44	1.41	1.33
2	B	241	NAD	O4D-C1D	4.22	1.46	1.40
2	A	241	NAD	C5A-C4A	-4.14	1.31	1.39
2	D	241	NAD	C2N-N1N	4.11	1.39	1.35
2	C	241	NAD	C2A-N1A	4.07	1.41	1.33
2	B	241	NAD	C5A-C4A	-4.02	1.31	1.39
2	A	241	NAD	C2A-N1A	3.95	1.40	1.33
2	D	241	NAD	C2A-N1A	3.86	1.40	1.33
2	D	241	NAD	C1B-N9A	-3.83	1.35	1.46
2	B	241	NAD	C2N-N1N	3.80	1.39	1.35
2	B	241	NAD	C2A-N3A	3.59	1.40	1.33
2	C	241	NAD	C2A-N3A	3.55	1.40	1.33
2	A	241	NAD	O4D-C1D	3.42	1.45	1.40
2	C	241	NAD	C2N-N1N	3.34	1.38	1.35
2	A	241	NAD	C2N-N1N	3.11	1.38	1.35
2	A	241	NAD	C2A-N3A	3.09	1.39	1.33
2	D	241	NAD	C2A-N3A	2.88	1.39	1.33
2	C	241	NAD	C7N-N7N	2.66	1.37	1.33
2	C	241	NAD	C1B-N9A	-2.55	1.39	1.46
2	A	241	NAD	C6A-N6A	2.39	1.40	1.34
2	B	241	NAD	C7N-N7N	2.33	1.37	1.33
2	D	241	NAD	C5A-C6A	-2.29	1.34	1.41
2	B	241	NAD	C8A-N9A	2.27	1.41	1.37
2	A	241	NAD	C5A-C6A	-2.15	1.35	1.41
2	C	241	NAD	C5A-C6A	-2.11	1.35	1.41
2	D	241	NAD	C8A-N9A	2.04	1.41	1.37
2	A	241	NAD	PA-O5B	2.03	1.67	1.59

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	241	NAD	N9A-C8A-N7A	-5.51	106.12	113.94
2	D	241	NAD	C4A-N9A-C1B	-5.37	114.07	126.63
2	D	241	NAD	N3A-C2A-N1A	-5.34	120.50	128.58
2	B	241	NAD	O4B-C1B-N9A	5.24	118.16	108.09
2	A	241	NAD	N9A-C8A-N7A	-4.83	107.08	113.94
2	A	241	NAD	N3A-C2A-N1A	-4.81	121.31	128.58
2	B	241	NAD	N3A-C2A-N1A	-4.59	121.63	128.58
2	C	241	NAD	N3A-C2A-N1A	-4.51	121.76	128.58
2	D	241	NAD	N9A-C8A-N7A	-4.37	107.73	113.94
2	B	241	NAD	N9A-C8A-N7A	-4.17	108.02	113.94
2	D	241	NAD	O7N-C7N-N7N	-4.05	116.77	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	241	NAD	C4A-N9A-C1B	-3.82	117.70	126.63
2	D	241	NAD	C5A-C4A-N9A	3.74	109.89	105.81
2	D	241	NAD	C1B-N9A-C8A	-3.73	118.81	127.09
2	B	241	NAD	C5A-C4A-N9A	3.73	109.88	105.81
2	A	241	NAD	C6A-C5A-C4A	3.42	121.85	117.18
2	C	241	NAD	C4A-N9A-C1B	-3.40	118.68	126.63
2	B	241	NAD	O7N-C7N-N7N	-3.32	117.81	122.62
2	C	241	NAD	C6A-C5A-C4A	3.31	121.70	117.18
2	C	241	NAD	C5A-C4A-N9A	3.30	109.41	105.81
2	B	241	NAD	C1B-N9A-C8A	-3.28	119.81	127.09
2	A	241	NAD	C5A-C4A-N9A	3.23	109.33	105.81
2	B	241	NAD	C6A-C5A-C4A	3.18	121.53	117.18
2	C	241	NAD	O7N-C7N-N7N	-3.14	118.08	122.62
2	A	241	NAD	C6A-C5A-N7A	-2.95	126.41	132.09
2	B	241	NAD	C6A-C5A-N7A	-2.87	126.55	132.09
2	D	241	NAD	C3N-C7N-N7N	2.87	121.27	117.74
2	D	241	NAD	C6A-C5A-C4A	2.87	121.09	117.18
2	C	241	NAD	C6A-C5A-N7A	-2.81	126.66	132.09
2	B	241	NAD	C3N-C7N-N7N	2.77	121.15	117.74
2	B	241	NAD	C6N-N1N-C1D	-2.73	114.37	119.73
2	B	241	NAD	C5B-C4B-C3B	-2.69	105.53	115.21
2	D	241	NAD	C6A-C5A-N7A	-2.64	127.00	132.09
2	A	241	NAD	O7N-C7N-N7N	-2.63	118.81	122.62
2	A	241	NAD	C4A-N9A-C1B	-2.57	120.63	126.63
2	C	241	NAD	C3N-C7N-N7N	2.32	120.60	117.74
2	A	241	NAD	O2A-PA-O3	2.20	113.21	107.27
2	A	241	NAD	C1B-N9A-C8A	-2.11	122.42	127.09
2	D	241	NAD	C6N-N1N-C1D	-2.10	115.60	119.73
2	D	241	NAD	O4B-C1B-N9A	-2.10	104.06	108.09
2	D	241	NAD	O2N-PN-O3	2.10	112.94	107.27
2	D	241	NAD	O2A-PA-O3	2.03	112.76	107.27

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	241	NAD	C2B-C1B-N9A-C8A
2	A	241	NAD	O4D-C1D-N1N-C2N
2	A	241	NAD	O4D-C1D-N1N-C6N
2	A	241	NAD	C2D-C1D-N1N-C6N
2	B	241	NAD	C5B-O5B-PA-O1A
2	B	241	NAD	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	B	241	NAD	C5B-O5B-PA-O3
2	B	241	NAD	O4D-C1D-N1N-C2N
2	B	241	NAD	C2D-C1D-N1N-C2N
2	C	241	NAD	O4D-C1D-N1N-C2N
2	D	241	NAD	C2B-C1B-N9A-C8A
2	D	241	NAD	O4D-C1D-N1N-C2N
2	D	241	NAD	C2D-C1D-N1N-C2N
2	B	241	NAD	O4B-C4B-C5B-O5B
2	B	241	NAD	C3B-C4B-C5B-O5B
2	C	241	NAD	C2B-C1B-N9A-C8A
2	D	241	NAD	PN-O3-PA-O1A
2	B	241	NAD	PN-O3-PA-O1A
2	C	241	NAD	C2D-C1D-N1N-C2N
2	C	241	NAD	O4B-C4B-C5B-O5B
2	C	241	NAD	O4D-C1D-N1N-C6N
2	B	241	NAD	PN-O3-PA-O2A
2	C	241	NAD	PN-O3-PA-O1A
2	A	241	NAD	O4D-C4D-C5D-O5D
2	C	241	NAD	PN-O3-PA-O2A
2	A	241	NAD	O4B-C1B-N9A-C8A
2	D	241	NAD	O4B-C4B-C5B-O5B
2	C	241	NAD	O4B-C1B-N9A-C8A
2	B	241	NAD	C4D-C5D-O5D-PN

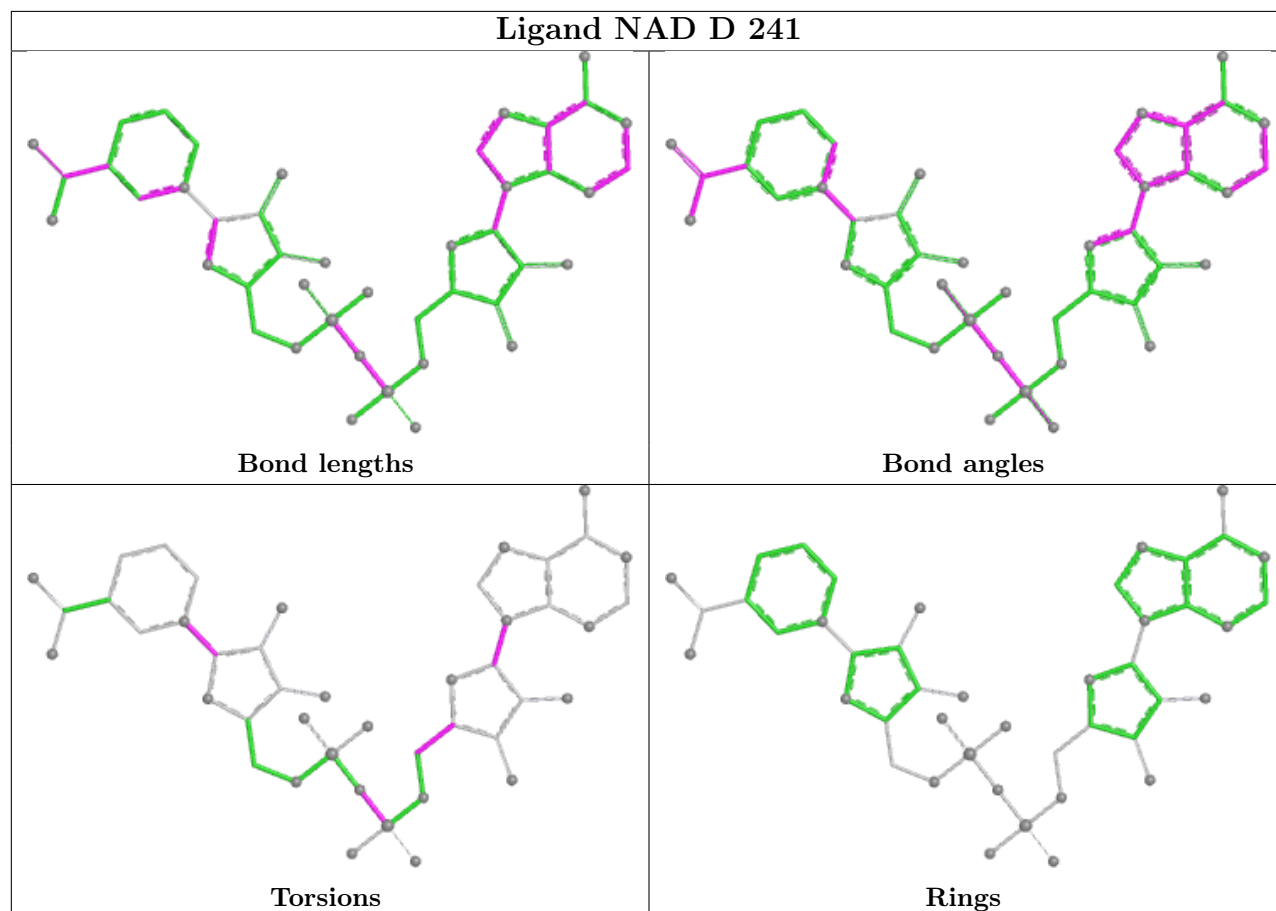
There are no ring outliers.

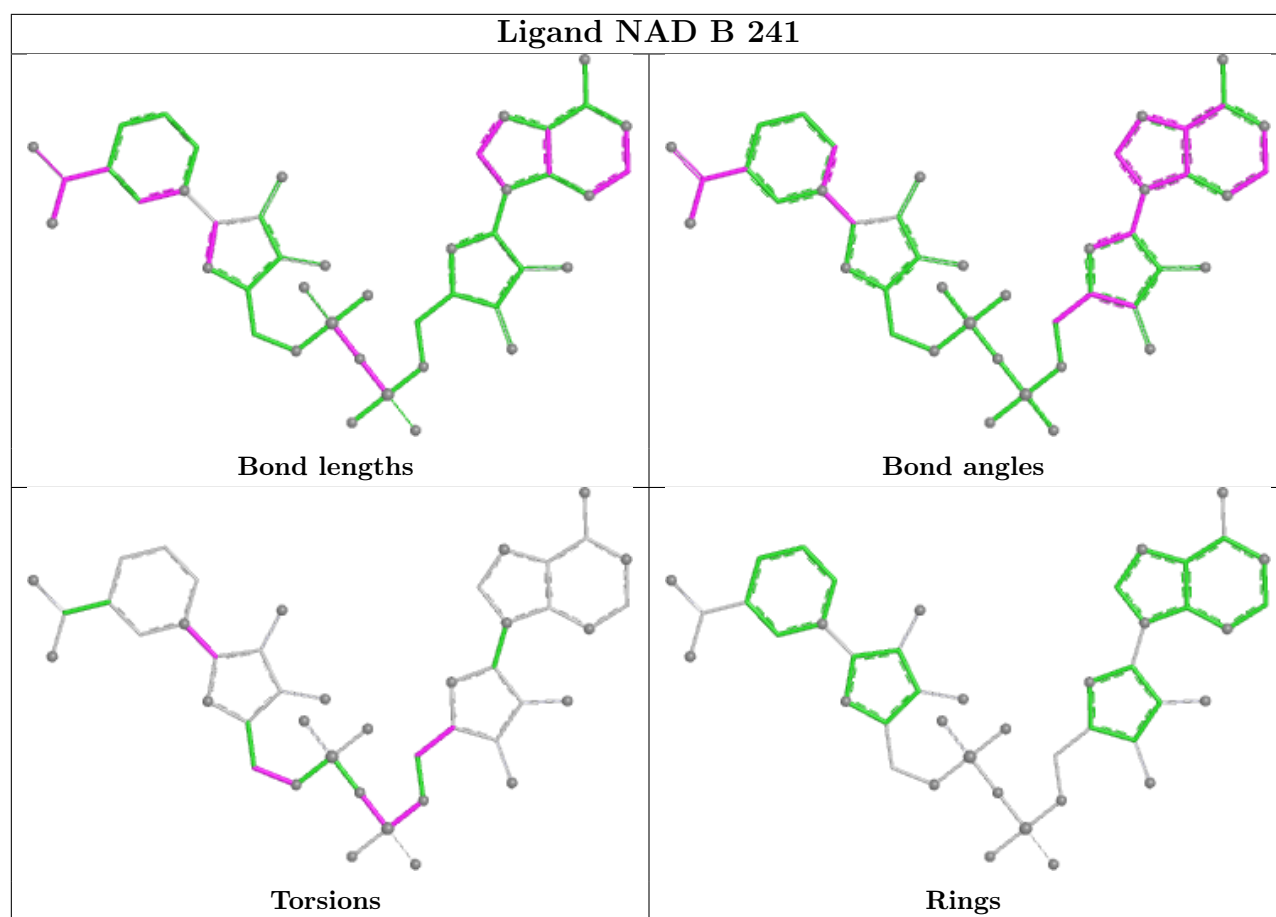
4 monomers are involved in 16 short contacts:

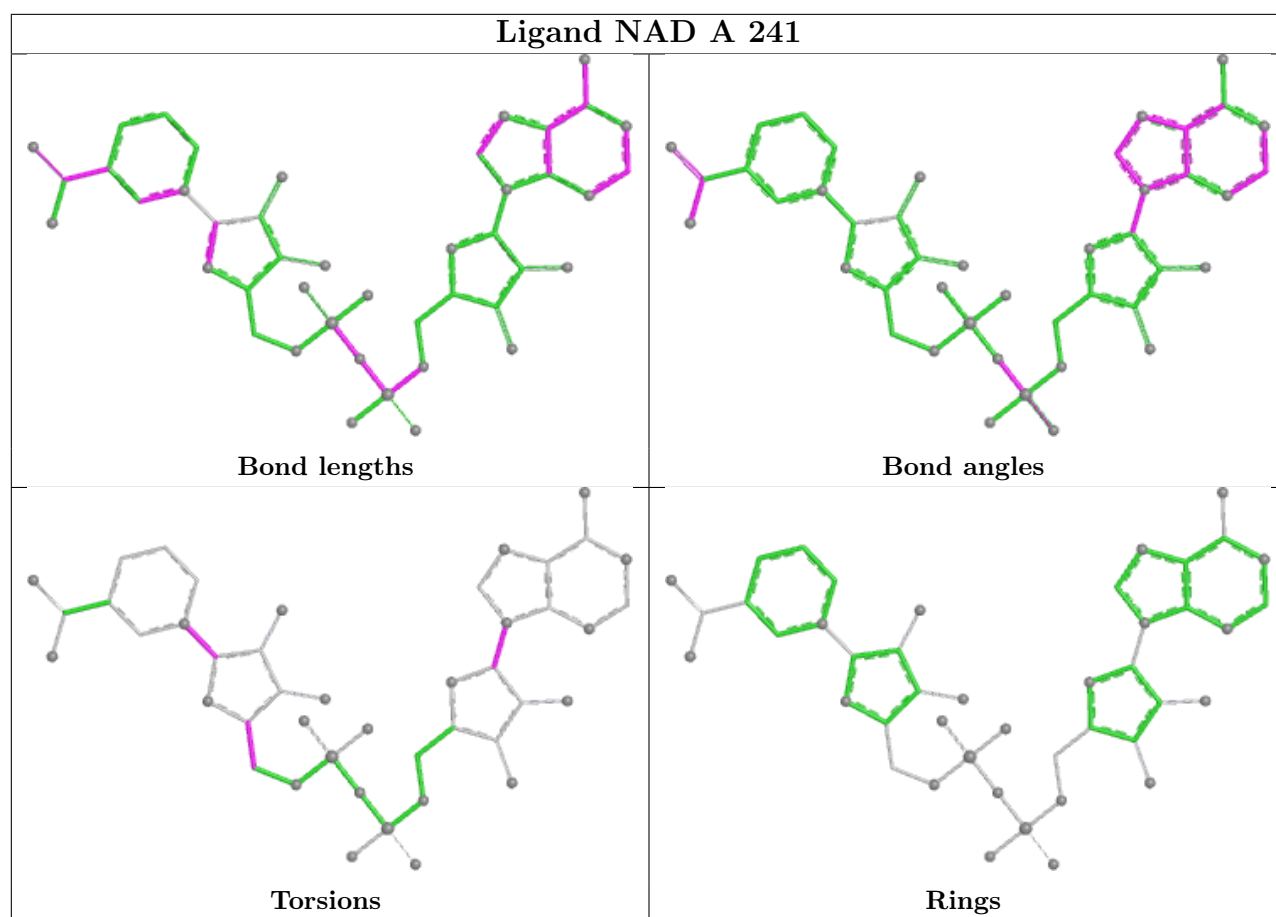
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	241	NAD	5	0
2	B	241	NAD	5	0
2	A	241	NAD	4	0
2	C	241	NAD	2	0

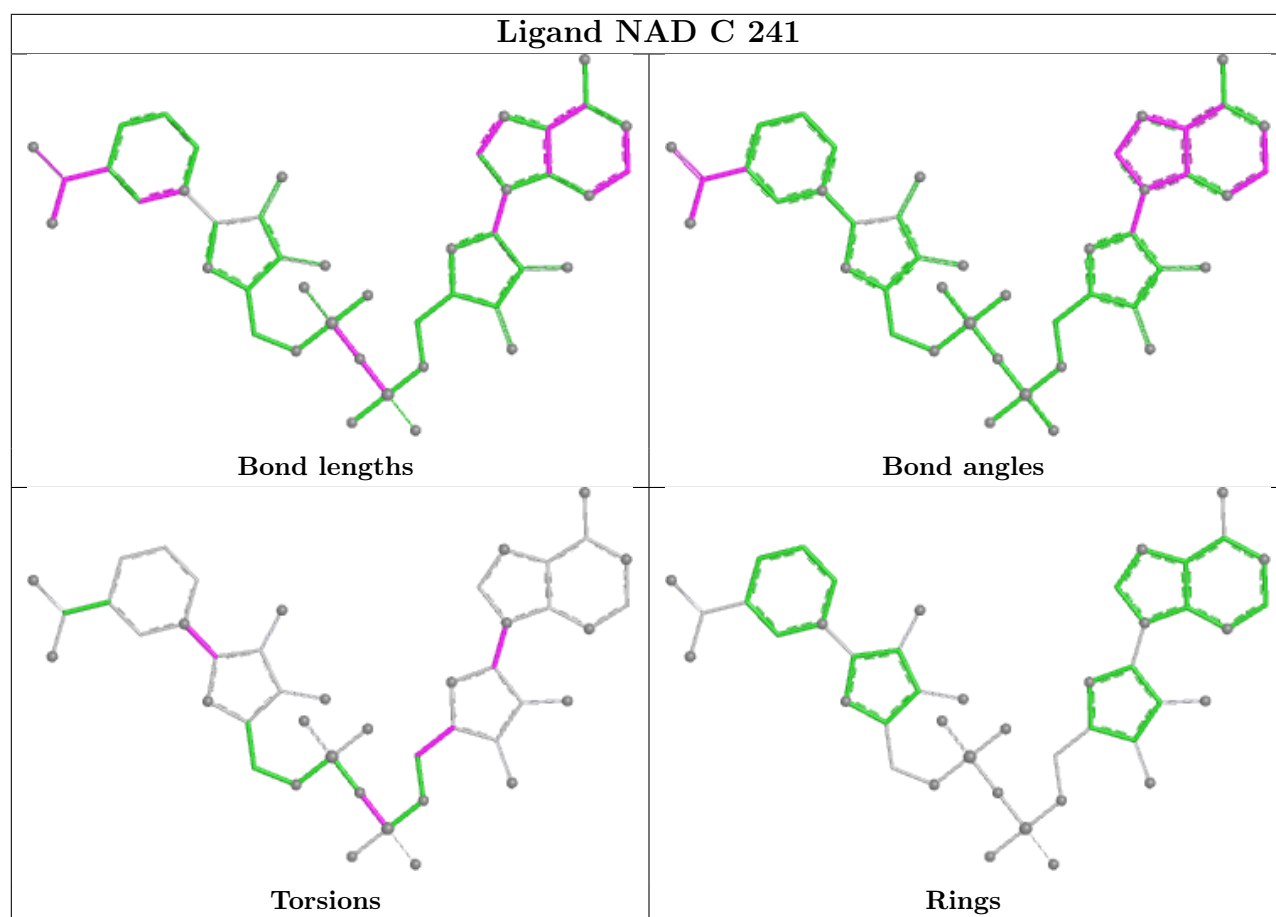
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 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	236/241 (97%)	0.61	12 (5%) 33 28	2, 16, 34, 52	0
1	B	236/241 (97%)	1.14	45 (19%) 3 2	3, 15, 31, 47	0
1	C	236/241 (97%)	1.07	28 (11%) 9 7	4, 15, 34, 53	0
1	D	236/241 (97%)	1.37	57 (24%) 2 1	5, 17, 38, 64	0
All	All	944/964 (97%)	1.05	142 (15%) 5 4	2, 16, 35, 64	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	68	GLY	6.2
1	D	76	VAL	5.1
1	B	228	THR	5.0
1	D	16	GLY	4.9
1	D	55	SER	4.6
1	D	60	ALA	4.3
1	B	233	THR	4.2
1	D	37	ASP	4.0
1	D	25	ALA	3.9
1	A	191	PRO	3.9
1	C	37	ASP	3.8
1	B	213	THR	3.7
1	B	189	SER	3.7
1	B	6	ALA	3.6
1	B	192	GLU	3.6
1	B	30	ASN	3.5
1	C	192	GLU	3.5
1	D	45	SER	3.5
1	C	189	SER	3.4
1	D	189	SER	3.4
1	B	195	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	197	SER	3.3
1	B	5	GLU	3.2
1	D	53	THR	3.2
1	D	19	GLY	3.2
1	C	95	SER	3.2
1	D	71	LEU	3.1
1	D	239	TYR	3.1
1	A	189	SER	3.1
1	B	44	ALA	3.1
1	B	230	ASP	3.0
1	B	216	LYS	3.0
1	B	207	THR	3.0
1	A	157	CYS	3.0
1	C	196	SER	2.9
1	B	210	ASP	2.9
1	D	85	GLY	2.9
1	C	193	ALA	2.9
1	B	196	SER	2.9
1	D	165	SER	2.9
1	D	229	THR	2.9
1	C	71	LEU	2.9
1	C	170	GLY	2.8
1	B	231	GLY	2.8
1	B	23	VAL	2.8
1	C	16	GLY	2.7
1	D	24	GLN	2.7
1	D	162	GLY	2.7
1	D	185	MET	2.7
1	D	46	ALA	2.7
1	C	184	PRO	2.7
1	B	209	HIS	2.7
1	C	40	GLU	2.7
1	B	78	ALA	2.7
1	D	149	ALA	2.7
1	A	192	GLU	2.6
1	D	20	SER	2.6
1	D	230	ASP	2.6
1	D	30	ASN	2.6
1	D	47	SER	2.6
1	B	101	ASP	2.6
1	B	234	GLU	2.6
1	B	204	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	74	GLN	2.5
1	C	93	SER	2.5
1	B	163	LYS	2.5
1	D	113	ILE	2.5
1	A	185	MET	2.5
1	D	100	CYS	2.4
1	D	84	GLY	2.4
1	D	6	ALA	2.4
1	C	164	ASN	2.4
1	C	52	MET	2.4
1	B	32	TRP	2.4
1	B	232	LYS	2.4
1	D	63	VAL	2.4
1	D	193	ALA	2.4
1	C	180	THR	2.4
1	A	165	SER	2.4
1	D	159	SER	2.4
1	D	125	GLY	2.4
1	B	84	GLY	2.3
1	B	8	ARG	2.3
1	B	238	ALA	2.3
1	C	25	ALA	2.3
1	A	69	LYS	2.3
1	B	157	CYS	2.3
1	D	34	ALA	2.3
1	B	183	THR	2.3
1	C	232	LYS	2.3
1	D	188	LYS	2.3
1	A	184	PRO	2.3
1	B	194	ASP	2.3
1	D	101	ASP	2.3
1	B	65	ALA	2.3
1	D	215	ASN	2.3
1	D	190	MET	2.2
1	B	229	THR	2.2
1	C	96	LEU	2.2
1	B	51	LYS	2.2
1	C	171	ALA	2.2
1	D	43	GLU	2.2
1	D	38	VAL	2.2
1	D	102	LEU	2.2
1	C	56	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	199	THR	2.2
1	B	215	ASN	2.2
1	B	16	GLY	2.2
1	A	95	SER	2.2
1	D	78	ALA	2.1
1	D	87	ALA	2.1
1	D	12	TYR	2.1
1	B	185	MET	2.1
1	C	185	MET	2.1
1	C	19	GLY	2.1
1	C	142	GLY	2.1
1	D	95	SER	2.1
1	D	169	SER	2.1
1	D	28	ALA	2.1
1	D	168	PRO	2.1
1	D	126	GLY	2.1
1	A	73	ASP	2.1
1	C	129	THR	2.1
1	B	71	LEU	2.1
1	A	170	GLY	2.1
1	C	68	GLY	2.1
1	B	26	PHE	2.1
1	B	138	ASP	2.1
1	C	118	ALA	2.1
1	B	74	GLN	2.1
1	D	40	GLU	2.0
1	C	55	SER	2.0
1	D	115	SER	2.0
1	D	171	ALA	2.0
1	D	112	THR	2.0
1	A	153	VAL	2.0
1	C	131	ALA	2.0
1	D	220	SER	2.0
1	B	140	THR	2.0
1	D	70	LEU	2.0
1	B	38	VAL	2.0
1	D	67	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

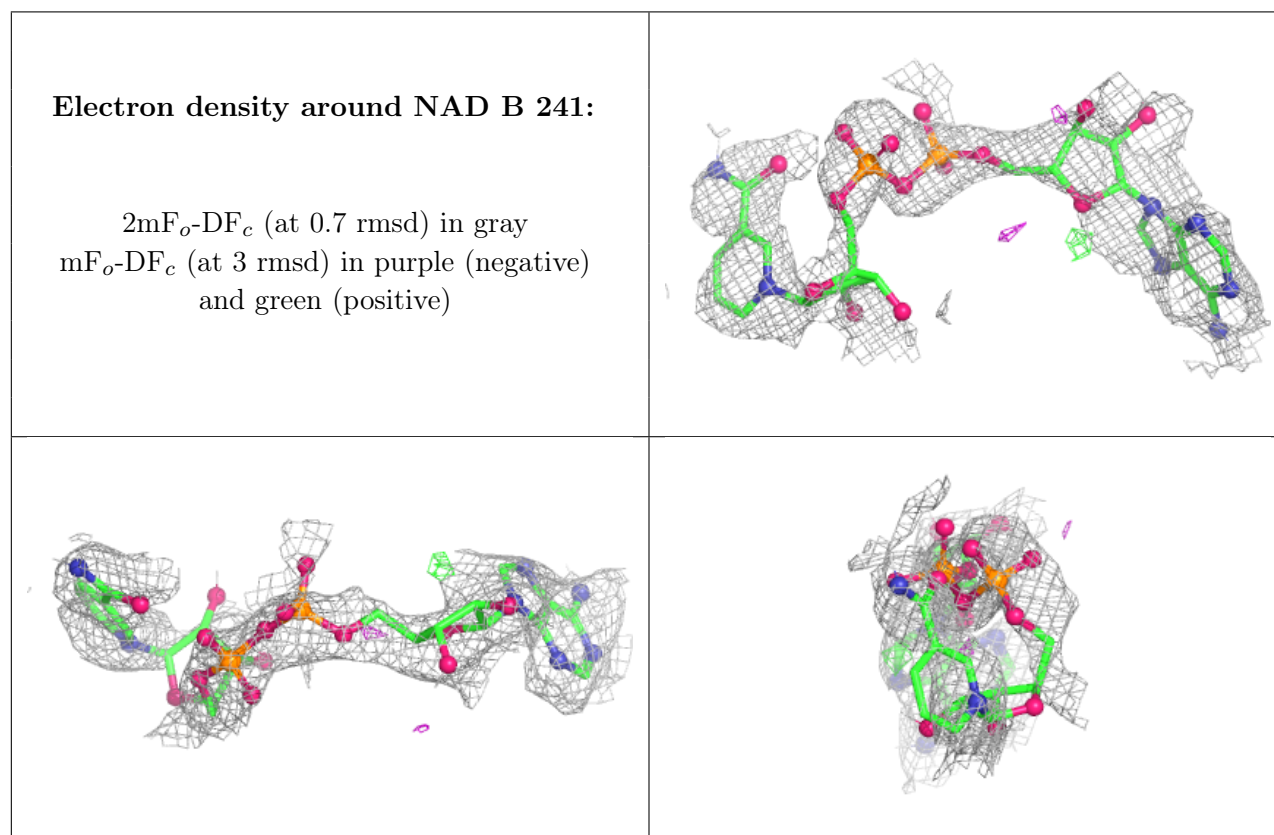
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

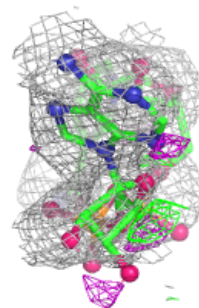
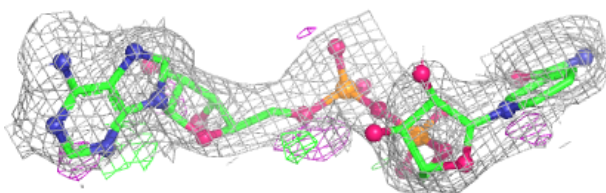
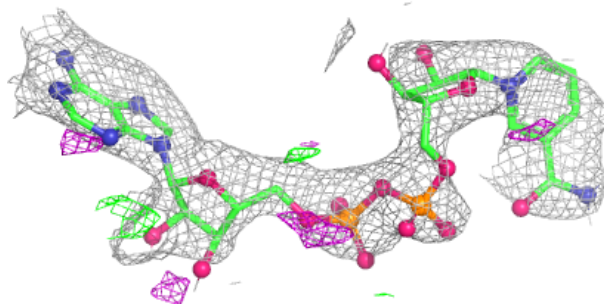
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	B	241	44/44	0.56	0.16	0,52,65,70	0
2	NAD	C	241	44/44	0.75	0.16	0,36,50,54	0
2	NAD	A	241	44/44	0.79	0.13	0,40,46,48	0
2	NAD	D	241	44/44	0.80	0.13	0,27,38,39	0

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.

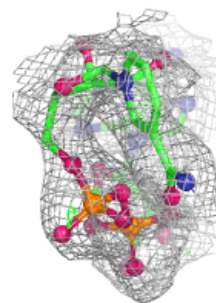
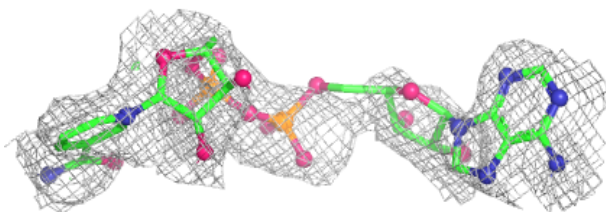
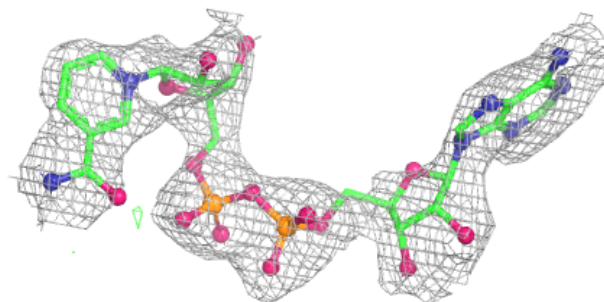


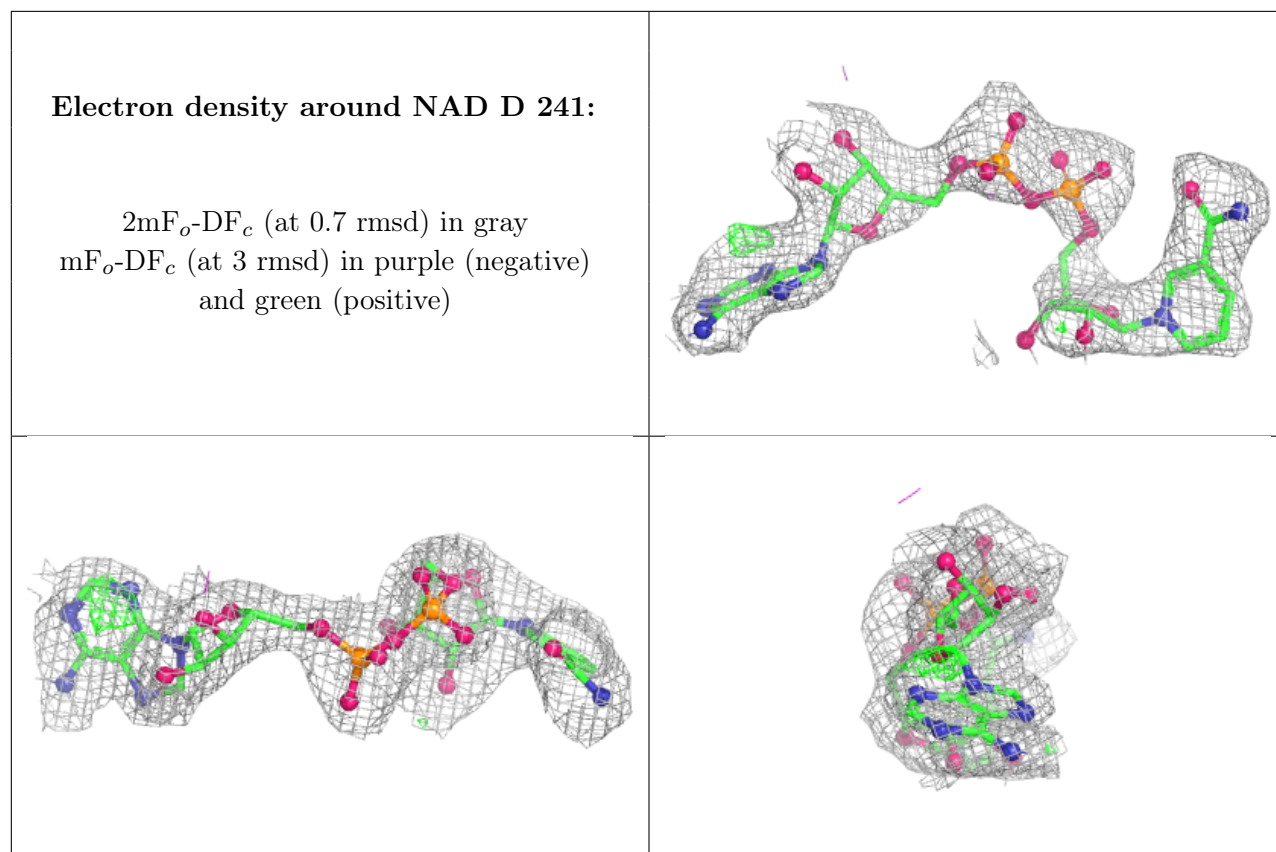
Electron density around NAD C 241:

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

**Electron density around NAD A 241:**

$2mF_o-DF_c$ (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.