



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:33 PM UTC

PDB ID : 1LDE / pdb_00001lde
Title : HORSE LIVER ALCOHOL DEHYDROGENASE COMPLEXED TO NADH
AND N-FORMYL PIPERDINE
Authors : Ramaswamy, S.; Plapp, B.V.
Deposited on : 1996-12-25
Resolution : 2.50 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

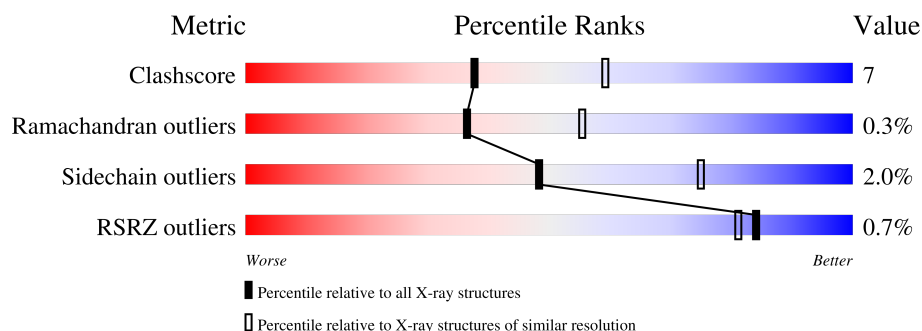
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	374	% 49% 43% 8% .
1	B	374	49% 43% 8%
1	C	374	% 52% 42% 6%
1	D	374	% 51% 40% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11912 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 LIVER ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2785	1769	472	521	23			
1	B	374	Total	C	N	O	S	0	0	0
			2785	1769	472	521	23			
1	C	374	Total	C	N	O	S	0	0	0
			2785	1769	472	521	23			
1	D	374	Total	C	N	O	S	0	0	0
			2785	1769	472	521	23			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

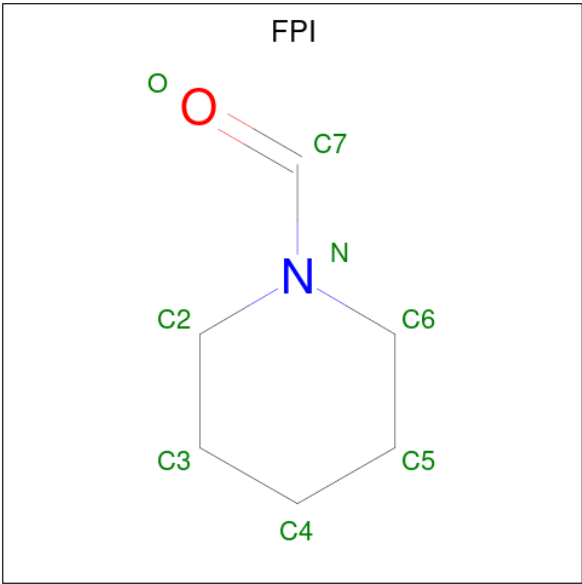
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 4 is N-FORMYLPIPERIDINE (CCD ID: FPI) (formula: C₆H₁₁NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	6	1	1		
4	B	1	Total	C	N	O	0	0
			8	6	1	1		
4	C	1	Total	C	N	O	0	0
			8	6	1	1		
4	D	1	Total	C	N	O	0	0
			8	6	1	1		

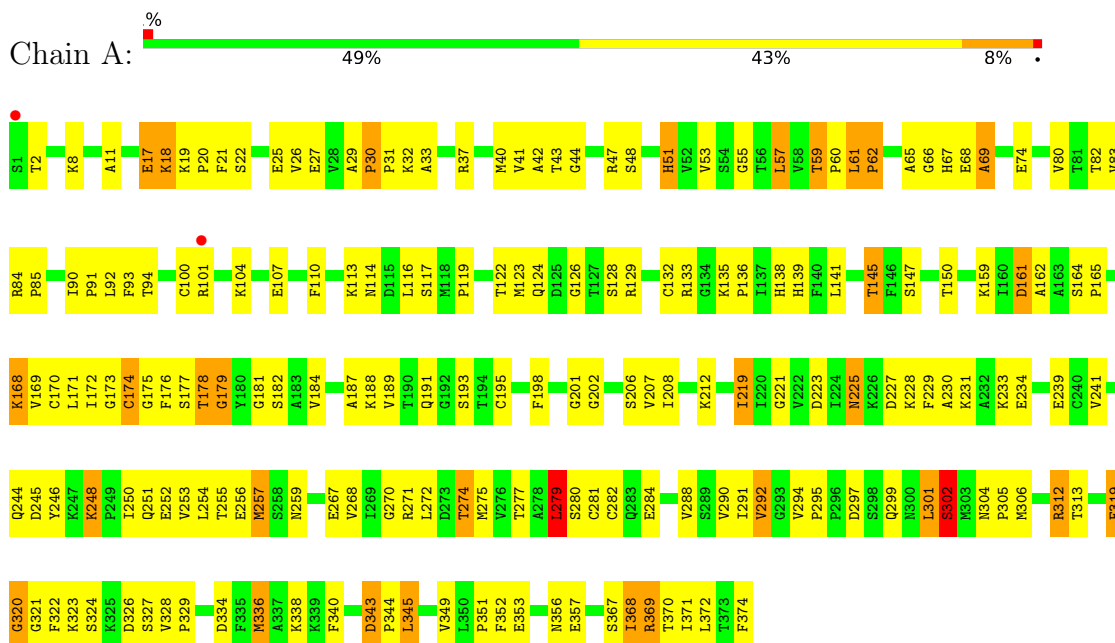
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	144	Total	O	0	0
			144	144		
5	B	144	Total	O	0	0
			144	144		
5	C	134	Total	O	0	0
			134	134		
5	D	134	Total	O	0	0
			134	134		

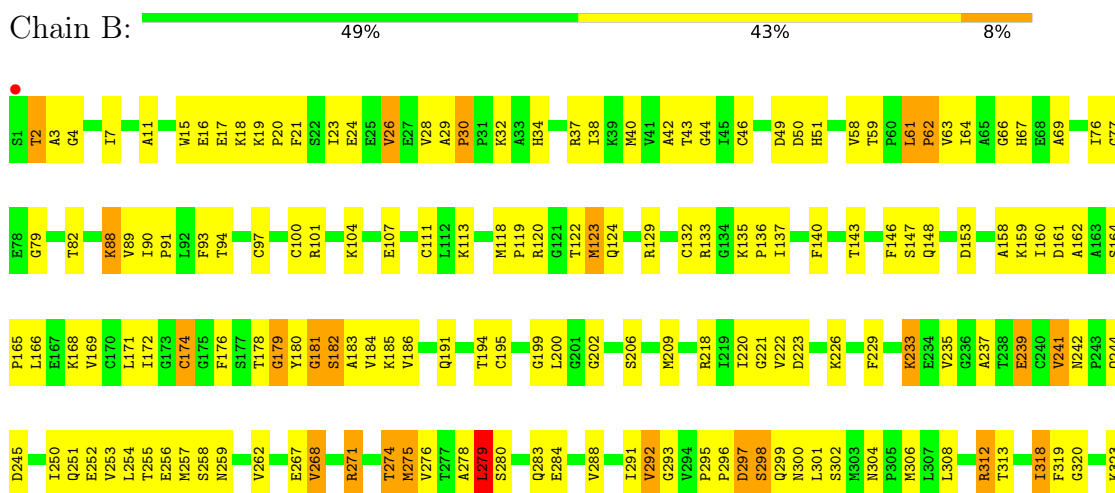
3 Residue-property plots

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: LIVER ALCOHOL DEHYDROGENASE

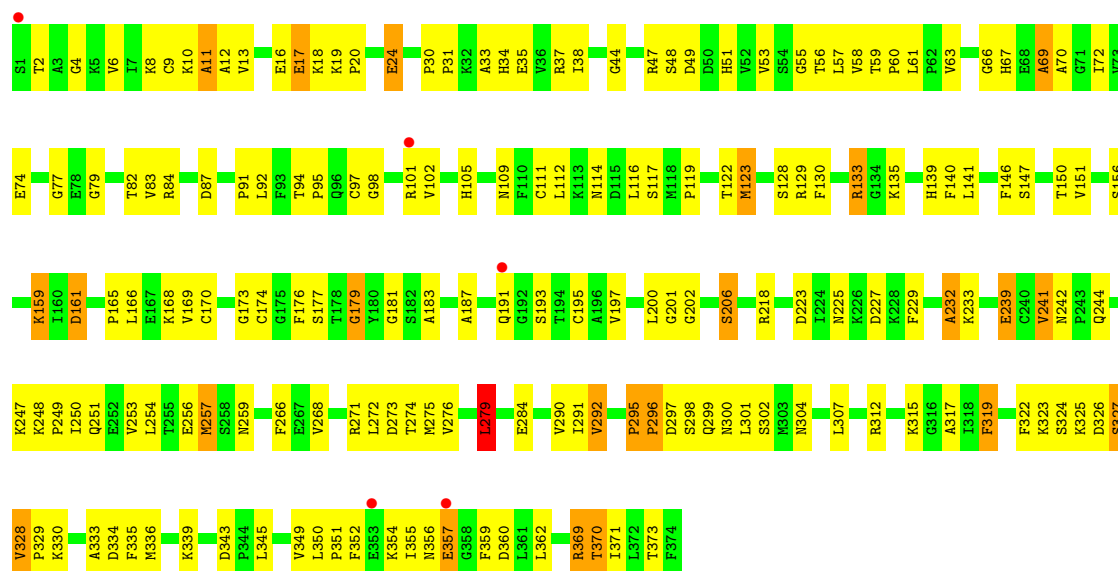


• Molecule 1: LIVER ALCOHOL DEHYDROGENASE

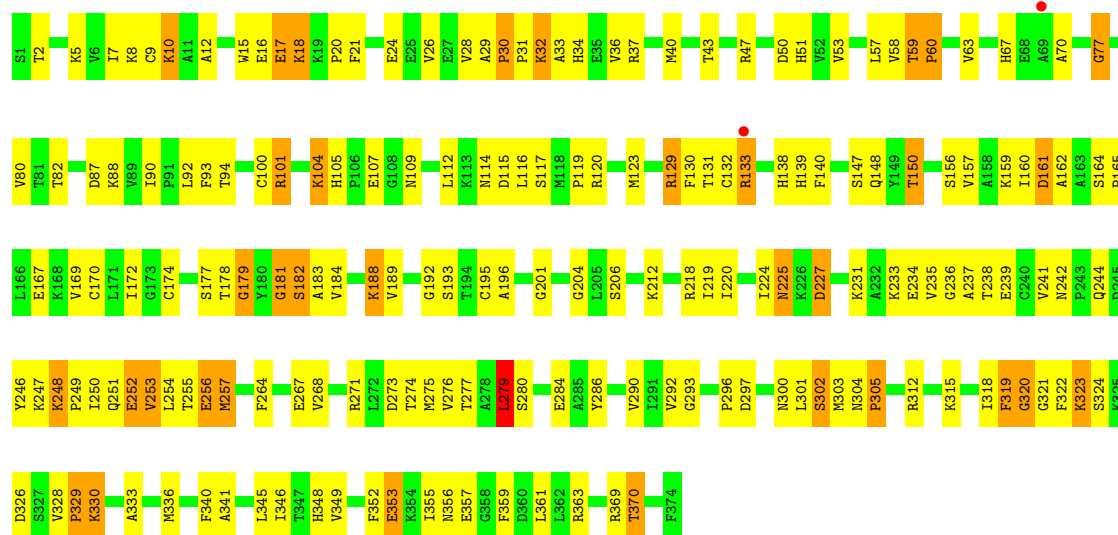




• Molecule 1: LIVER ALCOHOL DEHYDROGENASE



• Molecule 1: LIVER ALCOHOL DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.93Å 180.20Å 86.80Å 90.00° 106.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	88.8 (20.00-2.50) 88.1 (20.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.42 (at 2.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.256 0.189 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.764	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11912	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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 68.07 % 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 4.6440e-06. 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, ZN, FPI

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	1.88	45/2837 (1.6%)	2.53	201/3834 (5.2%)
1	B	1.87	42/2837 (1.5%)	2.48	212/3834 (5.5%)
1	C	1.86	38/2837 (1.3%)	2.48	191/3834 (5.0%)
1	D	1.88	50/2837 (1.8%)	2.49	201/3834 (5.2%)
All	All	1.87	175/11348 (1.5%)	2.49	805/15336 (5.2%)

All (175) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	HIS	CE1-NE2	12.26	1.44	1.32
1	B	122	THR	N-CA	-9.00	1.34	1.46
1	A	41	VAL	C-O	-8.82	1.14	1.23
1	C	84	ARG	CA-C	8.44	1.60	1.52
1	D	51	HIS	C-O	8.33	1.34	1.24
1	B	38	ILE	N-CA	-7.95	1.37	1.46
1	D	333	ALA	N-CA	7.79	1.55	1.46
1	D	183	ALA	N-CA	-7.77	1.37	1.46
1	A	27	GLU	N-CA	-7.63	1.36	1.46
1	C	84	ARG	C-O	7.55	1.30	1.24
1	C	170	CYS	C-O	-7.44	1.14	1.24
1	B	292	VAL	CA-C	7.36	1.60	1.52
1	B	220	ILE	C-N	7.30	1.40	1.33
1	B	23	ILE	C-O	-7.17	1.17	1.23
1	A	301	LEU	CA-C	7.02	1.61	1.52
1	C	369	ARG	NE-CZ	7.01	1.40	1.33
1	B	183	ALA	N-CA	-6.96	1.38	1.46
1	A	41	VAL	CA-C	-6.92	1.45	1.52
1	C	323	LYS	N-CA	6.71	1.54	1.46
1	C	67	HIS	ND1-CE1	6.71	1.39	1.32
1	D	58	VAL	N-CA	-6.70	1.37	1.46
1	D	267	GLU	N-CA	-6.70	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	HIS	CG-ND1	6.69	1.45	1.38
1	A	181	GLY	CA-C	6.67	1.59	1.52
1	D	348	HIS	N-CA	-6.66	1.38	1.46
1	A	323	LYS	CA-C	6.62	1.61	1.52
1	B	186	VAL	C-O	-6.62	1.17	1.24
1	B	293	GLY	CA-C	6.61	1.57	1.52
1	B	51	HIS	CE1-NE2	-6.60	1.25	1.32
1	A	122	THR	N-CA	-6.58	1.37	1.46
1	C	333	ALA	N-CA	6.58	1.54	1.46
1	B	262	VAL	CA-C	-6.57	1.46	1.53
1	A	288	VAL	C-O	6.56	1.30	1.24
1	C	111	CYS	CA-C	-6.53	1.44	1.52
1	D	172	ILE	C-N	-6.45	1.25	1.34
1	C	150	THR	N-CA	6.42	1.54	1.45
1	D	276	VAL	C-N	-6.41	1.25	1.33
1	B	140	PHE	CA-CB	-6.34	1.43	1.53
1	B	82	THR	CA-C	-6.22	1.44	1.52
1	C	105	HIS	CE1-NE2	6.21	1.38	1.32
1	C	44	GLY	C-O	6.17	1.32	1.23
1	B	90	ILE	N-CA	6.16	1.50	1.45
1	A	61	LEU	CA-CB	-6.14	1.44	1.53
1	B	28	VAL	N-CA	-6.13	1.38	1.46
1	B	66	GLY	C-N	6.13	1.42	1.33
1	D	162	ALA	C-O	6.10	1.31	1.24
1	D	359	PHE	N-CA	-6.09	1.38	1.46
1	D	355	ILE	N-CA	-6.05	1.39	1.46
1	D	225	ASN	C-N	-6.04	1.25	1.33
1	A	165	PRO	N-CD	6.03	1.56	1.47
1	C	13	VAL	N-CA	-6.02	1.39	1.46
1	A	272	LEU	C-N	-6.01	1.26	1.33
1	A	357	GLU	C-O	-5.96	1.16	1.24
1	D	10	LYS	C-O	5.91	1.31	1.23
1	A	67	HIS	N-CA	5.91	1.53	1.46
1	A	177	SER	CA-CB	-5.91	1.44	1.53
1	C	95	PRO	C-O	5.87	1.31	1.23
1	C	102	VAL	N-CA	5.85	1.53	1.46
1	D	30	PRO	CA-C	5.85	1.57	1.52
1	B	30	PRO	CA-CB	5.83	1.62	1.54
1	A	326	ASP	C-N	-5.83	1.25	1.33
1	D	63	VAL	CA-CB	5.80	1.64	1.55
1	D	63	VAL	N-CA	-5.78	1.40	1.46
1	D	28	VAL	C-O	5.78	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	195	CYS	C-N	-5.78	1.26	1.33
1	D	224	ILE	N-CA	-5.77	1.40	1.46
1	A	30	PRO	CA-CB	5.77	1.61	1.54
1	C	140	PHE	C-O	5.76	1.30	1.24
1	D	330	LYS	C-O	5.76	1.30	1.24
1	A	65	ALA	N-CA	5.75	1.52	1.46
1	C	12	ALA	N-CA	5.75	1.53	1.46
1	C	146	PHE	N-CA	5.74	1.53	1.46
1	A	324	SER	N-CA	-5.73	1.39	1.46
1	D	133	ARG	NE-CZ	5.71	1.39	1.33
1	D	150	THR	C-O	5.70	1.31	1.23
1	B	66	GLY	N-CA	-5.69	1.37	1.45
1	D	319	PHE	C-O	5.69	1.31	1.23
1	A	42	ALA	C-O	5.68	1.30	1.23
1	A	257	MET	CA-C	-5.64	1.44	1.52
1	A	82	THR	CA-C	-5.63	1.44	1.52
1	B	369	ARG	NE-CZ	5.63	1.39	1.33
1	C	169	VAL	C-O	5.62	1.30	1.24
1	A	101	ARG	C-N	-5.61	1.26	1.33
1	B	274	THR	C-O	-5.61	1.16	1.24
1	B	165	PRO	C-O	5.61	1.31	1.24
1	A	22	SER	C-O	-5.59	1.17	1.24
1	A	319	PHE	CA-CB	5.59	1.61	1.53
1	D	115	ASP	N-CA	5.59	1.52	1.46
1	C	183	ALA	C-O	5.58	1.30	1.24
1	B	176	PHE	N-CA	-5.57	1.39	1.46
1	C	299	GLN	N-CA	-5.55	1.39	1.46
1	D	321	GLY	CA-C	5.53	1.59	1.51
1	D	140	PHE	C-O	5.52	1.30	1.24
1	A	228	LYS	N-CA	-5.52	1.38	1.46
1	D	267	GLU	CA-C	5.50	1.59	1.52
1	C	371	ILE	CA-C	5.48	1.59	1.52
1	D	20	PRO	C-O	5.48	1.30	1.23
1	D	51	HIS	ND1-CE1	5.47	1.38	1.32
1	B	146	PHE	C-O	5.46	1.30	1.23
1	C	181	GLY	N-CA	-5.46	1.39	1.45
1	D	21	PHE	C-O	5.45	1.30	1.23
1	A	31	PRO	N-CA	-5.45	1.40	1.47
1	C	92	LEU	C-O	-5.45	1.17	1.24
1	A	345	LEU	C-N	5.44	1.40	1.33
1	B	301	LEU	C-N	-5.43	1.26	1.33
1	D	47	ARG	NE-CZ	5.42	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	275	MET	CA-C	5.42	1.59	1.52
1	B	304	ASN	C-N	-5.40	1.27	1.33
1	D	156	SER	N-CA	-5.40	1.39	1.46
1	A	313	THR	C-N	-5.38	1.26	1.33
1	D	119	PRO	CA-C	-5.38	1.46	1.52
1	C	63	VAL	CA-CB	5.38	1.63	1.55
1	B	59	THR	C-N	-5.38	1.27	1.33
1	C	57	LEU	C-N	-5.38	1.26	1.33
1	A	327	SER	CA-CB	5.37	1.62	1.53
1	B	180	TYR	C-N	-5.36	1.27	1.33
1	B	222	VAL	C-O	5.36	1.29	1.24
1	A	277	THR	C-O	5.35	1.30	1.24
1	A	74	GLU	C-N	-5.33	1.26	1.33
1	B	328	VAL	C-N	-5.32	1.26	1.34
1	D	159	LYS	N-CA	-5.32	1.39	1.46
1	B	46	CYS	C-O	5.32	1.30	1.23
1	B	111	CYS	CA-CB	5.31	1.62	1.53
1	D	181	GLY	CA-C	5.31	1.57	1.52
1	D	105	HIS	CA-C	-5.30	1.47	1.52
1	D	164	SER	CA-C	-5.30	1.46	1.53
1	A	66	GLY	C-N	5.29	1.41	1.33
1	B	90	ILE	CA-CB	-5.29	1.50	1.54
1	B	276	VAL	N-CA	-5.28	1.40	1.46
1	B	148	GLN	C-O	5.27	1.30	1.24
1	A	53	VAL	N-CA	-5.26	1.40	1.46
1	A	128	SER	CA-C	-5.25	1.46	1.52
1	D	286	TYR	N-CA	-5.25	1.41	1.46
1	B	153	ASP	C-O	5.23	1.30	1.23
1	C	77	GLY	N-CA	5.23	1.51	1.45
1	C	359	PHE	CA-CB	-5.22	1.45	1.53
1	D	320	GLY	C-O	-5.22	1.16	1.23
1	A	17	GLU	C-O	-5.21	1.16	1.23
1	A	44	GLY	C-N	-5.21	1.28	1.33
1	B	345	LEU	C-N	5.21	1.40	1.33
1	B	174	CYS	N-CA	-5.21	1.39	1.46
1	C	296	PRO	C-O	5.21	1.31	1.23
1	D	26	VAL	C-O	5.21	1.30	1.23
1	C	327	SER	CA-C	-5.20	1.45	1.52
1	A	138	HIS	CG-ND1	5.20	1.44	1.38
1	A	176	PHE	CA-CB	5.19	1.61	1.53
1	D	323	LYS	CA-C	5.18	1.59	1.52
1	A	68	GLU	N-CA	5.16	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	117	SER	CA-C	-5.15	1.46	1.52
1	C	69	ALA	CA-CB	5.15	1.62	1.53
1	B	326	ASP	C-N	-5.15	1.26	1.33
1	C	33	ALA	N-CA	5.14	1.52	1.46
1	D	201	GLY	CA-C	5.13	1.58	1.51
1	A	48	SER	N-CA	-5.13	1.39	1.46
1	D	253	VAL	N-CA	5.13	1.52	1.46
1	A	294	VAL	N-CA	5.12	1.51	1.46
1	C	19	LYS	C-O	-5.12	1.18	1.24
1	D	43	THR	N-CA	5.12	1.52	1.46
1	A	313	THR	CA-CB	-5.12	1.44	1.53
1	B	50	ASP	CA-C	5.11	1.59	1.52
1	B	21	PHE	N-CA	5.09	1.52	1.45
1	C	151	VAL	C-O	5.09	1.29	1.24
1	D	349	VAL	N-CA	5.08	1.52	1.46
1	C	44	GLY	N-CA	5.07	1.50	1.44
1	B	43	THR	C-N	5.07	1.40	1.33
1	A	170	CYS	N-CA	-5.07	1.40	1.46
1	B	185	LYS	C-N	-5.07	1.27	1.33
1	B	279	LEU	CA-C	5.07	1.59	1.52
1	C	195	CYS	N-CA	5.06	1.52	1.45
1	D	219	ILE	C-O	5.05	1.29	1.24
1	C	31	PRO	N-CD	-5.04	1.40	1.47
1	D	70	ALA	CA-C	5.03	1.58	1.52
1	C	128	SER	C-N	-5.03	1.27	1.33
1	D	292	VAL	CA-CB	-5.00	1.48	1.54
1	C	66	GLY	CA-C	5.00	1.58	1.51

All (805) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ARG	CD-NE-CZ	-19.18	97.55	124.40
1	A	101	ARG	NE-CZ-NH2	-18.95	102.14	119.20
1	B	259	ASN	OD1-CG-ND2	-14.73	107.87	122.60
1	C	191	GLN	OE1-CD-NE2	14.61	137.21	122.60
1	A	101	ARG	NH1-CZ-NH2	13.75	137.18	119.30
1	B	133	ARG	NE-CZ-NH2	13.67	131.50	119.20
1	C	251	GLN	OE1-CD-NE2	13.64	136.24	122.60
1	A	133	ARG	NE-CZ-NH2	12.82	130.74	119.20
1	A	101	ARG	CG-CD-NE	-12.64	84.18	112.00
1	D	59	THR	O-C-N	-12.00	112.47	121.83
1	C	59	THR	O-C-N	-11.98	112.48	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	PHE	CA-C-O	-11.75	108.67	121.00
1	B	101	ARG	NE-CZ-NH1	-11.14	110.36	121.50
1	C	328	VAL	N-CA-CB	-11.07	103.10	110.52
1	D	133	ARG	NE-CZ-NH2	10.82	128.94	119.20
1	A	161	ASP	CA-CB-CG	10.81	123.41	112.60
1	A	223	ASP	CA-C-O	-10.46	108.08	120.43
1	C	242	ASN	OD1-CG-ND2	-10.40	112.20	122.60
1	D	8	LYS	CA-C-O	-10.35	109.10	120.38
1	D	220	ILE	CA-C-N	-10.15	110.69	121.45
1	D	220	ILE	C-N-CA	-10.15	110.69	121.45
1	C	17	GLU	O-C-N	-9.92	111.48	122.79
1	C	101	ARG	NE-CZ-NH1	-9.66	111.84	121.50
1	A	93	PHE	CA-CB-CG	9.65	123.45	113.80
1	B	67	HIS	CA-CB-CG	-9.48	104.32	113.80
1	D	323	LYS	N-CA-C	-9.47	95.67	109.59
1	B	366	GLU	CA-C-O	-9.26	108.87	119.79
1	C	8	LYS	CA-C-O	-9.22	110.38	120.43
1	C	133	ARG	NE-CZ-NH2	9.21	127.49	119.20
1	D	324	SER	N-CA-C	9.19	122.23	111.02
1	C	251	GLN	N-CA-CB	9.17	123.61	110.12
1	A	312	ARG	NE-CZ-NH1	-9.14	112.36	121.50
1	A	221	GLY	CA-C-O	-9.09	113.00	120.91
1	D	192	GLY	CA-C-O	-9.04	109.45	119.04
1	B	179	GLY	CA-C-N	9.03	132.17	120.44
1	B	179	GLY	C-N-CA	9.03	132.17	120.44
1	A	370	THR	CA-C-O	-8.99	110.63	120.43
1	B	298	SER	N-CA-CB	-8.94	100.50	113.65
1	B	159	LYS	O-C-N	-8.91	112.61	123.04
1	B	326	ASP	CA-C-O	-8.84	111.05	120.42
1	C	161	ASP	CA-CB-CG	8.79	121.39	112.60
1	B	107	GLU	CA-C-N	-8.77	109.59	120.64
1	B	107	GLU	C-N-CA	-8.77	109.59	120.64
1	D	59	THR	CA-C-O	8.72	128.22	119.76
1	A	170	CYS	N-CA-C	-8.70	101.80	111.28
1	B	288	VAL	O-C-N	8.67	132.56	123.20
1	A	67	HIS	CA-CB-CG	-8.67	105.13	113.80
1	A	171	LEU	O-C-N	-8.64	112.34	122.20
1	D	179	GLY	CA-C-N	8.61	131.63	120.44
1	D	179	GLY	C-N-CA	8.61	131.63	120.44
1	D	363	ARG	NE-CZ-NH1	-8.54	112.96	121.50
1	D	239	GLU	CA-C-O	-8.51	112.14	121.33
1	A	17	GLU	O-C-N	-8.48	112.83	122.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	323	LYS	N-CA-C	-8.47	97.14	109.59
1	C	324	SER	N-CA-C	8.44	121.31	111.02
1	C	67	HIS	CA-CB-CG	-8.43	105.37	113.80
1	A	229	PHE	N-CA-C	8.40	120.44	111.28
1	D	333	ALA	CA-C-O	-8.38	111.94	120.90
1	A	323	LYS	N-CA-C	-8.36	97.11	109.15
1	A	372	LEU	O-C-N	8.35	132.71	123.27
1	B	184	VAL	CA-C-O	8.34	129.25	120.25
1	A	184	VAL	O-C-N	-8.33	112.39	121.80
1	A	135	LYS	CA-C-N	8.30	128.62	119.90
1	A	135	LYS	C-N-CA	8.30	128.62	119.90
1	C	362	LEU	O-C-N	8.29	130.66	122.03
1	D	101	ARG	NE-CZ-NH1	-8.25	113.25	121.50
1	B	283	GLN	CA-C-O	8.22	128.60	120.88
1	B	119	PRO	N-CA-CB	8.18	110.45	103.17
1	C	326	ASP	CA-C-O	-8.18	111.75	120.42
1	A	212	LYS	O-C-N	-8.15	113.48	122.12
1	B	172	ILE	O-C-N	-8.14	111.24	122.31
1	C	239	GLU	CA-C-O	-8.14	112.54	121.33
1	B	229	PHE	N-CA-C	8.13	119.77	111.07
1	B	172	ILE	CA-C-O	8.11	130.16	119.53
1	C	242	ASN	CA-C-O	8.09	127.32	119.55
1	C	114	ASN	OD1-CG-ND2	-8.05	114.55	122.60
1	A	284	GLU	CA-C-O	-8.02	111.22	120.20
1	A	176	PHE	CA-CB-CG	-8.00	105.80	113.80
1	C	129	ARG	NE-CZ-NH2	8.00	126.40	119.20
1	D	273	ASP	O-C-N	-7.98	113.66	122.12
1	D	9	CYS	O-C-N	7.89	131.44	122.99
1	C	101	ARG	NH1-CZ-NH2	7.86	129.52	119.30
1	D	239	GLU	O-C-N	7.83	132.18	123.25
1	B	304	ASN	CA-CB-CG	-7.81	104.79	112.60
1	A	176	PHE	CA-C-O	-7.80	112.81	121.00
1	B	101	ARG	NE-CZ-NH2	7.79	126.22	119.20
1	A	26	VAL	CA-C-O	-7.79	114.01	121.64
1	B	256	GLU	N-CA-CB	7.77	121.26	109.91
1	C	170	CYS	N-CA-C	-7.75	102.83	111.82
1	A	356	ASN	OD1-CG-ND2	-7.74	114.86	122.60
1	D	17	GLU	CA-C-O	7.72	130.37	121.87
1	B	255	THR	N-CA-C	-7.71	102.96	111.36
1	C	183	ALA	CB-CA-C	-7.71	99.01	110.95
1	B	323	LYS	N-CA-C	-7.70	98.06	109.15
1	B	89	VAL	CA-C-O	7.70	129.25	121.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	130	PHE	CA-CB-CG	7.67	121.47	113.80
1	B	356	ASN	OD1-CG-ND2	-7.66	114.94	122.60
1	C	17	GLU	CA-C-O	7.66	130.76	121.87
1	C	59	THR	CA-C-O	7.62	127.16	119.76
1	A	30	PRO	CA-C-N	7.62	127.38	119.76
1	A	30	PRO	C-N-CA	7.62	127.38	119.76
1	B	191	GLN	OE1-CD-NE2	7.61	130.21	122.60
1	B	308	LEU	CA-C-N	7.60	130.46	120.28
1	B	308	LEU	C-N-CA	7.60	130.46	120.28
1	A	327	SER	N-CA-C	7.59	121.02	111.69
1	A	374	PHE	CA-CB-CG	-7.59	106.21	113.80
1	A	37	ARG	NE-CZ-NH1	-7.58	113.92	121.50
1	C	291	ILE	CA-C-N	-7.56	115.33	122.66
1	C	291	ILE	C-N-CA	-7.56	115.33	122.66
1	A	8	LYS	CA-C-O	-7.53	112.73	120.71
1	A	184	VAL	N-CA-C	7.52	120.49	111.09
1	A	369	ARG	CA-C-O	7.51	128.57	120.38
1	B	300	ASN	OD1-CG-ND2	-7.50	115.10	122.60
1	B	351	PRO	N-CA-CB	7.50	110.32	103.34
1	D	292	VAL	CA-C-N	7.50	127.12	119.92
1	D	292	VAL	C-N-CA	7.50	127.12	119.92
1	C	146	PHE	CA-CB-CG	7.50	121.30	113.80
1	A	292	VAL	CA-C-N	7.50	127.22	120.10
1	A	292	VAL	C-N-CA	7.50	127.22	120.10
1	C	244	GLN	OE1-CD-NE2	-7.48	115.12	122.60
1	D	34	HIS	CA-CB-CG	-7.43	106.37	113.80
1	B	160	ILE	O-C-N	-7.42	115.18	122.97
1	D	17	GLU	O-C-N	-7.41	114.08	122.75
1	D	67	HIS	CA-CB-CG	-7.40	106.40	113.80
1	B	299	GLN	OE1-CD-NE2	-7.40	115.20	122.60
1	A	326	ASP	CA-C-O	-7.38	112.05	120.24
1	B	353	GLU	CB-CG-CD	7.38	125.14	112.60
1	B	184	VAL	O-C-N	-7.35	111.75	121.82
1	B	244	GLN	OE1-CD-NE2	7.35	129.95	122.60
1	A	291	ILE	CA-C-O	-7.34	112.06	120.65
1	C	47	ARG	CD-NE-CZ	-7.34	114.13	124.40
1	D	107	GLU	CA-C-N	-7.32	111.41	120.64
1	D	107	GLU	C-N-CA	-7.32	111.41	120.64
1	D	248	LYS	CA-C-N	7.32	127.37	119.90
1	D	248	LYS	C-N-CA	7.32	127.37	119.90
1	C	24	GLU	N-CA-CB	-7.31	99.77	111.62
1	A	231	LYS	CA-C-O	7.30	128.16	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	160	ILE	O-C-N	-7.29	113.46	122.57
1	D	120	ARG	N-CA-C	-7.28	104.66	113.97
1	B	15	TRP	CA-C-O	-7.27	111.09	119.60
1	B	218	ARG	NE-CZ-NH1	-7.27	114.23	121.50
1	B	304	ASN	CB-CG-ND2	-7.27	105.49	116.40
1	C	327	SER	N-CA-C	7.24	121.36	112.23
1	B	199	GLY	O-C-N	7.24	132.11	122.70
1	C	59	THR	CA-C-N	7.23	127.66	119.93
1	C	59	THR	C-N-CA	7.23	127.66	119.93
1	C	8	LYS	O-C-N	7.22	131.43	123.27
1	A	248	LYS	CA-C-N	7.20	127.24	119.90
1	A	248	LYS	C-N-CA	7.20	127.24	119.90
1	D	138	HIS	O-C-N	7.20	131.00	122.79
1	B	191	GLN	CG-CD-NE2	-7.19	105.61	116.40
1	B	4	GLY	CA-C-O	-7.19	110.05	119.25
1	C	201	GLY	O-C-N	-7.16	115.87	122.96
1	D	160	ILE	CA-C-O	7.13	129.69	120.78
1	A	353	GLU	CB-CG-CD	7.13	124.72	112.60
1	C	123	MET	N-CA-C	-7.11	100.29	110.59
1	B	160	ILE	CA-C-N	7.10	130.83	120.82
1	B	160	ILE	C-N-CA	7.10	130.83	120.82
1	A	352	PHE	CA-C-N	7.10	131.96	120.60
1	A	352	PHE	C-N-CA	7.10	131.96	120.60
1	C	291	ILE	CA-C-O	-7.09	112.35	120.65
1	D	37	ARG	CB-CA-C	7.07	121.42	109.75
1	D	219	ILE	CA-C-O	-7.07	113.92	120.22
1	D	292	VAL	CA-C-O	7.07	125.23	119.29
1	D	130	PHE	CA-CB-CG	7.06	120.86	113.80
1	B	158	ALA	CA-C-O	7.06	128.16	120.32
1	B	241	VAL	N-CA-CB	-7.05	99.87	111.44
1	A	135	LYS	CA-C-O	7.05	126.75	120.19
1	D	90	ILE	O-C-N	7.04	127.49	120.59
1	B	26	VAL	CA-C-O	-7.04	114.74	121.64
1	C	176	PHE	CA-CB-CG	-7.00	106.80	113.80
1	A	57	LEU	CA-C-O	-6.97	113.00	120.46
1	C	109	ASN	CB-CA-C	6.96	118.53	109.28
1	D	26	VAL	CA-C-N	-6.94	113.42	123.00
1	D	26	VAL	C-N-CA	-6.94	113.42	123.00
1	A	369	ARG	NE-CZ-NH2	-6.93	112.97	119.20
1	D	133	ARG	CD-NE-CZ	-6.92	114.72	124.40
1	D	303	MET	CA-C-O	6.89	128.60	121.23
1	C	37	ARG	CB-CA-C	6.89	121.48	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	PRO	N-CA-CB	6.85	109.83	103.39
1	B	324	SER	N-CA-C	6.84	119.36	111.02
1	D	16	GLU	CA-C-N	-6.84	109.31	120.87
1	D	16	GLU	C-N-CA	-6.84	109.31	120.87
1	C	6	VAL	O-C-N	-6.83	115.39	122.63
1	D	8	LYS	O-C-N	6.83	131.35	123.29
1	A	357	GLU	CA-C-N	6.81	127.54	119.98
1	A	357	GLU	C-N-CA	6.81	127.54	119.98
1	B	176	PHE	O-C-N	6.81	129.11	122.03
1	D	239	GLU	OE1-CD-OE2	6.81	139.24	122.90
1	C	291	ILE	O-C-N	6.80	131.23	122.94
1	A	179	GLY	CA-C-N	6.80	129.72	120.54
1	A	179	GLY	C-N-CA	6.80	129.72	120.54
1	C	266	PHE	O-C-N	-6.79	115.08	123.36
1	B	308	LEU	CA-C-O	6.79	128.28	120.00
1	C	343	ASP	O-C-N	-6.79	113.98	120.70
1	D	352	PHE	N-CA-C	6.78	119.54	111.33
1	A	62	PRO	CA-C-N	-6.78	113.63	122.51
1	A	62	PRO	C-N-CA	-6.78	113.63	122.51
1	A	255	THR	N-CA-C	-6.78	103.97	111.36
1	B	24	GLU	CB-CG-CD	6.78	124.12	112.60
1	B	15	TRP	O-C-N	6.77	131.97	122.36
1	D	156	SER	CA-C-N	-6.75	112.59	122.58
1	D	156	SER	C-N-CA	-6.75	112.59	122.58
1	B	172	ILE	CA-C-N	6.75	132.80	120.79
1	B	172	ILE	C-N-CA	6.75	132.80	120.79
1	D	7	ILE	CA-C-O	-6.74	112.79	120.67
1	B	88	LYS	N-CA-C	-6.74	98.64	109.96
1	D	117	SER	O-C-N	-6.73	115.13	122.07
1	D	315	LYS	CA-C-N	-6.73	114.34	121.48
1	D	315	LYS	C-N-CA	-6.73	114.34	121.48
1	D	60	PRO	CA-C-O	6.72	129.00	121.34
1	D	318	ILE	CA-C-N	6.72	131.91	122.36
1	D	318	ILE	C-N-CA	6.72	131.91	122.36
1	D	31	PRO	N-CA-CB	6.72	109.29	103.31
1	C	197	VAL	CA-C-O	-6.72	112.80	120.66
1	D	34	HIS	ND1-CG-CD2	6.68	112.78	106.10
1	B	136	PRO	N-CA-CB	6.68	109.28	103.27
1	C	242	ASN	CA-C-N	6.67	128.18	119.84
1	C	242	ASN	C-N-CA	6.67	128.18	119.84
1	A	244	GLN	OE1-CD-NE2	6.67	129.27	122.60
1	B	146	PHE	O-C-N	-6.67	113.81	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	PHE	CA-CB-CG	-6.65	107.15	113.80
1	C	273	ASP	N-CA-C	6.65	118.53	111.28
1	D	264	PHE	O-C-N	-6.65	115.24	123.36
1	A	94	THR	N-CA-C	-6.64	96.37	108.85
1	D	105	HIS	ND1-CG-CD2	6.63	112.73	106.10
1	D	326	ASP	CA-C-O	-6.63	112.88	120.24
1	D	218	ARG	CA-C-O	-6.63	113.04	120.66
1	C	4	GLY	CA-C-O	6.62	126.37	119.02
1	C	284	GLU	N-CA-C	6.62	120.23	111.75
1	A	259	ASN	OD1-CG-ND2	-6.62	115.98	122.60
1	B	226	LYS	O-C-N	-6.61	113.64	122.43
1	A	292	VAL	N-CA-C	-6.60	106.58	112.12
1	C	92	LEU	CA-C-O	6.59	127.32	120.40
1	A	191	GLN	OE1-CD-NE2	6.59	129.19	122.60
1	A	372	LEU	CA-C-O	-6.59	113.25	120.43
1	B	34	HIS	CA-CB-CG	-6.58	107.22	113.80
1	B	94	THR	N-CA-C	-6.58	98.15	109.15
1	B	319	PHE	CA-CB-CG	6.58	120.38	113.80
1	A	43	THR	CA-C-N	-6.57	114.46	122.15
1	A	43	THR	C-N-CA	-6.57	114.46	122.15
1	A	357	GLU	CA-C-O	6.57	127.52	119.97
1	A	123	MET	N-CA-C	-6.57	101.07	110.59
1	A	90	ILE	CA-C-O	6.56	123.35	119.94
1	B	30	PRO	CA-C-N	6.56	126.47	119.85
1	B	30	PRO	C-N-CA	6.56	126.47	119.85
1	B	162	ALA	CA-C-N	-6.56	112.37	122.60
1	B	162	ALA	C-N-CA	-6.56	112.37	122.60
1	A	126	GLY	CA-C-O	-6.56	111.72	119.06
1	C	111	CYS	CA-C-N	6.55	131.09	120.60
1	C	111	CYS	C-N-CA	6.55	131.09	120.60
1	C	9	CYS	O-C-N	6.55	130.00	122.99
1	A	20	PRO	O-C-N	6.54	130.82	122.91
1	A	51	HIS	N-CA-CB	6.53	120.28	110.22
1	D	184	VAL	N-CA-C	6.52	117.31	110.72
1	B	118	MET	N-CA-CB	-6.52	101.63	111.21
1	D	12	ALA	CB-CA-C	6.52	121.56	110.81
1	A	136	PRO	N-CA-CB	6.51	109.09	103.36
1	C	57	LEU	CA-C-N	6.50	130.50	122.37
1	C	57	LEU	C-N-CA	6.50	130.50	122.37
1	B	90	ILE	CA-C-O	6.48	123.31	119.94
1	C	356	ASN	OD1-CG-ND2	-6.47	116.13	122.60
1	D	277	THR	O-C-N	6.47	128.73	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	322	PHE	N-CA-C	6.47	119.66	109.96
1	A	124	GLN	CA-C-O	-6.45	112.81	120.10
1	C	10	LYS	CA-C-O	6.44	127.94	120.80
1	C	279	LEU	CB-CA-C	-6.43	100.78	110.88
1	B	148	GLN	OE1-CD-NE2	-6.43	116.17	122.60
1	C	300	ASN	O-C-N	6.43	130.30	123.03
1	B	251	GLN	OE1-CD-NE2	6.42	129.02	122.60
1	D	349	VAL	O-C-N	-6.41	116.33	123.26
1	B	245	ASP	CA-CB-CG	6.40	119.00	112.60
1	D	242	ASN	CA-C-N	6.39	127.83	119.84
1	D	242	ASN	C-N-CA	6.39	127.83	119.84
1	D	242	ASN	CA-C-O	6.39	125.47	119.59
1	D	296	PRO	O-C-N	-6.38	115.67	123.01
1	C	8	LYS	CA-C-N	-6.37	111.53	122.10
1	C	8	LYS	C-N-CA	-6.37	111.53	122.10
1	D	256	GLU	N-CA-CB	6.37	119.25	110.01
1	B	135	LYS	CA-C-O	6.37	127.37	120.05
1	A	357	GLU	CB-CG-CD	-6.35	101.81	112.60
1	A	320	GLY	O-C-N	-6.34	114.45	122.70
1	C	295	PRO	CA-C-N	6.34	126.72	119.93
1	C	295	PRO	C-N-CA	6.34	126.72	119.93
1	C	304	ASN	CA-C-N	6.34	126.03	119.56
1	C	304	ASN	C-N-CA	6.34	126.03	119.56
1	D	170	CYS	N-CA-C	-6.34	104.47	111.82
1	B	367	SER	N-CA-C	6.34	118.81	109.69
1	A	368	ILE	N-CA-C	-6.33	96.17	109.34
1	C	94	THR	N-CA-C	-6.33	98.59	109.15
1	D	181	GLY	N-CA-C	-6.33	105.16	112.50
1	B	123	MET	N-CA-CB	6.32	120.02	110.42
1	B	370	THR	N-CA-CB	6.32	120.72	110.42
1	D	132	CYS	O-C-N	-6.32	115.67	123.44
1	B	69	ALA	N-CA-C	6.31	117.81	108.60
1	A	90	ILE	CA-C-N	6.31	126.07	119.76
1	A	90	ILE	C-N-CA	6.31	126.07	119.76
1	D	162	ALA	CA-C-N	-6.31	112.57	122.73
1	D	162	ALA	C-N-CA	-6.31	112.57	122.73
1	C	257	MET	CA-CB-CG	6.31	126.71	114.10
1	B	135	LYS	CA-C-N	6.29	126.62	119.83
1	B	135	LYS	C-N-CA	6.29	126.62	119.83
1	B	174	CYS	CA-C-N	6.29	133.74	121.41
1	B	174	CYS	C-N-CA	6.29	133.74	121.41
1	D	290	VAL	O-C-N	-6.28	115.76	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	LYS	O-C-N	6.27	126.68	121.35
1	D	2	THR	CA-C-O	6.27	126.64	119.18
1	A	69	ALA	N-CA-C	6.27	117.39	108.74
1	B	237	ALA	CA-C-O	-6.27	113.60	120.81
1	C	95	PRO	CB-CA-C	-6.26	101.76	111.22
1	B	93	PHE	CA-CB-CG	6.26	120.06	113.80
1	D	101	ARG	NH1-CZ-NH2	6.26	127.44	119.30
1	B	300	ASN	CB-CG-ND2	6.25	125.77	116.40
1	D	277	THR	CA-C-O	-6.24	114.27	120.82
1	D	47	ARG	CD-NE-CZ	-6.24	115.67	124.40
1	B	49	ASP	N-CA-C	-6.23	104.57	111.36
1	B	69	ALA	O-C-N	6.23	129.80	123.26
1	B	251	GLN	N-CA-CB	6.23	119.28	110.12
1	C	49	ASP	N-CA-C	-6.23	104.57	111.36
1	A	139	HIS	O-C-N	-6.23	115.96	122.94
1	C	105	HIS	CA-C-N	6.22	125.91	119.56
1	C	105	HIS	C-N-CA	6.22	125.91	119.56
1	A	47	ARG	NE-CZ-NH2	6.22	124.80	119.20
1	C	11	ALA	CA-C-N	-6.22	114.15	122.42
1	C	11	ALA	C-N-CA	-6.22	114.15	122.42
1	A	2	THR	CA-C-O	6.21	126.58	119.18
1	D	359	PHE	N-CA-CB	6.21	119.35	110.16
1	C	343	ASP	CA-C-N	6.21	125.89	119.56
1	C	343	ASP	C-N-CA	6.21	125.89	119.56
1	B	2	THR	N-CA-C	-6.20	105.75	113.38
1	A	340	PHE	CA-CB-CG	6.19	119.99	113.80
1	C	55	GLY	N-CA-C	-6.19	106.88	114.92
1	D	93	PHE	CA-CB-CG	6.19	119.99	113.80
1	A	172	ILE	CA-C-N	6.18	131.61	120.79
1	A	172	ILE	C-N-CA	6.18	131.61	120.79
1	A	207	VAL	N-CA-CB	6.18	118.48	110.57
1	A	74	GLU	OE1-CD-OE2	-6.18	108.07	122.90
1	D	18	LYS	O-C-N	-6.18	114.28	122.00
1	B	258	SER	CA-C-O	6.18	126.79	119.56
1	D	159	LYS	O-C-N	-6.17	115.82	123.04
1	A	184	VAL	CA-C-O	6.17	127.13	120.47
1	A	282	CYS	O-C-N	-6.16	116.16	123.06
1	D	248	LYS	CB-CA-C	6.16	118.34	108.91
1	C	223	ASP	CA-C-O	-6.16	114.12	120.89
1	B	16	GLU	CA-C-N	-6.15	110.48	120.87
1	B	16	GLU	C-N-CA	-6.15	110.48	120.87
1	A	207	VAL	N-CA-C	-6.12	104.78	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	47	ARG	O-C-N	-6.12	115.23	122.20
1	D	80	VAL	CA-C-O	-6.11	114.07	121.04
1	B	184	VAL	N-CA-C	6.11	119.63	111.44
1	D	293	GLY	CA-C-N	-6.11	117.42	123.04
1	D	293	GLY	C-N-CA	-6.11	117.42	123.04
1	D	51	HIS	N-CA-C	-6.10	104.70	111.71
1	C	239	GLU	CB-CA-C	-6.09	97.35	110.45
1	B	209	MET	CA-C-O	-6.09	114.42	120.82
1	A	299	GLN	OE1-CD-NE2	-6.08	116.52	122.60
1	B	120	ARG	N-CA-CB	6.08	119.47	110.53
1	D	157	VAL	CA-C-O	-6.08	114.83	121.28
1	B	59	THR	N-CA-C	-6.08	100.27	108.11
1	D	123	MET	N-CA-C	-6.08	101.78	110.59
1	B	120	ARG	O-C-N	-6.07	114.36	122.49
1	D	318	ILE	O-C-N	-6.07	116.50	122.93
1	D	51	HIS	N-CA-CB	6.06	119.56	110.22
1	D	172	ILE	CA-C-N	6.06	131.40	120.79
1	D	172	ILE	C-N-CA	6.06	131.40	120.79
1	A	128	SER	O-C-N	-6.06	115.52	123.16
1	C	30	PRO	N-CA-C	-6.06	103.30	110.70
1	C	272	LEU	CA-C-O	-6.06	114.41	120.90
1	C	98	GLY	O-C-N	-6.06	114.82	122.70
1	A	312	ARG	NE-CZ-NH2	6.06	124.65	119.20
1	A	193	SER	N-CA-C	6.05	117.85	110.41
1	C	232	ALA	O-C-N	-6.05	115.71	122.12
1	C	79	GLY	CA-C-O	-6.05	112.63	119.04
1	C	373	THR	CA-C-O	6.05	127.12	120.71
1	C	169	VAL	N-CA-C	6.04	121.90	109.34
1	D	139	HIS	N-CA-C	-6.03	101.53	110.46
1	A	270	GLY	O-C-N	-6.03	114.86	122.70
1	B	40	MET	CA-C-O	6.03	127.91	121.16
1	C	156	SER	CA-C-N	-6.02	113.68	122.58
1	C	156	SER	C-N-CA	-6.02	113.68	122.58
1	C	343	ASP	CA-C-O	6.02	123.86	118.33
1	C	327	SER	CA-C-N	-6.01	114.66	120.43
1	C	327	SER	C-N-CA	-6.01	114.66	120.43
1	A	297	ASP	CA-CB-CG	-6.01	106.59	112.60
1	B	355	ILE	CA-C-O	-6.01	114.80	121.05
1	A	113	LYS	CA-C-O	-6.00	112.16	119.43
1	D	247	LYS	N-CA-C	-5.99	105.97	113.28
1	D	120	ARG	CA-CB-CG	5.99	126.08	114.10
1	A	198	PHE	CA-CB-CG	5.98	119.78	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	ASN	CA-C-N	5.98	126.41	119.47
1	B	242	ASN	C-N-CA	5.98	126.41	119.47
1	C	202	GLY	CA-C-N	-5.98	110.98	120.55
1	C	202	GLY	C-N-CA	-5.98	110.98	120.55
1	D	140	PHE	CA-CB-CG	5.97	119.77	113.80
1	C	357	GLU	CA-C-N	5.96	126.60	119.98
1	C	357	GLU	C-N-CA	5.96	126.60	119.98
1	C	159	LYS	CA-C-O	-5.96	113.89	120.69
1	A	110	PHE	CA-C-N	5.96	129.30	120.90
1	A	110	PHE	C-N-CA	5.96	129.30	120.90
1	C	16	GLU	CA-C-N	-5.95	110.14	120.97
1	C	16	GLU	C-N-CA	-5.95	110.14	120.97
1	C	370	THR	N-CA-C	-5.95	99.03	108.73
1	D	322	PHE	N-CA-C	5.95	118.97	110.10
1	B	244	GLN	CG-CD-NE2	-5.94	107.49	116.40
1	A	169	VAL	O-C-N	-5.94	114.86	122.22
1	D	31	PRO	CB-CA-C	-5.94	103.80	111.46
1	B	372	LEU	CA-C-O	-5.94	113.96	120.43
1	C	304	ASN	CA-C-O	5.94	123.71	119.32
1	D	87	ASP	CA-C-N	-5.94	113.01	121.50
1	D	87	ASP	C-N-CA	-5.94	113.01	121.50
1	B	202	GLY	N-CA-C	5.93	119.82	112.64
1	B	291	ILE	CA-C-N	-5.93	116.91	122.66
1	B	291	ILE	C-N-CA	-5.93	116.91	122.66
1	C	97	CYS	O-C-N	-5.92	114.29	122.46
1	A	295	PRO	CA-C-N	5.91	126.83	119.98
1	A	295	PRO	C-N-CA	5.91	126.83	119.98
1	D	116	LEU	CA-C-O	-5.90	114.24	120.55
1	B	296	PRO	CA-C-O	5.89	127.54	121.23
1	D	292	VAL	N-CA-C	-5.88	107.08	112.96
1	A	162	ALA	CA-C-O	-5.88	112.38	119.49
1	D	255	THR	N-CA-C	-5.87	104.78	111.07
1	B	338	LYS	N-CA-C	5.87	119.75	112.24
1	D	253	VAL	CA-CB-CG1	5.87	120.38	110.40
1	D	57	LEU	CA-C-N	5.87	130.32	122.93
1	D	57	LEU	C-N-CA	5.87	130.32	122.93
1	A	334	ASP	CA-CB-CG	-5.87	106.73	112.60
1	D	139	HIS	ND1-CG-CD2	5.84	111.94	106.10
1	A	55	GLY	CA-C-O	5.84	125.52	119.27
1	C	373	THR	OG1-CB-CG2	-5.84	97.62	109.30
1	B	326	ASP	CB-CA-C	-5.84	100.93	110.85
1	C	102	VAL	O-C-N	-5.84	115.82	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	GLU	N-CA-C	5.83	118.07	110.43
1	B	58	VAL	N-CA-C	5.83	117.17	108.54
1	C	355	ILE	O-C-N	-5.83	116.21	121.87
1	C	151	VAL	CB-CA-C	-5.83	102.55	110.42
1	A	47	ARG	NH1-CZ-NH2	-5.83	111.72	119.30
1	A	107	GLU	CA-C-N	-5.83	113.30	120.64
1	A	107	GLU	C-N-CA	-5.83	113.30	120.64
1	D	357	GLU	CB-CG-CD	5.81	122.48	112.60
1	A	301	LEU	N-CA-C	-5.81	101.60	110.14
1	B	235	VAL	CA-C-O	-5.81	112.16	119.48
1	B	79	GLY	O-C-N	-5.80	115.02	122.39
1	D	257	MET	CG-SD-CE	-5.80	88.13	100.90
1	B	43	THR	CA-C-N	-5.80	116.11	122.38
1	B	43	THR	C-N-CA	-5.80	116.11	122.38
1	B	239	GLU	CG-CD-OE2	-5.79	105.08	118.40
1	B	267	GLU	CB-CG-CD	5.79	122.45	112.60
1	C	297	ASP	N-CA-C	5.79	118.88	110.42
1	B	354	LYS	CD-CE-NZ	-5.79	93.38	111.90
1	B	296	PRO	O-C-N	-5.79	116.36	123.01
1	D	218	ARG	O-C-N	5.78	130.32	123.27
1	D	304	ASN	CA-C-N	5.78	125.46	119.56
1	D	304	ASN	C-N-CA	5.78	125.46	119.56
1	B	275	MET	CA-C-N	5.77	127.95	120.56
1	B	275	MET	C-N-CA	5.77	127.95	120.56
1	C	150	THR	CA-CB-OG1	-5.77	100.94	109.60
1	B	295	PRO	CB-CA-C	-5.77	103.88	110.92
1	D	319	PHE	N-CA-C	5.77	119.35	111.39
1	A	297	ASP	CA-C-O	5.76	126.71	120.95
1	C	325	LYS	CA-C-N	-5.76	112.12	120.29
1	C	325	LYS	C-N-CA	-5.76	112.12	120.29
1	C	60	PRO	CA-C-O	5.75	127.59	121.32
1	C	276	VAL	CA-C-O	5.75	127.27	121.17
1	D	5	LYS	N-CA-CB	-5.75	101.88	111.20
1	A	141	LEU	CB-CA-C	-5.75	103.41	111.80
1	C	251	GLN	CG-CD-NE2	-5.75	107.78	116.40
1	B	368	ILE	N-CA-C	-5.75	97.39	109.34
1	A	172	ILE	O-C-N	-5.74	115.11	122.22
1	B	332	VAL	N-CA-C	-5.74	105.14	110.53
1	D	239	GLU	CG-CD-OE1	-5.73	105.21	118.40
1	B	233	LYS	CA-CB-CG	5.73	125.55	114.10
1	D	356	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	C	229	PHE	N-CA-C	5.72	117.59	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	284	GLU	N-CA-C	5.71	118.28	111.71
1	A	324	SER	N-CA-C	5.71	120.73	111.37
1	B	143	THR	CA-C-O	-5.70	112.36	120.51
1	D	169	VAL	N-CA-C	5.70	121.20	109.34
1	B	268	VAL	O-C-N	-5.69	115.45	122.57
1	C	259	ASN	OD1-CG-ND2	-5.69	116.91	122.60
1	B	23	ILE	O-C-N	-5.68	116.27	122.64
1	A	353	GLU	CA-C-O	5.67	126.35	119.49
1	B	169	VAL	N-CA-C	5.66	119.95	112.76
1	D	8	LYS	N-CA-C	-5.66	99.96	109.07
1	B	343	ASP	CA-C-N	5.65	125.50	119.28
1	B	343	ASP	C-N-CA	5.65	125.50	119.28
1	B	329	PRO	N-CA-CB	5.65	109.54	103.33
1	D	227	ASP	CA-C-O	5.65	126.33	119.38
1	C	168	LYS	O-C-N	-5.64	115.53	122.19
1	B	199	GLY	CA-C-N	-5.64	114.76	123.17
1	B	199	GLY	C-N-CA	-5.64	114.76	123.17
1	C	102	VAL	CA-C-O	5.64	126.83	120.85
1	D	252	GLU	N-CA-CB	5.64	118.19	110.01
1	B	259	ASN	CB-CG-ND2	5.64	124.86	116.40
1	A	177	SER	N-CA-C	5.63	117.42	111.28
1	D	167	GLU	CA-C-N	5.63	131.01	122.56
1	D	167	GLU	C-N-CA	5.63	131.01	122.56
1	D	133	ARG	O-C-N	-5.63	112.47	122.21
1	C	275	MET	CA-C-N	5.62	127.65	120.56
1	C	275	MET	C-N-CA	5.62	127.65	120.56
1	A	343	ASP	CA-C-N	5.62	125.47	119.28
1	A	343	ASP	C-N-CA	5.62	125.47	119.28
1	C	72	ILE	CA-C-O	-5.62	114.40	120.36
1	C	187	ALA	CB-CA-C	-5.62	100.41	110.70
1	D	117	SER	N-CA-C	5.62	117.08	111.07
1	A	117	SER	N-CA-C	5.62	117.08	111.07
1	D	129	ARG	CB-CA-C	-5.61	101.23	110.72
1	A	133	ARG	CA-C-O	-5.61	113.86	120.81
1	C	370	THR	O-C-N	5.61	129.61	123.22
1	C	122	THR	CA-C-O	5.60	128.52	120.51
1	B	355	ILE	CA-C-N	5.60	128.34	120.28
1	B	355	ILE	C-N-CA	5.60	128.34	120.28
1	A	133	ARG	NH1-CZ-NH2	-5.60	112.03	119.30
1	D	15	TRP	O-C-N	5.59	129.82	122.33
1	A	304	ASN	CA-CB-CG	-5.59	107.01	112.60
1	A	280	SER	N-CA-C	5.59	117.45	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ASP	N-CA-C	5.58	118.57	110.42
1	A	371	ILE	O-C-N	-5.58	116.83	123.03
1	B	221	GLY	CA-C-O	-5.58	116.27	121.18
1	A	280	SER	CA-CB-OG	-5.58	99.94	111.10
1	C	119	PRO	N-CA-CB	5.58	108.13	103.17
1	D	256	GLU	CB-CA-C	-5.57	102.13	110.88
1	B	363	ARG	CD-NE-CZ	-5.57	116.61	124.40
1	A	302	SER	CA-CB-OG	-5.56	99.98	111.10
1	A	351	PRO	CA-C-O	-5.56	114.64	121.31
1	D	276	VAL	O-C-N	-5.56	116.46	121.91
1	B	146	PHE	CA-CB-CG	5.56	119.36	113.80
1	D	315	LYS	O-C-N	5.55	129.49	123.10
1	B	283	GLN	O-C-N	-5.55	116.01	122.89
1	C	334	ASP	CA-C-N	-5.54	112.42	120.29
1	C	334	ASP	C-N-CA	-5.54	112.42	120.29
1	D	251	GLN	N-CA-CB	5.54	118.26	110.12
1	B	320	GLY	O-C-N	-5.54	115.50	122.70
1	D	370	THR	N-CA-C	-5.54	100.22	109.24
1	A	357	GLU	O-C-N	-5.53	115.47	122.27
1	A	352	PHE	O-C-N	-5.53	115.23	122.59
1	A	349	VAL	O-C-N	-5.52	117.24	123.20
1	C	273	ASP	O-C-N	-5.52	116.27	122.12
1	A	80	VAL	O-C-N	-5.51	116.61	122.61
1	A	267	GLU	CB-CG-CD	5.51	121.97	112.60
1	D	322	PHE	CA-C-O	5.51	127.20	120.92
1	A	101	ARG	CB-CA-C	-5.51	100.44	110.63
1	D	356	ASN	CB-CG-ND2	5.51	124.66	116.40
1	A	8	LYS	N-CA-C	-5.50	100.73	109.59
1	D	353	GLU	CB-CG-CD	5.50	121.96	112.60
1	A	246	TYR	N-CA-C	5.50	118.67	110.14
1	A	132	CYS	CB-CA-C	5.50	118.27	110.24
1	C	31	PRO	CB-CA-C	-5.50	104.37	111.46
1	D	244	GLN	OE1-CD-NE2	5.49	128.09	122.60
1	A	369	ARG	O-C-N	-5.49	116.82	123.29
1	C	47	ARG	NH1-CZ-NH2	-5.49	112.17	119.30
1	C	301	LEU	CA-C-N	5.48	131.18	122.74
1	C	301	LEU	C-N-CA	5.48	131.18	122.74
1	B	7	ILE	CA-C-O	-5.48	114.08	121.32
1	A	299	GLN	O-C-N	-5.48	116.81	123.16
1	D	326	ASP	CB-CA-C	-5.48	100.68	110.70
1	A	259	ASN	CB-CG-ND2	5.48	124.61	116.40
1	D	138	HIS	CA-C-O	-5.47	115.52	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	GLN	CA-CB-CG	-5.47	103.16	114.10
1	D	236	GLY	O-C-N	-5.47	115.59	122.70
1	B	284	GLU	N-CA-C	5.47	118.00	111.71
1	C	82	THR	N-CA-C	5.47	120.01	113.23
1	C	74	GLU	N-CA-C	-5.45	106.30	113.12
1	D	82	THR	N-CA-C	5.44	119.97	113.23
1	B	62	PRO	CA-C-N	-5.43	115.39	122.51
1	B	62	PRO	C-N-CA	-5.43	115.39	122.51
1	D	63	VAL	N-CA-CB	-5.43	100.86	112.00
1	A	195	CYS	CA-C-O	-5.43	114.97	121.11
1	A	219	ILE	CA-C-O	-5.43	115.39	120.22
1	C	307	LEU	N-CA-C	-5.43	105.53	111.82
1	D	114	ASN	CA-C-N	-5.43	114.04	122.67
1	D	114	ASN	C-N-CA	-5.43	114.04	122.67
1	B	44	GLY	CA-C-N	-5.42	115.70	122.48
1	B	44	GLY	C-N-CA	-5.42	115.70	122.48
1	C	37	ARG	NE-CZ-NH1	-5.42	116.08	121.50
1	B	160	ILE	CA-C-O	5.42	127.42	121.67
1	C	369	ARG	NE-CZ-NH2	-5.41	114.33	119.20
1	D	182	SER	CA-C-N	5.41	127.99	120.63
1	D	182	SER	C-N-CA	5.41	127.99	120.63
1	D	30	PRO	CA-C-N	5.40	125.32	119.76
1	D	30	PRO	C-N-CA	5.40	125.32	119.76
1	D	94	THR	N-CA-C	-5.40	100.13	109.15
1	B	24	GLU	CB-CA-C	-5.40	98.69	111.65
1	D	20	PRO	N-CD-CG	-5.40	95.10	103.20
1	B	133	ARG	NH1-CZ-NH2	-5.39	112.29	119.30
1	A	372	LEU	CA-C-N	-5.39	115.11	122.93
1	A	372	LEU	C-N-CA	-5.39	115.11	122.93
1	D	297	ASP	CA-C-O	5.39	126.84	120.96
1	B	374	PHE	CA-CB-CG	-5.39	108.41	113.80
1	C	292	VAL	CA-C-N	5.39	125.22	120.10
1	C	292	VAL	C-N-CA	5.39	125.22	120.10
1	B	2	THR	CA-C-O	5.39	125.29	119.15
1	B	279	LEU	CB-CA-C	-5.39	102.42	110.88
1	C	275	MET	N-CA-C	-5.39	105.32	111.14
1	C	373	THR	O-C-N	-5.39	116.37	123.21
1	C	266	PHE	N-CA-CB	-5.38	101.76	110.81
1	C	298	SER	N-CA-C	5.38	119.68	113.38
1	D	249	PRO	N-CA-CB	5.38	107.98	103.25
1	C	165	PRO	O-C-N	-5.38	115.38	122.64
1	A	17	GLU	N-CA-C	5.37	117.47	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	THR	O-C-N	5.37	127.62	122.03
1	A	212	LYS	CA-C-O	5.37	126.24	120.55
1	A	322	PHE	O-C-N	-5.37	116.34	122.89
1	C	323	LYS	CB-CA-C	5.37	118.31	110.26
1	D	244	GLN	CG-CD-NE2	-5.37	108.35	116.40
1	B	122	THR	CA-C-N	5.37	132.81	122.03
1	B	122	THR	C-N-CA	5.37	132.81	122.03
1	D	147	SER	O-C-N	-5.37	117.47	123.48
1	D	235	VAL	CA-C-O	-5.35	114.09	120.78
1	A	30	PRO	N-CA-C	-5.35	104.17	110.70
1	C	87	ASP	CA-CB-CG	5.35	117.95	112.60
1	B	129	ARG	N-CA-C	-5.35	105.40	112.94
1	B	223	ASP	CA-C-N	-5.35	113.82	121.52
1	B	223	ASP	C-N-CA	-5.35	113.82	121.52
1	A	221	GLY	CA-C-N	-5.34	116.14	123.14
1	A	221	GLY	C-N-CA	-5.34	116.14	123.14
1	D	148	GLN	OE1-CD-NE2	5.34	127.94	122.60
1	B	252	GLU	CB-CG-CD	5.34	121.68	112.60
1	B	355	ILE	CB-CA-C	-5.33	105.05	112.04
1	B	91	PRO	N-CA-CB	5.33	108.30	103.34
1	D	305	PRO	O-C-N	-5.33	115.10	122.24
1	D	341	ALA	O-C-N	5.33	130.16	123.23
1	A	294	VAL	CA-C-O	5.32	123.09	119.20
1	C	74	GLU	CA-CB-CG	5.32	124.73	114.10
1	C	191	GLN	CG-CD-OE1	-5.31	110.17	120.80
1	B	306	MET	CA-C-N	5.31	127.93	120.28
1	B	306	MET	C-N-CA	5.31	127.93	120.28
1	B	180	TYR	CA-C-O	-5.31	115.25	120.82
1	B	42	ALA	CA-C-O	-5.31	114.01	120.54
1	B	239	GLU	CB-CA-C	-5.31	100.75	110.62
1	D	193	SER	N-CA-C	5.30	116.93	110.41
1	A	17	GLU	CA-C-O	5.30	127.70	121.87
1	B	124	GLN	CB-CG-CD	5.30	121.61	112.60
1	D	329	PRO	O-C-N	-5.29	115.88	122.23
1	D	115	ASP	CA-C-O	5.29	126.20	119.95
1	C	251	GLN	O-C-N	5.29	127.73	122.12
1	A	191	GLN	CG-CD-NE2	-5.29	108.47	116.40
1	B	133	ARG	NE-CZ-NH1	-5.29	116.21	121.50
1	C	179	GLY	CA-C-N	5.28	127.67	120.54
1	C	179	GLY	C-N-CA	5.28	127.67	120.54
1	D	50	ASP	O-C-N	-5.28	116.14	122.15
1	B	313	THR	CA-CB-OG1	-5.27	101.69	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	300	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	B	280	SER	CA-CB-OG	-5.27	100.56	111.10
1	D	204	GLY	O-C-N	-5.27	117.13	122.19
1	D	70	ALA	CA-C-O	-5.27	113.80	120.28
1	B	288	VAL	CA-C-N	-5.26	114.63	122.74
1	B	288	VAL	C-N-CA	-5.26	114.63	122.74
1	D	280	SER	O-C-N	5.26	128.38	122.22
1	B	304	ASN	CA-C-N	5.26	124.93	119.56
1	B	304	ASN	C-N-CA	5.26	124.93	119.56
1	C	317	ALA	N-CA-C	5.26	117.07	108.76
1	D	87	ASP	O-C-N	5.25	129.06	122.86
1	C	24	GLU	CB-CG-CD	5.25	121.53	112.60
1	C	111	CYS	O-C-N	-5.25	116.76	123.06
1	D	15	TRP	CA-C-O	-5.25	113.59	119.79
1	D	196	ALA	CA-C-O	5.25	125.80	120.24
1	C	61	LEU	CB-CA-C	5.25	116.71	108.63
1	C	328	VAL	CA-C-O	5.24	122.69	118.71
1	B	176	PHE	N-CA-CB	5.24	117.56	109.91
1	D	105	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	D	109	ASN	N-CA-C	-5.24	108.15	114.75
1	A	169	VAL	N-CA-C	5.24	119.41	112.76
1	D	246	TYR	N-CA-C	5.23	118.59	110.17
1	B	297	ASP	CA-CB-CG	-5.23	107.37	112.60
1	B	318	ILE	CA-C-O	-5.23	114.80	120.71
1	B	350	LEU	CA-C-N	5.23	124.99	119.76
1	B	350	LEU	C-N-CA	5.23	124.99	119.76
1	C	275	MET	CA-C-O	-5.23	115.31	120.70
1	A	274	THR	N-CA-C	-5.23	105.76	111.82
1	B	168	LYS	CB-CA-C	-5.23	102.57	110.83
1	A	251	GLN	N-CA-CB	5.22	117.79	110.12
1	A	119	PRO	CA-C-N	5.21	131.43	122.09
1	A	119	PRO	C-N-CA	5.21	131.43	122.09
1	A	114	ASN	N-CA-CB	5.21	117.38	110.29
1	C	218	ARG	CA-C-O	-5.21	114.67	120.66
1	A	116	LEU	CA-C-O	-5.21	113.80	120.31
1	C	241	VAL	O-C-N	-5.20	117.53	123.10
1	D	292	VAL	O-C-N	-5.20	116.47	122.04
1	B	164	SER	CA-C-N	5.20	126.34	119.84
1	B	164	SER	C-N-CA	5.20	126.34	119.84
1	B	293	GLY	N-CA-C	5.20	117.91	111.93
1	A	53	VAL	CB-CA-C	-5.20	105.05	112.22
1	B	19	LYS	O-C-N	5.19	125.87	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	GLY	CA-C-O	5.19	124.78	119.02
1	A	119	PRO	N-CA-CB	5.18	107.78	103.17
1	D	131	THR	OG1-CB-CG2	-5.18	98.93	109.30
1	A	129	ARG	N-CA-C	-5.18	105.63	112.94
1	D	147	SER	CA-C-O	5.18	126.59	120.89
1	A	2	THR	O-C-N	-5.18	115.06	122.41
1	C	319	PHE	N-CA-C	5.18	118.73	111.74
1	D	238	THR	N-CA-C	-5.18	107.01	113.38
1	C	58	VAL	N-CA-C	5.17	116.15	108.23
1	B	343	ASP	O-C-N	-5.17	115.58	120.70
1	A	59	THR	CB-CA-C	5.17	116.95	109.92
1	A	267	GLU	N-CA-C	-5.17	100.30	108.73
1	A	336	MET	CA-CB-CG	5.17	124.44	114.10
1	A	282	CYS	CB-CA-C	5.16	118.34	109.51
1	B	242	ASN	CA-C-O	5.16	124.34	119.59
1	C	135	LYS	CA-C-O	5.16	124.99	120.19
1	C	360	ASP	CA-CB-CG	-5.16	107.44	112.60
1	B	76	ILE	O-C-N	-5.16	117.61	123.03
1	B	271	ARG	CA-CB-CG	5.16	124.42	114.10
1	C	2	THR	N-CA-C	-5.15	106.99	113.28
1	C	139	HIS	N-CA-C	-5.15	103.12	110.59
1	D	346	ILE	CA-C-N	-5.15	113.66	122.11
1	D	346	ILE	C-N-CA	-5.15	113.66	122.11
1	D	20	PRO	CB-CA-C	-5.15	104.21	110.95
1	C	116	LEU	CA-C-N	5.14	127.13	120.44
1	C	116	LEU	C-N-CA	5.14	127.13	120.44
1	C	325	LYS	O-C-N	5.14	127.57	122.12
1	D	88	LYS	CA-C-O	-5.14	114.83	120.69
1	B	181	GLY	O-C-N	-5.14	117.25	122.19
1	C	193	SER	N-CA-C	5.14	116.73	110.41
1	A	291	ILE	CA-C-N	-5.14	117.38	122.77
1	A	291	ILE	C-N-CA	-5.14	117.38	122.77
1	B	195	CYS	CA-C-O	-5.14	115.36	121.16
1	B	200	LEU	N-CA-C	5.14	119.72	111.81
1	D	212	LYS	CA-C-O	-5.14	114.30	120.10
1	B	113	LYS	CA-CB-CG	-5.13	103.83	114.10
1	A	279	LEU	CB-CA-C	-5.13	102.27	110.79
1	B	182	SER	CA-C-N	5.13	127.61	120.63
1	B	182	SER	C-N-CA	5.13	127.61	120.63
1	A	173	GLY	N-CA-C	-5.13	108.30	114.66
1	C	112	LEU	O-C-N	-5.13	115.72	122.39
1	B	63	VAL	N-CA-C	5.12	116.38	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	GLU	CA-C-O	-5.12	115.03	120.92
1	C	4	GLY	O-C-N	-5.12	115.89	122.39
1	C	335	PHE	N-CA-C	-5.11	105.79	111.36
1	C	197	VAL	N-CA-C	5.11	114.94	107.37
1	A	92	LEU	N-CA-C	5.11	117.03	107.99
1	A	19	LYS	CB-CA-C	-5.11	101.27	109.08
1	A	202	GLY	O-C-N	5.11	127.09	122.19
1	D	340	PHE	CA-CB-CG	5.10	118.90	113.80
1	A	221	GLY	O-C-N	5.10	127.54	123.61
1	A	225	ASN	O-C-N	5.10	129.64	123.01
1	A	290	VAL	CA-C-O	5.10	125.74	120.39
1	A	174	CYS	O-C-N	-5.09	115.81	122.59
1	D	165	PRO	CA-C-N	5.09	127.61	120.28
1	D	165	PRO	C-N-CA	5.09	127.61	120.28
1	A	21	PHE	N-CA-CB	5.09	118.03	110.29
1	B	66	GLY	CA-C-N	-5.09	111.81	121.54
1	B	66	GLY	C-N-CA	-5.09	111.81	121.54
1	D	60	PRO	CB-CA-C	5.09	118.03	111.46
1	D	361	LEU	CD1-CG-CD2	-5.09	99.60	110.80
1	A	175	GLY	CA-C-N	5.09	127.37	120.65
1	A	175	GLY	C-N-CA	5.09	127.37	120.65
1	A	252	GLU	N-CA-CB	5.09	117.39	110.01
1	D	36	VAL	CA-C-O	-5.09	114.97	120.36
1	D	170	CYS	O-C-N	-5.09	116.01	122.27
1	C	259	ASN	CB-CG-OD1	5.09	130.97	120.80
1	B	369	ARG	N-CA-CB	5.08	118.55	110.57
1	B	89	VAL	O-C-N	-5.08	117.28	123.02
1	A	182	SER	CA-C-N	5.08	127.54	120.63
1	A	182	SER	C-N-CA	5.08	127.54	120.63
1	D	188	LYS	O-C-N	-5.08	116.48	122.58
1	B	312	ARG	N-CA-CB	5.08	118.04	109.92
1	A	306	MET	CA-C-O	5.07	125.63	119.49
1	A	133	ARG	CD-NE-CZ	5.07	131.50	124.40
1	C	360	ASP	CB-CG-OD1	5.07	130.06	118.40
1	B	325	LYS	CA-CB-CG	-5.07	103.97	114.10
1	C	141	LEU	CA-C-O	-5.07	115.66	121.54
1	B	37	ARG	CB-CA-C	5.07	118.11	109.75
1	A	338	LYS	N-CA-C	5.06	118.72	112.24
1	A	59	THR	N-CA-C	-5.06	101.58	108.11
1	A	367	SER	N-CA-C	5.06	117.23	109.95
1	B	356	ASN	O-C-N	5.06	128.14	122.22
1	D	59	THR	CA-C-N	5.06	124.97	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	59	THR	C-N-CA	5.06	124.97	119.76
1	D	104	LYS	CB-CA-C	-5.05	100.07	110.38
1	C	129	ARG	CB-CA-C	-5.05	102.18	110.72
1	A	145	THR	CA-C-O	-5.05	113.44	119.35
1	C	38	ILE	CA-C-N	5.05	129.49	122.77
1	C	38	ILE	C-N-CA	5.05	129.49	122.77
1	C	206	SER	CA-C-O	-5.05	114.16	119.97
1	B	353	GLU	O-C-N	-5.05	115.83	122.39
1	D	47	ARG	NE-CZ-NH2	-5.05	114.66	119.20
1	A	20	PRO	N-CA-CB	5.05	108.13	103.39
1	D	279	LEU	O-C-N	5.05	127.27	122.07
1	D	161	ASP	CA-CB-CG	5.04	117.64	112.60
1	C	112	LEU	CA-C-O	5.04	125.59	119.49
1	C	298	SER	CA-C-N	5.04	129.29	122.19
1	C	298	SER	C-N-CA	5.04	129.29	122.19
1	A	174	CYS	CA-C-N	5.04	131.28	121.41
1	A	174	CYS	C-N-CA	5.04	131.28	121.41
1	B	61	LEU	N-CA-CB	5.04	117.03	109.88
1	B	346	ILE	CA-C-O	5.03	126.58	120.74
1	C	37	ARG	NH1-CZ-NH2	5.03	125.84	119.30
1	C	117	SER	O-C-N	-5.03	116.89	122.07
1	B	239	GLU	CG-CD-OE1	5.02	129.96	118.40
1	A	280	SER	CB-CA-C	-5.02	102.31	110.85
1	C	352	PHE	CA-C-N	5.02	128.63	120.60
1	C	352	PHE	C-N-CA	5.02	128.63	120.60
1	D	77	GLY	N-CA-C	-5.02	104.77	112.85
1	B	194	THR	O-C-N	-5.02	117.45	123.27
1	C	156	SER	O-C-N	5.01	128.43	122.26
1	A	343	ASP	O-C-N	-5.01	115.74	120.70
1	C	34	HIS	CA-CB-CG	-5.01	108.79	113.80
1	A	225	ASN	CA-C-O	-5.01	114.99	120.70
1	A	370	THR	N-CA-CB	5.01	118.60	110.43
1	A	281	CYS	N-CA-C	-5.00	107.00	113.01
1	B	221	GLY	CA-C-N	-5.00	116.58	123.14
1	B	221	GLY	C-N-CA	-5.00	116.58	123.14
1	B	278	ALA	CB-CA-C	5.00	119.36	110.85
1	D	32	LYS	N-CA-CB	5.00	119.13	110.07
1	D	237	ALA	N-CA-CB	5.00	117.31	109.85

There are no chirality outliers.

There are no planarity outliers.

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	2785	0	2848	46	1
1	B	2785	0	2848	32	0
1	C	2785	0	2848	42	1
1	D	2785	0	2848	44	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	44	0	24	1	0
3	B	44	0	25	2	0
3	C	44	0	25	1	0
3	D	44	0	25	0	0
4	A	8	0	11	0	0
4	B	8	0	11	1	0
4	C	8	0	11	0	0
4	D	8	0	11	0	0
5	A	144	0	0	4	0
5	B	144	0	0	2	0
5	C	134	0	0	7	0
5	D	134	0	0	3	0
All	All	11912	0	11535	160	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 7.

All (160) 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:D:231:LYS:NZ	1:D:234:GLU:OE1	1.91	1.03
1:D:253:VAL:HG12	1:D:257:MET:HE2	1.54	0.89
1:B:253:VAL:HG12	1:B:257:MET:HE2	1.55	0.88
1:C:253:VAL:HG12	1:C:257:MET:HE2	1.56	0.87
1:D:253:VAL:HG12	1:D:257:MET:CE	2.12	0.79
1:A:253:VAL:HG12	1:A:257:MET:HE2	1.65	0.77
1:B:253:VAL:HG12	1:B:257:MET:CE	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:GLU:HG2	5:C:491:HOH:O	1.87	0.74
1:A:253:VAL:HG12	1:A:257:MET:CE	2.19	0.73
1:B:241:VAL:HG11	1:B:250:ILE:HD11	1.69	0.72
1:A:239:GLU:HG2	5:A:390:HOH:O	1.89	0.71
1:C:253:VAL:HG12	1:C:257:MET:CE	2.20	0.70
1:C:345:LEU:O	1:C:369:ARG:HB2	1.93	0.68
1:D:225:ASN:ND2	1:D:227:ASP:H	1.91	0.68
1:A:301:LEU:HD23	1:D:305:PRO:HG3	1.77	0.67
1:D:241:VAL:HG11	1:D:250:ILE:HD11	1.75	0.66
1:C:279:LEU:HD22	1:C:312:ARG:HD3	1.77	0.66
1:D:345:LEU:O	1:D:369:ARG:HB2	1.96	0.66
1:A:305:PRO:HG3	1:D:301:LEU:HD23	1.77	0.65
1:C:241:VAL:HG11	1:C:250:ILE:HD11	1.80	0.64
1:D:328:VAL:HB	1:D:329:PRO:HD3	1.80	0.64
1:D:40:MET:HE1	1:D:150:THR:HG22	1.80	0.64
1:C:330:LYS:HB3	5:C:469:HOH:O	1.98	0.63
1:A:161:ASP:OD2	1:A:336:MET:HG3	1.98	0.62
1:A:241:VAL:HG11	1:A:250:ILE:HD11	1.80	0.62
1:C:69:ALA:O	1:C:91:PRO:HD2	2.01	0.61
1:C:161:ASP:OD2	1:C:336:MET:HG3	2.01	0.60
1:C:83:VAL:HG12	1:C:159:LYS:HB2	1.84	0.60
1:C:350:LEU:HB3	1:C:351:PRO:HD2	1.85	0.59
1:D:279:LEU:HD22	1:D:312:ARG:HD3	1.82	0.59
1:A:302:SER:HA	1:D:301:LEU:O	2.03	0.59
1:D:10:LYS:NZ	1:D:353:GLU:HG3	2.19	0.57
1:C:239:GLU:HG2	5:C:399:HOH:O	2.04	0.56
1:C:24:GLU:OE2	1:C:133:ARG:NH2	2.39	0.56
1:C:17:GLU:O	1:C:18:LYS:HB2	2.06	0.55
1:C:328:VAL:HB	1:C:329:PRO:HD3	1.87	0.55
1:D:17:GLU:O	1:D:18:LYS:HB2	2.04	0.55
1:B:181:GLY:O	1:B:182:SER:C	2.48	0.55
1:D:17:GLU:HB2	1:D:53:VAL:O	2.06	0.55
1:C:241:VAL:HG21	1:C:257:MET:HE1	1.88	0.55
1:B:241:VAL:CG1	1:B:250:ILE:HD11	2.34	0.55
1:A:225:ASN:ND2	1:A:227:ASP:H	2.05	0.55
1:C:70:ALA:HB1	1:C:166:LEU:HD22	1.89	0.55
1:C:225:ASN:ND2	1:C:227:ASP:H	2.05	0.54
1:B:271:ARG:O	1:B:275:MET:HG3	2.07	0.54
1:B:161:ASP:OD2	1:B:336:MET:HG3	2.08	0.53
1:B:61:LEU:HB3	1:B:62:PRO:HA	1.90	0.53
1:B:179:GLY:HA3	1:B:206:SER:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:VAL:HG12	1:B:132:CYS:HB2	1.90	0.52
1:B:318:ILE:HD12	4:B:378:FPI:H41	1.92	0.52
1:C:17:GLU:HB2	1:C:53:VAL:O	2.09	0.52
1:B:297:ASP:O	1:B:298:SER:HB2	2.08	0.52
1:D:161:ASP:OD2	1:D:336:MET:HG3	2.10	0.52
1:D:32:LYS:O	1:D:77:GLY:HA3	2.10	0.51
1:C:20:PRO:HA	5:C:446:HOH:O	2.10	0.51
1:A:241:VAL:HG21	1:A:257:MET:HE1	1.93	0.51
1:C:351:PRO:HG2	1:C:354:LYS:HG3	1.93	0.50
1:C:357:GLU:CB	5:C:491:HOH:O	2.60	0.50
1:A:230:ALA:O	1:A:234:GLU:HG3	2.11	0.50
1:A:301:LEU:HD12	1:A:301:LEU:C	2.36	0.50
1:C:248:LYS:HE2	1:C:256:GLU:OE2	2.11	0.50
1:A:254:LEU:HA	1:A:257:MET:HG2	1.93	0.49
1:A:61:LEU:HA	1:A:62:PRO:C	2.38	0.49
1:D:271:ARG:HB2	1:D:274:THR:OG1	2.13	0.49
1:A:248:LYS:HE2	1:A:256:GLU:OE2	2.13	0.49
1:C:179:GLY:HA3	1:C:206:SER:HB2	1.94	0.49
1:D:10:LYS:HZ1	1:D:353:GLU:HG3	1.76	0.48
1:A:17:GLU:O	1:A:18:LYS:HB2	2.13	0.48
1:B:365:GLY:HA2	5:B:398:HOH:O	2.13	0.48
1:C:56:THR:HG23	1:C:296:PRO:HA	1.96	0.48
1:B:354:LYS:NZ	1:B:357:GLU:OE1	2.47	0.48
1:A:29:ALA:HB1	1:A:30:PRO:HD2	1.96	0.48
1:C:271:ARG:HB2	1:C:274:THR:OG1	2.13	0.48
1:A:69:ALA:O	1:A:91:PRO:HD2	2.15	0.47
1:D:179:GLY:HA3	1:D:206:SER:HB2	1.95	0.47
1:B:100:CYS:O	1:B:104:LYS:HG2	2.14	0.47
1:B:328:VAL:HB	1:B:329:PRO:HD3	1.96	0.47
1:C:177:SER:HB2	1:C:319:PHE:CE1	2.49	0.47
1:D:10:LYS:HZ1	1:D:353:GLU:CG	2.28	0.47
1:D:100:CYS:O	1:D:104:LYS:HG2	2.14	0.47
1:A:241:VAL:CG1	1:A:250:ILE:HD11	2.43	0.47
1:B:123:MET:HB3	1:B:123:MET:HE3	1.76	0.47
1:B:11:ALA:HA	1:B:147:SER:HA	1.97	0.46
1:B:279:LEU:HD22	1:B:312:ARG:HD3	1.96	0.46
1:D:177:SER:HB2	1:D:319:PHE:CE1	2.50	0.46
1:A:178:THR:HA	1:A:320:GLY:N	2.30	0.46
1:B:254:LEU:HA	1:B:257:MET:HG2	1.96	0.46
1:A:301:LEU:O	1:D:302:SER:HA	2.16	0.46
5:A:384:HOH:O	1:D:112:LEU:HD23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLY:HA2	5:A:397:HOH:O	2.16	0.46
1:B:171:LEU:HD13	1:B:345:LEU:HD12	1.97	0.46
1:D:241:VAL:CG1	1:D:250:ILE:HD11	2.43	0.46
1:A:279:LEU:HD22	1:A:312:ARG:HD3	1.97	0.45
1:D:248:LYS:HE2	1:D:256:GLU:OE2	2.16	0.45
1:C:254:LEU:HD23	1:C:257:MET:HE3	1.99	0.45
1:A:11:ALA:HA	1:A:147:SER:HA	1.98	0.45
1:A:345:LEU:O	1:A:369:ARG:HB2	2.16	0.45
1:C:292:VAL:O	3:C:377:NAD:H2N	2.17	0.45
1:B:32:LYS:O	1:B:77:GLY:HA3	2.16	0.45
1:D:254:LEU:HA	1:D:257:MET:HG2	1.98	0.45
1:B:178:THR:HG21	3:B:377:NAD:C4N	2.47	0.45
1:C:173:GLY:HA3	5:C:418:HOH:O	2.17	0.45
1:D:178:THR:HA	1:D:320:GLY:N	2.32	0.45
1:D:10:LYS:NZ	1:D:353:GLU:CG	2.80	0.44
1:D:92:LEU:CD2	1:D:328:VAL:HG21	2.48	0.44
1:B:29:ALA:HB1	1:B:30:PRO:HD2	1.99	0.44
1:A:187:ALA:O	1:A:188:LYS:HB2	2.18	0.44
1:A:69:ALA:HB3	1:A:145:THR:HG21	2.00	0.43
1:A:271:ARG:HB2	1:A:274:THR:OG1	2.18	0.43
1:A:292:VAL:O	3:A:377:NAD:H2N	2.17	0.43
5:A:522:HOH:O	1:D:101:ARG:HD2	2.18	0.43
1:B:292:VAL:O	3:B:377:NAD:H2N	2.17	0.43
1:B:338:LYS:HD3	5:B:484:HOH:O	2.17	0.43
1:D:188:LYS:O	1:D:189:VAL:C	2.60	0.43
1:B:2:THR:O	1:B:3:ALA:C	2.60	0.43
1:C:241:VAL:CG1	1:C:250:ILE:HD11	2.48	0.43
1:D:40:MET:CE	1:D:150:THR:HG22	2.45	0.43
1:D:301:LEU:C	1:D:301:LEU:HD12	2.44	0.43
1:D:330:LYS:HB3	5:D:500:HOH:O	2.19	0.43
1:B:254:LEU:HD23	1:B:257:MET:HE3	2.00	0.43
1:B:64:ILE:HG13	1:B:137:ILE:HG21	2.00	0.43
1:A:225:ASN:C	1:A:225:ASN:HD22	2.27	0.43
1:D:181:GLY:O	1:D:182:SER:C	2.62	0.43
1:C:48:SER:HA	1:C:51:HIS:CD2	2.53	0.42
1:A:32:LYS:O	1:A:33:ALA:C	2.61	0.42
1:A:40:MET:HE1	1:A:150:THR:HG22	2.01	0.42
1:A:51:HIS:HB3	1:A:57:LEU:HB2	2.01	0.42
1:B:271:ARG:HB2	1:B:274:THR:OG1	2.20	0.42
1:C:11:ALA:HA	1:C:147:SER:HA	2.00	0.42
1:D:24:GLU:OE2	1:D:133:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:LYS:HG2	5:D:456:HOH:O	2.18	0.42
1:A:83:VAL:HG12	1:A:159:LYS:HB2	2.02	0.42
1:B:88:LYS:HD3	1:B:166:LEU:HD21	2.00	0.42
1:D:29:ALA:HB1	1:D:30:PRO:HD2	2.01	0.42
1:A:208:ILE:HG23	1:A:219:ILE:HG21	2.00	0.42
1:A:328:VAL:HB	1:A:329:PRO:HD3	2.00	0.42
1:C:225:ASN:ND2	5:C:407:HOH:O	2.52	0.42
1:A:84:ARG:O	1:A:85:PRO:C	2.61	0.42
1:C:248:LYS:HB2	1:C:249:PRO:HD2	2.02	0.42
1:A:179:GLY:HA3	1:A:206:SER:HB2	2.00	0.41
1:A:225:ASN:ND2	1:A:225:ASN:C	2.77	0.41
1:A:100:CYS:O	1:A:104:LYS:HG2	2.20	0.41
1:A:188:LYS:O	1:A:189:VAL:C	2.63	0.41
1:C:200:LEU:HD13	1:C:232:ALA:HB2	2.01	0.41
1:D:59:THR:HA	1:D:60:PRO:HD3	1.91	0.41
1:C:35:GLU:CD	1:C:123:MET:HE2	2.45	0.41
1:C:123:MET:HB3	1:C:123:MET:HE3	1.76	0.41
1:B:350:LEU:HB3	1:B:351:PRO:HD2	2.02	0.41
1:C:290:VAL:HA	1:C:315:LYS:O	2.20	0.41
1:A:271:ARG:O	1:A:275:MET:HG3	2.20	0.41
1:C:339:LYS:HA	1:C:339:LYS:HE2	2.02	0.41
1:C:349:VAL:O	1:C:350:LEU:HD23	2.20	0.41
1:D:252:GLU:HG3	5:D:437:HOH:O	2.21	0.41
1:A:59:THR:HA	1:A:60:PRO:HD3	1.79	0.41
1:A:168:LYS:HE2	1:A:343:ASP:OD1	2.21	0.40
1:D:32:LYS:HD2	1:D:129:ARG:NH2	2.35	0.40
1:A:178:THR:OG1	1:A:319:PHE:HA	2.21	0.40
1:A:343:ASP:N	1:A:344:PRO:CD	2.83	0.40
1:C:295:PRO:HA	1:C:296:PRO:HD3	1.88	0.40
1:D:32:LYS:O	1:D:33:ALA:C	2.65	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)
1:A:245:ASP:O	1:C:247:LYS:N[1_554]	2.04	0.16

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	372/374 (100%)	351 (94%)	19 (5%)	2 (0%)	24	43
1	B	372/374 (100%)	353 (95%)	18 (5%)	1 (0%)	36	55
1	C	372/374 (100%)	351 (94%)	20 (5%)	1 (0%)	36	55
1	D	372/374 (100%)	347 (93%)	24 (6%)	1 (0%)	36	55
All	All	1488/1496 (100%)	1402 (94%)	81 (5%)	5 (0%)	36	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	CYS
1	C	174	CYS
1	D	174	CYS
1	B	174	CYS
1	A	368	ILE

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	308/308 (100%)	301 (98%)	7 (2%)	44	72
1	B	308/308 (100%)	301 (98%)	7 (2%)	44	72
1	C	308/308 (100%)	302 (98%)	6 (2%)	50	76
1	D	308/308 (100%)	303 (98%)	5 (2%)	55	79
All	All	1232/1232 (100%)	1207 (98%)	25 (2%)	48	75

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	164	SER
1	A	168	LYS
1	A	233	LYS
1	A	268	VAL
1	A	279	LEU
1	A	302	SER
1	B	18	LYS
1	B	97	CYS
1	B	233	LYS
1	B	239	GLU
1	B	268	VAL
1	B	279	LEU
1	B	302	SER
1	C	233	LYS
1	C	268	VAL
1	C	279	LEU
1	C	302	SER
1	C	327	SER
1	C	370	THR
1	D	233	LYS
1	D	268	VAL
1	D	279	LEU
1	D	302	SER
1	D	370	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	138	HIS
1	A	225	ASN
1	A	300	ASN
1	B	138	HIS
1	B	225	ASN
1	B	299	GLN
1	C	225	ASN
1	C	299	GLN
1	C	300	ASN
1	D	124	GLN
1	D	225	ASN

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Mol	Chain	Res	Type
1	D	299	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	FPI	B	378	2	8,8,8	1.55	1 (12%)	9,9,9	4.02	4 (44%)
3	NAD	D	377	-	46,48,48	2.65	20 (43%)	64,73,73	2.84	25 (39%)
4	FPI	C	378	2	8,8,8	1.78	1 (12%)	9,9,9	1.35	1 (11%)
3	NAD	A	377	-	46,48,48	2.43	21 (45%)	64,73,73	2.62	19 (29%)
3	NAD	B	377	-	46,48,48	2.30	17 (36%)	64,73,73	2.56	25 (39%)
3	NAD	C	377	-	46,48,48	2.24	18 (39%)	64,73,73	2.52	26 (40%)
4	FPI	D	378	2	8,8,8	1.43	2 (25%)	9,9,9	3.34	3 (33%)
4	FPI	A	378	2	8,8,8	1.68	2 (25%)	9,9,9	4.44	5 (55%)

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
4	FPI	B	378	2	-	0/2/10/10	0/1/1/1
3	NAD	D	377	-	-	5/30/62/62	0/5/5/5
4	FPI	C	378	2	-	0/2/10/10	0/1/1/1
3	NAD	A	377	-	-	5/30/62/62	0/5/5/5
3	NAD	B	377	-	-	5/30/62/62	0/5/5/5
3	NAD	C	377	-	-	6/30/62/62	0/5/5/5
4	FPI	D	378	2	-	0/2/10/10	0/1/1/1
4	FPI	A	378	2	-	0/2/10/10	0/1/1/1

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	377	NAD	O4D-C4D	7.98	1.62	1.45
3	D	377	NAD	C3N-C7N	6.24	1.59	1.50
3	D	377	NAD	PN-O3	6.03	1.66	1.59
3	B	377	NAD	C3N-C7N	5.40	1.58	1.50
3	A	377	NAD	O4D-C4D	5.07	1.56	1.45
3	C	377	NAD	C3N-C7N	4.96	1.58	1.50
3	D	377	NAD	C4N-C3N	4.81	1.46	1.39
3	B	377	NAD	O3B-C3B	4.64	1.54	1.43
3	A	377	NAD	PN-O3	-4.58	1.54	1.59
3	A	377	NAD	C4N-C3N	4.56	1.46	1.39
4	C	378	FPI	C2-N	4.46	1.53	1.46
3	C	377	NAD	O4B-C4B	4.28	1.54	1.45
3	C	377	NAD	O4D-C1D	4.27	1.46	1.40
3	A	377	NAD	C4A-N3A	4.19	1.42	1.34
3	D	377	NAD	C6N-N1N	4.09	1.44	1.35
3	B	377	NAD	C2A-N3A	3.92	1.40	1.33
3	A	377	NAD	O4B-C1B	-3.85	1.33	1.42
3	B	377	NAD	C6N-N1N	3.84	1.44	1.35
3	B	377	NAD	O4D-C1D	3.73	1.45	1.40
3	C	377	NAD	PN-O3	3.70	1.63	1.59
3	C	377	NAD	C2A-N3A	3.68	1.40	1.33
3	A	377	NAD	C5A-N7A	-3.66	1.32	1.39
3	A	377	NAD	O4D-C1D	3.60	1.45	1.40
4	B	378	FPI	C4-C3	3.60	1.64	1.51
3	B	377	NAD	PN-O3	3.60	1.63	1.59
3	A	377	NAD	O3B-C3B	3.54	1.51	1.43
3	C	377	NAD	C4N-C3N	3.52	1.44	1.39
3	D	377	NAD	C2A-N1A	-3.51	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	377	NAD	C5A-C6A	3.50	1.50	1.41
3	C	377	NAD	O4D-C4D	3.50	1.52	1.45
3	C	377	NAD	O3B-C3B	3.46	1.51	1.43
3	A	377	NAD	O2B-C2B	-3.43	1.34	1.43
3	C	377	NAD	O2B-C2B	-3.38	1.34	1.43
3	A	377	NAD	C5A-C6A	3.32	1.50	1.41
3	D	377	NAD	C8A-N7A	-3.31	1.25	1.31
3	A	377	NAD	C3N-C7N	3.30	1.55	1.50
3	B	377	NAD	O2B-C2B	-3.28	1.34	1.43
3	C	377	NAD	C5A-C6A	3.28	1.50	1.41
3	A	377	NAD	C2A-N3A	3.27	1.39	1.33
3	A	377	NAD	C2N-C3N	-3.26	1.33	1.39
3	B	377	NAD	C4A-N3A	3.23	1.40	1.34
3	C	377	NAD	PA-O3	-3.22	1.56	1.59
3	D	377	NAD	C2N-N1N	3.17	1.38	1.35
3	D	377	NAD	C5A-C6A	3.10	1.49	1.41
3	B	377	NAD	C5A-N7A	-3.10	1.33	1.39
3	B	377	NAD	C3D-C4D	3.08	1.60	1.53
3	D	377	NAD	O2B-C2B	-3.06	1.35	1.43
3	A	377	NAD	C5N-C4N	2.98	1.44	1.38
3	A	377	NAD	O3D-C3D	-2.98	1.35	1.43
3	D	377	NAD	O4B-C4B	2.96	1.51	1.45
3	D	377	NAD	PN-O2N	-2.96	1.41	1.55
3	B	377	NAD	PA-O3	-2.89	1.56	1.59
3	C	377	NAD	C3B-C4B	2.86	1.60	1.53
4	A	378	FPI	C4-C3	2.85	1.62	1.51
3	B	377	NAD	O4D-C4D	2.79	1.51	1.45
3	A	377	NAD	C2B-C3B	-2.77	1.45	1.53
3	D	377	NAD	C5N-C4N	2.76	1.43	1.38
3	B	377	NAD	PN-O1N	-2.68	1.41	1.50
3	C	377	NAD	PN-O2N	-2.66	1.43	1.55
3	D	377	NAD	O4D-C1D	2.66	1.44	1.40
4	A	378	FPI	C3-C2	2.65	1.60	1.51
3	A	377	NAD	C6N-N1N	2.55	1.41	1.35
3	B	377	NAD	O4B-C1B	-2.53	1.36	1.42
3	C	377	NAD	C6N-N1N	2.50	1.41	1.35
3	D	377	NAD	C4A-N3A	2.42	1.38	1.34
3	C	377	NAD	C2D-C3D	2.38	1.59	1.53
3	B	377	NAD	C5B-C4B	-2.38	1.44	1.51
3	A	377	NAD	C4A-N9A	2.32	1.42	1.37
3	C	377	NAD	O3D-C3D	-2.32	1.37	1.43
3	A	377	NAD	O4B-C4B	2.30	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	377	NAD	C5D-C4D	-2.28	1.44	1.51
3	D	377	NAD	C6N-C5N	-2.24	1.34	1.38
3	B	377	NAD	C5D-C4D	-2.22	1.44	1.51
3	A	377	NAD	PA-O2A	-2.17	1.45	1.55
3	C	377	NAD	C4A-N9A	2.17	1.42	1.37
3	A	377	NAD	PA-O3	-2.17	1.57	1.59
3	D	377	NAD	C3B-C4B	2.13	1.58	1.53
4	D	378	FPI	C6-N	2.11	1.49	1.46
3	D	377	NAD	C4A-N9A	2.09	1.42	1.37
4	D	378	FPI	C4-C3	2.03	1.59	1.51
3	D	377	NAD	C5A-N7A	-2.02	1.35	1.39
3	D	377	NAD	O2D-C2D	-2.02	1.38	1.43

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	377	NAD	C5N-C4N-C3N	-9.91	110.62	120.36
4	A	378	FPI	C2-N-C7	9.76	134.60	122.61
4	B	378	FPI	C2-N-C7	9.23	133.96	122.61
4	A	378	FPI	C6-N-C7	-8.03	112.75	122.61
3	A	377	NAD	C2N-C3N-C4N	7.61	127.11	118.26
3	D	377	NAD	C5N-C4N-C3N	-7.54	112.95	120.36
3	D	377	NAD	C2A-N1A-C6A	7.20	130.56	118.73
3	D	377	NAD	C2N-C3N-C4N	6.96	126.35	118.26
4	B	378	FPI	C6-N-C7	-6.66	114.44	122.61
3	C	377	NAD	C2A-N1A-C6A	6.57	129.53	118.73
3	C	377	NAD	C2N-C3N-C4N	6.57	125.90	118.26
3	B	377	NAD	C4A-N9A-C8A	-6.46	98.95	105.74
3	D	377	NAD	C3N-C7N-N7N	6.36	125.58	117.74
3	C	377	NAD	C6N-N1N-C2N	6.17	127.12	121.88
3	B	377	NAD	C2N-C3N-C4N	6.15	125.41	118.26
4	D	378	FPI	C6-N-C7	-5.99	115.25	122.61
3	A	377	NAD	C4A-N9A-C8A	-5.97	99.47	105.74
3	A	377	NAD	C3N-C7N-N7N	-5.96	110.40	117.74
3	D	377	NAD	C4A-N9A-C8A	-5.93	99.51	105.74
3	B	377	NAD	C5N-C4N-C3N	-5.88	114.58	120.36
4	D	378	FPI	C4-C5-C6	-5.58	100.87	111.19
3	A	377	NAD	O7N-C7N-C3N	5.42	126.23	119.60
3	C	377	NAD	C5N-C4N-C3N	-5.37	115.09	120.36
3	B	377	NAD	O2B-C2B-C3B	5.32	128.88	111.82
3	C	377	NAD	N3A-C2A-N1A	-5.31	120.54	128.58
3	D	377	NAD	O7N-C7N-N7N	-5.29	114.97	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	377	NAD	O7N-C7N-C3N	5.11	125.85	119.60
4	D	378	FPI	C2-N-C7	4.62	128.29	122.61
3	D	377	NAD	C6N-N1N-C2N	4.55	125.75	121.88
3	D	377	NAD	C2D-C3D-C4D	4.52	111.34	102.61
3	B	377	NAD	C2B-C3B-C4B	4.38	111.08	102.61
3	B	377	NAD	N9A-C8A-N7A	4.26	119.98	113.94
3	D	377	NAD	N9A-C8A-N7A	4.21	119.92	113.94
3	B	377	NAD	C2A-N1A-C6A	4.16	125.57	118.73
3	A	377	NAD	O2B-C2B-C3B	4.14	125.09	111.82
3	A	377	NAD	C2A-N1A-C6A	4.13	125.52	118.73
3	D	377	NAD	O4B-C1B-N9A	-4.13	100.16	108.09
3	D	377	NAD	N6A-C6A-N1A	4.04	127.37	118.38
3	B	377	NAD	C3N-C7N-N7N	-3.83	113.01	117.74
3	C	377	NAD	C2B-C3B-C4B	3.78	109.92	102.61
3	B	377	NAD	C2D-C3D-C4D	3.77	109.90	102.61
3	D	377	NAD	C6N-C5N-C4N	3.77	124.88	119.45
3	B	377	NAD	C6N-N1N-C1D	-3.73	112.41	119.73
3	C	377	NAD	O3-PA-O1A	-3.70	99.58	110.70
3	A	377	NAD	C6N-C5N-C4N	3.68	124.75	119.45
3	A	377	NAD	C2B-C3B-C4B	3.61	109.59	102.61
3	D	377	NAD	N3A-C2A-N1A	-3.60	123.14	128.58
3	D	377	NAD	O3-PA-O1A	-3.53	100.08	110.70
3	C	377	NAD	N6A-C6A-N1A	3.44	126.03	118.38
3	B	377	NAD	C5A-C4A-N3A	-3.42	122.00	126.72
3	A	377	NAD	C2D-C3D-C4D	3.40	109.17	102.61
3	C	377	NAD	O2A-PA-O1A	3.34	128.00	112.44
3	B	377	NAD	C5N-C6N-N1N	-3.34	115.83	120.38
3	A	377	NAD	N9A-C8A-N7A	3.30	118.62	113.94
3	B	377	NAD	C6N-N1N-C2N	3.27	124.66	121.88
3	B	377	NAD	C6A-C5A-C4A	3.22	121.57	117.18
3	D	377	NAD	C5N-C6N-N1N	-3.19	116.04	120.38
3	C	377	NAD	C5A-C4A-N3A	-3.16	122.37	126.72
3	C	377	NAD	C2D-C3D-C4D	3.12	108.65	102.61
3	C	377	NAD	C4A-N9A-C8A	-3.02	102.57	105.74
3	D	377	NAD	C5A-C6A-N1A	-2.96	110.01	117.51
3	D	377	NAD	C2B-C3B-C4B	2.94	108.28	102.61
3	D	377	NAD	O4D-C4D-C3D	-2.86	99.49	105.15
3	D	377	NAD	C1B-N9A-C8A	2.83	133.38	127.09
3	B	377	NAD	C6N-C5N-C4N	2.82	123.52	119.45
3	C	377	NAD	O4D-C4D-C5D	-2.82	100.31	109.33
3	C	377	NAD	O3B-C3B-C4B	-2.77	103.11	111.08
3	B	377	NAD	O3B-C3B-C4B	-2.77	103.13	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	377	NAD	C4B-O4B-C1B	-2.76	103.36	109.47
3	D	377	NAD	C4B-O4B-C1B	-2.73	103.44	109.47
3	A	377	NAD	O4D-C4D-C3D	-2.71	99.76	105.15
4	B	378	FPI	C5-C6-N	2.71	117.09	110.69
3	A	377	NAD	C6N-N1N-C1D	-2.66	114.51	119.73
4	C	378	FPI	C6-N-C7	-2.66	119.35	122.61
3	C	377	NAD	O4B-C1B-N9A	-2.64	103.03	108.09
3	C	377	NAD	C5A-C6A-N1A	-2.58	110.97	117.51
3	C	377	NAD	C3B-C2B-C1B	-2.58	96.59	101.46
3	B	377	NAD	C5A-C4A-N9A	2.57	108.61	105.81
3	C	377	NAD	O7N-C7N-N7N	-2.56	118.92	122.62
3	D	377	NAD	C5A-C4A-N3A	-2.55	123.20	126.72
3	C	377	NAD	C6A-C5A-C4A	2.55	120.66	117.18
3	B	377	NAD	O3D-C3D-C4D	-2.55	103.77	111.08
3	A	377	NAD	C6A-C5A-C4A	2.48	120.57	117.18
3	B	377	NAD	N6A-C6A-N1A	2.44	123.82	118.38
3	D	377	NAD	C2N-C3N-C7N	-2.42	112.47	119.46
3	A	377	NAD	C5A-C4A-N3A	-2.40	123.41	126.72
4	A	378	FPI	C5-C6-N	2.39	116.32	110.69
3	C	377	NAD	N3A-C4A-N9A	2.38	131.22	127.17
3	D	377	NAD	O2A-PA-O1A	2.37	123.46	112.44
4	A	378	FPI	C4-C3-C2	-2.34	106.86	111.19
3	C	377	NAD	O5D-PN-O1N	-2.34	99.66	108.94
3	C	377	NAD	C5D-C4D-C3D	2.32	123.57	115.21
3	B	377	NAD	O4D-C4D-C3D	-2.29	100.61	105.15
3	B	377	NAD	O4B-C4B-C3B	-2.28	100.63	105.15
3	D	377	NAD	O4B-C4B-C3B	-2.25	100.69	105.15
3	C	377	NAD	N9A-C8A-N7A	2.25	117.12	113.94
4	A	378	FPI	C4-C5-C6	-2.24	107.05	111.19
3	A	377	NAD	C5N-C6N-N1N	-2.23	117.34	120.38
4	B	378	FPI	C4-C5-C6	-2.23	107.06	111.19
3	B	377	NAD	C5A-C6A-N1A	-2.18	111.98	117.51
3	D	377	NAD	O3B-C3B-C4B	-2.16	104.86	111.08
3	C	377	NAD	C5N-C6N-N1N	-2.14	117.46	120.38
3	A	377	NAD	O2A-PA-O1A	2.12	122.31	112.44
3	C	377	NAD	C4D-O4D-C1D	2.11	111.86	109.92
3	B	377	NAD	N3A-C2A-N1A	-2.11	125.39	128.58
3	A	377	NAD	C1B-N9A-C8A	2.10	131.75	127.09
3	B	377	NAD	O3D-C3D-C2D	2.05	118.39	111.82
3	A	377	NAD	C5A-C6A-N1A	-2.02	112.39	117.51

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	377	NAD	C5B-O5B-PA-O1A
3	A	377	NAD	O4D-C1D-N1N-C2N
3	A	377	NAD	O4D-C1D-N1N-C6N
3	A	377	NAD	C2D-C1D-N1N-C2N
3	A	377	NAD	C2D-C1D-N1N-C6N
3	B	377	NAD	O4D-C1D-N1N-C2N
3	B	377	NAD	O4D-C1D-N1N-C6N
3	B	377	NAD	C2D-C1D-N1N-C2N
3	B	377	NAD	C2D-C1D-N1N-C6N
3	C	377	NAD	O4D-C1D-N1N-C2N
3	C	377	NAD	O4D-C1D-N1N-C6N
3	C	377	NAD	C2D-C1D-N1N-C2N
3	C	377	NAD	C2D-C1D-N1N-C6N
3	D	377	NAD	O4D-C1D-N1N-C2N
3	D	377	NAD	O4D-C1D-N1N-C6N
3	D	377	NAD	C2D-C1D-N1N-C2N
3	D	377	NAD	C2D-C1D-N1N-C6N
3	C	377	NAD	C3D-C4D-C5D-O5D
3	D	377	NAD	C3D-C4D-C5D-O5D
3	B	377	NAD	O4B-C4B-C5B-O5B
3	C	377	NAD	PA-O3-PN-O1N

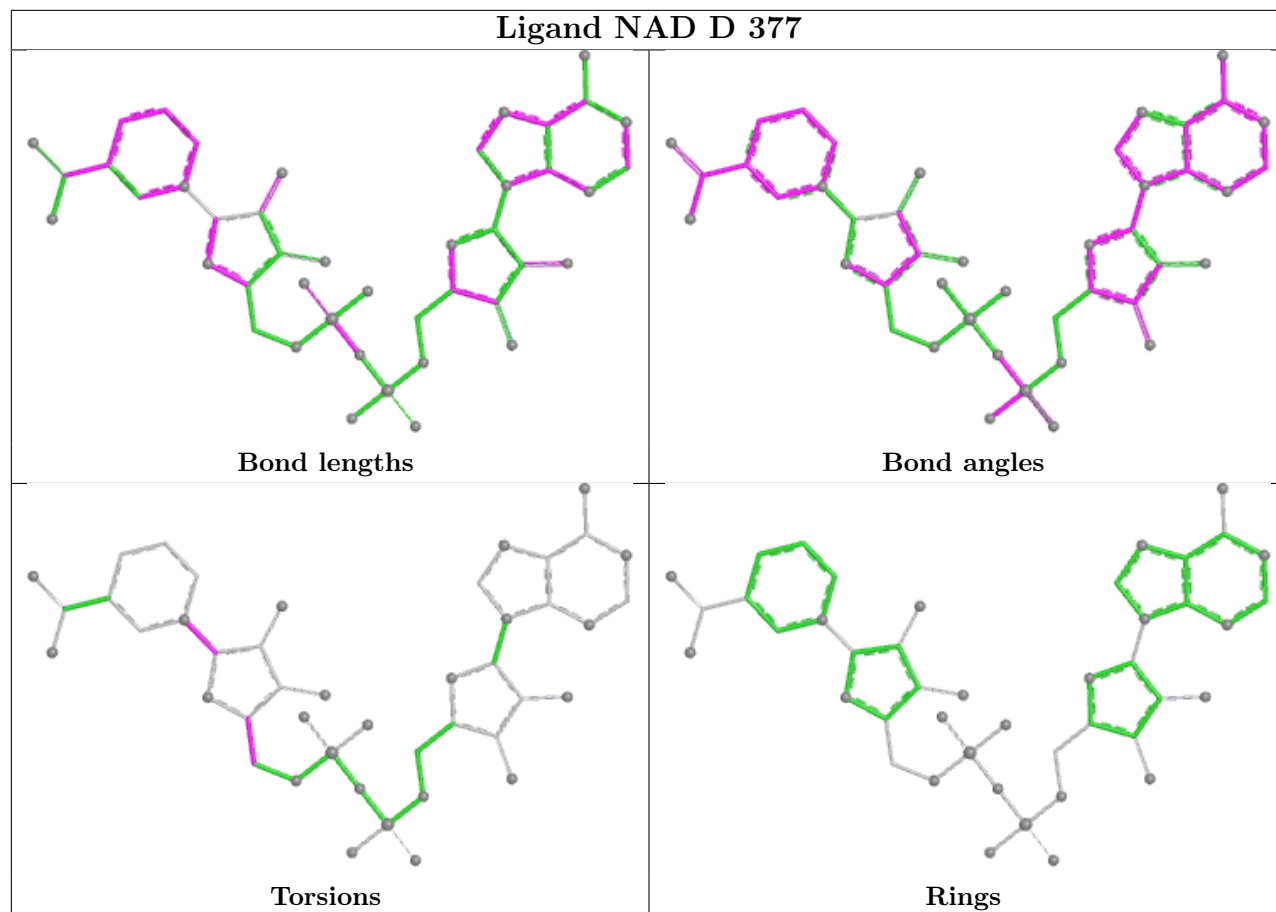
There are no ring outliers.

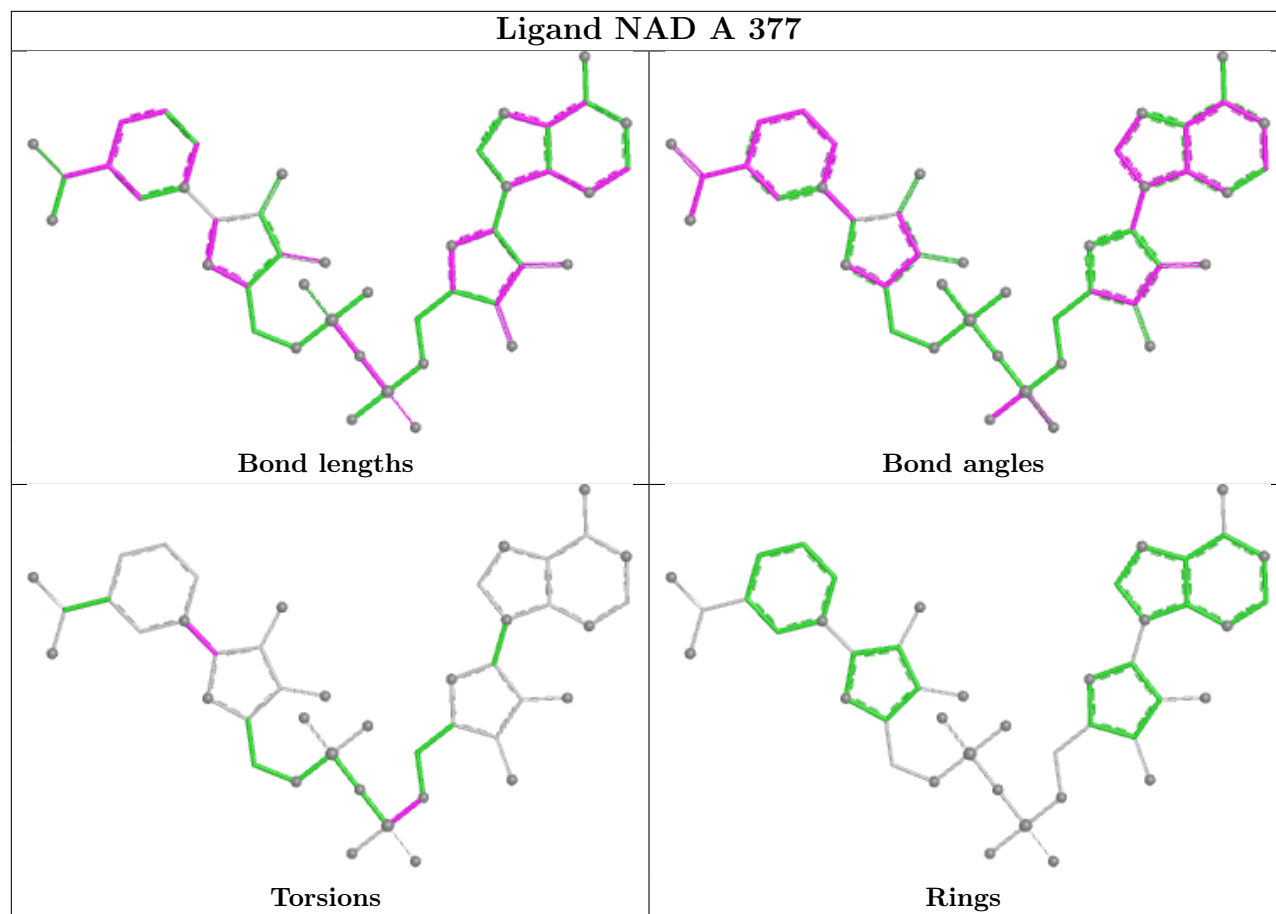
4 monomers are involved in 5 short contacts:

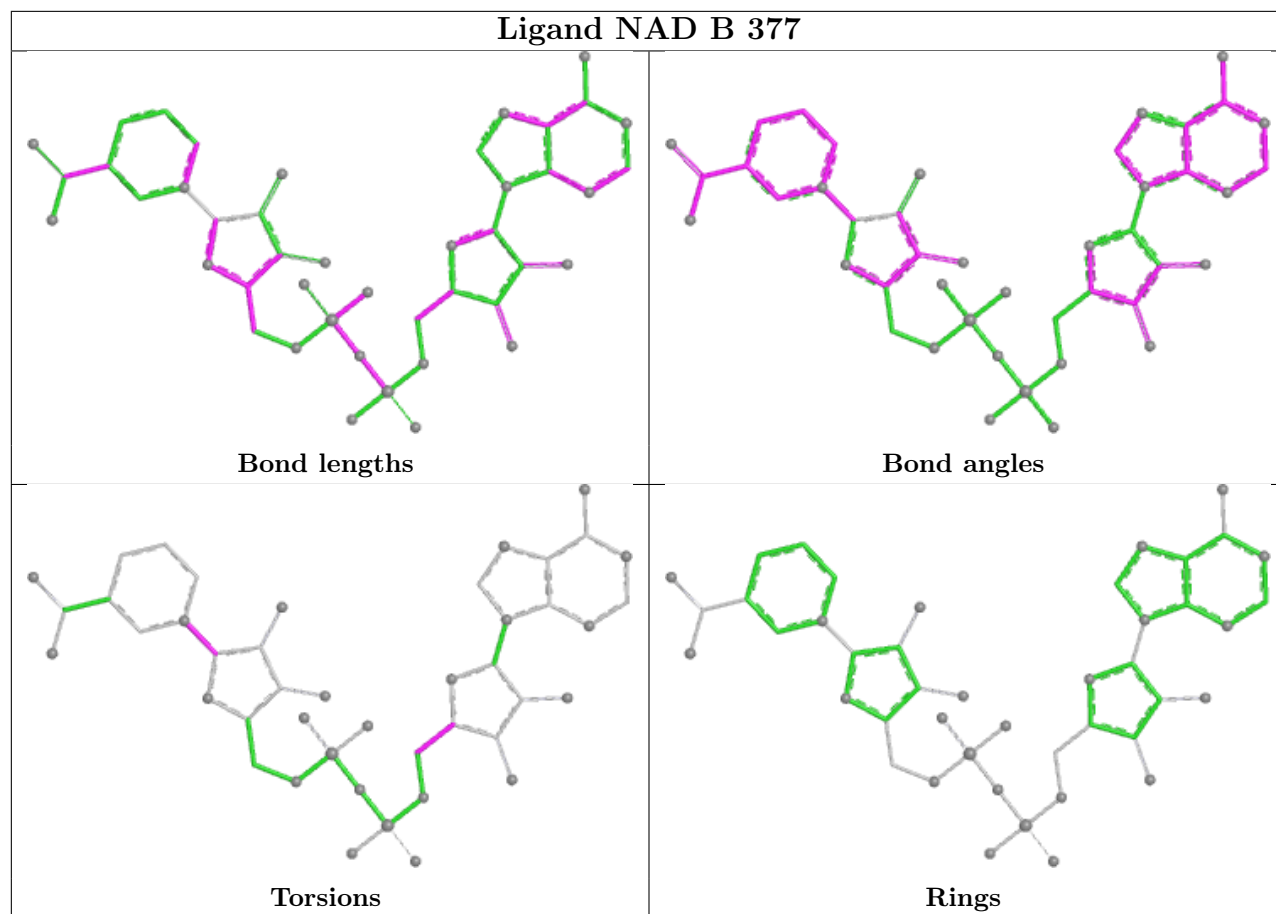
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	378	FPI	1	0
3	A	377	NAD	1	0
3	B	377	NAD	2	0
3	C	377	NAD	1	0

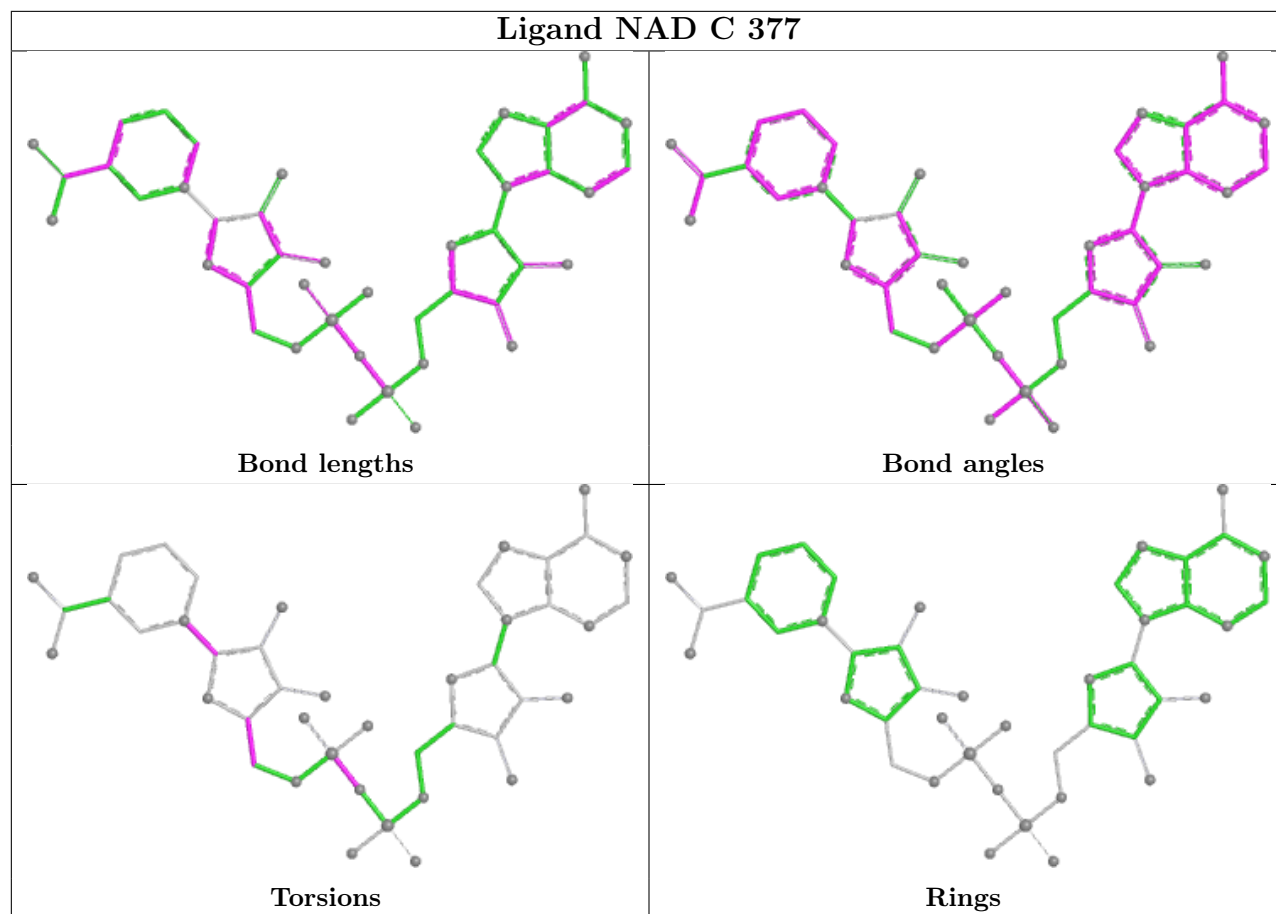
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	374/374 (100%)	-0.20	2 (0%) 87 85	8, 16, 32, 43	0
1	B	374/374 (100%)	-0.20	1 (0%) 90 87	8, 16, 31, 42	0
1	C	374/374 (100%)	-0.10	5 (1%) 75 71	8, 16, 31, 43	0
1	D	374/374 (100%)	-0.16	2 (0%) 87 85	8, 16, 31, 43	0
All	All	1496/1496 (100%)	-0.17	10 (0%) 84 81	8, 16, 32, 43	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	SER	2.8
1	C	191	GLN	2.6
1	C	353	GLU	2.6
1	C	101	ARG	2.5
1	D	69	ALA	2.5
1	C	357	GLU	2.5
1	C	1	SER	2.3
1	A	101	ARG	2.3
1	D	133	ARG	2.2
1	B	1	SER	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

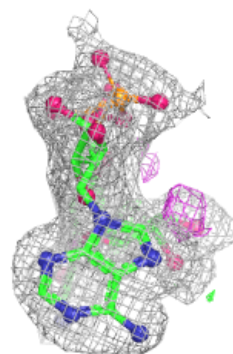
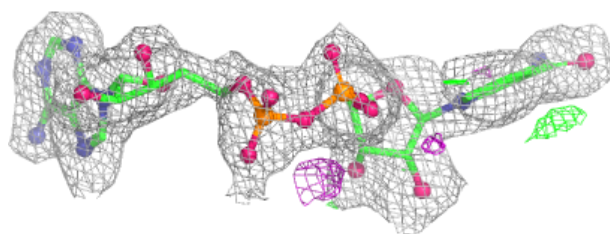
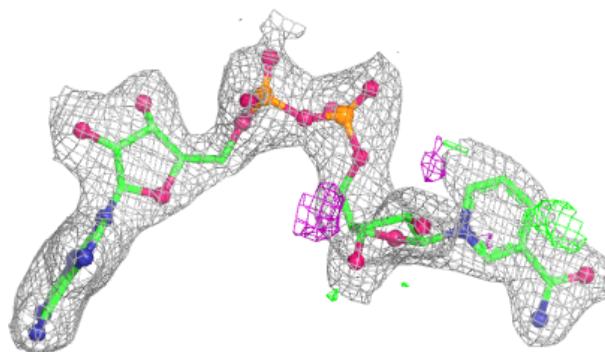
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FPI	D	378	8/8	0.88	0.11	6,9,10,11	0
4	FPI	C	378	8/8	0.93	0.09	6,8,10,11	0
4	FPI	A	378	8/8	0.93	0.09	7,8,9,10	0
3	NAD	D	377	44/44	0.95	0.08	8,13,20,21	0
4	FPI	B	378	8/8	0.95	0.07	6,8,9,10	0
3	NAD	C	377	44/44	0.96	0.07	8,13,20,21	0
2	ZN	B	376	1/1	0.96	0.04	19,19,19,19	0
2	ZN	A	376	1/1	0.97	0.03	20,20,20,20	0
3	NAD	A	377	44/44	0.97	0.07	7,14,21,22	0
3	NAD	B	377	44/44	0.98	0.05	7,13,21,21	0
2	ZN	C	375	1/1	0.99	0.02	13,13,13,13	0
2	ZN	C	376	1/1	0.99	0.02	21,21,21,21	0
2	ZN	D	375	1/1	0.99	0.02	14,14,14,14	0
2	ZN	D	376	1/1	0.99	0.02	20,20,20,20	0
2	ZN	B	375	1/1	0.99	0.02	12,12,12,12	0
2	ZN	A	375	1/1	0.99	0.02	12,12,12,12	0

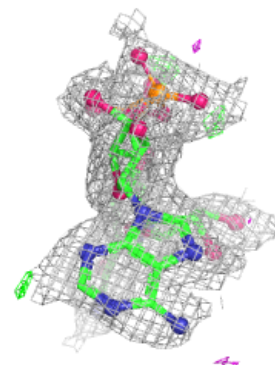
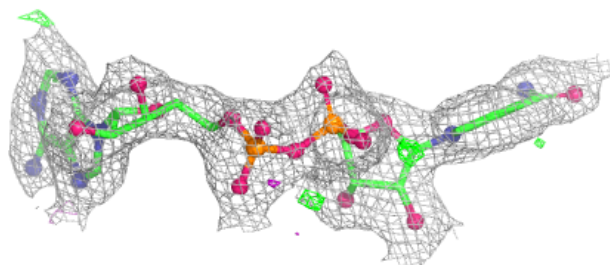
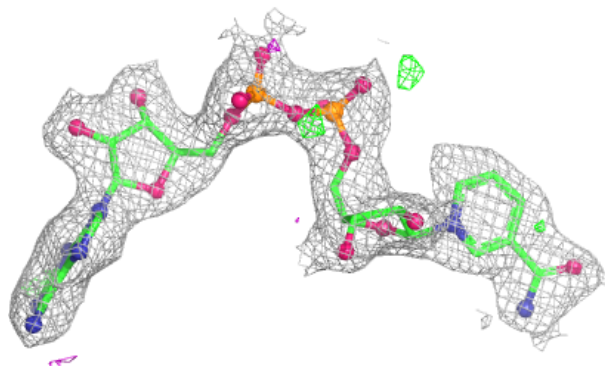
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD D 377:

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

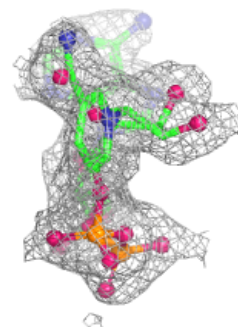
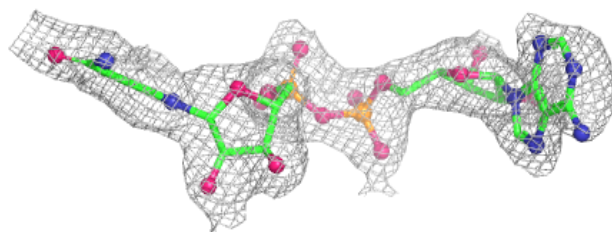
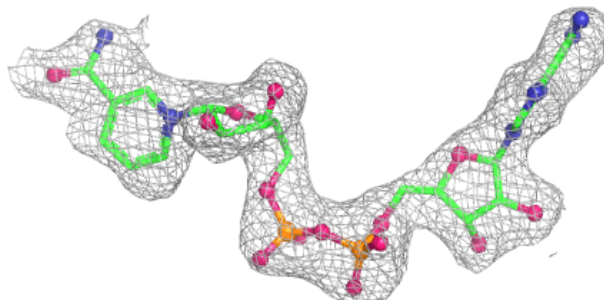
**Electron density around NAD C 377:**

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

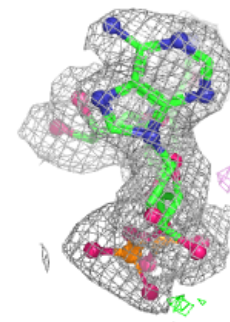
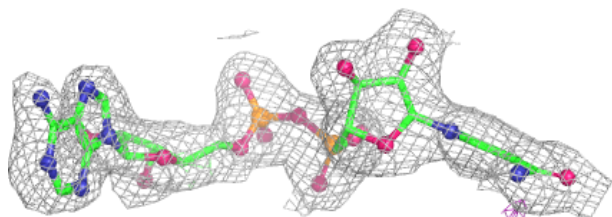
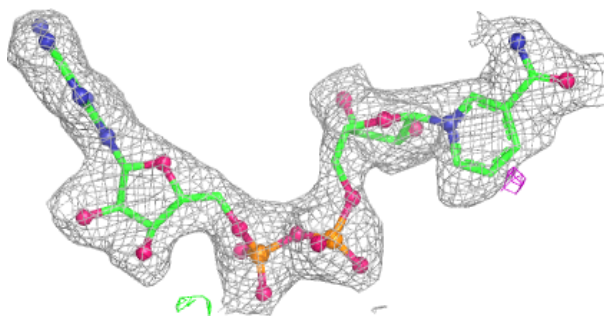


Electron density around NAD A 377:

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

**Electron density around NAD B 377:**

$2mF_o-DF_c$ (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.