



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:04 PM UTC

PDB ID : 2Q2Q / pdb_00002q2q
Title : Structure of D-3-Hydroxybutyrate Dehydrogenase from Pseudomonas putida
Authors : Paithankar, K.S.; Feller, C.; Kuettner, E.B.; Keim, A.; Grunow, M.; Strater, N.
Deposited on : 2007-05-29
Resolution : 2.02 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

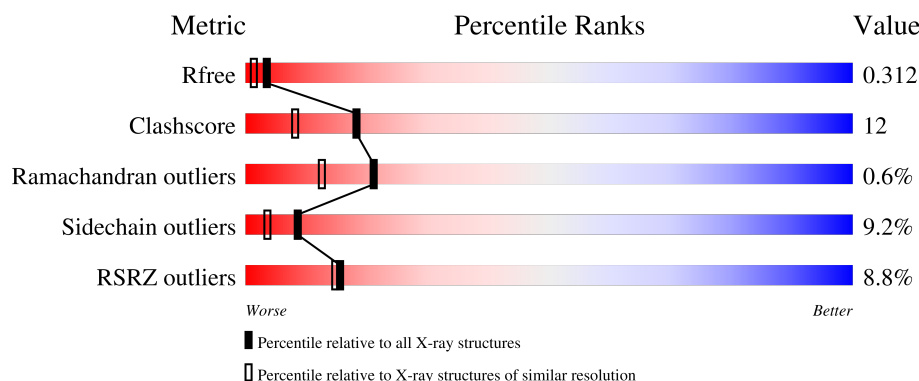
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	255	9% 66% 27% 5%
1	B	255	7% 73% 21% • •
1	C	255	15% 63% 28% • 5%
1	D	255	4% 71% 25% •
1	E	255	9% 63% 30% • •

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Mol	Chain	Length	Quality of chain
1	F	255	6% 66% 21% 6% 7%
1	G	255	8% 71% 22% 5%
1	H	255	10% 64% 25% 5% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15261 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 Beta-D-hydroxybutyrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1843	1171	330	338	4			
1	B	252	Total	C	N	O	S	0	0	0
			1852	1176	332	340	4			
1	C	243	Total	C	N	O	S	0	0	0
			1784	1137	319	324	4			
1	D	255	Total	C	N	O	S	0	0	0
			1869	1185	336	344	4			
1	E	249	Total	C	N	O	S	0	0	0
			1833	1165	329	335	4			
1	F	238	Total	C	N	O	S	0	0	0
			1742	1110	311	317	4			
1	G	251	Total	C	N	O	S	0	0	0
			1845	1173	331	337	4			
1	H	240	Total	C	N	O	S	0	0	0
			1758	1120	314	320	4			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total	O	0	0
			61	61		
3	B	83	Total	O	0	0
			83	83		
3	C	37	Total	O	0	0
			37	37		
3	D	70	Total	O	0	0
			70	70		
3	E	55	Total	O	0	0
			55	55		
3	F	50	Total	O	0	0
			50	50		

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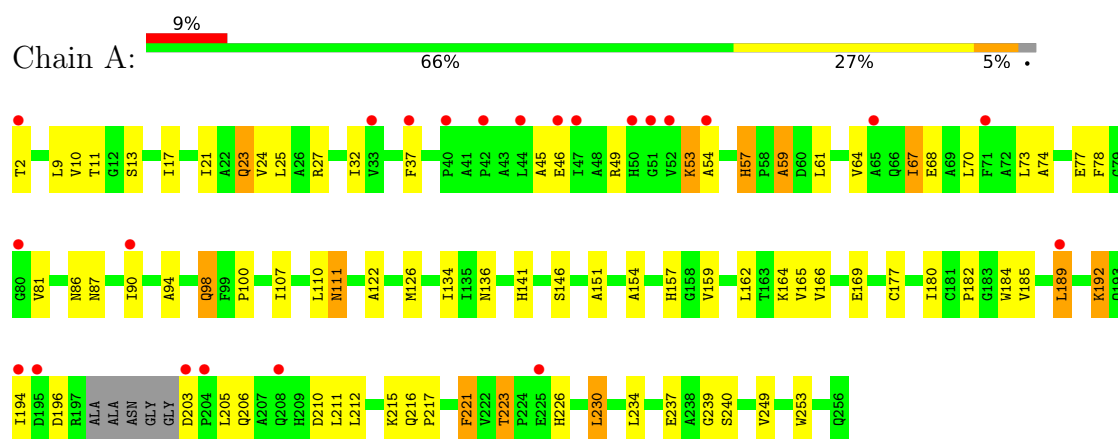
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	71	Total	O	0	0
			71	71		
3	H	44	Total	O	0	0
			44	44		

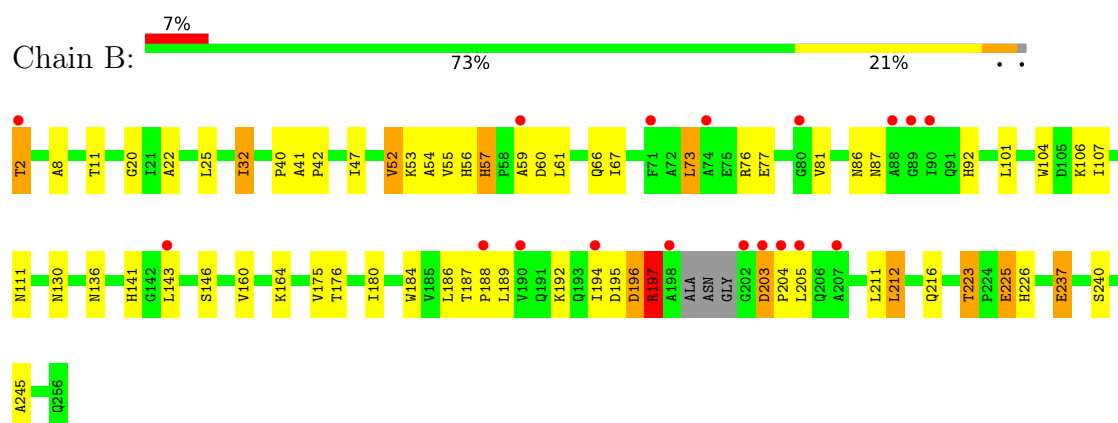
3 Residue-property plots [i](#)

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.

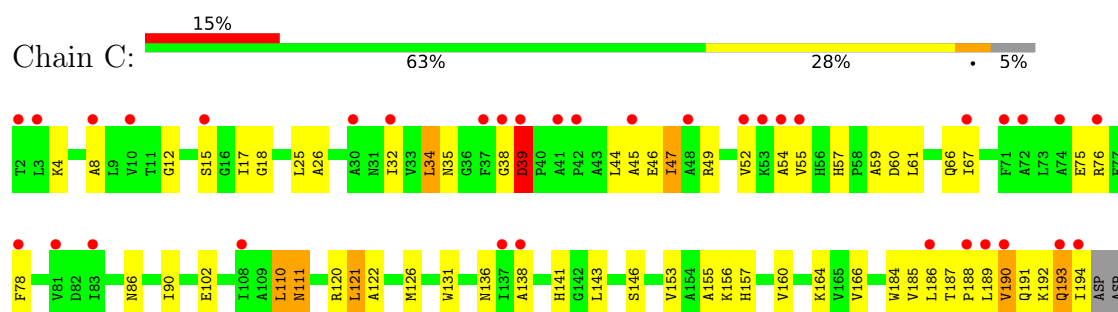
- Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

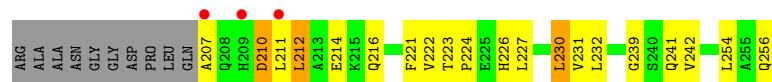


- Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

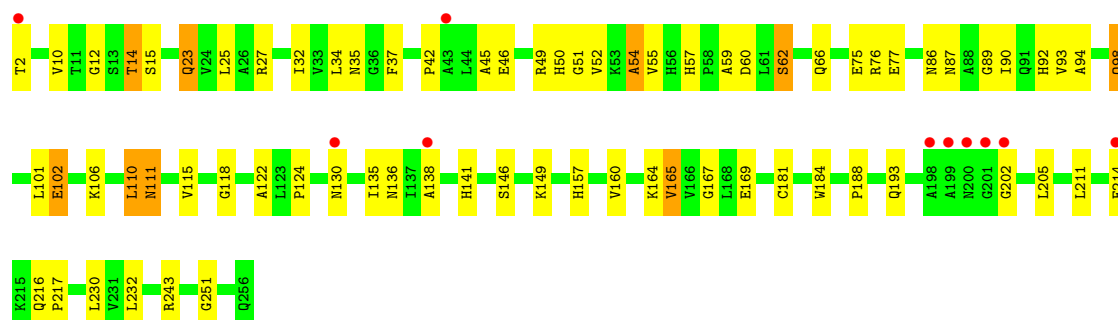


- Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

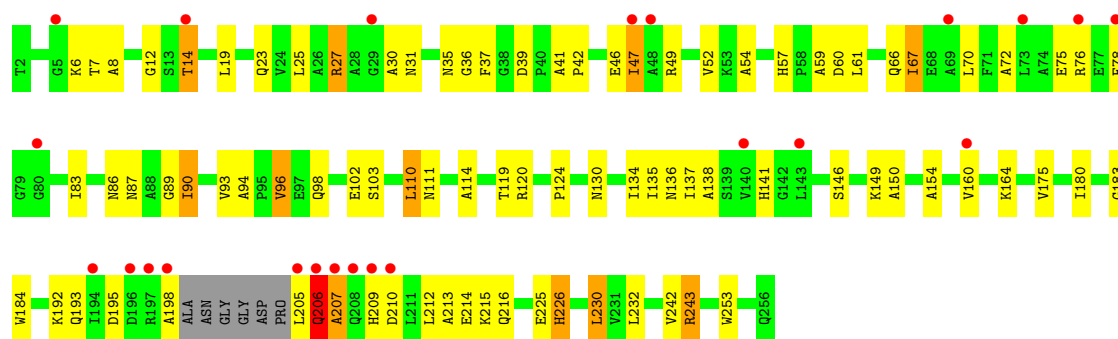




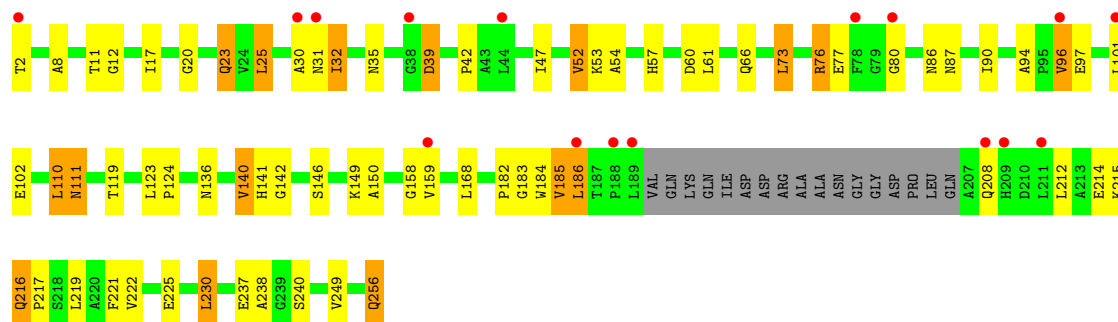
• Molecule 1: Beta-D-hydroxybutyrate dehydrogenase



• Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

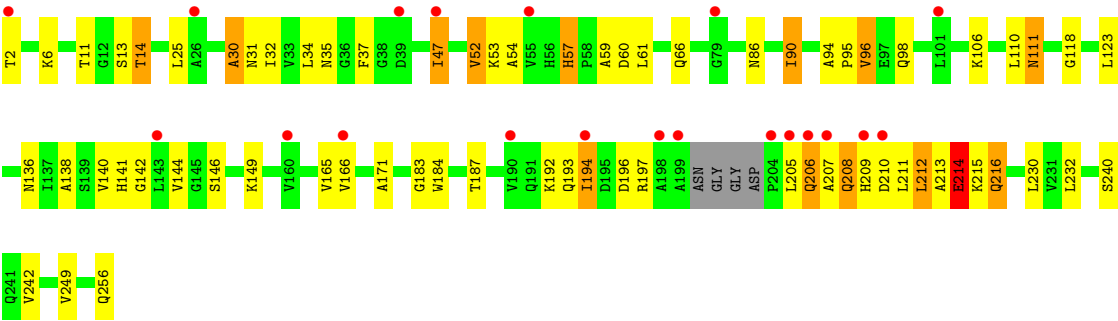


• Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

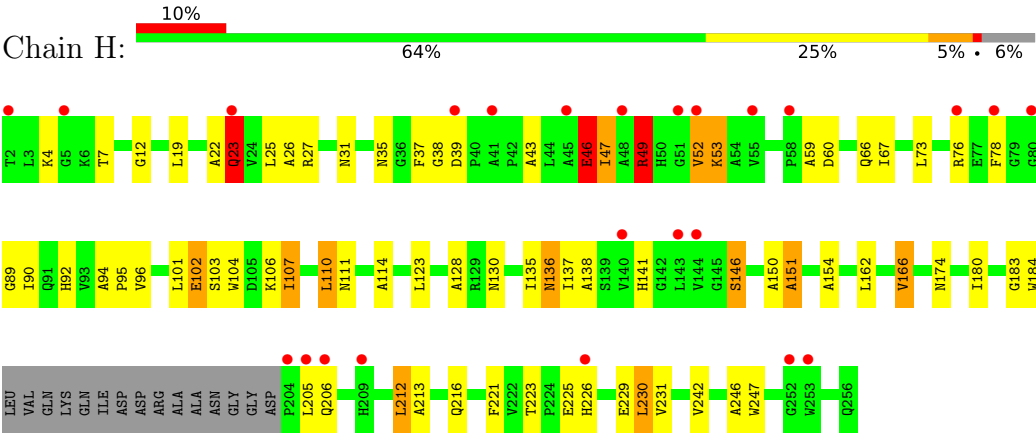


• Molecule 1: Beta-D-hydroxybutyrate dehydrogenase





● Molecule 1: Beta-D-hydroxybutyrate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	261.46Å 59.91Å 116.52Å 90.00° 113.70° 90.00°	Depositor
Resolution (Å)	30.00 – 2.02 30.00 – 2.02	Depositor EDS
% Data completeness (in resolution range)	96.4 (30.00-2.02) 96.3 (30.00-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.03Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.199 , 0.274 0.254 , 0.312	Depositor DCC
R_{free} test set	5241 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.009 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15261	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5024e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
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	1.49	10/1879 (0.5%)	1.36	12/2560 (0.5%)
1	B	1.52	14/1888 (0.7%)	1.35	8/2572 (0.3%)
1	C	1.38	8/1819 (0.4%)	1.33	6/2478 (0.2%)
1	D	1.64	14/1906 (0.7%)	1.41	8/2598 (0.3%)
1	E	1.71	14/1868 (0.7%)	1.45	17/2544 (0.7%)
1	F	1.60	15/1777 (0.8%)	1.35	9/2422 (0.4%)
1	G	1.83	12/1881 (0.6%)	1.49	19/2562 (0.7%)
1	H	1.65	19/1794 (1.1%)	1.46	18/2445 (0.7%)
All	All	1.61	106/14812 (0.7%)	1.40	97/20181 (0.5%)

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	E	0	2
1	H	0	2
All	All	0	4

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	209	HIS	CE1-NE2	32.35	1.65	1.32
1	G	209	HIS	CG-ND1	20.87	1.61	1.38
1	E	206	GLN	CD-OE1	18.27	1.58	1.23
1	E	206	GLN	CD-NE2	15.94	1.66	1.33
1	G	209	HIS	CG-CD2	11.67	1.48	1.35
1	G	165	VAL	CA-CB	9.75	1.65	1.54
1	G	30	ALA	CA-CB	8.26	1.66	1.53
1	H	146	SER	N-CA	8.06	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	209	HIS	CE1-NE2	7.90	1.40	1.32
1	E	93	VAL	CA-CB	7.89	1.63	1.54
1	H	242	VAL	CA-CB	7.50	1.62	1.53
1	H	23	GLN	CG-CD	7.47	1.70	1.52
1	E	209	HIS	CG-ND1	7.34	1.46	1.38
1	D	75	GLU	CG-CD	7.31	1.70	1.52
1	H	67	ILE	CA-CB	7.27	1.62	1.54
1	C	46	GLU	C-O	7.26	1.33	1.24
1	E	90	ILE	C-O	7.20	1.32	1.23
1	F	168	LEU	N-CA	7.08	1.54	1.46
1	C	155	ALA	CA-CB	7.03	1.64	1.53
1	G	249	VAL	CA-CB	6.93	1.61	1.53
1	H	94	ALA	CA-CB	6.88	1.64	1.54
1	A	9	LEU	C-O	-6.79	1.16	1.24
1	D	122	ALA	CA-CB	-6.60	1.43	1.53
1	G	242	VAL	CA-CB	6.48	1.61	1.53
1	A	24	VAL	CA-CB	6.43	1.62	1.54
1	B	160	VAL	CA-CB	-6.41	1.46	1.54
1	C	44	LEU	C-O	6.41	1.32	1.24
1	E	206	GLN	C-O	6.38	1.32	1.24
1	H	94	ALA	N-CA	6.35	1.52	1.46
1	D	10	VAL	CA-CB	6.34	1.62	1.54
1	F	256	GLN	C-OXT	6.31	1.36	1.23
1	C	166	VAL	CA-C	6.26	1.60	1.52
1	H	137	ILE	CA-CB	-6.22	1.47	1.53
1	B	104	TRP	C-O	-6.22	1.17	1.24
1	H	85	VAL	CA-CB	6.12	1.61	1.53
1	F	216	GLN	CA-C	6.09	1.58	1.52
1	A	221	PHE	CA-C	-6.03	1.44	1.52
1	B	92	HIS	N-CA	6.02	1.53	1.46
1	E	213	ALA	CA-CB	5.97	1.62	1.53
1	F	238	ALA	C-O	5.95	1.31	1.24
1	C	164	LYS	C-O	-5.94	1.17	1.24
1	F	39	ASP	N-CA	5.89	1.52	1.46
1	B	176	THR	N-CA	-5.87	1.38	1.45
1	H	221	PHE	CA-C	-5.85	1.45	1.53
1	H	154	ALA	CA-CB	5.79	1.62	1.53
1	F	158	GLY	N-CA	5.78	1.53	1.45
1	A	67	ILE	CA-CB	5.77	1.61	1.54
1	A	74	ALA	CA-CB	5.73	1.62	1.53
1	F	230	LEU	C-O	-5.71	1.17	1.24
1	D	214	GLU	CG-CD	5.68	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	188	PRO	C-O	5.68	1.34	1.23
1	G	140	VAL	CA-CB	5.67	1.62	1.54
1	E	30	ALA	CA-CB	5.67	1.62	1.53
1	F	140	VAL	CA-CB	5.62	1.62	1.54
1	B	245	ALA	CA-CB	-5.62	1.44	1.53
1	F	32	ILE	CA-CB	5.60	1.61	1.54
1	B	143	LEU	N-CA	5.55	1.53	1.46
1	H	23	GLN	CD-NE2	5.55	1.44	1.33
1	H	246	ALA	CA-C	5.54	1.59	1.53
1	D	135	ILE	CA-CB	5.53	1.61	1.54
1	B	175	VAL	N-CA	5.51	1.53	1.46
1	H	95	PRO	N-CA	5.51	1.53	1.47
1	B	237	GLU	C-O	-5.47	1.17	1.24
1	F	185	VAL	CA-C	5.45	1.59	1.52
1	D	54	ALA	C-O	-5.44	1.17	1.23
1	A	57	HIS	CA-C	5.43	1.57	1.52
1	D	118	GLY	N-CA	5.41	1.52	1.45
1	B	2	THR	CB-CG2	5.41	1.70	1.52
1	B	32	ILE	CA-CB	5.38	1.61	1.54
1	D	181	CYS	CA-C	-5.36	1.47	1.52
1	D	115	VAL	CB-CG1	5.36	1.70	1.52
1	D	124	PRO	C-O	-5.34	1.17	1.24
1	G	142	GLY	N-CA	5.34	1.53	1.45
1	F	214	GLU	CB-CG	5.33	1.68	1.52
1	F	102	GLU	CB-CG	5.32	1.68	1.52
1	C	241	GLN	N-CA	5.32	1.52	1.46
1	E	137	ILE	CA-C	5.31	1.58	1.53
1	D	23	GLN	CD-NE2	5.30	1.44	1.33
1	F	249	VAL	CA-CB	5.30	1.61	1.53
1	E	135	ILE	CA-CB	5.29	1.60	1.54
1	E	175	VAL	CA-CB	5.28	1.60	1.54
1	G	166	VAL	CA-CB	5.27	1.60	1.54
1	H	151	ALA	CA-CB	5.26	1.61	1.53
1	G	118	GLY	C-O	5.25	1.30	1.23
1	E	67	ILE	CA-CB	5.24	1.60	1.54
1	A	81	VAL	CA-CB	5.20	1.60	1.54
1	A	239	GLY	N-CA	5.19	1.52	1.45
1	C	160	VAL	C-O	-5.19	1.18	1.24
1	B	22	ALA	CA-CB	5.18	1.61	1.53
1	D	165	VAL	C-O	-5.14	1.18	1.24
1	A	151	ALA	CA-CB	5.13	1.61	1.53
1	H	136	ASN	C-O	-5.10	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	ALA	N-CA	5.09	1.52	1.46
1	G	90	ILE	C-O	5.09	1.29	1.23
1	H	19	LEU	CA-C	5.09	1.59	1.52
1	B	180	ILE	C-O	-5.08	1.18	1.24
1	B	223	THR	CA-C	5.08	1.59	1.52
1	F	215	LYS	N-CA	5.08	1.52	1.46
1	D	23	GLN	CG-CD	5.07	1.64	1.52
1	D	92	HIS	CA-C	5.07	1.58	1.52
1	H	107	ILE	CG1-CD1	-5.06	1.32	1.51
1	F	219	LEU	N-CA	5.06	1.53	1.46
1	H	128	ALA	C-O	-5.02	1.18	1.24
1	B	81	VAL	CA-CB	-5.01	1.48	1.54
1	C	230	LEU	C-O	5.01	1.29	1.24
1	E	36	GLY	C-O	5.01	1.27	1.23

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	39	ASP	CA-C-N	10.66	130.49	119.19
1	H	39	ASP	C-N-CA	10.66	130.49	119.19
1	A	94	ALA	CA-C-N	-10.34	108.85	119.92
1	A	94	ALA	C-N-CA	-10.34	108.85	119.92
1	F	183	GLY	N-CA-C	-9.07	96.99	112.77
1	A	98	GLN	CB-CA-C	-8.70	96.01	110.72
1	G	96	VAL	CB-CA-C	-8.59	98.85	112.16
1	D	62	SER	CB-CA-C	-7.72	96.34	110.63
1	G	144	VAL	CA-C-N	-7.66	114.41	122.30
1	G	144	VAL	C-N-CA	-7.66	114.41	122.30
1	E	94	ALA	CA-C-N	-7.29	112.12	119.92
1	E	94	ALA	C-N-CA	-7.29	112.12	119.92
1	E	206	GLN	OE1-CD-NE2	6.81	129.41	122.60
1	E	183	GLY	N-CA-C	-6.75	101.03	112.77
1	H	166	VAL	N-CA-C	-6.68	104.25	110.53
1	G	213	ALA	N-CA-C	6.56	118.43	111.28
1	E	243	ARG	NE-CZ-NH2	-6.51	113.34	119.20
1	E	154	ALA	N-CA-C	-6.47	104.14	111.07
1	C	242	VAL	N-CA-C	-6.39	98.66	107.99
1	B	240	SER	N-CA-C	6.38	119.92	111.75
1	H	226	HIS	N-CA-C	-6.38	104.33	111.28
1	G	209	HIS	ND1-CG-CD2	6.33	112.43	106.10
1	E	41	ALA	CA-C-N	-6.32	112.03	119.05
1	E	41	ALA	C-N-CA	-6.32	112.03	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	57	HIS	CA-C-N	-6.32	113.73	120.94
1	G	57	HIS	C-N-CA	-6.32	113.73	120.94
1	G	205	LEU	N-CA-C	-6.29	105.63	113.55
1	H	229	GLU	N-CA-C	6.19	118.03	111.28
1	E	206	GLN	CG-CD-NE2	-6.18	107.13	116.40
1	H	183	GLY	N-CA-C	-6.14	102.09	112.77
1	G	123	LEU	N-CA-C	6.08	121.16	113.25
1	F	240	SER	N-CA-C	6.02	118.63	111.71
1	F	208	GLN	N-CA-C	-5.99	104.39	111.03
1	E	243	ARG	CG-CD-NE	-5.89	99.05	112.00
1	C	121	LEU	N-CA-C	5.87	117.48	111.14
1	G	194	ILE	CB-CA-C	-5.86	104.23	112.14
1	B	52	VAL	CB-CA-C	5.83	120.02	110.69
1	E	96	VAL	N-CA-C	5.83	116.48	110.36
1	G	187	THR	CA-C-N	-5.83	113.81	119.87
1	G	187	THR	C-N-CA	-5.83	113.81	119.87
1	H	212	LEU	N-CA-C	5.78	117.25	111.07
1	C	39	ASP	CA-C-N	5.74	126.61	120.47
1	C	39	ASP	C-N-CA	5.74	126.61	120.47
1	E	226	HIS	CB-CA-C	-5.73	100.94	110.68
1	D	75	GLU	CA-CB-CG	5.69	125.49	114.10
1	B	203	ASP	CA-C-N	5.67	125.20	119.19
1	B	203	ASP	C-N-CA	5.67	125.20	119.19
1	G	183	GLY	N-CA-C	-5.64	102.95	112.77
1	G	171	ALA	N-CA-C	5.61	118.11	111.33
1	G	212	LEU	N-CA-C	5.57	117.81	111.02
1	B	212	LEU	N-CA-C	5.56	119.33	112.54
1	H	213	ALA	N-CA-C	5.52	118.22	111.82
1	G	214	GLU	CB-CA-C	-5.49	101.34	110.68
1	G	240	SER	N-CA-C	5.48	118.77	111.75
1	F	159	VAL	N-CA-C	5.48	116.21	110.62
1	C	239	GLY	N-CA-C	-5.48	106.08	115.61
1	D	167	GLY	N-CA-C	-5.42	106.23	112.73
1	H	7	THR	N-CA-C	5.37	118.00	109.24
1	F	94	ALA	N-CA-C	5.36	112.95	108.13
1	H	123	LEU	CA-C-N	-5.33	113.14	119.05
1	H	123	LEU	C-N-CA	-5.33	113.14	119.05
1	F	119	THR	N-CA-C	5.31	117.48	111.11
1	D	102	GLU	N-CA-C	5.31	119.01	112.54
1	C	222	VAL	N-CA-C	-5.30	102.23	109.55
1	B	20	GLY	N-CA-C	-5.29	106.37	112.50
1	F	142	GLY	N-CA-C	-5.28	106.60	115.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	26	ALA	CA-C-N	5.27	128.08	120.38
1	H	26	ALA	C-N-CA	5.27	128.08	120.38
1	D	211	LEU	N-CA-C	-5.26	105.44	111.07
1	H	23	GLN	CB-CG-CD	5.23	121.49	112.60
1	D	75	GLU	N-CA-C	-5.21	105.50	111.07
1	D	243	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	G	94	ALA	CA-C-N	-5.18	114.44	119.78
1	G	94	ALA	C-N-CA	-5.18	114.44	119.78
1	A	159	VAL	N-CA-C	5.18	115.39	110.42
1	A	240	SER	N-CA-C	5.17	117.65	111.71
1	A	59	ALA	N-CA-C	5.16	117.57	110.35
1	B	57	HIS	CA-C-N	-5.15	113.40	119.84
1	B	57	HIS	C-N-CA	-5.15	113.40	119.84
1	E	213	ALA	CA-C-N	-5.15	112.12	121.14
1	E	213	ALA	C-N-CA	-5.15	112.12	121.14
1	A	210	ASP	N-CA-C	-5.15	105.79	111.71
1	A	223	THR	CA-C-N	5.14	124.59	119.24
1	A	223	THR	C-N-CA	5.14	124.59	119.24
1	D	98	GLN	CB-CA-C	-5.12	101.51	110.17
1	E	243	ARG	NE-CZ-NH1	5.11	126.61	121.50
1	A	157	HIS	CA-C-N	5.10	125.74	120.03
1	A	157	HIS	C-N-CA	5.10	125.74	120.03
1	H	4	LYS	N-CA-C	5.09	117.23	111.02
1	E	39	ASP	CA-C-N	-5.07	114.56	120.04
1	E	39	ASP	C-N-CA	-5.07	114.56	120.04
1	H	22	ALA	CA-C-N	5.05	127.36	120.54
1	H	22	ALA	C-N-CA	5.05	127.36	120.54
1	H	247	TRP	N-CA-C	-5.02	101.05	109.24
1	F	256	GLN	CA-C-O	-5.02	105.93	121.00
1	A	67	ILE	N-CA-CB	5.01	116.99	110.57
1	F	80	GLY	N-CA-C	5.01	117.15	112.04

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	206	GLN	Sidechain
1	E	207	ALA	Peptide
1	H	38	GLY	Peptide
1	H	49	ARG	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	1843	0	1865	60	0
1	B	1852	0	1873	34	0
1	C	1784	0	1814	57	0
1	D	1869	0	1888	47	0
1	E	1833	0	1859	51	0
1	F	1742	0	1765	48	0
1	G	1845	0	1872	33	0
1	H	1758	0	1781	39	0
2	C	44	0	26	1	0
2	D	44	0	26	2	0
2	E	44	0	26	4	0
2	F	44	0	26	3	0
2	G	44	0	26	2	0
2	H	44	0	26	1	0
3	A	61	0	0	2	0
3	B	83	0	0	1	0
3	C	37	0	0	1	0
3	D	70	0	0	4	0
3	E	55	0	0	1	1
3	F	50	0	0	1	0
3	G	71	0	0	1	1
3	H	44	0	0	2	0
All	All	15261	0	14873	359	1

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 (359) 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:C:32:ILE:HG22	1:C:34:LEU:HD13	1.27	1.08
1:F:186:LEU:HD23	1:F:186:LEU:H	1.19	1.07
1:C:32:ILE:HG22	1:C:34:LEU:CD1	1.90	1.01
1:E:184:TRP:H	1:E:216:GLN:HE22	1.09	1.00
1:C:32:ILE:CG2	1:C:34:LEU:CD1	2.39	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:TRP:H	1:F:216:GLN:HE22	1.08	0.98
1:F:141:HIS:HE1	1:F:146:SER:OG	1.49	0.94
1:H:184:TRP:H	1:H:216:GLN:HE22	1.10	0.94
1:D:14:THR:HG21	1:D:37:PHE:O	1.68	0.92
1:F:186:LEU:H	1:F:186:LEU:CD2	1.83	0.90
1:C:32:ILE:CG2	1:C:34:LEU:HD13	2.03	0.87
1:D:42:PRO:O	1:D:46:GLU:HG2	1.74	0.87
1:F:256:GLN:OXT	3:F:317:HOH:O	1.93	0.87
1:H:96:VAL:HG12	1:H:150:ALA:HB2	1.57	0.87
1:A:184:TRP:H	1:A:216:GLN:HE22	1.17	0.87
1:C:184:TRP:H	1:C:216:GLN:HE22	1.23	0.86
1:G:184:TRP:H	1:G:216:GLN:HE22	1.24	0.86
1:E:27:ARG:NH1	3:E:342:HOH:O	2.09	0.86
1:B:184:TRP:H	1:B:216:GLN:HE22	1.25	0.84
1:G:141:HIS:HE1	1:G:146:SER:OG	1.62	0.83
1:A:189:LEU:HD12	1:A:189:LEU:O	1.79	0.83
1:G:14:THR:HG21	1:G:37:PHE:O	1.77	0.82
1:C:45:ALA:O	1:C:49:ARG:HG2	1.80	0.81
1:A:57:HIS:CE1	1:A:59:ALA:HB2	2.15	0.81
1:D:184:TRP:H	1:D:216:GLN:HE22	1.27	0.80
1:C:32:ILE:HG21	1:C:34:LEU:CD1	2.12	0.80
1:D:51:GLY:HA2	1:F:53:LYS:HD3	1.65	0.79
1:G:57:HIS:HD2	1:G:59:ALA:H	1.31	0.79
1:E:86:ASN:HD22	1:E:136:ASN:HD21	1.32	0.78
3:D:365:HOH:O	1:H:92:HIS:HD2	1.65	0.78
1:E:90:ILE:H	1:E:111:ASN:HD21	1.33	0.77
1:C:32:ILE:HG21	1:C:34:LEU:HD11	1.68	0.76
1:G:95:PRO:HG2	1:G:98:GLN:OE1	1.86	0.75
1:A:53:LYS:HG3	1:A:78:PHE:HE1	1.52	0.75
1:E:14:THR:HG22	2:E:300:NAD:O3B	1.87	0.74
1:H:90:ILE:H	1:H:111:ASN:HD21	1.33	0.74
1:A:111:ASN:HD22	1:A:111:ASN:N	1.83	0.74
1:B:86:ASN:HD22	1:B:136:ASN:HD21	1.34	0.74
1:E:184:TRP:N	1:E:216:GLN:HE22	1.85	0.74
1:F:141:HIS:CE1	1:F:146:SER:OG	2.38	0.74
1:C:76:ARG:NE	1:C:76:ARG:HA	2.03	0.73
1:B:86:ASN:HD22	1:B:136:ASN:ND2	1.85	0.73
1:F:90:ILE:H	1:F:111:ASN:HD21	1.34	0.73
1:E:72:ALA:O	1:E:76:ARG:HG3	1.88	0.73
1:G:57:HIS:CD2	1:G:59:ALA:H	2.06	0.72
1:G:47:ILE:HD11	1:G:54:ALA:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:HIS:HB2	1:B:73:LEU:HD12	1.70	0.71
1:B:101:LEU:HD12	1:B:101:LEU:H	1.54	0.71
1:F:186:LEU:HD23	1:F:186:LEU:N	1.99	0.71
1:C:38:GLY:O	1:C:39:ASP:CB	2.38	0.71
1:G:86:ASN:HD22	1:G:136:ASN:ND2	1.88	0.71
1:D:90:ILE:H	1:D:111:ASN:HD21	1.38	0.70
1:A:184:TRP:H	1:A:216:GLN:NE2	1.90	0.69
1:E:14:THR:HG21	1:E:37:PHE:O	1.91	0.69
1:A:86:ASN:HD22	1:A:136:ASN:ND2	1.91	0.69
1:E:96:VAL:HG22	1:E:150:ALA:HB2	1.74	0.69
1:A:57:HIS:HB2	1:A:73:LEU:HD23	1.73	0.69
1:E:49:ARG:HD3	1:E:49:ARG:C	2.17	0.69
1:A:141:HIS:HE1	1:A:146:SER:OG	1.76	0.69
1:G:90:ILE:H	1:G:111:ASN:HD21	1.42	0.68
1:F:73:LEU:HD22	1:F:77:GLU:HG2	1.75	0.68
1:B:164:LYS:NZ	1:C:157:HIS:HE1	1.92	0.68
1:C:111:ASN:N	1:C:111:ASN:HD22	1.91	0.68
1:F:30:ALA:O	1:F:52:VAL:HG11	1.94	0.67
1:F:184:TRP:N	1:F:216:GLN:HE22	1.87	0.67
1:H:90:ILE:HG13	1:H:107:ILE:CD1	2.25	0.67
1:E:86:ASN:HD22	1:E:136:ASN:ND2	1.93	0.67
1:H:184:TRP:N	1:H:216:GLN:HE22	1.90	0.66
1:D:12:GLY:H	1:D:35:ASN:HD22	1.42	0.66
1:G:86:ASN:HD22	1:G:136:ASN:HD21	1.42	0.66
1:C:60:ASP:H	1:C:66:GLN:NE2	1.93	0.65
1:F:47:ILE:CG2	1:F:54:ALA:HB2	2.25	0.65
1:C:57:HIS:HD2	1:C:59:ALA:H	1.45	0.65
1:F:186:LEU:HD22	1:F:221:PHE:HB3	1.78	0.65
1:H:60:ASP:H	1:H:66:GLN:NE2	1.95	0.65
1:B:55:VAL:HG11	1:B:77:GLU:HG3	1.79	0.64
3:D:365:HOH:O	1:H:92:HIS:CD2	2.46	0.64
1:H:102:GLU:C	1:H:106:LYS:HE3	2.23	0.64
1:F:184:TRP:H	1:F:216:GLN:NE2	1.89	0.63
1:D:138:ALA:O	2:D:300:NAD:H6N	1.98	0.63
1:E:47:ILE:CG1	1:E:54:ALA:HB2	2.28	0.63
1:H:141:HIS:HE1	1:H:146:SER:OG	1.80	0.63
1:E:184:TRP:H	1:E:216:GLN:NE2	1.88	0.63
1:A:90:ILE:HG22	1:A:111:ASN:HD21	1.63	0.62
1:C:184:TRP:N	1:C:216:GLN:HE22	1.93	0.62
1:E:47:ILE:HD11	1:E:54:ALA:HB2	1.79	0.62
1:H:73:LEU:HD12	1:H:76:ARG:NH2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:225:GLU:H	1:H:225:GLU:CD	2.08	0.62
1:C:143:LEU:HD12	1:C:254:LEU:CD1	2.29	0.62
1:D:45:ALA:O	1:D:49:ARG:HD2	1.99	0.62
1:G:256:GLN:OXT	3:G:310:HOH:O	2.16	0.62
1:A:90:ILE:HB	1:A:110:LEU:HD23	1.82	0.61
1:D:51:GLY:HA2	1:F:53:LYS:CD	2.29	0.61
1:H:102:GLU:O	1:H:106:LYS:HE3	2.01	0.61
1:A:86:ASN:HD22	1:A:136:ASN:HD21	1.47	0.61
1:C:61:LEU:HD22	1:C:67:ILE:HG12	1.83	0.61
1:F:47:ILE:HG22	1:F:54:ALA:HB2	1.81	0.60
1:H:86:ASN:HD22	1:H:136:ASN:HD21	1.50	0.60
1:D:141:HIS:HE1	1:D:146:SER:OG	1.83	0.60
1:E:138:ALA:O	2:E:300:NAD:H6N	2.02	0.60
1:E:206:GLN:C	1:E:206:GLN:CD	2.69	0.60
1:A:164:LYS:NZ	1:D:157:HIS:HE1	2.00	0.60
1:D:57:HIS:CD2	1:D:59:ALA:HB2	2.36	0.60
1:D:60:ASP:OD1	1:D:62:SER:HB2	2.02	0.60
1:A:180:ILE:HG12	1:A:230:LEU:HD13	1.84	0.59
1:H:92:HIS:HE1	3:H:338:HOH:O	1.83	0.59
1:G:47:ILE:CD1	1:G:52:VAL:HG12	2.33	0.59
1:A:184:TRP:N	1:A:216:GLN:HE22	1.95	0.59
1:F:31:ASN:HA	1:F:52:VAL:HG13	1.85	0.59
1:C:110:LEU:HB3	1:C:111:ASN:HD22	1.68	0.59
1:B:225:GLU:CD	1:B:225:GLU:H	2.10	0.58
1:H:184:TRP:H	1:H:216:GLN:NE2	1.92	0.58
1:D:98:GLN:HA	1:D:98:GLN:HE21	1.66	0.58
1:C:47:ILE:HG22	1:C:54:ALA:HB2	1.84	0.58
1:B:61:LEU:O	1:B:67:ILE:HD11	2.04	0.58
1:B:164:LYS:HZ2	1:C:157:HIS:HE1	1.50	0.58
1:C:38:GLY:O	1:C:39:ASP:HB3	2.03	0.58
1:D:98:GLN:HA	1:D:98:GLN:NE2	2.19	0.58
1:E:86:ASN:HB2	1:E:136:ASN:HD22	1.67	0.58
1:A:37:PHE:HB2	3:A:315:HOH:O	2.03	0.58
1:D:149:LYS:NZ	1:D:193:GLN:HE22	2.02	0.58
1:E:31:ASN:OD1	1:E:52:VAL:HG22	2.04	0.58
1:F:12:GLY:H	1:F:35:ASN:HD22	1.52	0.57
1:H:86:ASN:HD22	1:H:136:ASN:ND2	2.00	0.57
1:H:31:ASN:HA	1:H:52:VAL:HG13	1.86	0.57
1:G:206:GLN:OE1	1:G:206:GLN:HA	2.04	0.57
1:B:184:TRP:N	1:B:216:GLN:HE22	1.97	0.57
1:B:141:HIS:HE1	1:B:146:SER:OG	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:12:GLY:H	1:H:35:ASN:HD22	1.51	0.57
1:E:8:ALA:HA	1:E:83:ILE:O	2.05	0.56
1:H:46:GLU:O	1:H:49:ARG:HG3	2.05	0.56
1:E:149:LYS:NZ	1:E:193:GLN:HE22	2.03	0.56
1:B:60:ASP:H	1:B:66:GLN:NE2	2.03	0.56
1:D:86:ASN:HD22	1:D:136:ASN:ND2	2.03	0.56
1:F:35:ASN:HD21	2:F:300:NAD:H2A	1.71	0.56
1:C:8:ALA:HB3	1:C:32:ILE:HD13	1.88	0.55
1:E:110:LEU:HB3	1:E:111:ASN:HD22	1.70	0.55
1:H:180:ILE:HG12	1:H:230:LEU:HD13	1.88	0.55
1:E:89:GLY:HA2	1:E:110:LEU:HD13	1.88	0.55
1:A:46:GLU:OE2	1:A:49:ARG:NH1	2.40	0.55
1:C:143:LEU:HD12	1:C:254:LEU:HD13	1.89	0.55
1:C:17:ILE:HD11	1:C:185:VAL:HG21	1.88	0.55
1:G:214:GLU:HB3	1:G:215:LYS:HG2	1.89	0.55
1:F:141:HIS:HE1	1:F:146:SER:HG	1.55	0.54
1:C:12:GLY:H	1:C:35:ASN:HD22	1.55	0.54
1:F:17:ILE:HD11	1:F:185:VAL:HG21	1.88	0.54
1:A:45:ALA:O	1:A:49:ARG:HG2	2.08	0.54
1:D:57:HIS:HD2	1:D:59:ALA:H	1.56	0.54
1:H:43:ALA:O	1:H:47:ILE:HG12	2.08	0.54
1:A:100:PRO:HB3	1:H:37:PHE:CD2	2.43	0.53
1:D:111:ASN:N	1:D:111:ASN:HD22	2.07	0.53
1:A:90:ILE:HG23	1:A:107:ILE:HG12	1.90	0.53
1:E:47:ILE:CD1	1:E:54:ALA:HB2	2.39	0.53
1:B:184:TRP:H	1:B:216:GLN:NE2	2.02	0.53
1:E:207:ALA:O	1:E:210:ASP:HB2	2.09	0.53
1:A:53:LYS:HG3	1:A:78:PHE:CE1	2.38	0.53
1:D:98:GLN:NE2	1:D:98:GLN:CA	2.67	0.52
1:C:141:HIS:HE1	1:C:146:SER:OG	1.92	0.52
1:H:89:GLY:HA2	1:H:110:LEU:HD13	1.91	0.52
1:A:23:GLN:NE2	1:A:46:GLU:HG3	2.24	0.52
1:H:223:THR:HB	1:H:225:GLU:OE1	2.09	0.52
1:C:184:TRP:H	1:C:216:GLN:NE2	2.00	0.52
1:E:42:PRO:O	1:E:46:GLU:HG2	2.09	0.52
1:C:138:ALA:HA	1:C:156:LYS:HD2	1.92	0.51
1:C:256:GLN:O	3:C:332:HOH:O	2.19	0.51
1:C:184:TRP:CD1	1:C:212:LEU:HD12	2.45	0.51
1:D:86:ASN:HD22	1:D:136:ASN:HD21	1.57	0.51
1:C:26:ALA:HB2	1:C:32:ILE:HG13	1.93	0.51
1:H:135:ILE:HD12	1:H:231:VAL:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:TRP:CZ3	1:A:211:LEU:HD21	2.46	0.51
1:A:57:HIS:HB3	1:A:70:LEU:HD13	1.92	0.51
1:B:107:ILE:HG23	1:B:111:ASN:HD22	1.75	0.51
1:F:90:ILE:HG12	1:F:110:LEU:HD12	1.93	0.51
1:H:53:LYS:HG2	1:H:78:PHE:CE2	2.46	0.51
1:C:17:ILE:HA	1:C:224:PRO:HB3	1.92	0.50
1:D:98:GLN:HE21	1:D:98:GLN:CA	2.24	0.50
1:F:47:ILE:HG21	1:F:54:ALA:HB2	1.92	0.50
1:A:61:LEU:O	1:A:67:ILE:HD11	2.12	0.50
1:E:141:HIS:HE1	1:E:146:SER:OG	1.94	0.50
1:D:165:VAL:O	1:D:169:GLU:HG3	2.11	0.50
1:G:11:THR:HB	1:G:61:LEU:HD11	1.93	0.50
1:E:19:LEU:O	1:E:23:GLN:HG3	2.12	0.49
1:A:141:HIS:CE1	1:A:146:SER:OG	2.62	0.49
1:C:138:ALA:O	2:C:300:NAD:H6N	2.12	0.49
1:D:184:TRP:H	1:D:216:GLN:NE2	2.03	0.49
1:E:49:ARG:C	1:E:49:ARG:CD	2.85	0.49
1:H:73:LEU:HD12	1:H:76:ARG:HH21	1.75	0.49
1:C:191:GLN:HA	1:C:194:ILE:CD1	2.42	0.49
1:D:32:ILE:O	1:D:54:ALA:HA	2.12	0.49
1:A:23:GLN:NE2	1:A:46:GLU:O	2.45	0.49
1:C:55:VAL:CG2	1:C:78:PHE:HE2	2.25	0.49
1:E:206:GLN:CD	1:E:207:ALA:N	2.70	0.49
1:E:207:ALA:HA	1:E:210:ASP:OD1	2.12	0.49
1:C:141:HIS:HB3	1:C:153:VAL:HG22	1.94	0.49
1:E:57:HIS:CD2	1:E:59:ALA:HB2	2.48	0.49
1:A:64:VAL:O	1:A:68:GLU:HG3	2.13	0.49
1:C:207:ALA:O	1:C:210:ASP:HB2	2.12	0.49
1:E:87:ASN:O	2:E:300:NAD:H4D	2.13	0.49
1:G:14:THR:HG22	2:G:300:NAD:O3B	2.13	0.49
1:G:184:TRP:N	1:G:216:GLN:HE22	2.02	0.49
1:D:27:ARG:HG3	1:D:50:HIS:CE1	2.48	0.48
1:D:86:ASN:HB2	1:D:136:ASN:HD22	1.77	0.48
1:B:40:PRO:HB3	1:B:56:HIS:CG	2.48	0.48
1:E:195:ASP:O	1:E:198:ALA:HB3	2.13	0.48
1:F:225:GLU:CD	1:F:225:GLU:H	2.21	0.48
1:A:194:ILE:HD11	1:A:221:PHE:CZ	2.49	0.48
1:D:149:LYS:HZ3	1:D:193:GLN:HE22	1.60	0.48
1:A:73:LEU:HD12	1:A:77:GLU:CG	2.43	0.48
1:A:57:HIS:HB2	1:A:73:LEU:CD2	2.43	0.48
1:E:214:GLU:HG3	1:E:215:LYS:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:ASN:OD1	1:E:52:VAL:CG2	2.62	0.48
1:A:192:LYS:O	1:A:196:ASP:OD2	2.32	0.48
1:G:57:HIS:CD2	1:G:59:ALA:HB2	2.49	0.48
1:C:191:GLN:HA	1:C:194:ILE:HD12	1.95	0.47
1:B:41:ALA:HB3	1:B:42:PRO:HD3	1.96	0.47
1:A:73:LEU:HD12	1:A:77:GLU:HG2	1.94	0.47
1:A:57:HIS:HE1	1:A:59:ALA:HB2	1.71	0.47
1:D:57:HIS:CD2	1:D:59:ALA:H	2.33	0.47
1:F:20:GLY:O	1:F:23:GLN:NE2	2.47	0.47
1:G:30:ALA:O	1:G:52:VAL:HG11	2.15	0.47
1:C:75:GLU:OE1	1:C:76:ARG:NH1	2.47	0.47
1:G:86:ASN:HB2	1:G:136:ASN:HD22	1.80	0.47
1:C:184:TRP:HD1	1:C:212:LEU:HD12	1.79	0.47
1:D:46:GLU:OE2	1:D:49:ARG:NH1	2.47	0.47
1:F:39:ASP:O	1:F:42:PRO:HD2	2.13	0.47
1:F:73:LEU:HD23	1:F:76:ARG:NH2	2.29	0.47
1:F:185:VAL:HG13	1:F:222:VAL:O	2.15	0.47
1:G:194:ILE:HG21	1:G:208:GLN:HB3	1.95	0.47
1:B:223:THR:H	1:B:226:HIS:CD2	2.33	0.47
1:D:160:VAL:HG12	1:D:164:LYS:HE3	1.96	0.47
1:F:11:THR:HB	1:F:61:LEU:HD11	1.97	0.47
1:F:86:ASN:HD22	1:F:136:ASN:ND2	2.11	0.47
1:C:12:GLY:O	1:C:18:GLY:HA3	2.15	0.47
1:A:86:ASN:HB2	1:A:136:ASN:HD22	1.80	0.46
1:D:87:ASN:O	2:D:300:NAD:H4D	2.16	0.46
1:E:226:HIS:HE1	1:F:237:GLU:OE1	1.98	0.46
1:A:32:ILE:O	1:A:54:ALA:HA	2.15	0.46
1:H:130:ASN:O	1:H:174:ASN:HB2	2.15	0.46
1:A:215:LYS:HB3	1:A:253:TRP:CE2	2.50	0.46
1:G:149:LYS:NZ	1:G:193:GLN:HE22	2.13	0.46
1:G:197:ARG:NH2	1:G:214:GLU:OE2	2.42	0.46
1:C:190:VAL:O	1:C:193:GLN:N	2.49	0.46
1:C:227:LEU:O	1:C:231:VAL:HG23	2.14	0.46
1:G:47:ILE:CD1	1:G:54:ALA:HB2	2.44	0.46
1:G:61:LEU:HG	2:G:300:NAD:H2A	1.98	0.46
1:A:192:LYS:N	1:A:192:LYS:HE3	2.30	0.46
1:E:47:ILE:CD1	1:E:52:VAL:HG13	2.46	0.46
1:A:17:ILE:HG22	1:A:21:ILE:HD12	1.97	0.46
1:A:90:ILE:HG22	1:A:111:ASN:ND2	2.30	0.46
1:F:87:ASN:O	2:F:300:NAD:H4D	2.16	0.46
1:A:141:HIS:HD2	3:A:316:HOH:O	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:HIS:HD2	1:D:59:ALA:HB2	1.79	0.45
1:F:60:ASP:H	1:F:66:GLN:NE2	2.14	0.45
1:A:17:ILE:HG12	1:A:185:VAL:HG11	1.99	0.45
1:E:57:HIS:HD2	1:E:59:ALA:H	1.63	0.45
1:A:90:ILE:H	1:A:111:ASN:HD21	1.63	0.45
1:C:143:LEU:CD1	1:C:254:LEU:HD13	2.46	0.45
1:F:96:VAL:HG12	1:F:150:ALA:HB2	1.99	0.45
1:C:86:ASN:HD22	1:C:136:ASN:ND2	2.14	0.45
1:G:31:ASN:OD1	1:G:53:LYS:HB2	2.17	0.45
1:H:162:LEU:O	1:H:166:VAL:HG23	2.17	0.45
1:A:73:LEU:CD1	1:A:77:GLU:HG3	2.46	0.45
1:A:134:ILE:O	1:A:177:CYS:HA	2.16	0.45
1:B:101:LEU:HD21	1:C:120:ARG:CZ	2.47	0.45
1:E:60:ASP:H	1:E:66:GLN:NE2	2.15	0.45
1:E:61:LEU:HG	2:E:300:NAD:H2A	1.99	0.45
1:A:203:ASP:HB3	1:A:206:GLN:HB3	1.99	0.45
1:E:180:ILE:HG12	1:E:230:LEU:HD13	1.98	0.45
1:C:122:ALA:HB1	1:C:126:MET:HE3	1.99	0.44
1:F:86:ASN:HB2	1:F:136:ASN:HD22	1.82	0.44
1:B:61:LEU:HD22	1:B:67:ILE:HG12	1.99	0.44
1:B:211:LEU:HD12	1:B:211:LEU:HA	1.83	0.44
1:D:27:ARG:CG	1:D:50:HIS:CE1	3.00	0.44
1:F:73:LEU:HD23	1:F:76:ARG:HH21	1.82	0.44
1:B:187:THR:HB	1:B:188:PRO:CD	2.47	0.44
1:D:184:TRP:N	1:D:216:GLN:HE22	2.05	0.44
1:E:12:GLY:H	1:E:35:ASN:HD22	1.64	0.44
1:E:57:HIS:HB3	1:E:70:LEU:HD13	1.99	0.44
1:A:111:ASN:N	1:A:111:ASN:ND2	2.56	0.44
1:C:38:GLY:O	1:C:39:ASP:HB2	2.16	0.44
1:H:23:GLN:OE1	1:H:27:ARG:NH2	2.51	0.44
1:A:234:LEU:HD23	1:A:234:LEU:HA	1.83	0.44
1:C:75:GLU:HG3	1:C:76:ARG:HD2	2.00	0.44
1:B:73:LEU:CD2	1:B:77:GLU:HG2	2.49	0.43
1:F:61:LEU:HB2	1:F:110:LEU:HD23	2.00	0.43
1:D:46:GLU:CD	1:D:49:ARG:NH1	2.76	0.43
1:F:186:LEU:HD22	1:F:221:PHE:CB	2.45	0.43
1:H:90:ILE:HG13	1:H:107:ILE:HD12	2.00	0.43
1:A:162:LEU:O	1:A:166:VAL:HG23	2.18	0.43
1:B:11:THR:O	1:B:87:ASN:HB3	2.18	0.43
1:E:216:GLN:HE21	1:E:253:TRP:HE3	1.65	0.43
1:H:104:TRP:CE3	1:H:151:ALA:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ILE:CB	1:A:110:LEU:HD23	2.46	0.43
1:B:212:LEU:N	1:B:212:LEU:HD23	2.34	0.43
1:E:242:VAL:C	1:E:243:ARG:HG3	2.42	0.43
1:A:164:LYS:HZ2	1:D:157:HIS:HE1	1.67	0.43
1:D:93:VAL:O	1:D:94:ALA:HB2	2.19	0.43
1:G:141:HIS:CE1	1:G:146:SER:OG	2.54	0.43
1:B:47:ILE:HG21	1:B:54:ALA:HB2	2.02	0.42
1:C:187:THR:O	1:C:188:PRO:C	2.61	0.42
1:D:55:VAL:HG11	1:D:77:GLU:CD	2.44	0.42
1:D:45:ALA:O	1:D:49:ARG:CD	2.66	0.42
1:H:23:GLN:HE22	1:H:225:GLU:HG3	1.84	0.42
1:A:223:THR:H	1:A:226:HIS:CD2	2.36	0.42
1:D:60:ASP:H	1:D:66:GLN:NE2	2.18	0.42
1:H:138:ALA:O	2:H:300:NAD:H6N	2.20	0.42
1:A:122:ALA:HB1	1:A:126:MET:HE3	2.00	0.42
1:F:86:ASN:HD22	1:F:136:ASN:HD21	1.68	0.42
1:H:59:ALA:HA	1:H:66:GLN:HE21	1.84	0.42
1:B:196:ASP:O	1:B:197:ARG:HG2	2.19	0.42
1:F:8:ALA:HB3	1:F:32:ILE:HD13	2.00	0.42
1:D:89:GLY:HA2	1:D:110:LEU:HD13	2.02	0.42
1:F:12:GLY:H	1:F:35:ASN:ND2	2.18	0.42
1:A:165:VAL:O	1:A:169:GLU:HG3	2.20	0.41
1:F:25:LEU:HD12	1:F:25:LEU:HA	1.93	0.41
1:A:11:THR:O	1:A:87:ASN:HB3	2.19	0.41
1:B:164:LYS:HZ1	1:C:157:HIS:HE1	1.67	0.41
1:D:130:ASN:ND2	3:D:360:HOH:O	2.53	0.41
1:F:149:LYS:O	1:F:150:ALA:C	2.63	0.41
1:B:59:ALA:CB	1:B:66:GLN:O	2.68	0.41
1:D:217:PRO:HD2	1:D:251:GLY:O	2.21	0.41
1:E:160:VAL:HG12	1:E:164:LYS:HE3	2.02	0.41
1:G:47:ILE:HD12	1:G:47:ILE:O	2.21	0.41
1:A:10:VAL:HG12	1:A:13:SER:HB3	2.03	0.41
1:A:189:LEU:HD12	1:A:189:LEU:C	2.44	0.41
1:B:11:THR:HB	1:B:61:LEU:HD11	2.01	0.41
1:G:32:ILE:HG22	1:G:34:LEU:HG	2.02	0.41
1:B:141:HIS:HD2	3:B:282:HOH:O	2.02	0.41
1:C:223:THR:H	1:C:226:HIS:CD2	2.39	0.41
1:D:110:LEU:HB3	1:D:111:ASN:HD22	1.85	0.41
1:F:57:HIS:HB2	1:F:73:LEU:HD12	2.03	0.41
1:B:8:ALA:HB3	1:B:32:ILE:HD13	2.02	0.41
1:C:90:ILE:H	1:C:111:ASN:HD21	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:103:SER:O	1:H:104:TRP:C	2.60	0.41
1:H:110:LEU:O	1:H:114:ALA:HB3	2.21	0.41
1:A:215:LYS:HB3	1:A:253:TRP:CZ2	2.56	0.41
1:A:73:LEU:HD11	1:A:77:GLU:HG3	2.03	0.41
1:E:7:THR:HG21	1:E:78:PHE:HB2	2.03	0.41
1:E:86:ASN:HB2	1:E:136:ASN:ND2	2.33	0.41
1:F:123:LEU:N	1:F:124:PRO:CD	2.83	0.41
1:H:92:HIS:CE1	3:H:338:HOH:O	2.64	0.41
1:B:187:THR:HB	1:B:188:PRO:HD2	2.03	0.41
1:C:186:LEU:HD22	1:C:221:PHE:CE1	2.55	0.41
1:E:110:LEU:O	1:E:114:ALA:HB3	2.21	0.41
1:E:119:THR:HG23	1:E:134:ILE:HD13	2.01	0.41
1:A:182:PRO:HA	1:A:249:VAL:O	2.21	0.40
1:D:90:ILE:HD11	1:D:106:LYS:HG3	2.03	0.40
1:E:61:LEU:HD22	1:E:67:ILE:HG12	2.03	0.40
1:G:47:ILE:HD12	1:G:52:VAL:HG12	2.02	0.40
1:C:57:HIS:HD2	1:C:59:ALA:N	2.17	0.40
1:C:86:ASN:HD22	1:C:136:ASN:HD21	1.69	0.40
1:F:111:ASN:HD22	1:F:111:ASN:N	2.19	0.40
1:G:35:ASN:HA	1:G:57:HIS:O	2.21	0.40
1:G:60:ASP:H	1:G:66:GLN:NE2	2.19	0.40
1:B:203:ASP:HA	1:B:204:PRO:HD2	1.92	0.40
1:C:121:LEU:HD23	1:C:121:LEU:HA	1.93	0.40
1:F:182:PRO:HB2	2:F:300:NAD:C5N	2.51	0.40
1:G:14:THR:CG2	1:G:37:PHE:O	2.60	0.40
1:D:57:HIS:HE1	3:D:363:HOH:O	2.05	0.40

All (1) 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)
3:E:336:HOH:O	3:G:332:HOH:O[2_555]	1.98	0.22

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	246/255 (96%)	237 (96%)	9 (4%)	0	100	100
1	B	248/255 (97%)	230 (93%)	15 (6%)	3 (1%)	10	4
1	C	239/255 (94%)	224 (94%)	13 (5%)	2 (1%)	16	8
1	D	253/255 (99%)	244 (96%)	8 (3%)	1 (0%)	30	22
1	E	245/255 (96%)	233 (95%)	11 (4%)	1 (0%)	30	22
1	F	234/255 (92%)	226 (97%)	8 (3%)	0	100	100
1	G	247/255 (97%)	237 (96%)	7 (3%)	3 (1%)	10	4
1	H	236/255 (92%)	220 (93%)	14 (6%)	2 (1%)	16	8
All	All	1948/2040 (96%)	1851 (95%)	85 (4%)	12 (1%)	21	12

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	39	ASP
1	H	46	GLU
1	H	47	ILE
1	G	207	ALA
1	B	196	ASP
1	B	130	ASN
1	B	197	ARG
1	G	138	ALA
1	C	131	TRP
1	D	202	GLY
1	E	206	GLN
1	G	206	GLN

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	188/189 (100%)	174 (93%)	14 (7%)	13 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	188/189 (100%)	172 (92%)	16 (8%)	10	4
1	C	181/189 (96%)	162 (90%)	19 (10%)	6	2
1	D	189/189 (100%)	173 (92%)	16 (8%)	10	4
1	E	186/189 (98%)	166 (89%)	20 (11%)	6	2
1	F	176/189 (93%)	160 (91%)	16 (9%)	9	4
1	G	187/189 (99%)	166 (89%)	21 (11%)	6	1
1	H	178/189 (94%)	165 (93%)	13 (7%)	13	7
All	All	1473/1512 (97%)	1338 (91%)	135 (9%)	8	3

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	23	GLN
1	A	25	LEU
1	A	27	ARG
1	A	53	LYS
1	A	98	GLN
1	A	111	ASN
1	A	189	LEU
1	A	192	LYS
1	A	205	LEU
1	A	212	LEU
1	A	217	PRO
1	A	230	LEU
1	A	237	GLU
1	B	2	THR
1	B	25	LEU
1	B	52	VAL
1	B	53	LYS
1	B	73	LEU
1	B	76	ARG
1	B	106	LYS
1	B	186	LEU
1	B	189	LEU
1	B	192	LYS
1	B	194	ILE
1	B	195	ASP
1	B	197	ARG
1	B	205	LEU

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Mol	Chain	Res	Type
1	B	225	GLU
1	B	237	GLU
1	C	4	LYS
1	C	15	SER
1	C	25	LEU
1	C	34	LEU
1	C	47	ILE
1	C	52	VAL
1	C	102	GLU
1	C	110	LEU
1	C	111	ASN
1	C	189	LEU
1	C	190	VAL
1	C	192	LYS
1	C	193	GLN
1	C	210	ASP
1	C	211	LEU
1	C	212	LEU
1	C	214	GLU
1	C	230	LEU
1	C	232	LEU
1	D	2	THR
1	D	14	THR
1	D	15	SER
1	D	23	GLN
1	D	25	LEU
1	D	34	LEU
1	D	52	VAL
1	D	76	ARG
1	D	101	LEU
1	D	102	GLU
1	D	110	LEU
1	D	111	ASN
1	D	188	PRO
1	D	205	LEU
1	D	230	LEU
1	D	232	LEU
1	E	6	LYS
1	E	14	THR
1	E	25	LEU
1	E	27	ARG
1	E	47	ILE

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Mol	Chain	Res	Type
1	E	75	GLU
1	E	98	GLN
1	E	102	GLU
1	E	103	SER
1	E	110	LEU
1	E	120	ARG
1	E	124	PRO
1	E	130	ASN
1	E	192	LYS
1	E	205	LEU
1	E	206	GLN
1	E	212	LEU
1	E	225	GLU
1	E	230	LEU
1	E	232	LEU
1	F	2	THR
1	F	23	GLN
1	F	25	LEU
1	F	52	VAL
1	F	73	LEU
1	F	76	ARG
1	F	96	VAL
1	F	97	GLU
1	F	101	LEU
1	F	110	LEU
1	F	111	ASN
1	F	140	VAL
1	F	186	LEU
1	F	212	LEU
1	F	217	PRO
1	F	230	LEU
1	G	2	THR
1	G	6	LYS
1	G	13	SER
1	G	14	THR
1	G	25	LEU
1	G	47	ILE
1	G	52	VAL
1	G	96	VAL
1	G	106	LYS
1	G	110	LEU
1	G	111	ASN

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Mol	Chain	Res	Type
1	G	192	LYS
1	G	196	ASP
1	G	208	GLN
1	G	210	ASP
1	G	211	LEU
1	G	212	LEU
1	G	214	GLU
1	G	216	GLN
1	G	230	LEU
1	G	232	LEU
1	H	23	GLN
1	H	25	LEU
1	H	46	GLU
1	H	49	ARG
1	H	52	VAL
1	H	53	LYS
1	H	101	LEU
1	H	102	GLU
1	H	110	LEU
1	H	205	LEU
1	H	206	GLN
1	H	212	LEU
1	H	230	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	66	GLN
1	A	86	ASN
1	A	111	ASN
1	A	136	ASN
1	A	141	HIS
1	A	193	GLN
1	A	206	GLN
1	A	216	GLN
1	A	256	GLN
1	B	50	HIS
1	B	66	GLN
1	B	86	ASN
1	B	111	ASN
1	B	136	ASN

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Mol	Chain	Res	Type
1	B	141	HIS
1	B	206	GLN
1	B	216	GLN
1	B	226	HIS
1	B	256	GLN
1	C	23	GLN
1	C	35	ASN
1	C	57	HIS
1	C	66	GLN
1	C	111	ASN
1	C	136	ASN
1	C	141	HIS
1	C	157	HIS
1	C	191	GLN
1	C	193	GLN
1	C	216	GLN
1	D	35	ASN
1	D	57	HIS
1	D	66	GLN
1	D	98	GLN
1	D	111	ASN
1	D	130	ASN
1	D	136	ASN
1	D	141	HIS
1	D	157	HIS
1	D	193	GLN
1	D	206	GLN
1	D	216	GLN
1	E	35	ASN
1	E	50	HIS
1	E	57	HIS
1	E	66	GLN
1	E	86	ASN
1	E	111	ASN
1	E	136	ASN
1	E	141	HIS
1	E	157	HIS
1	E	193	GLN
1	E	216	GLN
1	E	226	HIS
1	E	256	GLN
1	F	23	GLN

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Mol	Chain	Res	Type
1	F	31	ASN
1	F	35	ASN
1	F	66	GLN
1	F	92	HIS
1	F	111	ASN
1	F	136	ASN
1	F	141	HIS
1	F	157	HIS
1	F	208	GLN
1	F	216	GLN
1	G	35	ASN
1	G	57	HIS
1	G	66	GLN
1	G	92	HIS
1	G	111	ASN
1	G	136	ASN
1	G	141	HIS
1	G	191	GLN
1	G	193	GLN
1	G	208	GLN
1	G	216	GLN
1	G	256	GLN
1	H	31	ASN
1	H	35	ASN
1	H	66	GLN
1	H	92	HIS
1	H	111	ASN
1	H	130	ASN
1	H	136	ASN
1	H	141	HIS
1	H	157	HIS
1	H	216	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	H	300	-	46,48,48	1.97	10 (21%)	64,73,73	2.13	17 (26%)
2	NAD	D	300	-	46,48,48	1.47	7 (15%)	64,73,73	2.54	20 (31%)
2	NAD	C	300	-	46,48,48	2.09	8 (17%)	64,73,73	1.66	12 (18%)
2	NAD	G	300	-	46,48,48	1.72	5 (10%)	64,73,73	1.98	18 (28%)
2	NAD	F	300	-	46,48,48	1.94	8 (17%)	64,73,73	1.91	16 (25%)
2	NAD	E	300	-	46,48,48	1.88	9 (19%)	64,73,73	1.98	16 (25%)

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	H	300	-	-	8/30/62/62	0/5/5/5
2	NAD	D	300	-	-	5/30/62/62	0/5/5/5
2	NAD	C	300	-	-	4/30/62/62	0/5/5/5
2	NAD	G	300	-	-	6/30/62/62	0/5/5/5
2	NAD	F	300	-	-	12/30/62/62	0/5/5/5
2	NAD	E	300	-	-	6/30/62/62	0/5/5/5

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	300	NAD	O7N-C7N	10.14	1.43	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	300	NAD	O7N-C7N	8.19	1.39	1.24
2	F	300	NAD	O7N-C7N	7.31	1.37	1.24
2	G	300	NAD	O7N-C7N	6.62	1.36	1.24
2	E	300	NAD	O7N-C7N	6.48	1.36	1.24
2	F	300	NAD	PA-O3	5.15	1.65	1.59
2	E	300	NAD	PA-O3	4.84	1.64	1.59
2	C	300	NAD	PA-O3	4.82	1.64	1.59
2	G	300	NAD	PA-O3	4.76	1.64	1.59
2	H	300	NAD	C2N-N1N	4.74	1.40	1.35
2	G	300	NAD	C2A-N1A	4.60	1.42	1.33
2	F	300	NAD	C2N-N1N	4.22	1.39	1.35
2	D	300	NAD	O7N-C7N	4.15	1.31	1.24
2	D	300	NAD	C2A-N1A	4.10	1.41	1.33
2	H	300	NAD	PN-O3	4.00	1.63	1.59
2	E	300	NAD	C2N-N1N	3.94	1.39	1.35
2	E	300	NAD	C5N-C4N	3.78	1.45	1.38
2	F	300	NAD	C2A-N1A	3.65	1.40	1.33
2	E	300	NAD	PN-O3	-3.47	1.55	1.59
2	F	300	NAD	O4D-C1D	3.15	1.45	1.40
2	H	300	NAD	C2A-N1A	3.13	1.39	1.33
2	F	300	NAD	C8A-N7A	3.09	1.37	1.31
2	C	300	NAD	C2A-N1A	3.07	1.39	1.33
2	D	300	NAD	O4D-C1D	3.01	1.44	1.40
2	D	300	NAD	C2N-C3N	-2.98	1.34	1.39
2	C	300	NAD	C2N-N1N	2.92	1.38	1.35
2	E	300	NAD	O4D-C1D	2.81	1.44	1.40
2	H	300	NAD	PA-O3	2.80	1.62	1.59
2	F	300	NAD	C2A-N3A	2.74	1.38	1.33
2	C	300	NAD	C2A-N3A	2.66	1.38	1.33
2	H	300	NAD	C2N-C3N	2.64	1.43	1.39
2	C	300	NAD	PN-O3	2.59	1.62	1.59
2	E	300	NAD	C3N-C7N	2.49	1.54	1.50
2	C	300	NAD	C8A-N7A	2.45	1.36	1.31
2	G	300	NAD	C2N-N1N	2.42	1.37	1.35
2	H	300	NAD	C4A-N3A	2.40	1.38	1.34
2	H	300	NAD	C2A-N3A	2.39	1.38	1.33
2	D	300	NAD	PA-O3	2.31	1.62	1.59
2	H	300	NAD	O4D-C1D	2.27	1.43	1.40
2	H	300	NAD	C8A-N7A	2.25	1.36	1.31
2	E	300	NAD	C8A-N7A	2.22	1.35	1.31
2	F	300	NAD	C2N-C3N	2.21	1.42	1.39
2	C	300	NAD	O4D-C1D	2.18	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	300	NAD	C4A-N3A	2.17	1.38	1.34
2	G	300	NAD	C5D-C4D	2.05	1.57	1.51
2	D	300	NAD	C5A-N7A	-2.02	1.35	1.39
2	D	300	NAD	PA-O2A	-2.01	1.46	1.55

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	300	NAD	C3N-C7N-N7N	10.56	130.74	117.74
2	E	300	NAD	C3N-C7N-N7N	7.87	127.43	117.74
2	H	300	NAD	N3A-C2A-N1A	-7.25	117.61	128.58
2	D	300	NAD	O7N-C7N-N7N	-5.98	113.97	122.62
2	C	300	NAD	N3A-C2A-N1A	-5.58	120.13	128.58
2	D	300	NAD	N9A-C8A-N7A	-5.31	106.41	113.94
2	H	300	NAD	O3-PN-O1N	-5.28	94.81	110.70
2	F	300	NAD	C3N-C7N-N7N	5.23	124.18	117.74
2	H	300	NAD	N9A-C8A-N7A	-5.15	106.63	113.94
2	E	300	NAD	N3A-C2A-N1A	-5.06	120.93	128.58
2	G	300	NAD	N9A-C8A-N7A	-4.99	106.86	113.94
2	E	300	NAD	O7N-C7N-C3N	-4.85	113.67	119.60
2	F	300	NAD	N3A-C2A-N1A	-4.84	121.25	128.58
2	G	300	NAD	O7N-C7N-C3N	-4.71	113.83	119.60
2	G	300	NAD	C5A-C4A-N3A	-4.70	120.25	126.72
2	G	300	NAD	O3-PN-O1N	-4.68	96.64	110.70
2	D	300	NAD	C4D-O4D-C1D	-4.64	105.67	109.92
2	E	300	NAD	O3-PA-O1A	-4.47	97.26	110.70
2	D	300	NAD	C5A-N7A-C8A	4.45	110.44	103.45
2	F	300	NAD	N9A-C8A-N7A	-4.26	107.89	113.94
2	H	300	NAD	C3N-C7N-N7N	4.23	122.94	117.74
2	D	300	NAD	N3A-C2A-N1A	-4.14	122.31	128.58
2	G	300	NAD	C3N-C7N-N7N	4.14	122.84	117.74
2	G	300	NAD	C6A-C5A-C4A	4.13	122.81	117.18
2	D	300	NAD	C3B-C2B-C1B	-4.10	93.70	101.46
2	D	300	NAD	C5A-C4A-N3A	-3.99	121.22	126.72
2	C	300	NAD	C5A-C4A-N3A	-3.95	121.27	126.72
2	F	300	NAD	C5A-C4A-N3A	-3.88	121.38	126.72
2	H	300	NAD	C4A-N9A-C8A	3.82	109.75	105.74
2	G	300	NAD	N3A-C4A-N9A	3.79	133.62	127.17
2	C	300	NAD	N9A-C8A-N7A	-3.74	108.63	113.94
2	F	300	NAD	C6N-N1N-C2N	-3.68	118.74	121.88
2	C	300	NAD	N3A-C4A-N9A	3.64	133.37	127.17
2	H	300	NAD	C2A-N1A-C6A	3.63	124.70	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	300	NAD	O7N-C7N-C3N	-3.61	115.19	119.60
2	F	300	NAD	C4A-N9A-C8A	3.58	109.50	105.74
2	D	300	NAD	C4A-N9A-C8A	3.53	109.44	105.74
2	E	300	NAD	N9A-C8A-N7A	-3.51	108.95	113.94
2	D	300	NAD	O3D-C3D-C2D	-3.49	100.62	111.82
2	H	300	NAD	C5A-N7A-C8A	3.45	108.86	103.45
2	H	300	NAD	C4A-N9A-C1B	-3.44	118.60	126.63
2	H	300	NAD	O3-PA-O1A	-3.41	100.46	110.70
2	F	300	NAD	N3A-C4A-N9A	3.34	132.85	127.17
2	G	300	NAD	C5A-N7A-C8A	3.32	108.66	103.45
2	H	300	NAD	O2A-PA-O3	3.31	116.21	107.27
2	D	300	NAD	N3A-C4A-N9A	3.29	132.75	127.17
2	G	300	NAD	C4A-N9A-C8A	3.22	109.12	105.74
2	G	300	NAD	O4B-C1B-N9A	3.14	114.11	108.09
2	F	300	NAD	O7N-C7N-N7N	-3.05	118.21	122.62
2	C	300	NAD	C4A-N9A-C8A	3.04	108.93	105.74
2	G	300	NAD	N3A-C2A-N1A	-3.01	124.03	128.58
2	E	300	NAD	C5A-C4A-N3A	-3.00	122.59	126.72
2	F	300	NAD	O3-PA-O1A	-2.93	101.90	110.70
2	C	300	NAD	O3-PA-O1A	-2.92	101.92	110.70
2	E	300	NAD	C4D-O4D-C1D	-2.84	107.32	109.92
2	C	300	NAD	C2A-N3A-C4A	2.83	118.73	111.83
2	D	300	NAD	O3-PA-O1A	-2.82	102.23	110.70
2	D	300	NAD	O3B-C3B-C4B	-2.82	103.00	111.08
2	G	300	NAD	O3-PA-O1A	-2.79	102.31	110.70
2	H	300	NAD	C4D-O4D-C1D	2.78	112.47	109.92
2	E	300	NAD	C5A-N7A-C8A	2.77	107.81	103.45
2	E	300	NAD	O7N-C7N-N7N	-2.74	118.66	122.62
2	F	300	NAD	O3-PN-O1N	-2.73	102.50	110.70
2	C	300	NAD	C5A-C6A-N6A	-2.72	116.55	123.29
2	D	300	NAD	C4A-C5A-N7A	-2.66	107.54	110.58
2	D	300	NAD	C2A-N3A-C4A	2.61	118.20	111.83
2	F	300	NAD	C2A-N3A-C4A	2.60	118.17	111.83
2	E	300	NAD	C2A-N1A-C6A	2.59	122.98	118.73
2	D	300	NAD	O3-PN-O1N	-2.58	102.93	110.70
2	D	300	NAD	C5N-C6N-N1N	-2.53	116.94	120.38
2	E	300	NAD	O2N-PN-O3	2.52	114.09	107.27
2	G	300	NAD	C4D-O4D-C1D	-2.48	107.66	109.92
2	H	300	NAD	C2A-N3A-C4A	2.42	117.74	111.83
2	E	300	NAD	N3A-C4A-N9A	2.40	131.25	127.17
2	D	300	NAD	O2N-PN-O1N	2.40	123.61	112.44
2	E	300	NAD	O3B-C3B-C2B	-2.38	104.18	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	300	NAD	O5B-PA-O1A	-2.37	99.55	108.94
2	F	300	NAD	O5D-PN-O1N	-2.29	99.85	108.94
2	E	300	NAD	C2A-N3A-C4A	2.29	117.42	111.83
2	F	300	NAD	C5A-N7A-C8A	2.27	107.02	103.45
2	D	300	NAD	O2A-PA-O3	2.26	113.38	107.27
2	F	300	NAD	O2B-C2B-C3B	2.21	118.90	111.82
2	G	300	NAD	C3B-C2B-C1B	-2.19	97.31	101.46
2	F	300	NAD	O2N-PN-O3	2.19	113.19	107.27
2	H	300	NAD	O7N-C7N-N7N	-2.19	119.45	122.62
2	H	300	NAD	C6N-N1N-C2N	-2.18	120.03	121.88
2	C	300	NAD	O3-PN-O1N	-2.17	104.17	110.70
2	G	300	NAD	C6A-C5A-N7A	-2.16	127.93	132.09
2	E	300	NAD	O2B-C2B-C3B	2.14	118.69	111.82
2	H	300	NAD	C5N-C4N-C3N	-2.14	118.27	120.36
2	C	300	NAD	O5D-PN-O1N	2.13	117.39	108.94
2	C	300	NAD	C6A-C5A-C4A	2.09	120.04	117.18
2	G	300	NAD	C2A-N3A-C4A	2.08	116.92	111.83
2	E	300	NAD	C4A-N9A-C8A	2.06	107.90	105.74
2	H	300	NAD	C1B-N9A-C8A	2.05	131.64	127.09
2	C	300	NAD	C2B-C1B-N9A	-2.04	108.23	113.30
2	G	300	NAD	O2N-PN-O1N	2.03	121.90	112.44
2	F	300	NAD	O4B-C1B-N9A	2.01	111.95	108.09
2	H	300	NAD	O3B-C3B-C4B	-2.01	105.31	111.08

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	300	NAD	C5D-O5D-PN-O3
2	C	300	NAD	C5D-O5D-PN-O1N
2	D	300	NAD	C5D-O5D-PN-O3
2	D	300	NAD	C5D-O5D-PN-O2N
2	E	300	NAD	C5D-O5D-PN-O3
2	E	300	NAD	C5D-O5D-PN-O1N
2	E	300	NAD	C5D-O5D-PN-O2N
2	E	300	NAD	O4D-C1D-N1N-C2N
2	F	300	NAD	C5B-O5B-PA-O1A
2	F	300	NAD	C5B-O5B-PA-O2A
2	F	300	NAD	O4D-C1D-N1N-C2N
2	G	300	NAD	C5D-O5D-PN-O2N
2	G	300	NAD	O4D-C1D-N1N-C2N
2	H	300	NAD	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
2	H	300	NAD	C5D-O5D-PN-O2N
2	H	300	NAD	O4D-C1D-N1N-C2N
2	F	300	NAD	O4D-C4D-C5D-O5D
2	F	300	NAD	O4B-C4B-C5B-O5B
2	F	300	NAD	C3D-C4D-C5D-O5D
2	F	300	NAD	PN-O3-PA-O1A
2	F	300	NAD	C3B-C4B-C5B-O5B
2	C	300	NAD	PA-O3-PN-O2N
2	H	300	NAD	PA-O3-PN-O2N
2	D	300	NAD	C5D-O5D-PN-O1N
2	F	300	NAD	C5B-O5B-PA-O3
2	G	300	NAD	C5D-O5D-PN-O3
2	H	300	NAD	C5D-O5D-PN-O1N
2	F	300	NAD	PA-O3-PN-O2N
2	E	300	NAD	O4D-C1D-N1N-C6N
2	F	300	NAD	O4D-C1D-N1N-C6N
2	G	300	NAD	O4D-C1D-N1N-C6N
2	H	300	NAD	O4D-C1D-N1N-C6N
2	F	300	NAD	PN-O3-PA-O2A
2	D	300	NAD	PA-O3-PN-O1N
2	G	300	NAD	PA-O3-PN-O1N
2	G	300	NAD	PA-O3-PN-O2N
2	H	300	NAD	PA-O3-PN-O1N
2	D	300	NAD	PA-O3-PN-O2N
2	E	300	NAD	PA-O3-PN-O1N
2	C	300	NAD	O4B-C4B-C5B-O5B
2	H	300	NAD	O4B-C4B-C5B-O5B

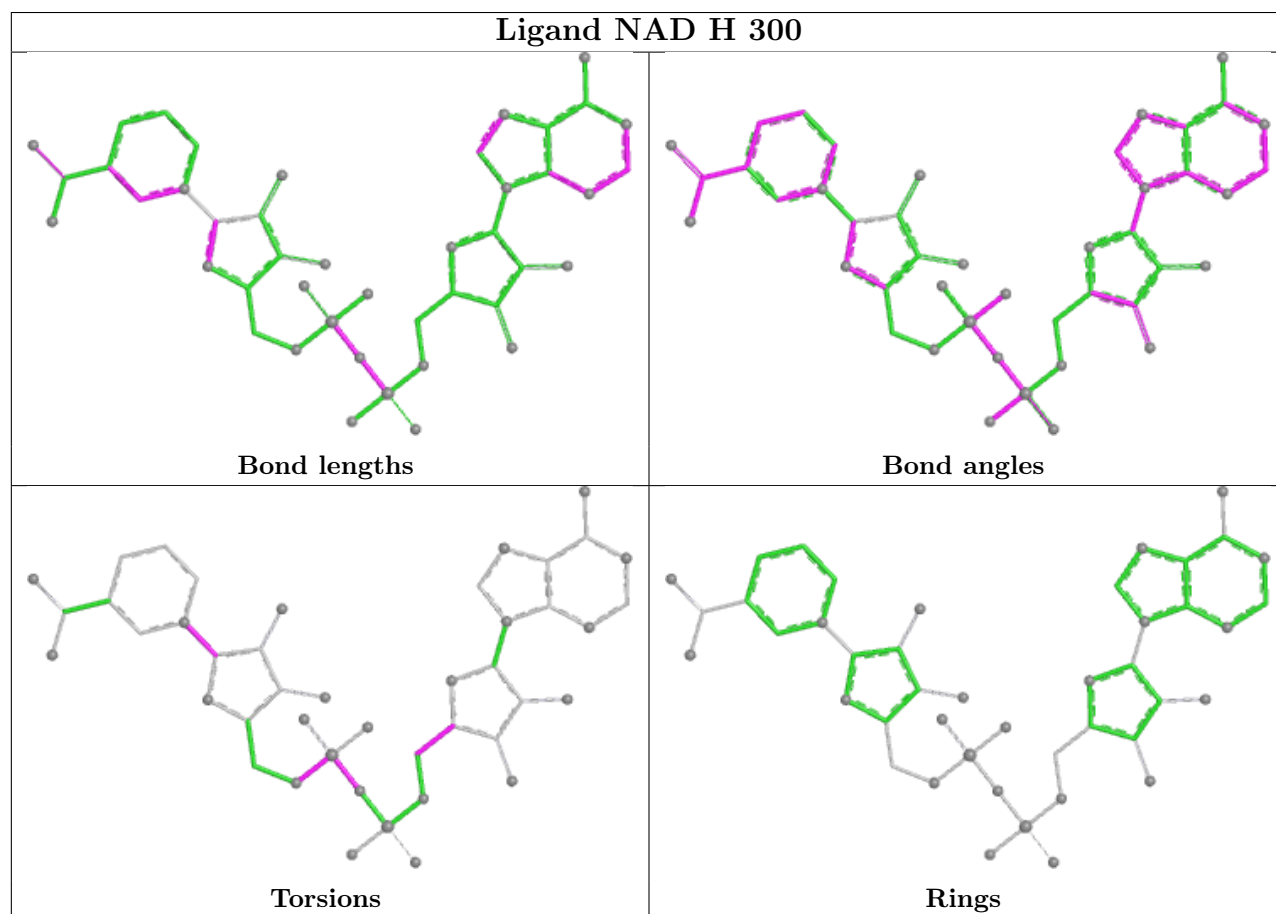
There are no ring outliers.

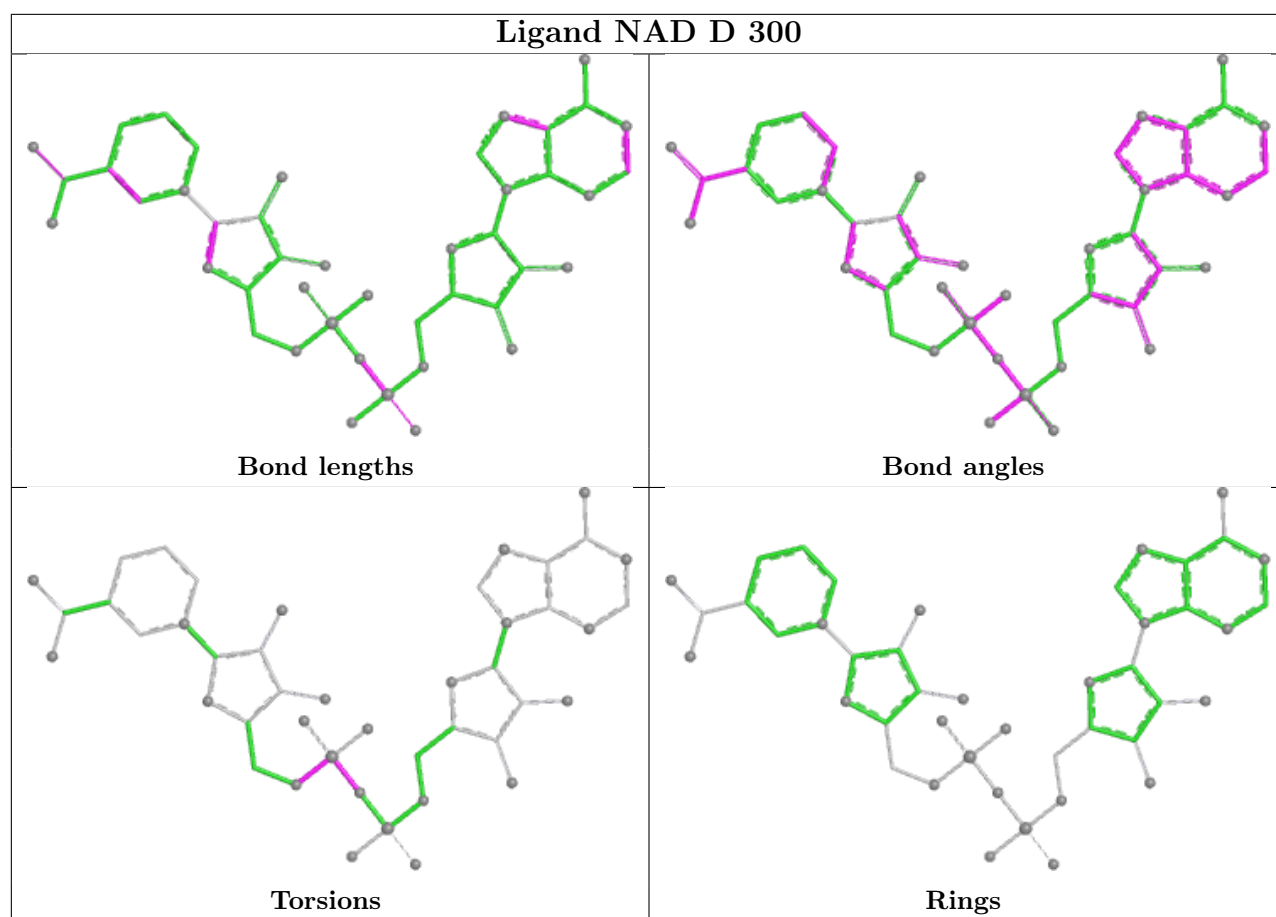
6 monomers are involved in 13 short contacts:

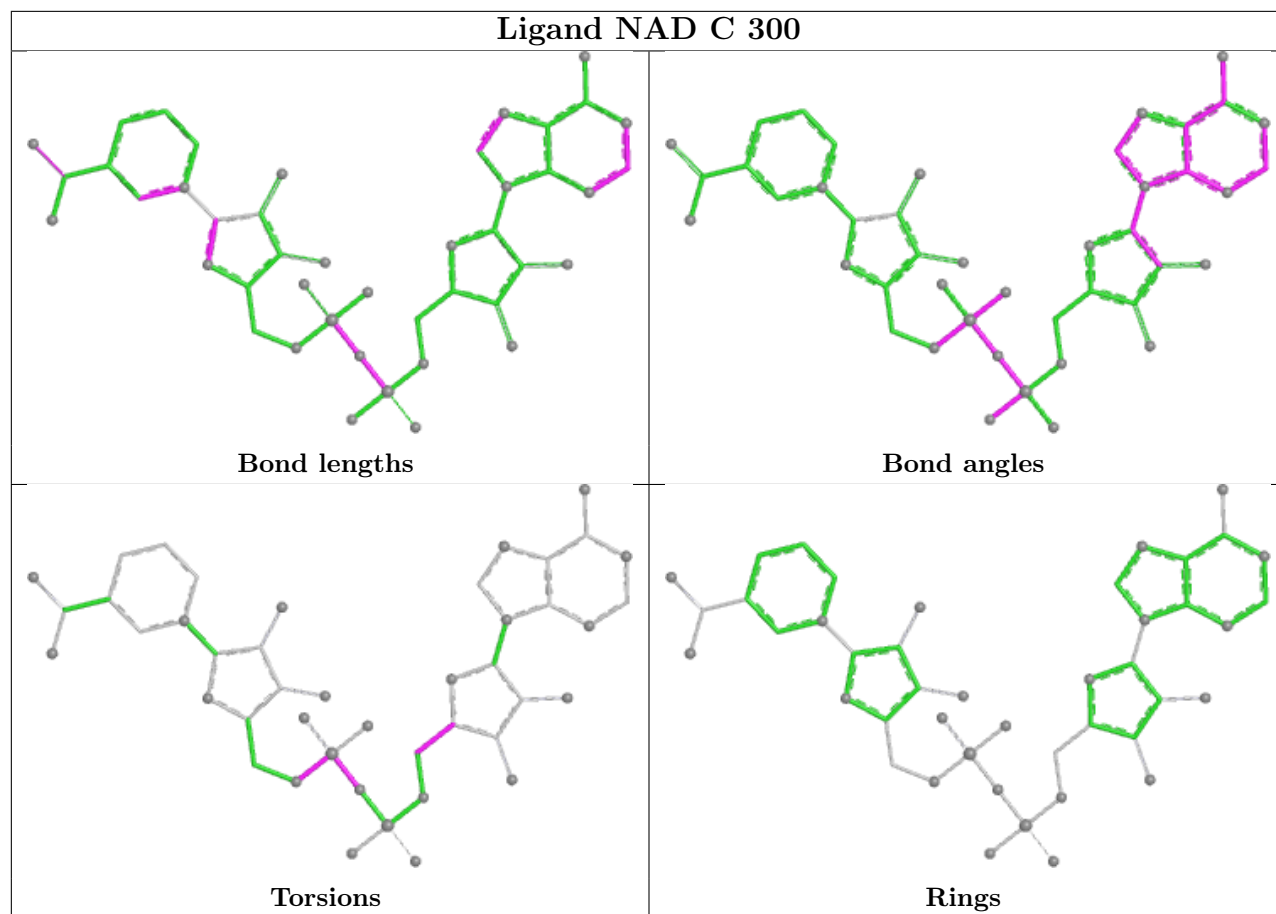
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	300	NAD	1	0
2	D	300	NAD	2	0
2	C	300	NAD	1	0
2	G	300	NAD	2	0
2	F	300	NAD	3	0
2	E	300	NAD	4	0

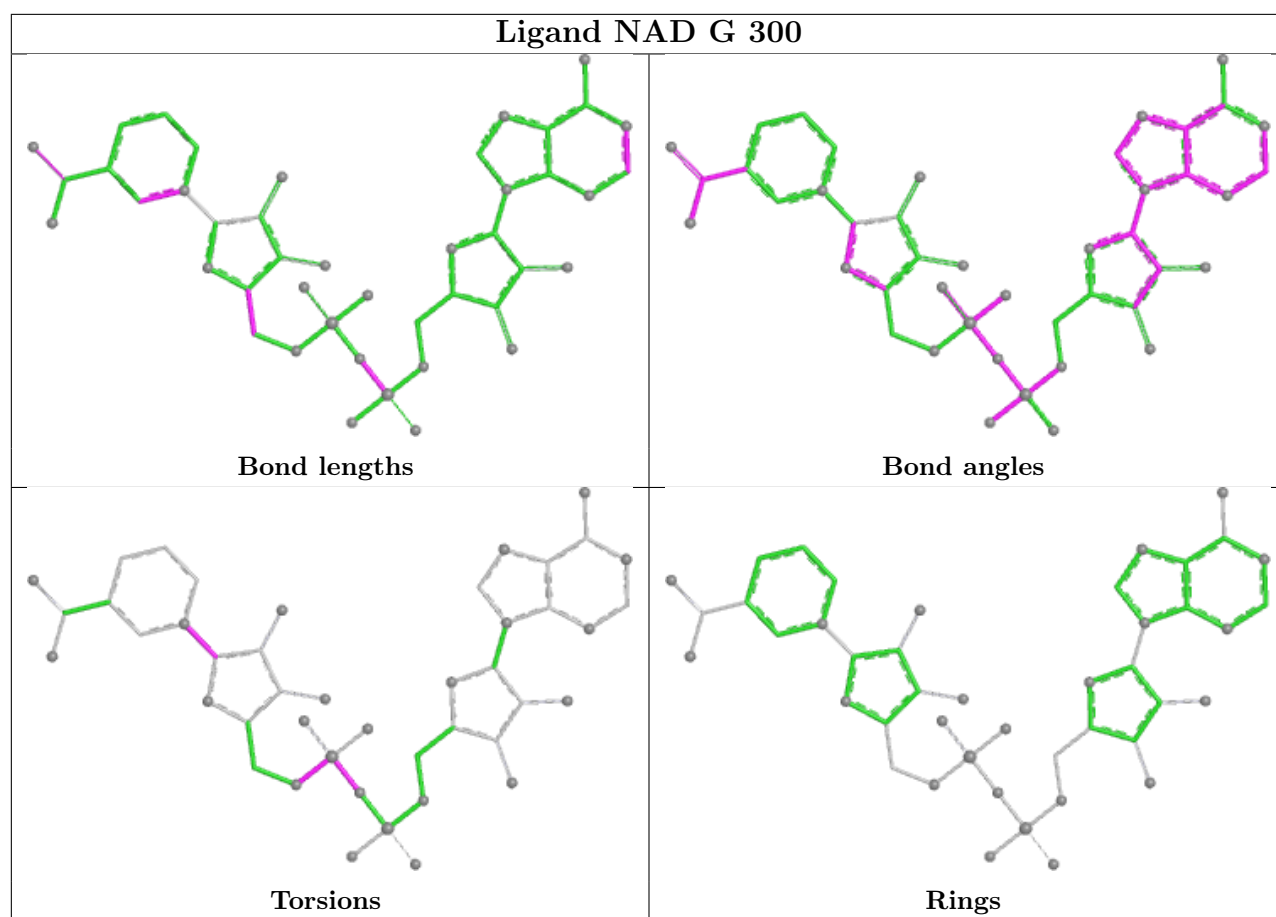
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

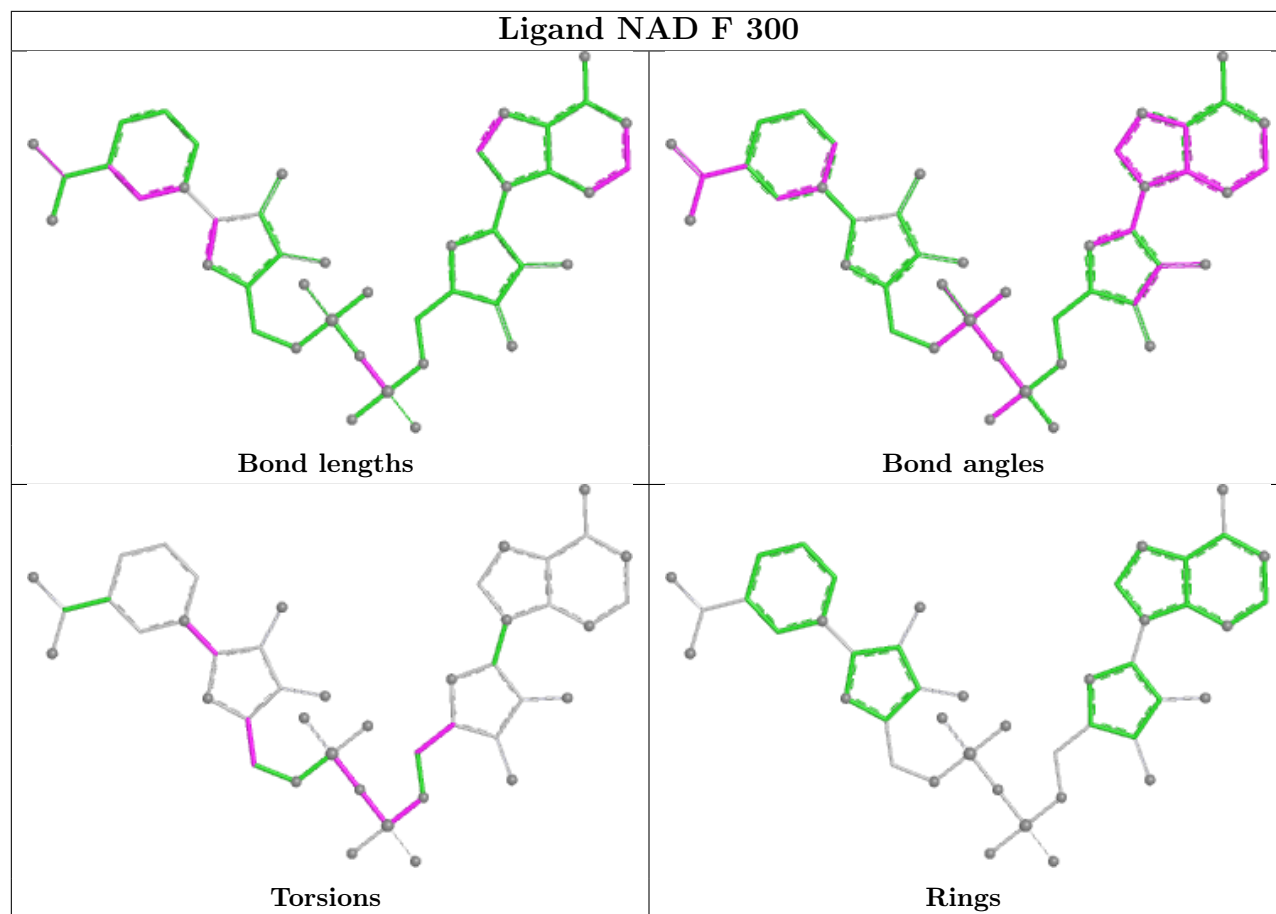
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

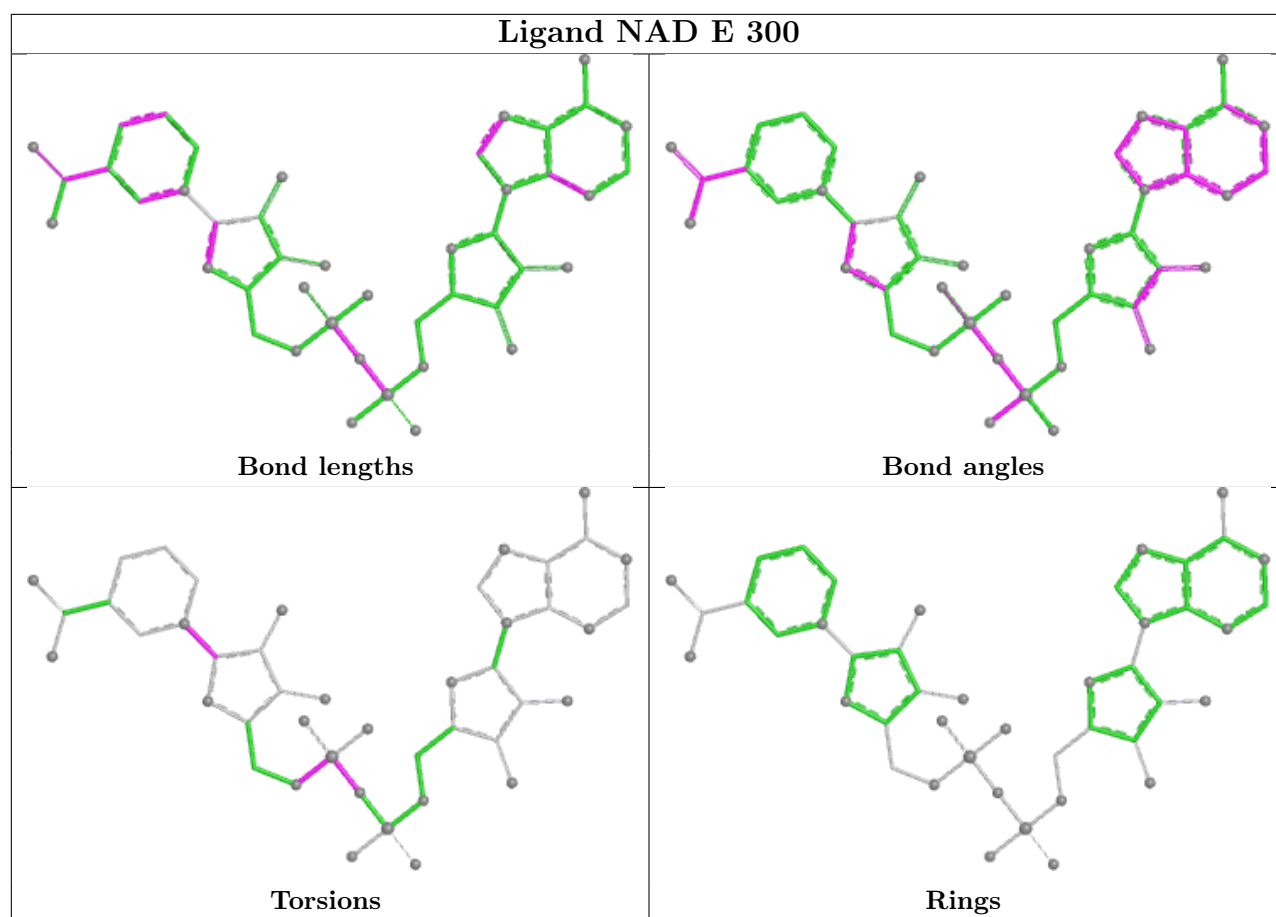












5.7 Other polymers [i](#)

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	250/255 (98%)	0.96	23 (9%) 14 13	36, 42, 52, 60	0
1	B	252/255 (98%)	0.90	18 (7%) 22 21	35, 42, 48, 59	0
1	C	243/255 (95%)	1.20	38 (15%) 5 4	35, 42, 50, 57	0
1	D	255/255 (100%)	0.86	10 (3%) 43 43	37, 42, 50, 59	0
1	E	249/255 (97%)	0.97	23 (9%) 14 13	36, 42, 48, 57	0
1	F	238/255 (93%)	0.95	16 (6%) 24 23	35, 42, 50, 55	0
1	G	251/255 (98%)	1.01	20 (7%) 18 17	35, 42, 49, 56	0
1	H	240/255 (94%)	1.03	26 (10%) 11 10	36, 42, 53, 63	0
All	All	1978/2040 (96%)	0.98	174 (8%) 15 15	35, 42, 50, 63	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	205	LEU	5.7
1	C	190	VAL	5.5
1	G	204	PRO	5.2
1	G	198	ALA	4.8
1	C	189	LEU	4.7
1	H	188	PRO	4.7
1	F	38	GLY	4.5
1	E	207	ALA	4.3
1	E	198	ALA	4.2
1	G	205	LEU	4.1
1	G	206	GLN	4.0
1	D	201	GLY	3.8
1	F	186	LEU	3.8
1	G	2	THR	3.7
1	B	198	ALA	3.7
1	D	130	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	199	ALA	3.7
1	H	80	GLY	3.5
1	H	52	VAL	3.5
1	C	2	THR	3.5
1	B	203	ASP	3.5
1	H	41	ALA	3.4
1	D	200	ASN	3.4
1	H	205	LEU	3.4
1	C	194	ILE	3.4
1	G	55	VAL	3.4
1	E	5	GLY	3.2
1	A	52	VAL	3.2
1	F	96	VAL	3.2
1	B	202	GLY	3.2
1	F	188	PRO	3.2
1	E	194	ILE	3.2
1	C	38	GLY	3.1
1	E	48	ALA	3.1
1	E	196	ASP	3.1
1	C	15	SER	3.1
1	H	206	GLN	3.0
1	A	2	THR	3.0
1	A	37	PHE	3.0
1	B	89	GLY	2.9
1	B	194	ILE	2.9
1	C	42	PRO	2.9
1	D	199	ALA	2.9
1	H	45	ALA	2.9
1	C	188	PRO	2.9
1	A	54	ALA	2.9
1	H	204	PRO	2.9
1	A	65	ALA	2.9
1	F	189	LEU	2.8
1	G	194	ILE	2.8
1	G	79	GLY	2.8
1	B	205	LEU	2.8
1	C	81	VAL	2.8
1	A	40	PRO	2.8
1	B	204	PRO	2.8
1	B	90	ILE	2.8
1	A	195	ASP	2.7
1	G	39	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	48	ALA	2.7
1	C	209	HIS	2.7
1	C	41	ALA	2.6
1	C	207	ALA	2.6
1	H	55	VAL	2.6
1	H	51	GLY	2.6
1	C	45	ALA	2.6
1	G	207	ALA	2.6
1	C	37	PHE	2.6
1	G	160	VAL	2.6
1	B	80	GLY	2.6
1	B	143	LEU	2.6
1	H	186	LEU	2.6
1	C	76	ARG	2.6
1	B	59	ALA	2.6
1	C	8	ALA	2.6
1	C	74	ALA	2.6
1	A	204	PRO	2.6
1	B	207	ALA	2.5
1	C	32	ILE	2.5
1	H	2	THR	2.5
1	A	44	LEU	2.5
1	E	143	LEU	2.5
1	H	78	PHE	2.5
1	C	55	VAL	2.5
1	H	76	ARG	2.5
1	E	14	THR	2.4
1	D	43	ALA	2.4
1	D	198	ALA	2.4
1	F	30	ALA	2.4
1	A	51	GLY	2.4
1	A	80	GLY	2.4
1	C	72	ALA	2.4
1	E	69	ALA	2.4
1	F	44	LEU	2.4
1	E	80	GLY	2.4
1	C	39	ASP	2.4
1	A	33	VAL	2.4
1	G	166	VAL	2.4
1	B	2	THR	2.4
1	B	74	ALA	2.3
1	F	101	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	202	GLY	2.3
1	E	210	ASP	2.3
1	H	144	VAL	2.3
1	F	208	GLN	2.3
1	H	23	GLN	2.3
1	H	48	ALA	2.3
1	F	80	GLY	2.3
1	G	143	LEU	2.3
1	B	190	VAL	2.3
1	F	31	ASN	2.3
1	C	186	LEU	2.3
1	E	197	ARG	2.3
1	G	210	ASP	2.3
1	C	108	ILE	2.3
1	E	47	ILE	2.3
1	C	52	VAL	2.3
1	E	160	VAL	2.3
1	C	54	ALA	2.3
1	D	214	GLU	2.2
1	C	193	GLN	2.2
1	A	71	PHE	2.2
1	B	71	PHE	2.2
1	D	2	THR	2.2
1	H	58	PRO	2.2
1	G	26	ALA	2.2
1	A	189	LEU	2.2
1	A	50	HIS	2.2
1	E	209	HIS	2.2
1	H	209	HIS	2.2
1	G	47	ILE	2.2
1	A	225	GLU	2.2
1	C	3	LEU	2.2
1	C	211	LEU	2.2
1	G	101	LEU	2.2
1	H	143	LEU	2.2
1	A	208	GLN	2.2
1	A	194	ILE	2.2
1	E	78	PHE	2.2
1	H	252	GLY	2.2
1	B	88	ALA	2.2
1	H	253	TRP	2.2
1	B	188	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	39	ASP	2.2
1	A	90	ILE	2.1
1	E	140	VAL	2.1
1	F	159	VAL	2.1
1	H	226	HIS	2.1
1	C	30	ALA	2.1
1	C	138	ALA	2.1
1	C	53	LYS	2.1
1	C	71	PHE	2.1
1	F	78	PHE	2.1
1	G	190	VAL	2.1
1	F	2	THR	2.1
1	A	42	PRO	2.1
1	E	29	GLY	2.1
1	A	47	ILE	2.1
1	C	137	ILE	2.1
1	C	10	VAL	2.1
1	C	78	PHE	2.1
1	E	73	LEU	2.0
1	E	208	GLN	2.0
1	E	76	ARG	2.0
1	G	209	HIS	2.0
1	C	67	ILE	2.0
1	C	83	ILE	2.0
1	A	46	GLU	2.0
1	H	140	VAL	2.0
1	D	138	ALA	2.0
1	E	206	GLN	2.0
1	F	211	LEU	2.0
1	A	203	ASP	2.0
1	F	209	HIS	2.0
1	H	5	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

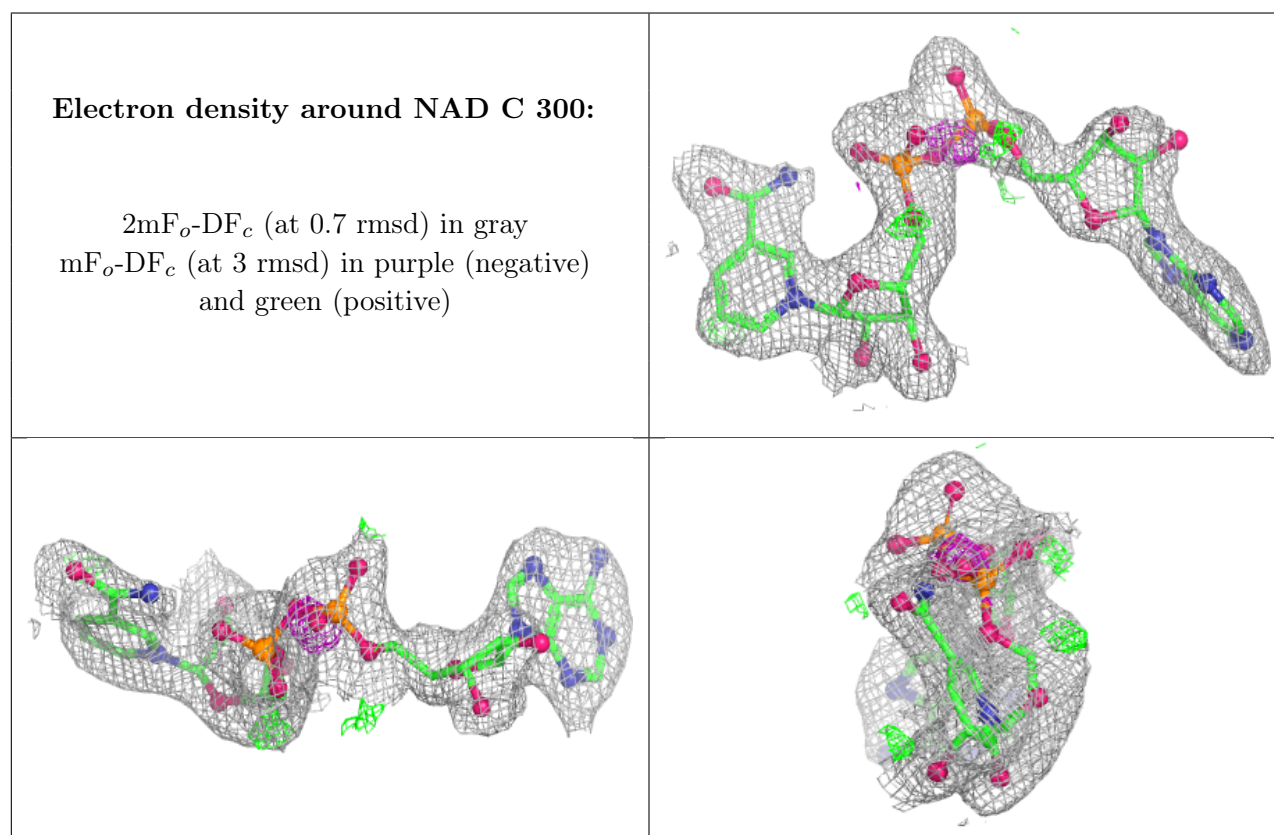
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

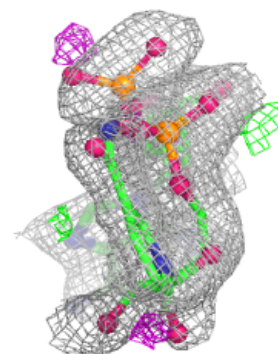
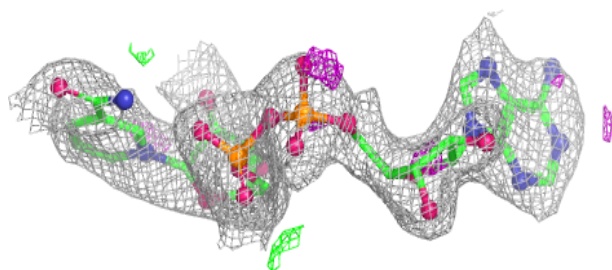
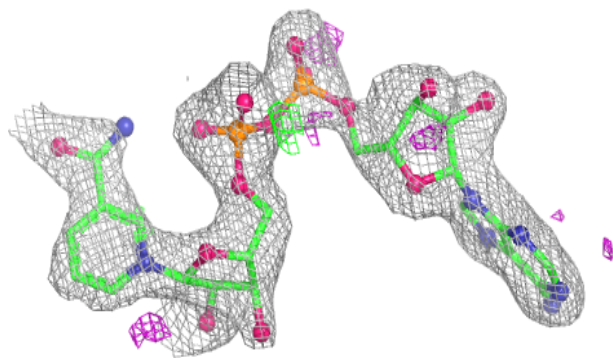
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAD	C	300	44/44	0.76	0.14	47,62,73,77	0
2	NAD	F	300	44/44	0.85	0.11	39,51,56,59	0
2	NAD	H	300	44/44	0.91	0.08	33,42,47,51	0
2	NAD	G	300	44/44	0.92	0.07	35,42,48,52	0
2	NAD	E	300	44/44	0.94	0.07	30,39,45,49	0
2	NAD	D	300	44/44	0.95	0.07	25,35,41,44	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.

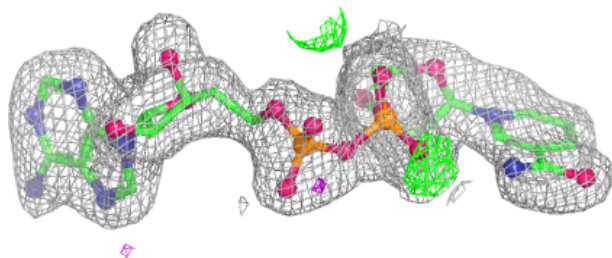
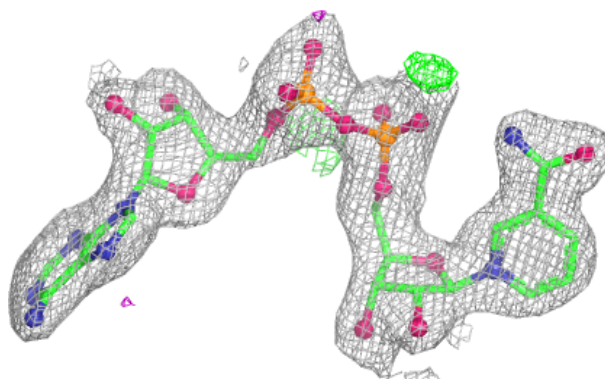


Electron density around NAD F 300:

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

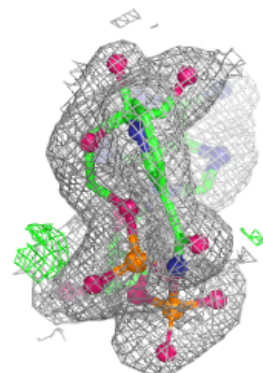
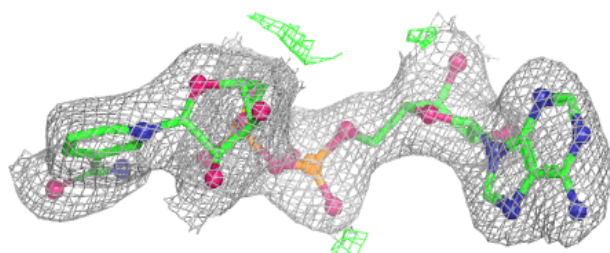
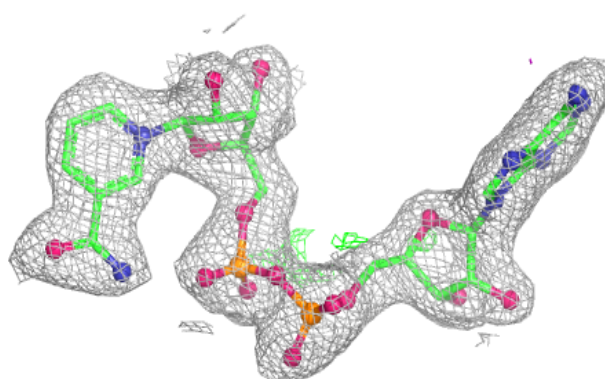
**Electron density around NAD H 300:**

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

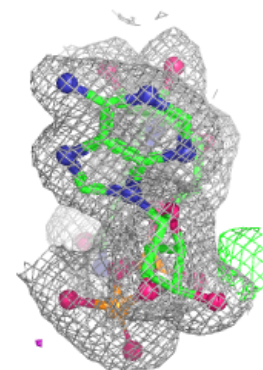
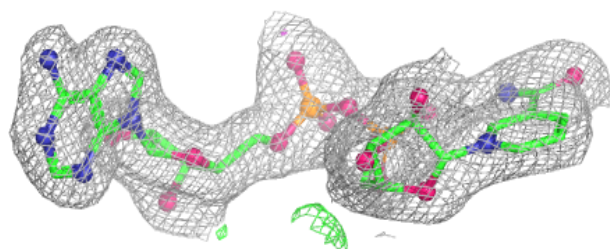
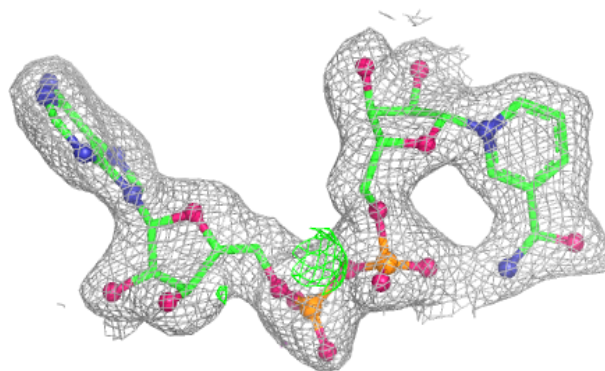


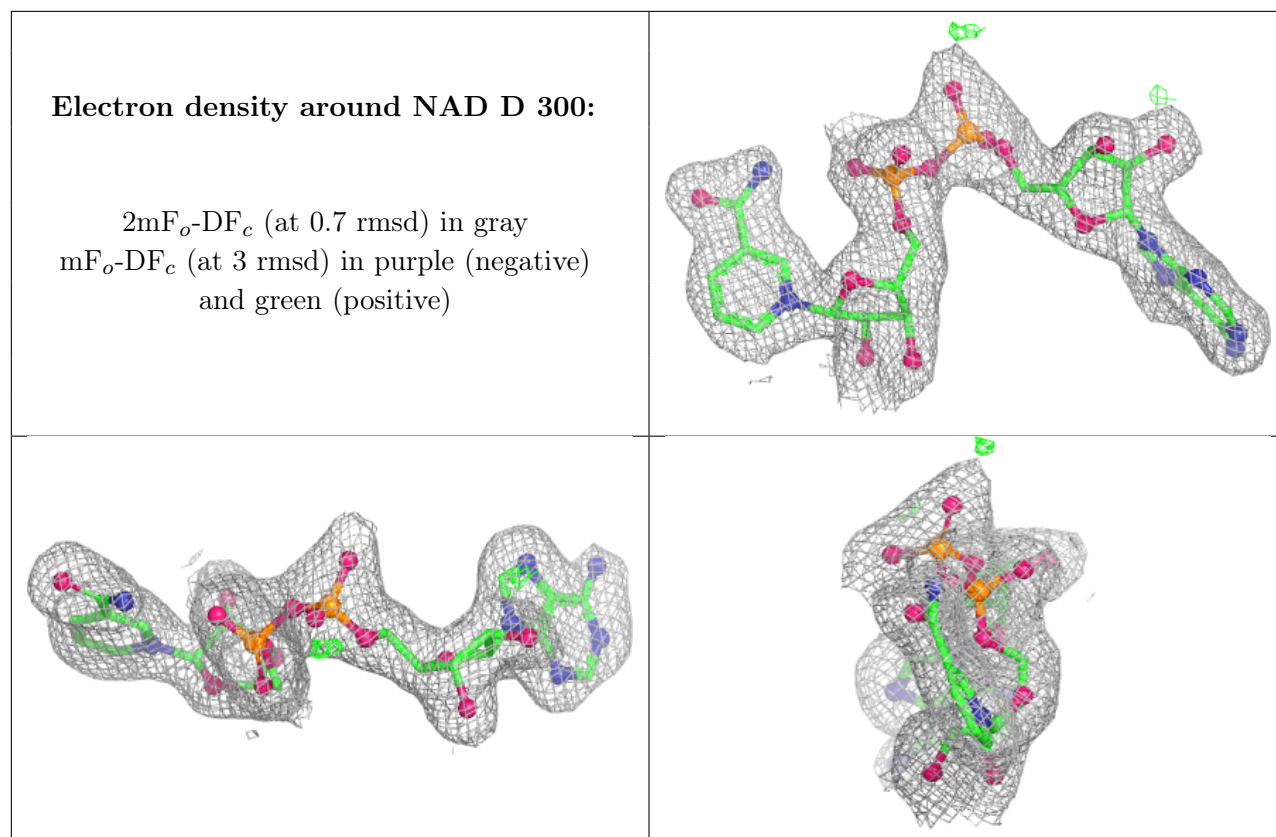
Electron density around NAD G 300:

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

**Electron density around NAD E 300:**

$2mF_o-DF_c$ (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.