



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:06 AM UTC

PDB ID : 1LDY / pdb_00001ldy
Title : HORSE LIVER ALCOHOL DEHYDROGENASE COMPLEXED TO NADH
AND CYCLOHEXYL FORMAMIDE (CXF)
Authors : Ramaswamy, S.; Plapp, B.V.
Deposited on : 1996-12-23
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

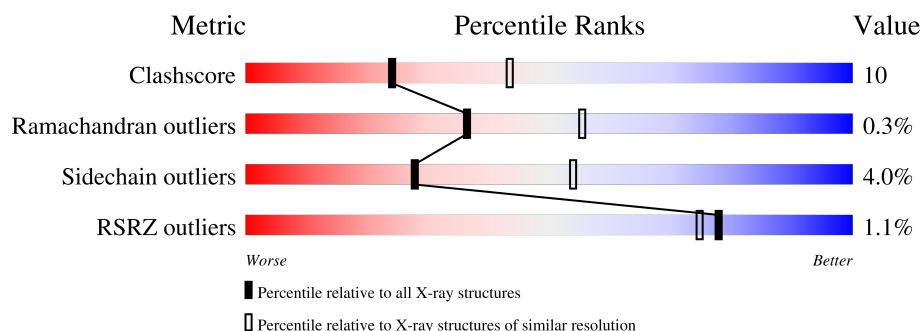
1 Overall quality at a glance

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	
1	B	374	
1	C	374	
1	D	374	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12372 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 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).

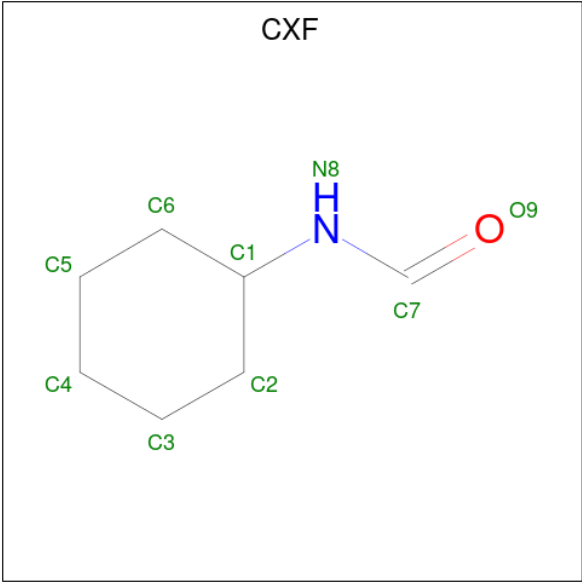
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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 CYCLOHEXYLFORMAMIDE (CCD ID: CXF) (formula: C₇H₁₃NO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 9 7 1 1	0	0
4	B	1	Total C N O 9 7 1 1	0	0
4	C	1	Total C N O 9 7 1 1	0	0
4	D	1	Total C N O 9 7 1 1	0	0

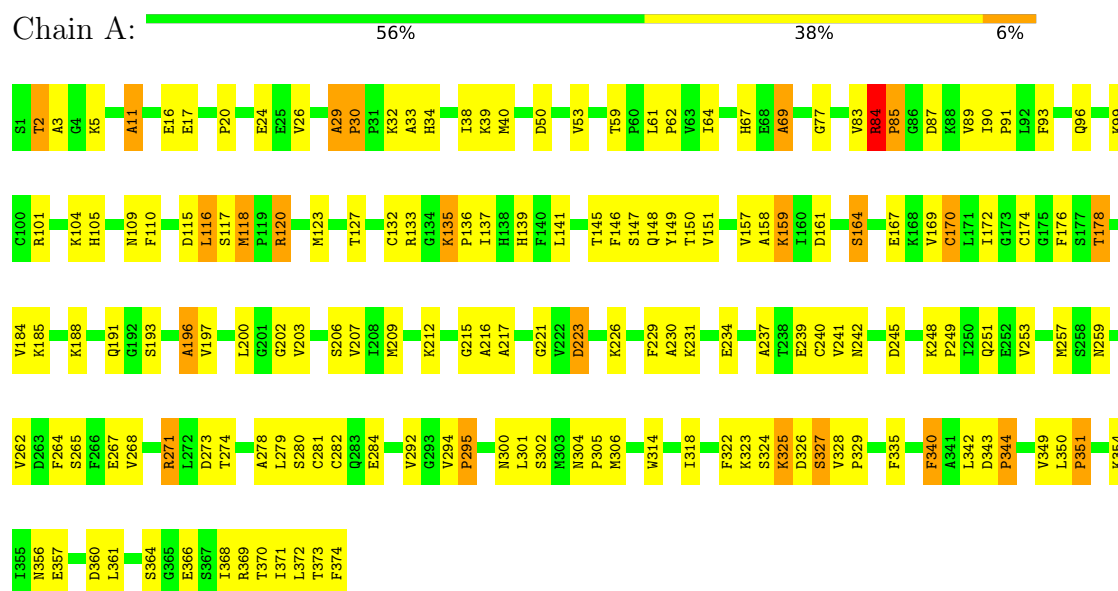
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	250	Total O 250 250	0	0
5	B	249	Total O 249 249	0	0
5	C	257	Total O 257 257	0	0
5	D	256	Total O 256 256	0	0

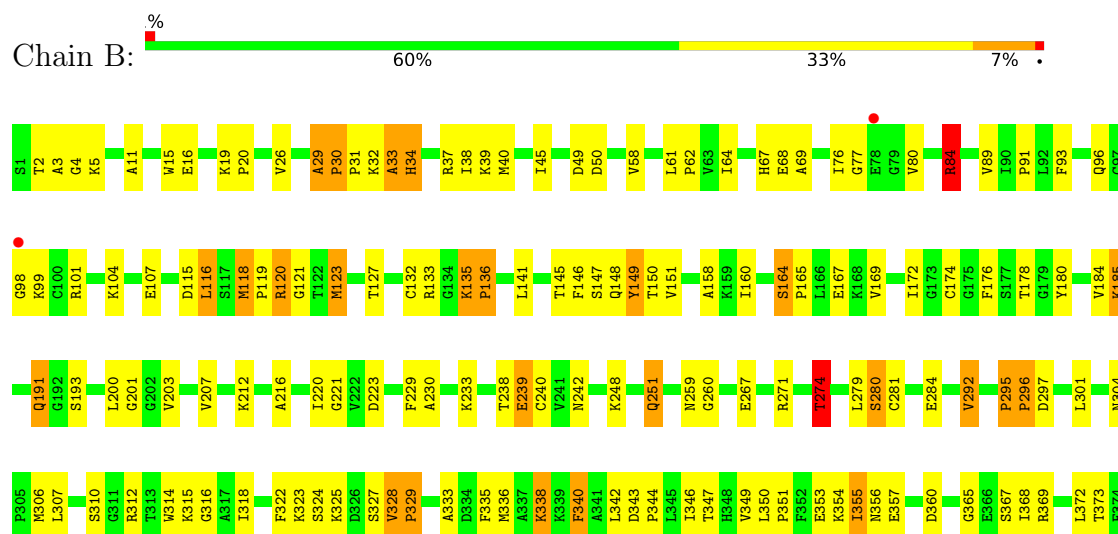
3 Residue-property plots

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.

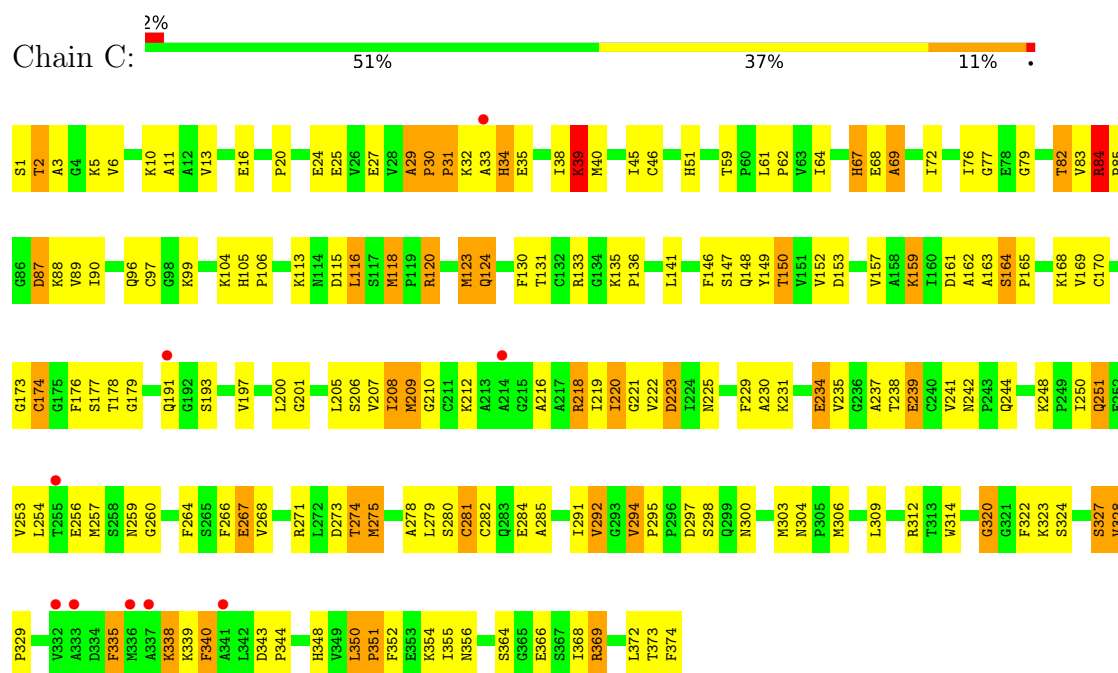
• Molecule 1: ALCOHOL DEHYDROGENASE



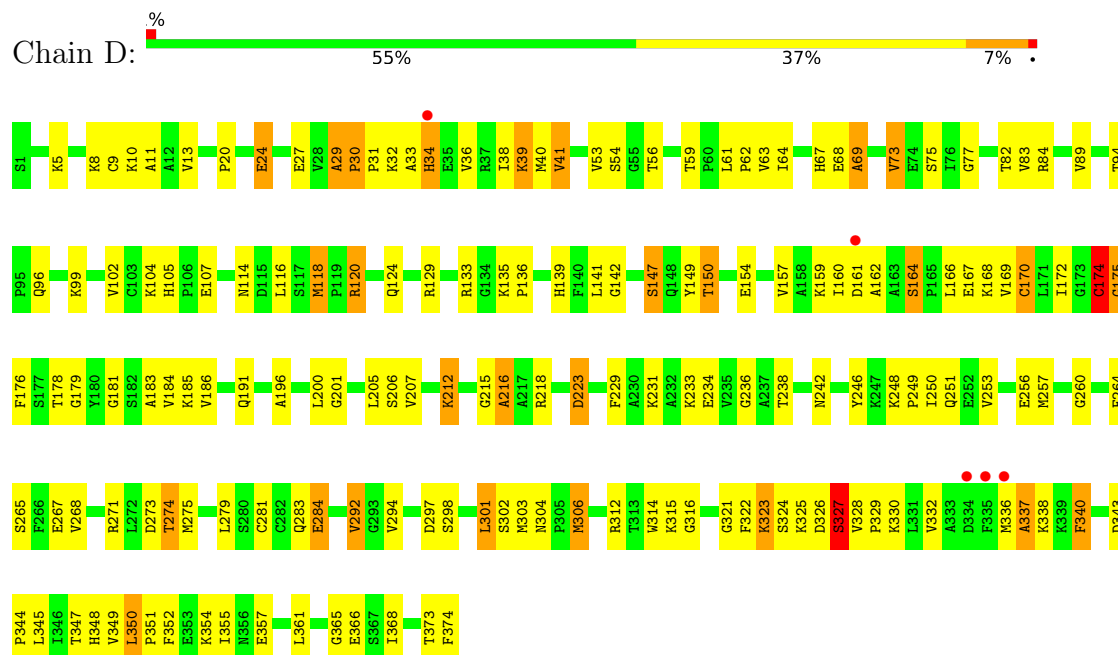
• Molecule 1: ALCOHOL DEHYDROGENASE



• Molecule 1: ALCOHOL DEHYDROGENASE



- Molecule 1: 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)	12.00 – 2.50 12.00 – 2.51	Depositor EDS
% Data completeness (in resolution range)	89.8 (12.00-2.50) 91.6 (12.00-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.40 (at 2.52Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.207 , (Not available) 0.199 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	1.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 71.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12372	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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 87.48 % 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 6.7562e-08. 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.19	3/2837 (0.1%)	2.28	149/3834 (3.9%)
1	B	1.19	2/2837 (0.1%)	2.30	145/3834 (3.8%)
1	C	1.27	2/2837 (0.1%)	2.39	175/3834 (4.6%)
1	D	1.24	2/2837 (0.1%)	2.35	139/3834 (3.6%)
All	All	1.22	9/11348 (0.1%)	2.33	608/15336 (4.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	30	PRO	CA-C	5.94	1.56	1.52
1	B	304	ASN	C-N	-5.68	1.27	1.34
1	B	329	PRO	C-O	5.64	1.31	1.24
1	A	30	PRO	CA-C	5.48	1.55	1.52
1	A	59	THR	C-N	-5.33	1.27	1.33
1	D	102	VAL	C-N	5.33	1.41	1.34
1	D	330	LYS	C-O	5.22	1.30	1.24
1	C	51	HIS	ND1-CE1	-5.17	1.27	1.32
1	A	323	LYS	CA-C	5.03	1.59	1.52

All (608) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	ARG	NE-CZ-NH2	14.78	132.50	119.20
1	D	218	ARG	NE-CZ-NH2	12.76	130.69	119.20
1	D	34	HIS	CA-CB-CG	-12.26	101.54	113.80
1	C	34	HIS	CA-CB-CG	-12.17	101.63	113.80
1	A	221	GLY	CA-C-O	-11.60	111.36	120.76
1	B	34	HIS	CA-CB-CG	-11.05	102.75	113.80
1	A	34	HIS	CA-CB-CG	-10.71	103.09	113.80
1	B	242	ASN	OD1-CG-ND2	-10.67	111.93	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	239	GLU	CA-C-O	-10.43	110.06	121.33
1	B	30	PRO	O-C-N	-10.21	116.35	121.15
1	A	229	PHE	N-CA-C	9.90	122.07	111.28
1	D	218	ARG	NE-CZ-NH1	-9.86	111.64	121.50
1	A	67	HIS	CA-CB-CG	-9.86	103.94	113.80
1	B	292	VAL	CA-C-N	9.72	129.34	120.10
1	B	292	VAL	C-N-CA	9.72	129.34	120.10
1	C	328	VAL	CA-C-O	9.62	125.14	118.69
1	A	148	GLN	OE1-CD-NE2	-9.55	113.05	122.60
1	D	176	PHE	O-C-N	9.46	131.87	122.03
1	A	172	ILE	O-C-N	-9.29	109.67	122.31
1	B	67	HIS	CA-CB-CG	-9.27	104.53	113.80
1	A	30	PRO	N-CA-CB	9.26	108.03	103.22
1	C	312	ARG	NE-CZ-NH2	-9.19	110.93	119.20
1	C	30	PRO	N-CA-CB	9.18	107.99	103.22
1	A	16	GLU	CA-C-O	-9.14	111.45	121.33
1	D	292	VAL	CA-C-N	9.00	129.49	120.31
1	D	292	VAL	C-N-CA	9.00	129.49	120.31
1	C	165	PRO	N-CA-CB	8.97	107.94	102.92
1	A	324	SER	N-CA-C	8.92	121.90	111.02
1	C	207	VAL	N-CA-C	-8.85	102.21	110.53
1	A	90	ILE	CA-C-O	8.80	124.52	119.94
1	A	239	GLU	CA-C-O	-8.76	111.87	121.33
1	D	160	ILE	CA-C-O	8.75	130.94	121.67
1	B	172	ILE	CA-C-O	8.72	130.95	119.53
1	A	151	VAL	CA-C-O	8.71	129.59	120.36
1	B	221	GLY	CA-C-O	-8.68	113.54	121.18
1	A	207	VAL	N-CA-C	-8.66	101.98	110.72
1	B	121	GLY	O-C-N	-8.60	113.77	122.54
1	D	324	SER	N-CA-C	8.58	121.48	111.02
1	B	172	ILE	O-C-N	-8.54	110.70	122.31
1	B	324	SER	N-CA-C	8.50	121.39	111.02
1	C	324	SER	N-CA-C	8.50	121.39	111.02
1	B	239	GLU	CA-C-O	-8.34	112.33	121.33
1	C	39	LYS	O-C-N	8.33	132.72	123.22
1	C	248	LYS	CA-C-N	8.33	128.40	119.90
1	C	248	LYS	C-N-CA	8.33	128.40	119.90
1	A	241	VAL	CA-C-O	-8.31	111.36	120.67
1	C	320	GLY	O-C-N	-8.30	111.91	122.70
1	B	207	VAL	N-CA-C	-8.29	102.74	110.53
1	A	292	VAL	CA-C-N	8.26	127.95	120.10
1	A	292	VAL	C-N-CA	8.26	127.95	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	ILE	CA-C-O	8.23	130.31	119.53
1	C	176	PHE	O-C-N	8.19	130.54	122.03
1	D	176	PHE	CA-CB-CG	-8.18	105.62	113.80
1	D	29	ALA	CA-C-N	8.16	125.53	119.66
1	D	29	ALA	C-N-CA	8.16	125.53	119.66
1	C	218	ARG	NE-CZ-NH2	8.12	126.51	119.20
1	C	275	MET	CA-C-O	-8.11	112.30	120.82
1	A	176	PHE	CA-CB-CG	-8.09	105.71	113.80
1	C	208	ILE	O-C-N	-8.08	114.03	121.87
1	A	158	ALA	CA-C-O	8.05	129.05	120.36
1	C	322	PHE	N-CA-C	8.01	121.97	109.96
1	A	109	ASN	OD1-CG-ND2	7.98	130.58	122.60
1	C	6	VAL	O-C-N	-7.96	114.55	122.67
1	D	176	PHE	CA-C-O	-7.95	112.66	121.00
1	B	304	ASN	CA-C-N	7.95	127.61	119.82
1	B	304	ASN	C-N-CA	7.95	127.61	119.82
1	B	160	ILE	CA-C-O	7.85	129.99	121.67
1	C	64	ILE	N-CA-CB	7.84	121.48	111.83
1	C	133	ARG	NE-CZ-NH2	7.81	126.23	119.20
1	C	67	HIS	CA-CB-CG	-7.81	105.99	113.80
1	C	59	THR	O-C-N	-7.80	115.75	121.83
1	D	30	PRO	CA-C-N	7.79	128.25	119.83
1	D	30	PRO	C-N-CA	7.79	128.25	119.83
1	A	64	ILE	N-CA-CB	7.79	120.95	111.60
1	A	30	PRO	CA-C-N	7.77	127.76	119.76
1	A	30	PRO	C-N-CA	7.77	127.76	119.76
1	D	54	SER	CA-C-O	-7.75	109.19	119.11
1	D	323	LYS	N-CA-C	-7.71	98.05	109.15
1	A	340	PHE	CA-C-O	-7.71	113.01	121.33
1	C	229	PHE	N-CA-C	7.70	120.65	111.33
1	D	67	HIS	CA-CB-CG	-7.67	106.13	113.80
1	D	275	MET	O-C-N	7.64	130.34	122.09
1	C	260	GLY	CA-C-O	-7.63	110.50	118.97
1	A	191	GLN	OE1-CD-NE2	-7.57	115.03	122.60
1	C	242	ASN	CA-C-N	7.57	128.25	119.47
1	C	242	ASN	C-N-CA	7.57	128.25	119.47
1	D	322	PHE	N-CA-C	7.54	121.28	109.96
1	C	275	MET	N-CA-C	-7.53	103.02	111.07
1	C	161	ASP	CA-CB-CG	7.51	120.11	112.60
1	C	218	ARG	NE-CZ-NH1	-7.49	114.02	121.50
1	C	374	PHE	CA-CB-CG	-7.46	106.34	113.80
1	B	158	ALA	CA-C-O	7.43	128.39	120.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	ALA	CA-C-O	-7.43	113.02	121.19
1	A	271	ARG	NE-CZ-NH2	7.41	125.87	119.20
1	C	369	ARG	CD-NE-CZ	-7.38	114.07	124.40
1	C	238	THR	O-C-N	-7.37	112.36	122.46
1	A	248	LYS	CA-C-N	7.36	127.41	119.90
1	A	248	LYS	C-N-CA	7.36	127.41	119.90
1	C	150	THR	CA-CB-OG1	-7.34	98.59	109.60
1	D	133	ARG	NE-CZ-NH2	7.34	125.80	119.20
1	A	372	LEU	O-C-N	7.31	131.53	123.27
1	C	212	LYS	O-C-N	-7.30	114.55	122.07
1	C	212	LYS	CA-C-O	7.29	128.47	120.82
1	C	251	GLN	OE1-CD-NE2	7.28	129.88	122.60
1	B	93	PHE	CA-CB-CG	7.26	121.06	113.80
1	D	355	ILE	CA-C-O	-7.26	113.72	121.27
1	C	201	GLY	N-CA-C	-7.24	99.82	112.55
1	D	120	ARG	CA-C-O	7.24	127.42	119.24
1	D	264	PHE	O-C-N	-7.23	114.54	123.36
1	B	151	VAL	CA-C-O	7.23	127.57	120.27
1	D	24	GLU	CB-CG-CD	-7.19	100.38	112.60
1	B	30	PRO	N-CA-CB	7.14	106.94	103.22
1	C	39	LYS	CA-C-O	-7.13	112.73	120.36
1	A	29	ALA	CA-C-N	7.12	124.79	119.66
1	A	29	ALA	C-N-CA	7.12	124.79	119.66
1	C	177	SER	O-C-N	7.12	129.49	122.09
1	D	212	LYS	CA-C-O	-7.10	113.36	120.82
1	B	355	ILE	CA-C-O	-7.10	113.89	121.27
1	B	38	ILE	CA-C-O	7.08	127.83	120.39
1	C	267	GLU	CB-CG-CD	7.07	124.62	112.60
1	B	30	PRO	CA-C-O	7.07	126.31	120.73
1	C	79	GLY	CA-C-O	-7.06	111.56	119.04
1	C	30	PRO	O-C-N	7.05	124.46	121.15
1	C	165	PRO	O-C-N	-7.01	117.75	122.73
1	A	372	LEU	CA-C-O	-7.01	112.79	120.43
1	D	304	ASN	CA-C-O	7.00	124.50	119.32
1	C	209	MET	CG-SD-CE	-6.99	85.53	100.90
1	D	207	VAL	N-CA-C	-6.98	103.97	110.53
1	D	160	ILE	O-C-N	-6.97	115.65	122.97
1	A	178	THR	O-C-N	6.96	129.32	122.09
1	C	221	GLY	CA-C-O	-6.90	115.29	121.64
1	C	87	ASP	CA-C-O	-6.89	114.05	121.56
1	A	292	VAL	O-C-N	-6.89	114.94	121.97
1	D	201	GLY	N-CA-C	-6.87	100.46	112.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	312	ARG	NE-CZ-NH1	6.84	128.34	121.50
1	D	34	HIS	ND1-CG-CD2	6.83	112.93	106.10
1	B	229	PHE	N-CA-C	6.83	118.38	111.07
1	B	31	PRO	CB-CA-C	-6.83	102.66	111.46
1	D	191	GLN	O-C-N	-6.83	114.49	122.95
1	B	316	GLY	O-C-N	-6.81	116.23	123.45
1	A	212	LYS	O-C-N	-6.81	115.06	122.07
1	C	123	MET	N-CA-C	-6.76	101.81	110.53
1	B	327	SER	CA-C-N	-6.76	114.92	120.33
1	B	327	SER	C-N-CA	-6.76	114.92	120.33
1	A	101	ARG	NE-CZ-NH1	-6.75	114.75	121.50
1	C	303	MET	O-C-N	-6.75	115.56	123.25
1	A	304	ASN	OD1-CG-ND2	6.75	129.34	122.60
1	D	248	LYS	CA-C-N	6.74	126.77	119.90
1	D	248	LYS	C-N-CA	6.74	126.77	119.90
1	C	309	LEU	O-C-N	-6.73	114.35	122.22
1	C	30	PRO	N-CA-C	-6.72	103.39	110.58
1	D	275	MET	N-CA-C	-6.72	103.88	111.14
1	C	281	CYS	CA-C-O	-6.72	111.12	119.38
1	B	89	VAL	CA-C-N	-6.72	117.01	122.85
1	B	89	VAL	C-N-CA	-6.72	117.01	122.85
1	B	327	SER	O-C-N	6.72	131.33	122.33
1	C	136	PRO	N-CA-CB	6.70	109.57	103.34
1	D	350	LEU	CA-C-O	6.70	126.67	120.50
1	D	347	THR	O-C-N	-6.68	114.40	122.48
1	C	76	ILE	O-C-N	-6.66	115.87	123.00
1	B	356	ASN	CA-C-N	6.64	129.07	120.44
1	B	356	ASN	C-N-CA	6.64	129.07	120.44
1	B	307	LEU	N-CA-CB	6.63	119.86	110.12
1	A	349	VAL	N-CA-CB	6.62	121.18	111.52
1	B	176	PHE	CA-C-O	-6.60	114.07	121.00
1	D	174	CYS	CA-C-O	6.60	129.95	120.51
1	D	306	MET	CB-CG-SD	6.60	132.49	112.70
1	D	229	PHE	N-CA-C	6.57	118.45	111.28
1	A	116	LEU	CA-C-N	6.57	128.97	120.44
1	A	116	LEU	C-N-CA	6.57	128.97	120.44
1	D	283	GLN	OE1-CD-NE2	-6.57	116.03	122.60
1	A	306	MET	CB-CG-SD	6.56	132.38	112.70
1	C	291	ILE	O-C-N	6.55	130.42	122.95
1	C	300	ASN	CA-CB-CG	-6.52	106.08	112.60
1	A	292	VAL	CA-C-O	6.52	126.27	120.34
1	A	93	PHE	CA-CB-CG	6.51	120.31	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	170	CYS	N-CA-C	-6.51	104.27	111.82
1	C	266	PHE	CA-C-N	-6.51	114.12	122.77
1	C	266	PHE	C-N-CA	-6.51	114.12	122.77
1	D	172	ILE	CA-C-O	6.51	128.05	119.53
1	A	323	LYS	N-CA-C	-6.49	99.81	109.15
1	B	280	SER	N-CA-CB	6.48	120.19	110.22
1	A	284	GLU	N-CA-C	6.47	120.04	111.75
1	C	335	PHE	CA-C-O	6.47	127.28	120.42
1	A	368	ILE	N-CA-C	-6.47	95.89	109.34
1	D	96	GLN	CA-CB-CG	-6.47	101.17	114.10
1	D	273	ASP	CB-CG-OD1	6.46	133.26	118.40
1	B	242	ASN	CA-C-N	6.46	126.96	119.47
1	B	242	ASN	C-N-CA	6.46	126.96	119.47
1	A	151	VAL	O-C-N	-6.46	116.23	123.20
1	A	271	ARG	NH1-CZ-NH2	-6.46	110.91	119.30
1	D	216	ALA	CA-C-O	-6.45	114.10	121.19
1	A	24	GLU	CB-CG-CD	-6.43	101.66	112.60
1	A	369	ARG	CA-C-O	6.43	127.31	120.36
1	A	371	ILE	O-C-N	-6.43	115.89	123.03
1	B	37	ARG	CA-C-N	6.43	131.57	123.14
1	B	37	ARG	C-N-CA	6.43	131.57	123.14
1	C	176	PHE	CA-CB-CG	-6.43	107.37	113.80
1	B	323	LYS	N-CA-C	-6.43	99.41	109.25
1	D	129	ARG	NE-CZ-NH2	-6.43	113.41	119.20
1	A	84	ARG	CA-C-O	6.43	126.42	120.50
1	C	356	ASN	O-C-N	-6.43	115.31	122.12
1	A	374	PHE	CA-CB-CG	-6.43	107.37	113.80
1	B	267	GLU	CB-CG-CD	6.43	123.53	112.60
1	C	96	GLN	CA-CB-CG	-6.42	101.26	114.10
1	C	323	LYS	N-CA-C	-6.42	99.91	109.15
1	D	136	PRO	N-CA-CB	6.42	109.31	103.34
1	B	248	LYS	CA-C-N	6.41	126.44	119.90
1	B	248	LYS	C-N-CA	6.41	126.44	119.90
1	D	30	PRO	N-CA-CB	6.41	106.55	103.22
1	A	148	GLN	CA-C-O	6.41	127.34	120.10
1	D	216	ALA	CB-CA-C	-6.40	99.09	109.72
1	C	304	ASN	CA-C-N	6.40	126.09	119.82
1	C	304	ASN	C-N-CA	6.40	126.09	119.82
1	D	150	THR	CA-CB-OG1	-6.39	100.01	109.60
1	A	69	ALA	N-CA-C	6.39	117.00	108.38
1	D	169	VAL	N-CA-C	6.38	122.61	109.34
1	A	123	MET	N-CA-C	-6.36	102.33	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	VAL	N-CA-C	6.36	119.03	111.09
1	D	312	ARG	NE-CZ-NH2	-6.34	113.49	119.20
1	C	292	VAL	CA-C-N	6.34	126.36	120.34
1	C	292	VAL	C-N-CA	6.34	126.36	120.34
1	C	163	ALA	CA-C-N	-6.33	111.05	120.68
1	C	163	ALA	C-N-CA	-6.33	111.05	120.68
1	C	223	ASP	O-C-N	-6.33	116.39	123.48
1	B	30	PRO	CA-C-N	6.32	126.27	119.76
1	B	30	PRO	C-N-CA	6.32	126.27	119.76
1	C	120	ARG	CA-C-O	6.32	126.38	119.24
1	A	101	ARG	NE-CZ-NH2	6.31	124.88	119.20
1	C	39	LYS	N-CA-C	-6.31	98.44	108.73
1	B	15	TRP	CA-C-O	-6.30	112.31	120.00
1	A	251	GLN	CA-C-O	-6.30	112.98	120.10
1	A	161	ASP	CA-CB-CG	6.30	118.90	112.60
1	A	240	CYS	CA-C-O	-6.29	113.42	120.66
1	A	325	LYS	CA-C-O	-6.29	113.75	120.42
1	A	356	ASN	CB-CG-ND2	6.29	125.83	116.40
1	C	176	PHE	CA-C-O	-6.29	114.40	121.00
1	A	304	ASN	CA-C-N	6.27	125.96	119.56
1	A	304	ASN	C-N-CA	6.27	125.96	119.56
1	C	45	ILE	CA-C-O	6.27	128.01	120.74
1	B	176	PHE	CA-CB-CG	-6.27	107.53	113.80
1	B	146	PHE	O-C-N	-6.25	114.05	122.68
1	B	50	ASP	O-C-N	-6.25	115.50	122.12
1	B	369	ARG	N-CA-CB	6.24	120.39	110.65
1	B	20	PRO	N-CA-CB	6.24	109.93	103.38
1	B	312	ARG	NE-CZ-NH2	-6.23	113.59	119.20
1	C	124	GLN	OE1-CD-NE2	-6.22	116.38	122.60
1	B	146	PHE	CA-CB-CG	6.22	120.02	113.80
1	A	172	ILE	CA-C-N	6.21	131.66	120.79
1	A	172	ILE	C-N-CA	6.21	131.66	120.79
1	A	327	SER	N-CA-C	6.21	120.06	112.23
1	C	10	LYS	CA-C-O	6.21	128.61	121.28
1	A	30	PRO	N-CA-C	-6.21	103.93	110.58
1	D	294	VAL	O-C-N	6.21	126.30	121.46
1	C	219	ILE	CA-C-O	-6.21	113.02	120.78
1	A	217	ALA	CA-C-O	-6.20	112.43	120.00
1	C	275	MET	O-C-N	6.20	128.46	122.07
1	C	278	ALA	CA-C-O	-6.20	113.98	120.55
1	C	350	LEU	CA-C-O	6.20	126.20	120.50
1	D	120	ARG	N-CA-C	-6.20	106.26	113.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	VAL	O-C-N	6.19	129.61	122.99
1	B	346	ILE	O-C-N	-6.19	115.09	122.77
1	B	365	GLY	N-CA-C	-6.18	107.17	115.21
1	A	87	ASP	CA-CB-CG	6.18	118.78	112.60
1	D	216	ALA	N-CA-CB	6.18	119.16	109.83
1	B	327	SER	CA-C-O	-6.16	112.52	119.79
1	C	284	GLU	N-CA-C	6.16	119.64	111.75
1	D	321	GLY	CA-C-O	6.16	125.86	119.02
1	D	120	ARG	NH1-CZ-NH2	6.16	127.31	119.30
1	C	130	PHE	CA-C-O	6.16	127.35	120.70
1	B	149	TYR	O-C-N	6.15	130.77	123.33
1	A	304	ASN	CB-CG-ND2	-6.14	107.18	116.40
1	D	94	THR	CB-CA-C	-6.14	103.35	110.17
1	B	29	ALA	CA-C-N	6.13	124.07	119.66
1	B	29	ALA	C-N-CA	6.13	124.07	119.66
1	C	90	ILE	O-C-N	6.09	126.56	120.59
1	A	89	VAL	CA-C-N	-6.09	117.55	122.85
1	A	89	VAL	C-N-CA	-6.09	117.55	122.85
1	B	148	GLN	CA-C-O	6.09	126.98	120.10
1	B	260	GLY	CA-C-O	-6.09	112.34	118.86
1	D	352	PHE	N-CA-C	6.08	118.68	111.33
1	C	179	GLY	O-C-N	-6.07	114.81	122.70
1	D	275	MET	CA-C-O	-6.07	114.45	120.70
1	C	355	ILE	CA-C-O	-6.05	114.97	121.27
1	D	205	LEU	N-CA-CB	6.05	119.01	110.12
1	A	16	GLU	O-C-N	6.04	130.14	123.25
1	D	102	VAL	CA-C-N	-6.04	111.58	120.28
1	D	102	VAL	C-N-CA	-6.04	111.58	120.28
1	C	259	ASN	OD1-CG-ND2	6.04	128.64	122.60
1	A	193	SER	N-CA-CB	-6.04	102.11	110.38
1	C	130	PHE	CA-CB-CG	6.04	119.84	113.80
1	B	123	MET	N-CA-C	-6.04	102.74	110.53
1	B	284	GLU	N-CA-C	6.04	118.65	111.71
1	B	349	VAL	N-CA-CB	6.03	120.32	111.52
1	A	50	ASP	CA-C-O	6.01	126.89	120.10
1	B	240	CYS	CA-C-O	-6.00	113.39	120.60
1	B	119	PRO	N-CA-CB	6.00	109.55	103.25
1	B	322	PHE	N-CA-C	5.99	119.15	110.28
1	C	368	ILE	N-CA-C	-5.99	96.89	109.34
1	B	191	GLN	OE1-CD-NE2	-5.99	116.61	122.60
1	B	306	MET	CB-CG-SD	5.98	130.65	112.70
1	D	184	VAL	N-CA-C	5.98	119.45	111.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	337	ALA	CA-C-O	5.98	126.95	119.12
1	B	148	GLN	OE1-CD-NE2	-5.97	116.63	122.60
1	C	306	MET	N-CA-C	-5.96	105.26	112.54
1	C	146	PHE	CA-CB-CG	5.96	119.76	113.80
1	C	256	GLU	CA-C-O	-5.96	114.56	120.82
1	B	347	THR	O-C-N	-5.96	115.27	122.48
1	B	115	ASP	CA-C-O	5.95	127.15	119.95
1	C	24	GLU	CA-CB-CG	5.94	125.98	114.10
1	A	136	PRO	N-CA-CB	5.94	108.59	103.36
1	C	352	PHE	CA-C-N	5.94	130.10	120.60
1	C	352	PHE	C-N-CA	5.94	130.10	120.60
1	B	151	VAL	O-C-N	-5.92	117.02	123.18
1	D	365	GLY	N-CA-C	-5.92	107.23	114.92
1	B	101	ARG	CD-NE-CZ	-5.90	116.14	124.40
1	B	64	ILE	CA-C-O	-5.90	113.95	120.97
1	B	346	ILE	CA-C-O	5.89	127.94	120.75
1	B	16	GLU	CA-C-O	-5.89	114.75	121.40
1	C	264	PHE	CA-CB-CG	-5.88	107.92	113.80
1	A	96	GLN	CA-CB-CG	-5.88	102.34	114.10
1	B	84	ARG	CA-C-O	5.87	125.90	120.50
1	D	124	GLN	O-C-N	-5.86	115.91	122.12
1	A	242	ASN	CA-C-N	5.86	126.27	119.47
1	A	242	ASN	C-N-CA	5.86	126.27	119.47
1	A	300	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	B	133	ARG	NH1-CZ-NH2	-5.85	111.69	119.30
1	A	267	GLU	CB-CG-CD	5.85	122.55	112.60
1	B	145	THR	CA-C-O	-5.85	112.48	119.15
1	B	342	LEU	CA-C-O	5.85	126.37	119.06
1	C	131	THR	CA-CB-CG2	-5.84	100.56	110.50
1	C	16	GLU	N-CA-CB	-5.83	101.93	111.66
1	C	159	LYS	CA-C-O	-5.83	114.11	120.81
1	B	307	LEU	N-CA-C	-5.82	104.94	111.28
1	B	274	THR	CA-C-N	5.81	128.00	120.44
1	B	274	THR	C-N-CA	5.81	128.00	120.44
1	A	259	ASN	CB-CG-OD1	-5.80	109.19	120.80
1	B	58	VAL	O-C-N	-5.80	116.33	122.95
1	A	169	VAL	O-C-N	-5.80	115.03	122.22
1	A	164	SER	CA-C-O	5.80	127.02	120.70
1	D	242	ASN	CA-C-O	5.78	125.06	119.62
1	D	273	ASP	OD1-CG-OD2	-5.78	109.02	122.90
1	D	345	LEU	CA-C-O	5.78	126.03	119.27
1	C	120	ARG	N-CA-C	-5.77	106.79	113.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	THR	CA-C-O	5.76	125.72	119.15
1	D	105	HIS	CA-C-O	5.76	126.10	120.23
1	A	38	ILE	CB-CA-C	-5.75	102.05	110.62
1	C	238	THR	CA-C-O	5.75	126.00	119.27
1	A	33	ALA	CB-CA-C	-5.74	100.94	109.90
1	B	116	LEU	CA-C-N	5.74	127.90	120.44
1	B	116	LEU	C-N-CA	5.74	127.90	120.44
1	C	372	LEU	CA-C-O	-5.74	114.17	120.43
1	D	41	VAL	CA-C-O	5.73	124.10	119.29
1	D	114	ASN	CA-C-O	5.72	128.16	121.87
1	A	259	ASN	OD1-CG-ND2	5.72	128.32	122.60
1	A	370	THR	CA-C-O	-5.71	114.20	120.43
1	A	223	ASP	CA-C-O	-5.71	113.69	120.43
1	B	185	LYS	CA-C-O	-5.71	113.11	119.67
1	D	63	VAL	CA-C-O	5.71	127.16	121.45
1	C	87	ASP	CA-CB-CG	5.70	118.30	112.60
1	C	45	ILE	O-C-N	-5.70	114.39	122.76
1	D	231	LYS	CA-C-O	-5.69	114.51	120.55
1	B	133	ARG	NE-CZ-NH1	-5.69	115.81	121.50
1	A	115	ASP	CA-C-O	5.68	126.66	119.95
1	A	322	PHE	N-CA-C	5.68	118.69	110.28
1	A	344	PRO	O-C-N	-5.68	115.30	122.17
1	B	233	LYS	O-C-N	5.68	128.14	122.12
1	C	234	GLU	CA-C-N	-5.68	113.34	121.52
1	C	234	GLU	C-N-CA	-5.68	113.34	121.52
1	B	149	TYR	CA-C-O	-5.68	113.79	120.60
1	C	46	CYS	O-C-N	-5.67	116.58	123.10
1	A	146	PHE	CA-CB-CG	5.67	119.47	113.80
1	C	162	ALA	CA-C-O	-5.66	112.64	119.49
1	B	98	GLY	CA-C-O	-5.66	112.66	119.00
1	D	250	ILE	CA-C-O	-5.65	114.52	120.57
1	C	306	MET	CB-CG-SD	5.65	129.64	112.70
1	D	181	GLY	O-C-N	-5.64	116.77	122.19
1	D	304	ASN	CA-C-N	5.64	125.32	119.56
1	D	304	ASN	C-N-CA	5.64	125.32	119.56
1	D	265	SER	CA-C-O	5.63	127.70	121.11
1	D	303	MET	O-C-N	-5.63	116.83	123.25
1	B	203	VAL	CA-C-O	-5.62	114.18	120.25
1	B	325	LYS	CA-CB-CG	-5.62	102.86	114.10
1	C	191	GLN	CB-CG-CD	5.62	122.15	112.60
1	D	366	GLU	O-C-N	-5.61	115.75	122.15
1	C	340	PHE	CA-CB-CG	5.61	119.41	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	196	ALA	CA-C-O	5.60	126.17	120.24
1	C	148	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	C	285	ALA	CA-C-N	-5.59	112.01	121.18
1	C	285	ALA	C-N-CA	-5.59	112.01	121.18
1	B	360	ASP	O-C-N	5.59	128.04	122.12
1	D	327	SER	N-CA-C	5.59	120.16	113.23
1	A	301	LEU	N-CA-CB	5.58	119.26	110.56
1	D	168	LYS	N-CA-C	-5.58	105.58	112.72
1	D	303	MET	CA-C-O	5.58	127.36	121.33
1	B	50	ASP	CA-C-O	5.58	126.46	120.55
1	C	369	ARG	NE-CZ-NH2	-5.58	114.18	119.20
1	D	59	THR	O-C-N	-5.57	117.95	121.85
1	B	167	GLU	CB-CG-CD	5.56	122.05	112.60
1	A	278	ALA	CA-C-O	-5.56	114.66	120.55
1	D	13	VAL	O-C-N	-5.56	117.04	122.93
1	D	82	THR	N-CA-C	5.56	120.06	113.28
1	A	280	SER	N-CA-CB	5.55	118.28	110.12
1	B	251	GLN	CA-C-O	-5.55	113.83	120.10
1	B	4	GLY	CA-C-O	-5.55	112.78	119.00
1	D	340	PHE	CA-CB-CG	5.55	119.35	113.80
1	D	374	PHE	CA-CB-CG	-5.54	108.25	113.80
1	D	105	HIS	CA-C-N	5.54	125.38	119.28
1	D	105	HIS	C-N-CA	5.54	125.38	119.28
1	C	115	ASP	CA-C-O	5.54	127.25	120.55
1	A	148	GLN	O-C-N	-5.54	115.74	122.22
1	C	69	ALA	N-CA-CB	-5.54	102.49	111.24
1	D	284	GLU	N-CA-C	5.53	118.83	111.75
1	B	64	ILE	N-CA-CB	5.53	118.23	111.60
1	C	31	PRO	CB-CA-C	-5.52	104.34	111.46
1	A	294	VAL	CA-C-N	5.52	126.06	120.38
1	A	294	VAL	C-N-CA	5.52	126.06	120.38
1	B	340	PHE	CA-CB-CG	5.51	119.31	113.80
1	A	301	LEU	N-CA-C	-5.51	101.88	110.42
1	D	24	GLU	N-CA-C	5.51	117.35	109.14
1	A	282	CYS	CB-CA-C	5.50	118.83	109.53
1	D	38	ILE	N-CA-C	5.50	116.41	108.48
1	D	56	THR	N-CA-C	-5.49	105.38	111.36
1	A	203	VAL	CA-C-O	-5.48	115.04	120.85
1	C	242	ASN	CA-C-O	5.47	124.80	119.55
1	B	38	ILE	CB-CA-C	-5.46	102.54	110.63
1	B	367	SER	N-CA-C	5.46	117.82	109.95
1	C	162	ALA	CA-C-N	-5.46	114.08	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	162	ALA	C-N-CA	-5.46	114.08	122.60
1	C	292	VAL	CA-C-O	5.46	125.31	120.34
1	A	133	ARG	NE-CZ-NH2	5.46	124.11	119.20
1	C	105	HIS	CA-C-N	5.46	125.28	119.28
1	C	105	HIS	C-N-CA	5.46	125.28	119.28
1	C	264	PHE	CA-C-O	-5.46	114.26	120.32
1	B	203	VAL	O-C-N	5.46	129.30	121.82
1	C	25	GLU	CA-C-O	5.46	126.91	120.69
1	C	242	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	D	64	ILE	N-CA-C	-5.46	99.10	106.85
1	C	222	VAL	O-C-N	-5.45	117.37	123.26
1	B	296	PRO	N-CA-CB	5.45	108.18	103.27
1	C	273	ASP	CB-CG-OD1	5.45	130.94	118.40
1	A	169	VAL	N-CA-C	5.45	119.68	112.76
1	A	203	VAL	O-C-N	5.44	127.44	121.83
1	B	238	THR	N-CA-C	-5.44	106.48	113.23
1	B	160	ILE	O-C-N	-5.43	117.27	122.97
1	B	193	SER	N-CA-CB	-5.43	102.94	110.38
1	D	20	PRO	CB-CA-C	-5.43	104.11	111.12
1	C	64	ILE	N-CA-C	-5.43	99.14	106.85
1	D	326	ASP	CA-C-O	-5.43	114.21	120.24
1	B	96	GLN	CA-CB-CG	-5.42	103.25	114.10
1	D	265	SER	N-CA-C	-5.42	100.93	109.50
1	D	368	ILE	N-CA-C	-5.42	98.06	109.34
1	C	84	ARG	NE-CZ-NH1	5.42	126.92	121.50
1	C	27	GLU	N-CA-CB	5.42	119.06	110.55
1	C	282	CYS	CB-CA-C	5.42	119.42	109.46
1	C	193	SER	CA-C-O	-5.41	115.82	121.99
1	C	295	PRO	CA-C-N	5.41	125.67	119.83
1	C	295	PRO	C-N-CA	5.41	125.67	119.83
1	C	225	ASN	N-CA-CB	5.40	119.60	110.69
1	D	53	VAL	O-C-N	-5.40	116.28	121.90
1	A	26	VAL	CA-C-N	5.40	130.61	123.05
1	A	26	VAL	C-N-CA	5.40	130.61	123.05
1	A	139	HIS	N-CA-C	-5.40	102.76	110.59
1	B	259	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	A	349	VAL	O-C-N	-5.39	117.38	123.20
1	B	301	LEU	N-CA-C	-5.39	102.07	110.42
1	C	267	GLU	O-C-N	-5.38	117.08	123.22
1	A	249	PRO	N-CA-CB	5.37	107.98	103.25
1	D	83	VAL	CA-C-N	-5.37	113.50	123.11
1	D	83	VAL	C-N-CA	-5.37	113.50	123.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	VAL	CA-C-N	-5.37	113.77	121.98
1	B	80	VAL	C-N-CA	-5.37	113.77	121.98
1	C	351	PRO	N-CA-C	-5.37	102.72	111.68
1	C	235	VAL	CA-C-N	-5.36	110.90	121.41
1	C	235	VAL	C-N-CA	-5.36	110.90	121.41
1	D	107	GLU	CA-C-O	-5.36	113.16	119.05
1	D	301	LEU	N-CA-C	-5.35	102.12	110.42
1	D	73	VAL	O-C-N	5.35	128.50	122.67
1	A	117	SER	CB-CA-C	-5.34	102.49	110.88
1	D	75	SER	O-C-N	-5.34	117.65	123.26
1	D	31	PRO	CB-CA-C	-5.34	104.91	111.64
1	D	172	ILE	O-C-N	-5.34	115.05	122.31
1	D	242	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	A	356	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	C	197	VAL	CA-C-N	5.33	129.51	122.42
1	C	197	VAL	C-N-CA	5.33	129.51	122.42
1	A	326	ASP	CB-CA-C	-5.33	100.95	110.70
1	A	191	GLN	CG-CD-OE1	5.32	131.44	120.80
1	C	38	ILE	CB-CA-C	-5.32	102.63	110.82
1	C	327	SER	N-CA-C	5.32	118.93	112.23
1	A	188	LYS	CA-C-N	5.32	127.83	120.49
1	A	188	LYS	C-N-CA	5.32	127.83	120.49
1	D	316	GLY	O-C-N	-5.32	119.05	123.73
1	B	15	TRP	N-CA-CB	5.31	118.17	110.26
1	D	9	CYS	O-C-N	5.31	128.67	122.99
1	B	76	ILE	O-C-N	-5.30	117.33	123.00
1	A	265	SER	O-C-N	-5.30	116.72	123.24
1	A	120	ARG	N-CA-C	-5.30	107.36	113.88
1	D	139	HIS	N-CA-C	-5.29	102.92	110.59
1	A	273	ASP	CB-CG-OD1	5.29	130.56	118.40
1	C	210	GLY	CA-C-O	-5.27	114.50	120.30
1	B	33	ALA	CB-CA-C	-5.27	100.97	109.72
1	C	82	THR	N-CA-C	5.27	119.71	113.28
1	C	13	VAL	O-C-N	-5.26	116.95	122.95
1	C	220	ILE	CB-CA-C	-5.26	104.59	110.96
1	B	295	PRO	CA-C-N	5.26	125.51	119.83
1	B	295	PRO	C-N-CA	5.26	125.51	119.83
1	B	69	ALA	N-CA-C	5.26	115.48	108.38
1	C	69	ALA	CA-C-O	5.26	126.93	121.31
1	A	170	CYS	N-CA-C	-5.25	105.67	111.71
1	A	91	PRO	N-CA-CB	5.25	108.22	103.34
1	A	20	PRO	N-CA-CB	5.24	108.89	103.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	PRO	CA-C-N	5.24	125.49	119.83
1	A	295	PRO	C-N-CA	5.24	125.49	119.83
1	D	233	LYS	O-C-N	5.24	127.67	122.12
1	D	246	TYR	CA-C-N	-5.23	112.45	121.66
1	D	246	TYR	C-N-CA	-5.23	112.45	121.66
1	D	267	GLU	CA-C-O	5.23	125.96	120.36
1	D	349	VAL	N-CA-CB	5.23	119.15	111.52
1	C	116	LEU	CA-C-N	5.22	127.23	120.44
1	C	116	LEU	C-N-CA	5.22	127.23	120.44
1	D	174	CYS	O-C-N	-5.22	115.65	122.59
1	B	91	PRO	N-CA-CB	5.21	108.19	103.34
1	D	34	HIS	CG-CD2-NE2	-5.21	101.99	107.20
1	A	110	PHE	CA-CB-CG	5.21	119.01	113.80
1	A	202	GLY	N-CA-C	5.21	118.98	112.73
1	C	169	VAL	N-CA-C	5.21	120.17	109.34
1	B	297	ASP	N-CA-C	5.21	118.02	110.42
1	B	368	ILE	N-CA-C	-5.21	98.51	109.34
1	B	67	HIS	CB-CA-C	5.20	117.14	109.29
1	C	280	SER	CB-CA-C	-5.20	102.16	110.79
1	A	360	ASP	CA-CB-CG	-5.20	107.40	112.60
1	D	68	GLU	O-C-N	-5.20	116.48	122.87
1	A	158	ALA	O-C-N	-5.19	117.12	123.30
1	D	249	PRO	N-CA-CB	5.19	107.82	103.25
1	C	294	VAL	CA-C-N	5.19	125.72	120.38
1	C	294	VAL	C-N-CA	5.19	125.72	120.38
1	B	136	PRO	N-CA-CB	5.18	108.16	103.34
1	B	220	ILE	CB-CG1-CD1	5.18	124.68	113.80
1	B	184	VAL	N-CA-C	5.17	118.37	111.44
1	C	208	ILE	CA-C-N	-5.17	113.36	120.28
1	C	208	ILE	C-N-CA	-5.17	113.36	120.28
1	B	201	GLY	N-CA-C	-5.16	103.46	112.55
1	D	133	ARG	O-C-N	-5.15	113.94	122.23
1	C	284	GLU	CA-C-O	-5.15	114.43	120.20
1	C	260	GLY	O-C-N	5.15	128.35	122.33
1	A	105	HIS	CA-C-N	5.14	124.94	119.28
1	A	105	HIS	C-N-CA	5.14	124.94	119.28
1	C	2	THR	CA-C-O	5.14	125.02	119.15
1	C	237	ALA	CA-C-O	-5.14	115.53	121.19
1	C	84	ARG	CA-C-O	5.13	125.22	120.50
1	D	332	VAL	N-CA-C	-5.13	105.70	110.53
1	D	8	LYS	CA-C-O	-5.13	114.83	120.43
1	B	328	VAL	CA-C-O	5.13	122.13	118.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	183	ALA	O-C-N	5.13	127.63	122.09
1	B	120	ARG	N-CA-C	-5.12	107.58	113.88
1	C	225	ASN	CB-CA-C	-5.12	102.62	111.23
1	A	351	PRO	N-CA-C	-5.12	102.56	111.32
1	C	72	ILE	CA-C-N	-5.12	113.82	120.63
1	C	72	ILE	C-N-CA	-5.12	113.82	120.63
1	A	167	GLU	CB-CG-CD	5.12	121.30	112.60
1	A	342	LEU	CA-C-O	5.11	125.45	119.06
1	C	216	ALA	CB-CA-C	-5.11	100.47	109.62
1	D	260	GLY	CA-C-O	-5.11	113.30	118.97
1	A	237	ALA	CA-C-O	-5.11	115.10	120.92
1	C	29	ALA	CA-C-N	5.11	123.34	119.66
1	C	29	ALA	C-N-CA	5.11	123.34	119.66
1	D	238	THR	O-C-N	-5.10	115.16	122.41
1	B	31	PRO	N-CA-CB	5.10	107.85	103.31
1	C	85	PRO	N-CA-CB	5.09	107.78	103.19
1	D	223	ASP	CA-C-O	-5.09	115.29	120.89
1	A	135	LYS	CA-C-O	5.09	125.90	120.05
1	A	159	LYS	CA-C-O	-5.09	114.96	120.81
1	B	49	ASP	N-CA-C	-5.09	105.64	111.14
1	A	146	PHE	O-C-N	-5.09	115.66	122.68
1	B	68	GLU	CA-C-O	-5.09	115.69	121.39
1	D	147	SER	O-C-N	-5.09	117.78	123.48
1	A	340	PHE	CA-CB-CG	5.08	118.88	113.80
1	B	220	ILE	CA-C-N	-5.07	116.65	121.57
1	B	220	ILE	C-N-CA	-5.07	116.65	121.57
1	B	191	GLN	CG-CD-OE1	5.07	130.93	120.80
1	B	353	GLU	CB-CG-CD	5.07	121.21	112.60
1	A	264	PHE	CA-CB-CG	-5.06	108.74	113.80
1	C	244	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	B	169	VAL	N-CA-C	5.06	119.87	109.34
1	A	11	ALA	CA-C-O	-5.06	115.33	120.99
1	B	338	LYS	N-CA-CB	-5.05	104.79	112.47
1	D	69	ALA	N-CA-C	5.05	115.19	108.38
1	A	196	ALA	CA-C-O	5.04	125.59	120.24
1	D	256	GLU	CA-CB-CG	-5.04	104.01	114.10
1	C	201	GLY	CA-C-N	5.04	125.68	120.03
1	C	201	GLY	C-N-CA	5.04	125.68	120.03
1	D	105	HIS	ND1-CG-CD2	5.04	111.14	106.10
1	D	238	THR	N-CA-C	-5.04	107.13	113.28
1	C	267	GLU	CB-CA-C	5.04	118.35	110.19
1	D	129	ARG	N-CA-C	-5.03	106.73	112.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	ILE	O-C-N	-5.03	115.60	122.59
1	A	356	ASN	CA-C-N	5.03	126.98	120.44
1	A	356	ASN	C-N-CA	5.03	126.98	120.44
1	B	230	ALA	O-C-N	5.03	127.46	122.08
1	C	351	PRO	CB-CA-C	5.02	117.81	110.63
1	A	85	PRO	O-C-N	-5.02	116.73	122.85
1	B	180	TYR	CA-C-O	-5.02	115.55	120.82
1	A	267	GLU	N-CA-C	-5.01	100.56	108.73
1	D	13	VAL	CA-C-O	5.01	126.65	120.84
1	B	19	LYS	O-C-N	5.00	126.10	121.80
1	D	236	GLY	O-C-N	-5.00	116.20	122.70
1	C	106	PRO	N-CA-CB	5.00	108.79	103.39

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	50	0
1	B	2785	0	2848	50	0
1	C	2785	0	2848	72	0
1	D	2785	0	2848	61	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	25	1	0
3	B	44	0	25	2	0
3	C	44	0	23	1	0
3	D	44	0	24	2	0
4	A	9	0	13	1	0
4	B	9	0	13	2	0
4	C	9	0	13	3	0
4	D	9	0	13	0	0
5	A	250	0	0	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	249	0	0	13	0
5	C	257	0	0	23	0
5	D	256	0	0	20	0
All	All	12372	0	11541	229	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (229) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:HD12	1:A:223:ASP:HB2	1.56	0.84
1:B:200:LEU:HD12	1:B:223:ASP:HB2	1.61	0.81
1:D:200:LEU:HD12	1:D:223:ASP:HB2	1.68	0.76
1:D:154:GLU:HB3	5:D:556:HOH:O	1.88	0.74
1:C:218:ARG:NH2	5:C:554:HOH:O	2.18	0.72
1:D:32:LYS:HE3	5:D:552:HOH:O	1.91	0.69
1:C:200:LEU:HD12	1:C:223:ASP:HB2	1.74	0.68
1:C:120:ARG:HB2	5:C:562:HOH:O	1.94	0.68
1:A:340:PHE:HB2	5:A:397:HOH:O	1.94	0.67
1:B:99:LYS:O	1:B:104:LYS:HE3	1.94	0.67
1:B:178:THR:HG21	3:B:377:NAD:C4N	2.27	0.65
1:B:340:PHE:HB2	5:B:398:HOH:O	1.94	0.65
1:C:350:LEU:HB3	1:C:351:PRO:HD2	1.79	0.65
1:D:39:LYS:HB2	1:D:149:TYR:CE2	2.31	0.65
1:C:83:VAL:HG12	1:C:159:LYS:HB2	1.79	0.65
1:A:132:CYS:HB3	1:A:137:ILE:HD11	1.80	0.64
1:A:209:MET:SD	5:A:397:HOH:O	2.55	0.64
1:B:191:GLN:HE22	1:D:302:SER:HB3	1.62	0.64
1:B:351:PRO:HG2	1:B:354:LYS:HD2	1.81	0.62
1:C:364:SER:OG	1:C:366:GLU:HG3	2.00	0.62
1:D:162:ALA:HB2	5:D:488:HOH:O	2.01	0.61
1:C:39:LYS:NZ	5:C:559:HOH:O	2.33	0.61
1:A:84:ARG:HD3	5:A:467:HOH:O	2.01	0.61
1:B:39:LYS:HB2	1:B:149:TYR:CE2	2.36	0.60
1:A:178:THR:HG21	3:A:377:NAD:C4N	2.32	0.60
1:C:84:ARG:HD3	5:C:479:HOH:O	2.01	0.59
1:A:32:LYS:HE3	5:A:540:HOH:O	2.01	0.59
1:A:231:LYS:HB3	5:A:538:HOH:O	2.02	0.59
1:B:120:ARG:HB2	5:B:551:HOH:O	2.03	0.58
1:D:340:PHE:HB2	5:D:408:HOH:O	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ASP:O	1:D:164:SER:OG	2.22	0.58
1:C:173:GLY:HA3	5:C:429:HOH:O	2.02	0.58
1:D:116:LEU:HG	1:D:141:LEU:HD22	1.86	0.57
1:C:338:LYS:HA	5:C:502:HOH:O	2.04	0.57
1:B:32:LYS:HE3	5:B:541:HOH:O	2.05	0.57
1:D:24:GLU:HB2	5:D:474:HOH:O	2.05	0.57
1:C:241:VAL:HA	5:C:402:HOH:O	2.03	0.57
1:B:350:LEU:HB3	1:B:351:PRO:HD2	1.86	0.57
1:C:239:GLU:HA	5:C:403:HOH:O	2.05	0.56
1:B:338:LYS:NZ	5:B:379:HOH:O	2.29	0.56
1:D:351:PRO:HG2	1:D:354:LYS:HD2	1.87	0.56
1:C:1:SER:O	1:C:5:LYS:NZ	2.29	0.56
1:C:39:LYS:HB2	1:C:149:TYR:CE2	2.40	0.56
1:A:99:LYS:O	1:A:104:LYS:HE3	2.06	0.55
1:A:351:PRO:HG2	1:A:354:LYS:HD2	1.87	0.55
1:C:340:PHE:HB2	5:C:408:HOH:O	2.06	0.55
1:A:127:THR:HB	5:A:507:HOH:O	2.06	0.55
1:D:40:MET:HE1	1:D:150:THR:HG22	1.88	0.55
1:B:279:LEU:HD13	1:B:314:TRP:CG	2.42	0.55
1:C:116:LEU:HG	1:C:141:LEU:HD22	1.88	0.55
1:D:336:MET:HB2	5:D:557:HOH:O	2.06	0.55
1:C:205:LEU:HD21	5:C:527:HOH:O	2.07	0.55
1:C:339:LYS:HD3	5:C:609:HOH:O	2.05	0.55
1:B:318:ILE:HD12	4:B:378:CXF:H31	1.88	0.54
1:A:17:GLU:OE2	1:B:338:LYS:HE3	2.08	0.54
1:A:116:LEU:HG	1:A:141:LEU:HD22	1.90	0.54
1:D:89:VAL:HG12	1:D:159:LYS:HA	1.89	0.54
1:D:178:THR:HG21	3:D:377:NAD:C4N	2.37	0.54
1:B:116:LEU:HD23	4:B:378:CXF:H41	1.90	0.53
1:B:116:LEU:HG	1:B:141:LEU:HD22	1.91	0.53
1:B:351:PRO:CG	1:B:354:LYS:HD2	2.39	0.53
1:A:157:VAL:O	1:A:325:LYS:HE3	2.09	0.52
1:C:32:LYS:HB2	1:C:35:GLU:CD	2.35	0.52
1:D:32:LYS:HB3	5:D:592:HOH:O	2.08	0.52
1:D:33:ALA:O	1:D:34:HIS:HB2	2.09	0.52
1:C:11:ALA:HA	1:C:147:SER:HA	1.92	0.51
1:B:61:LEU:HB3	1:B:62:PRO:HA	1.92	0.51
1:A:253:VAL:O	1:A:257:MET:HG3	2.10	0.51
1:C:33:ALA:O	1:C:34:HIS:HB2	2.11	0.50
1:A:295:PRO:HG2	5:A:427:HOH:O	2.12	0.50
1:C:328:VAL:N	1:C:329:PRO:CD	2.73	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ALA:HA	1:A:147:SER:HA	1.93	0.50
1:D:10:LYS:HE3	5:D:532:HOH:O	2.11	0.50
1:D:61:LEU:HB3	1:D:62:PRO:HA	1.94	0.49
1:B:212:LYS:NZ	5:B:503:HOH:O	2.37	0.49
1:C:40:MET:HE1	1:C:150:THR:CG2	2.43	0.49
1:C:152:VAL:HG21	1:C:157:VAL:HB	1.94	0.49
1:A:32:LYS:O	1:A:77:GLY:HA3	2.12	0.49
1:D:30:PRO:O	5:D:504:HOH:O	2.20	0.49
1:D:40:MET:HE1	1:D:150:THR:CG2	2.43	0.49
1:B:33:ALA:O	1:B:34:HIS:HB2	2.11	0.49
1:C:88:LYS:NZ	1:C:164:SER:O	2.44	0.49
1:C:231:LYS:HB3	5:C:411:HOH:O	2.12	0.49
1:D:284:GLU:OE1	5:D:611:HOH:O	2.19	0.49
1:B:239:GLU:OE1	5:B:513:HOH:O	2.18	0.48
1:D:350:LEU:HB3	1:D:351:PRO:HD2	1.95	0.48
1:A:271:ARG:HB2	1:A:274:THR:OG1	2.13	0.48
1:A:364:SER:OG	1:A:366:GLU:HG3	2.12	0.48
1:B:271:ARG:HB2	1:B:274:THR:OG1	2.14	0.48
1:C:31:PRO:HD2	5:C:470:HOH:O	2.11	0.48
1:C:124:GLN:N	1:C:153:ASP:OD2	2.40	0.48
1:D:157:VAL:O	1:D:325:LYS:HE3	2.12	0.48
1:A:39:LYS:HB2	1:A:149:TYR:CE2	2.48	0.48
1:B:292:VAL:O	3:B:377:NAD:H2N	2.14	0.48
1:B:344:PRO:HA	5:B:400:HOH:O	2.14	0.48
1:A:61:LEU:HB3	1:A:62:PRO:HA	1.95	0.48
1:C:208:ILE:O	1:C:209:MET:C	2.54	0.47
1:C:351:PRO:HG2	1:C:354:LYS:HD2	1.96	0.47
1:C:32:LYS:HE3	5:C:552:HOH:O	2.13	0.47
1:A:335:PHE:O	5:A:490:HOH:O	2.20	0.47
1:C:271:ARG:HB2	1:C:274:THR:OG1	2.15	0.47
1:D:343:ASP:N	1:D:344:PRO:CD	2.78	0.47
1:B:315:LYS:NZ	5:B:610:HOH:O	2.47	0.47
1:C:40:MET:HE1	1:C:150:THR:HG22	1.96	0.47
1:D:323:LYS:O	1:D:327:SER:OG	2.33	0.47
1:D:337:ALA:O	1:D:338:LYS:CB	2.60	0.47
1:D:27:GLU:HG3	5:D:564:HOH:O	2.15	0.47
1:B:32:LYS:O	1:B:77:GLY:HA3	2.15	0.46
1:D:351:PRO:CG	1:D:354:LYS:HD2	2.44	0.46
1:B:123:MET:HE3	1:B:123:MET:HB3	1.81	0.46
1:D:32:LYS:O	1:D:77:GLY:HA3	2.16	0.46
1:D:306:MET:HB3	5:D:531:HOH:O	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LEU:HD13	1:A:314:TRP:CG	2.50	0.46
1:B:40:MET:HE1	1:B:150:THR:CG2	2.46	0.46
1:B:185:LYS:HE2	5:B:415:HOH:O	2.15	0.46
1:D:29:ALA:HB1	1:D:30:PRO:HD2	1.97	0.46
1:C:294:VAL:HG21	4:C:378:CXF:H52	1.97	0.46
1:A:305:PRO:HG3	1:D:301:LEU:HD23	1.96	0.46
1:D:253:VAL:O	1:D:257:MET:HG3	2.16	0.46
1:C:89:VAL:HG12	1:C:159:LYS:HA	1.98	0.46
1:D:11:ALA:HA	1:D:147:SER:HA	1.96	0.46
1:A:350:LEU:HB3	1:A:351:PRO:HD2	1.98	0.46
1:B:11:ALA:HA	1:B:147:SER:HA	1.98	0.45
1:A:120:ARG:HB2	5:A:550:HOH:O	2.16	0.45
1:C:220:ILE:HG21	1:C:254:LEU:HD21	1.99	0.45
1:A:69:ALA:HB3	1:A:145:THR:HG21	1.98	0.45
1:C:294:VAL:CG2	4:C:378:CXF:H32	2.46	0.45
1:D:142:GLY:HA3	5:D:448:HOH:O	2.17	0.45
1:D:120:ARG:HB2	5:D:562:HOH:O	2.17	0.45
1:D:279:LEU:HD13	1:D:314:TRP:CG	2.51	0.45
1:C:118:MET:HE3	1:C:118:MET:HB3	1.84	0.45
1:C:32:LYS:CE	5:C:552:HOH:O	2.65	0.44
1:D:167:GLU:HB2	5:D:483:HOH:O	2.16	0.44
1:C:61:LEU:HB3	1:C:62:PRO:HA	2.00	0.44
1:D:118:MET:HE3	1:D:118:MET:HB3	1.80	0.44
1:B:164:SER:HA	1:B:165:PRO:HD3	1.81	0.44
1:C:67:HIS:CD2	4:C:378:CXF:H7	2.52	0.44
1:B:2:THR:O	1:B:3:ALA:C	2.59	0.44
1:D:271:ARG:HB2	1:D:274:THR:OG1	2.18	0.44
1:D:154:GLU:N	5:D:445:HOH:O	2.50	0.44
1:B:127:THR:HB	5:B:508:HOH:O	2.17	0.44
1:C:32:LYS:O	1:C:77:GLY:HA3	2.18	0.44
1:C:335:PHE:HB2	1:C:340:PHE:CZ	2.52	0.44
1:C:178:THR:HA	1:C:320:GLY:N	2.33	0.44
1:C:369:ARG:HH11	1:C:369:ARG:HD3	1.63	0.44
1:D:292:VAL:O	3:D:377:NAD:H2N	2.16	0.44
1:A:118:MET:HE3	1:A:118:MET:HB3	1.80	0.44
1:C:2:THR:HG22	5:C:561:HOH:O	2.17	0.43
1:C:29:ALA:HB1	1:C:30:PRO:HD2	2.00	0.43
1:C:279:LEU:HD13	1:C:314:TRP:CG	2.53	0.43
1:B:328:VAL:HB	1:B:329:PRO:HD3	1.99	0.43
1:A:351:PRO:CG	1:A:354:LYS:HD2	2.48	0.43
1:B:107:GLU:HG3	5:C:388:HOH:O	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:ASP:N	1:B:344:PRO:CD	2.81	0.43
1:A:361:LEU:HD23	5:A:563:HOH:O	2.18	0.43
1:B:26:VAL:HG12	1:B:132:CYS:HB2	2.00	0.43
1:B:343:ASP:N	1:B:344:PRO:HD2	2.33	0.43
1:D:348:HIS:CD2	1:D:361:LEU:HD13	2.53	0.43
1:C:343:ASP:N	1:C:344:PRO:CD	2.81	0.43
1:A:69:ALA:HA	1:A:170:CYS:HB2	2.01	0.43
1:B:296:PRO:HG2	5:B:617:HOH:O	2.19	0.43
1:C:351:PRO:CG	1:C:354:LYS:HD2	2.49	0.43
1:B:118:MET:HE3	1:B:118:MET:HB3	1.78	0.43
1:C:97:CYS:HB3	1:C:113:LYS:HG3	2.00	0.43
1:D:328:VAL:HB	1:D:329:PRO:HD3	2.01	0.43
1:D:328:VAL:N	1:D:329:PRO:CD	2.81	0.43
1:C:350:LEU:HB3	1:C:351:PRO:CD	2.47	0.43
1:B:335:PHE:HB2	1:B:340:PHE:CZ	2.54	0.42
1:D:174:CYS:HB3	1:D:175:GLY:H	1.62	0.42
1:D:179:GLY:HA3	1:D:206:SER:HB2	2.00	0.42
1:A:196:ALA:HB2	1:A:262:VAL:HG11	2.01	0.42
1:B:29:ALA:HB1	1:B:30:PRO:HD2	2.00	0.42
1:A:226:LYS:HG2	5:A:473:HOH:O	2.18	0.42
1:A:343:ASP:N	1:A:344:PRO:CD	2.82	0.42
1:C:297:ASP:O	1:C:298:SER:HB2	2.19	0.42
1:D:99:LYS:O	1:D:104:LYS:HE3	2.19	0.42
1:C:253:VAL:O	1:C:257:MET:HG3	2.19	0.42
1:D:41:VAL:HG21	1:D:166:LEU:HD12	2.00	0.42
1:C:2:THR:O	1:C:3:ALA:C	2.62	0.42
1:A:185:LYS:HE2	5:A:414:HOH:O	2.19	0.42
1:A:245:ASP:OD2	5:A:390:HOH:O	2.22	0.42
1:A:230:ALA:O	1:A:234:GLU:HG3	2.20	0.42
1:A:302:SER:HA	1:D:301:LEU:O	2.20	0.42
1:D:212:LYS:NZ	5:D:513:HOH:O	2.53	0.42
1:C:124:GLN:HG2	1:C:153:ASP:CG	2.45	0.42
1:C:231:LYS:NZ	1:C:344:PRO:O	2.39	0.42
1:A:318:ILE:HD12	4:A:378:CXF:H31	2.02	0.42
1:A:215:GLY:O	1:A:216:ALA:C	2.63	0.41
1:D:234:GLU:OE1	5:D:617:HOH:O	2.22	0.41
1:C:20:PRO:HD2	5:C:581:HOH:O	2.20	0.41
1:B:120:ARG:NH1	5:B:605:HOH:O	2.46	0.41
1:C:68:GLU:OE2	1:C:174:CYS:HB3	2.21	0.41
1:A:53:VAL:HG11	5:A:449:HOH:O	2.20	0.41
1:B:84:ARG:HG3	5:B:547:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:ALA:O	1:B:336:MET:HB2	2.21	0.41
1:D:120:ARG:NH1	5:D:619:HOH:O	2.41	0.41
1:C:250:ILE:HG22	5:C:399:HOH:O	2.20	0.41
1:C:343:ASP:N	1:C:344:PRO:HD2	2.36	0.41
1:D:186:VAL:HG12	1:D:315:LYS:HE2	2.02	0.41
1:A:2:THR:O	1:A:3:ALA:C	2.61	0.41
1:A:84:ARG:O	1:A:85:PRO:C	2.63	0.41
1:C:82:THR:HB	5:C:573:HOH:O	2.19	0.41
1:A:257:MET:HB3	1:A:257:MET:HE2	1.81	0.41
1:B:295:PRO:HG2	5:C:383:HOH:O	2.21	0.41
1:C:292:VAL:O	3:C:377:NAD:H2N	2.20	0.41
1:D:69:ALA:HA	1:D:170:CYS:HB2	2.02	0.41
1:D:215:GLY:O	1:D:216:ALA:C	2.62	0.41
1:A:29:ALA:HB1	1:A:30:PRO:HD2	2.02	0.41
1:B:328:VAL:N	1:B:329:PRO:CD	2.83	0.41
1:B:355:ILE:HG13	1:B:372:LEU:HD11	2.02	0.41
1:C:123:MET:HE3	1:C:123:MET:HB3	1.89	0.41
1:C:267:GLU:HG3	1:C:275:MET:HA	2.02	0.41
1:C:348:HIS:HA	5:C:530:HOH:O	2.20	0.41
1:D:185:LYS:HE2	5:D:425:HOH:O	2.20	0.41
1:C:84:ARG:N	1:C:87:ASP:OD2	2.47	0.41
1:A:328:VAL:HB	1:A:329:PRO:HD3	2.03	0.40
1:C:230:ALA:O	1:C:234:GLU:HG3	2.21	0.40
1:A:40:MET:HE1	1:A:150:THR:CG2	2.51	0.40
1:A:335:PHE:HB2	1:A:340:PHE:CZ	2.56	0.40
1:B:135:LYS:HA	1:B:136:PRO:HD3	1.99	0.40
1:C:69:ALA:HA	1:C:170:CYS:HB2	2.02	0.40
1:D:297:ASP:O	1:D:298:SER:HB2	2.21	0.40
1:A:83:VAL:HG12	1:A:159:LYS:HB2	2.04	0.40
1:C:99:LYS:O	1:C:104:LYS:HE3	2.21	0.40
1:D:36:VAL:HG13	1:D:73:VAL:HG13	2.04	0.40
1:D:301:LEU:HD12	1:D:301:LEU:C	2.47	0.40
1:B:40:MET:HE1	1:B:150:THR:HG22	2.03	0.40
1:C:168:LYS:HE3	5:C:608:HOH:O	2.22	0.40
1:C:328:VAL:HB	1:C:329:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	372/374 (100%)	353 (95%)	18 (5%)	1 (0%)	36	55
1	B	372/374 (100%)	353 (95%)	18 (5%)	1 (0%)	36	55
1	C	372/374 (100%)	355 (95%)	16 (4%)	1 (0%)	36	55
1	D	372/374 (100%)	357 (96%)	13 (4%)	2 (0%)	24	43
All	All	1488/1496 (100%)	1418 (95%)	65 (4%)	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	D	175	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	308/308 (100%)	297 (96%)	11 (4%)	31	58
1	B	308/308 (100%)	296 (96%)	12 (4%)	28	55
1	C	308/308 (100%)	295 (96%)	13 (4%)	26	52
1	D	308/308 (100%)	295 (96%)	13 (4%)	26	52
All	All	1232/1232 (100%)	1183 (96%)	49 (4%)	28	54

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	84	ARG
1	A	118	MET
1	A	135	LYS
1	A	164	SER
1	A	206	SER
1	A	268	VAL
1	A	281	CYS
1	A	327	SER
1	A	357	GLU
1	A	373	THR
1	B	5	LYS
1	B	84	ARG
1	B	118	MET
1	B	135	LYS
1	B	164	SER
1	B	251	GLN
1	B	274	THR
1	B	280	SER
1	B	281	CYS
1	B	310	SER
1	B	357	GLU
1	B	373	THR
1	C	39	LYS
1	C	84	ARG
1	C	118	MET
1	C	135	LYS
1	C	164	SER
1	C	206	SER
1	C	251	GLN
1	C	268	VAL
1	C	274	THR
1	C	281	CYS
1	C	327	SER
1	C	338	LYS
1	C	373	THR
1	D	5	LYS
1	D	39	LYS
1	D	84	ARG
1	D	118	MET
1	D	135	LYS
1	D	164	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	251	GLN
1	D	268	VAL
1	D	274	THR
1	D	281	CYS
1	D	327	SER
1	D	357	GLU
1	D	373	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	138	HIS
1	B	124	GLN
1	B	138	HIS
1	B	191	GLN
1	D	251	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	CXF	B	378	2	9,9,9	1.64	2 (22%)	9,10,10	2.11	4 (44%)
4	CXF	A	378	2	9,9,9	1.40	1 (11%)	9,10,10	1.92	4 (44%)
3	NAD	B	377	-	46,48,48	1.97	16 (34%)	64,73,73	2.37	18 (28%)
3	NAD	A	377	-	46,48,48	2.00	14 (30%)	64,73,73	2.14	15 (23%)
3	NAD	C	377	-	46,48,48	1.97	13 (28%)	64,73,73	2.64	24 (37%)
4	CXF	C	378	2	9,9,9	1.33	1 (11%)	9,10,10	1.38	2 (22%)
3	NAD	D	377	-	46,48,48	2.28	17 (36%)	64,73,73	2.65	25 (39%)
4	CXF	D	378	2	9,9,9	1.67	3 (33%)	9,10,10	2.73	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	CXF	B	378	2	-	1/3/11/11	0/1/1/1
4	CXF	A	378	2	-	1/3/11/11	0/1/1/1
3	NAD	B	377	-	-	10/30/62/62	0/5/5/5
3	NAD	A	377	-	-	6/30/62/62	0/5/5/5
3	NAD	C	377	-	-	8/30/62/62	0/5/5/5
4	CXF	C	378	2	-	0/3/11/11	0/1/1/1
3	NAD	D	377	-	-	5/30/62/62	0/5/5/5
4	CXF	D	378	2	-	0/3/11/11	0/1/1/1

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	377	NAD	C3N-C7N	5.22	1.58	1.50
3	D	377	NAD	O4D-C4D	5.18	1.56	1.45
3	C	377	NAD	C3N-C7N	5.12	1.58	1.50
3	D	377	NAD	O4D-C1D	4.90	1.47	1.40
3	C	377	NAD	O4D-C1D	4.41	1.46	1.40
3	D	377	NAD	O2B-C2B	-4.30	1.32	1.43
3	A	377	NAD	C3N-C7N	4.08	1.56	1.50
3	B	377	NAD	PA-O3	-3.92	1.55	1.59
3	C	377	NAD	PA-O3	-3.88	1.55	1.59
3	B	377	NAD	PN-O3	3.84	1.63	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	377	NAD	O2B-C2B	-3.80	1.33	1.43
3	A	377	NAD	PA-O3	-3.66	1.55	1.59
3	D	377	NAD	PA-O3	-3.63	1.55	1.59
3	A	377	NAD	O2B-C2B	-3.57	1.34	1.43
3	B	377	NAD	C3N-C7N	3.53	1.55	1.50
3	B	377	NAD	O4D-C4D	3.53	1.52	1.45
3	A	377	NAD	C4A-N3A	3.53	1.41	1.34
3	A	377	NAD	O4D-C1D	3.46	1.45	1.40
4	D	378	CXF	C6-C1	3.45	1.59	1.52
3	D	377	NAD	C2N-N1N	3.44	1.38	1.35
3	D	377	NAD	C5N-C4N	3.40	1.44	1.38
3	A	377	NAD	C5N-C4N	3.39	1.44	1.38
3	D	377	NAD	C2N-C3N	-3.35	1.33	1.39
3	A	377	NAD	O4D-C4D	3.34	1.52	1.45
3	B	377	NAD	O2B-C2B	-3.31	1.34	1.43
3	C	377	NAD	O4D-C4D	3.19	1.52	1.45
3	A	377	NAD	C2N-C3N	-3.18	1.34	1.39
3	B	377	NAD	O4D-C1D	3.12	1.45	1.40
3	A	377	NAD	C2A-N3A	3.11	1.39	1.33
3	A	377	NAD	C5A-C6A	3.08	1.49	1.41
4	B	378	CXF	C6-C1	3.05	1.59	1.52
3	B	377	NAD	C5N-C4N	3.00	1.44	1.38
3	D	377	NAD	C2A-N3A	2.98	1.39	1.33
3	B	377	NAD	C5A-N7A	-2.93	1.33	1.39
3	B	377	NAD	C4A-N3A	2.92	1.39	1.34
3	B	377	NAD	C5A-C6A	2.89	1.49	1.41
3	D	377	NAD	C3B-C4B	2.88	1.60	1.53
3	C	377	NAD	O3D-C3D	-2.87	1.35	1.43
4	B	378	CXF	C2-C1	2.80	1.58	1.52
3	B	377	NAD	C2N-N1N	2.79	1.38	1.35
3	C	377	NAD	C4A-N9A	2.78	1.43	1.37
3	C	377	NAD	O3B-C3B	2.71	1.49	1.43
3	A	377	NAD	O3B-C3B	2.70	1.49	1.43
3	B	377	NAD	C2A-N3A	2.67	1.38	1.33
3	C	377	NAD	C2A-N3A	2.64	1.38	1.33
3	D	377	NAD	C5A-C4A	2.63	1.43	1.39
3	A	377	NAD	O4B-C1B	-2.61	1.36	1.42
3	D	377	NAD	C5A-N7A	-2.59	1.34	1.39
3	C	377	NAD	C5A-N7A	-2.56	1.34	1.39
3	D	377	NAD	O3D-C3D	-2.54	1.36	1.43
3	D	377	NAD	C5A-C6A	2.53	1.48	1.41
4	D	378	CXF	C2-C1	2.53	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	377	NAD	C5A-C6A	2.47	1.47	1.41
4	A	378	CXF	C2-C1	2.46	1.57	1.52
3	B	377	NAD	O3B-C3B	2.41	1.48	1.43
3	D	377	NAD	C3D-C4D	2.28	1.58	1.53
3	D	377	NAD	O3B-C3B	2.26	1.48	1.43
3	C	377	NAD	C5D-C4D	-2.15	1.45	1.51
3	B	377	NAD	C5A-C4A	2.15	1.42	1.39
3	B	377	NAD	C5B-C4B	-2.11	1.45	1.51
3	D	377	NAD	PN-O3	2.10	1.61	1.59
4	C	378	CXF	C5-C6	2.09	1.58	1.53
3	A	377	NAD	C5A-N7A	-2.08	1.35	1.39
3	C	377	NAD	C3B-C4B	2.05	1.58	1.53
3	B	377	NAD	O3D-C3D	-2.04	1.37	1.43
4	D	378	CXF	C1-N8	-2.02	1.45	1.47
3	A	377	NAD	C3D-C4D	2.00	1.58	1.53

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	377	NAD	C5N-C4N-C3N	-9.23	111.29	120.36
3	D	377	NAD	C2N-C3N-C4N	9.17	128.92	118.26
3	C	377	NAD	C2N-C3N-C4N	9.13	128.88	118.26
3	B	377	NAD	C2N-C3N-C4N	8.35	127.97	118.26
3	C	377	NAD	C5N-C4N-C3N	-7.64	112.85	120.36
3	B	377	NAD	C5N-C4N-C3N	-7.55	112.94	120.36
3	A	377	NAD	C2N-C3N-C4N	7.46	126.93	118.26
3	A	377	NAD	C5N-C4N-C3N	-7.44	113.05	120.36
3	C	377	NAD	C6N-N1N-C2N	5.78	126.80	121.88
3	B	377	NAD	C2A-N1A-C6A	5.76	128.20	118.73
4	D	378	CXF	O9-C7-N8	-5.69	110.62	125.32
3	D	377	NAD	C2A-N1A-C6A	5.69	128.07	118.73
3	A	377	NAD	C2A-N1A-C6A	5.41	127.62	118.73
3	C	377	NAD	C2A-N1A-C6A	5.11	127.12	118.73
3	C	377	NAD	C4A-N9A-C8A	-5.00	100.49	105.74
3	C	377	NAD	O2N-PN-O3	4.81	120.26	107.27
3	D	377	NAD	C6N-N1N-C2N	4.69	125.86	121.88
3	B	377	NAD	C6N-N1N-C2N	4.53	125.73	121.88
3	A	377	NAD	C4A-N9A-C8A	-4.40	101.12	105.74
3	B	377	NAD	O2B-C2B-C3B	4.22	125.35	111.82
4	B	378	CXF	C6-C1-N8	-4.18	102.00	110.39
3	D	377	NAD	C4A-N9A-C8A	-4.11	101.43	105.74
3	B	377	NAD	C4A-N9A-C8A	-4.02	101.52	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	377	NAD	O2A-PA-O1A	3.99	131.03	112.44
3	D	377	NAD	C3N-C7N-N7N	3.94	122.60	117.74
3	D	377	NAD	N6A-C6A-N1A	3.93	127.13	118.38
3	C	377	NAD	N3A-C2A-N1A	-3.78	122.86	128.58
3	C	377	NAD	O2A-PA-O3	-3.70	97.26	107.27
3	A	377	NAD	O2B-C2B-C3B	3.67	123.58	111.82
3	D	377	NAD	N9A-C8A-N7A	3.66	119.13	113.94
3	A	377	NAD	N3A-C2A-N1A	-3.53	123.24	128.58
3	A	377	NAD	N9A-C8A-N7A	3.36	118.70	113.94
4	A	378	CXF	O9-C7-N8	-3.29	116.82	125.32
3	D	377	NAD	N3A-C2A-N1A	-3.28	123.62	128.58
3	B	377	NAD	N3A-C2A-N1A	-3.25	123.67	128.58
3	C	377	NAD	N9A-C8A-N7A	3.17	118.44	113.94
3	B	377	NAD	C2B-C3B-C4B	3.10	108.59	102.61
3	D	377	NAD	C6N-C5N-C4N	3.09	123.90	119.45
3	C	377	NAD	N6A-C6A-N1A	3.08	125.24	118.38
3	C	377	NAD	C2D-C3D-C4D	3.07	108.55	102.61
3	C	377	NAD	C2N-C3N-C7N	-3.04	110.68	119.46
3	D	377	NAD	C5N-C6N-N1N	-3.01	116.28	120.38
3	C	377	NAD	C5D-C4D-C3D	2.99	125.96	115.21
3	D	377	NAD	C2N-C3N-C7N	-2.97	110.89	119.46
3	B	377	NAD	C1B-N9A-C8A	2.95	133.65	127.09
4	B	378	CXF	C2-C1-N8	-2.95	104.47	110.39
3	D	377	NAD	O2B-C2B-C3B	2.94	121.25	111.82
3	B	377	NAD	N6A-C6A-N1A	2.90	124.83	118.38
3	B	377	NAD	C6N-N1N-C1D	-2.90	114.04	119.73
3	B	377	NAD	N9A-C8A-N7A	2.90	118.04	113.94
3	C	377	NAD	C5A-C4A-N3A	-2.89	122.73	126.72
3	D	377	NAD	C2B-C3B-C4B	2.89	108.19	102.61
3	A	377	NAD	O2N-PN-O3	2.88	115.05	107.27
4	D	378	CXF	C6-C1-C2	-2.87	105.84	110.80
4	D	378	CXF	C6-C1-N8	-2.85	104.66	110.39
3	D	377	NAD	O7N-C7N-C3N	-2.84	116.13	119.60
3	D	377	NAD	C5A-C4A-N3A	-2.74	122.94	126.72
3	C	377	NAD	C6A-C5A-C4A	2.74	120.91	117.18
3	B	377	NAD	C2N-C3N-C7N	-2.72	111.60	119.46
4	C	378	CXF	C6-C1-C2	2.66	115.39	110.80
3	A	377	NAD	C1B-N9A-C8A	2.64	132.95	127.09
4	D	378	CXF	C5-C6-C1	-2.62	106.39	111.09
3	D	377	NAD	O3B-C3B-C4B	-2.62	103.57	111.08
4	B	378	CXF	O9-C7-N8	-2.61	118.58	125.32
3	B	377	NAD	C5D-C4D-C3D	2.58	124.51	115.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	377	NAD	C1B-N9A-C8A	2.56	132.78	127.09
3	A	377	NAD	C2N-C3N-C7N	-2.55	112.10	119.46
3	A	377	NAD	C2B-C3B-C4B	2.50	107.45	102.61
3	D	377	NAD	C5A-C6A-N1A	-2.50	111.16	117.51
3	B	377	NAD	C5A-C6A-N1A	-2.48	111.22	117.51
3	C	377	NAD	C5A-C6A-N1A	-2.47	111.24	117.51
3	A	377	NAD	O2A-PA-O1A	2.45	123.86	112.44
4	B	378	CXF	C6-C1-C2	-2.43	106.61	110.80
3	C	377	NAD	C2B-C3B-C4B	2.42	107.29	102.61
3	C	377	NAD	O4D-C4D-C3D	-2.40	100.39	105.15
3	C	377	NAD	O4B-C1B-C2B	2.38	111.71	106.62
3	A	377	NAD	C5A-C4A-N3A	-2.36	123.46	126.72
3	D	377	NAD	N3A-C4A-N9A	2.35	131.17	127.17
3	D	377	NAD	C4D-O4D-C1D	-2.33	107.79	109.92
3	C	377	NAD	C1B-N9A-C8A	2.33	132.26	127.09
3	C	377	NAD	O3B-C3B-C4B	-2.27	104.56	111.08
3	C	377	NAD	O4B-C1B-N9A	2.26	112.43	108.09
3	A	377	NAD	N6A-C6A-N1A	2.24	123.37	118.38
4	A	378	CXF	C6-C1-C2	-2.23	106.96	110.80
3	D	377	NAD	C2D-C3D-C4D	2.21	106.88	102.61
4	A	378	CXF	C4-C3-C2	-2.18	106.94	111.42
3	D	377	NAD	O2B-C2B-C1B	2.17	117.59	110.10
3	A	377	NAD	C6N-N1N-C1D	-2.17	115.47	119.73
3	D	377	NAD	O2A-PA-O1A	2.16	122.48	112.44
4	A	378	CXF	C6-C1-N8	-2.15	106.07	110.39
3	B	377	NAD	O2N-PN-O3	2.15	113.08	107.27
3	D	377	NAD	C6A-C5A-C4A	2.11	120.05	117.18
3	B	377	NAD	C2D-C3D-C4D	2.10	106.67	102.61
4	D	378	CXF	C2-C1-N8	-2.09	106.18	110.39
3	B	377	NAD	O3B-C3B-C4B	-2.09	105.08	111.08
4	C	378	CXF	C2-C1-N8	-2.08	106.22	110.39
3	C	377	NAD	O2B-C2B-C3B	2.06	118.44	111.82

There are no chirality outliers.

All (31) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	377	NAD	C5B-O5B-PA-O1A
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	O4D-C4D-C5D-O5D
3	C	377	NAD	C3D-C4D-C5D-O5D
3	B	377	NAD	C3D-C4D-C5D-O5D
3	B	377	NAD	C5B-O5B-PA-O3
4	A	378	CXF	C2-C1-N8-C7
4	B	378	CXF	C2-C1-N8-C7
3	D	377	NAD	C3D-C4D-C5D-O5D
3	A	377	NAD	PA-O3-PN-O1N
3	C	377	NAD	PA-O3-PN-O1N
3	B	377	NAD	C2B-C1B-N9A-C8A
3	B	377	NAD	O4D-C4D-C5D-O5D
3	C	377	NAD	O4B-C1B-N9A-C8A
3	B	377	NAD	PA-O3-PN-O1N

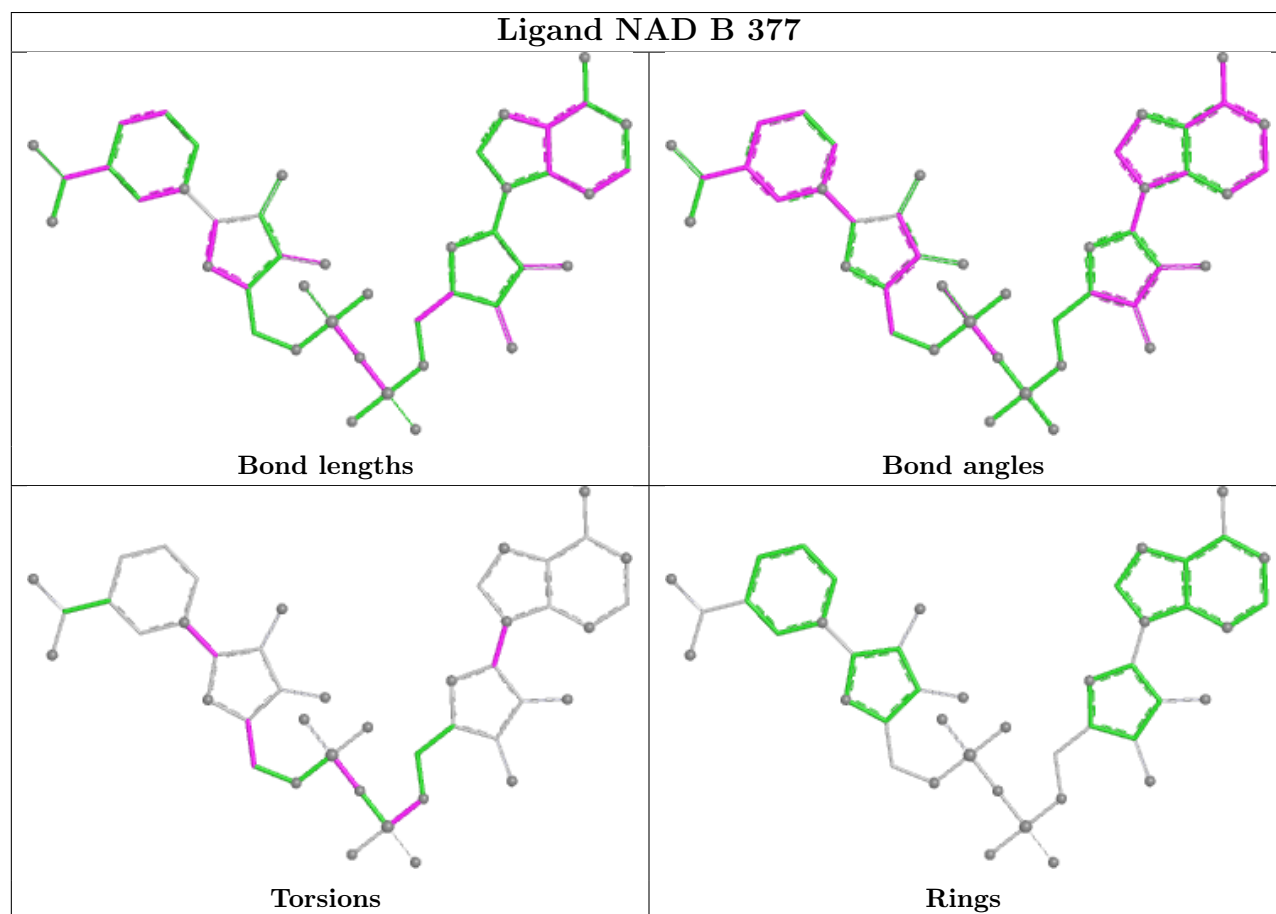
There are no ring outliers.

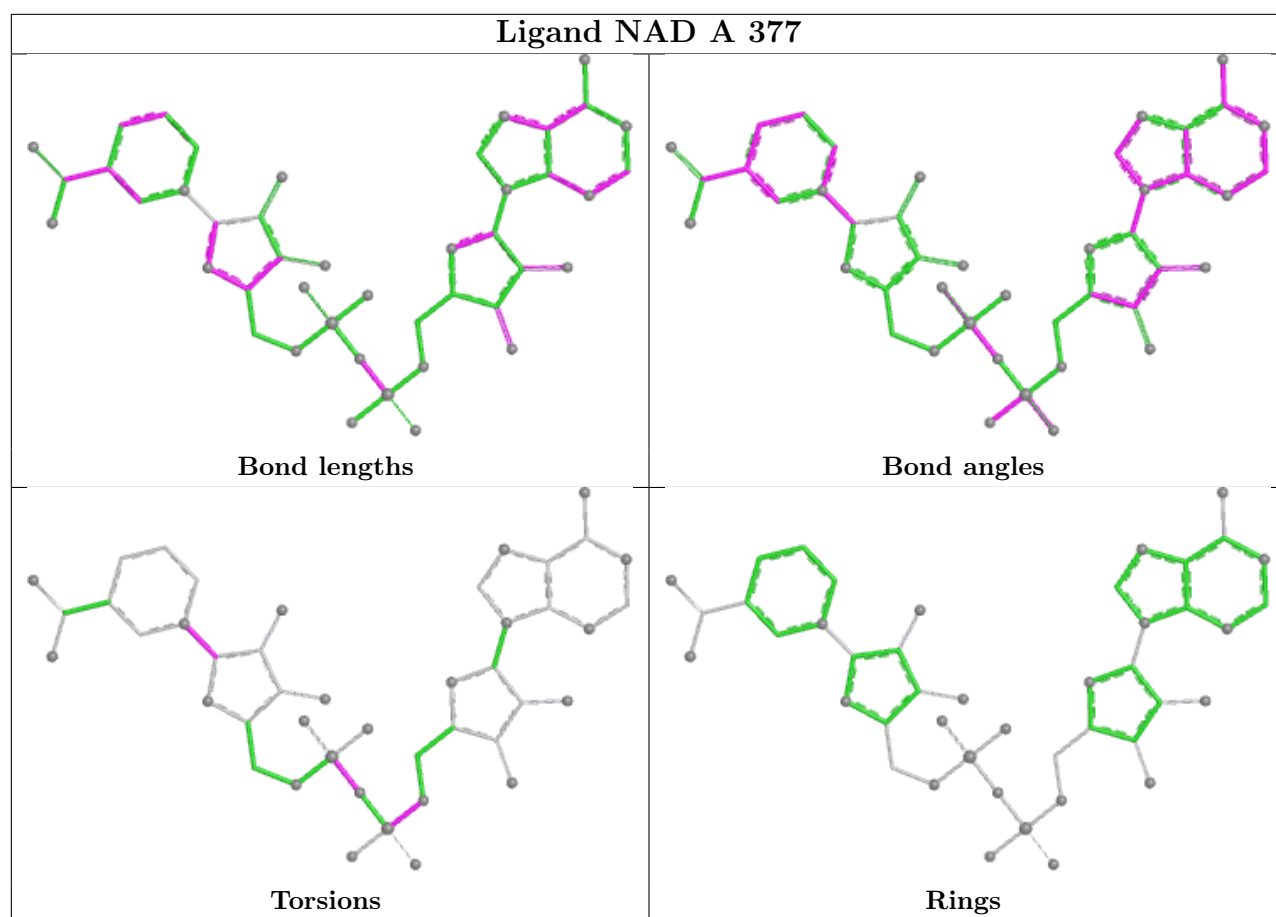
7 monomers are involved in 12 short contacts:

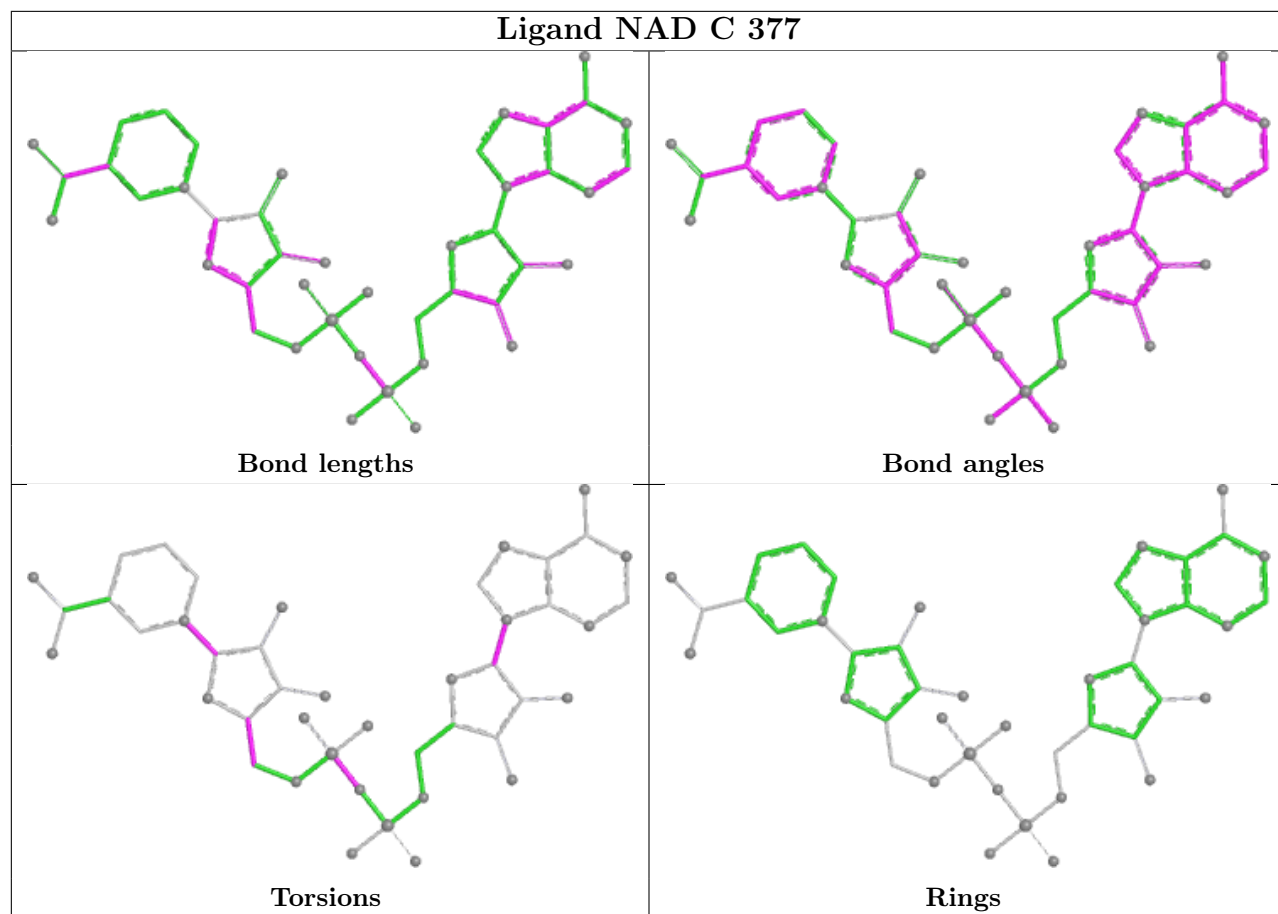
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	378	CXF	2	0
4	A	378	CXF	1	0
3	B	377	NAD	2	0
3	A	377	NAD	1	0
3	C	377	NAD	1	0
4	C	378	CXF	3	0
3	D	377	NAD	2	0

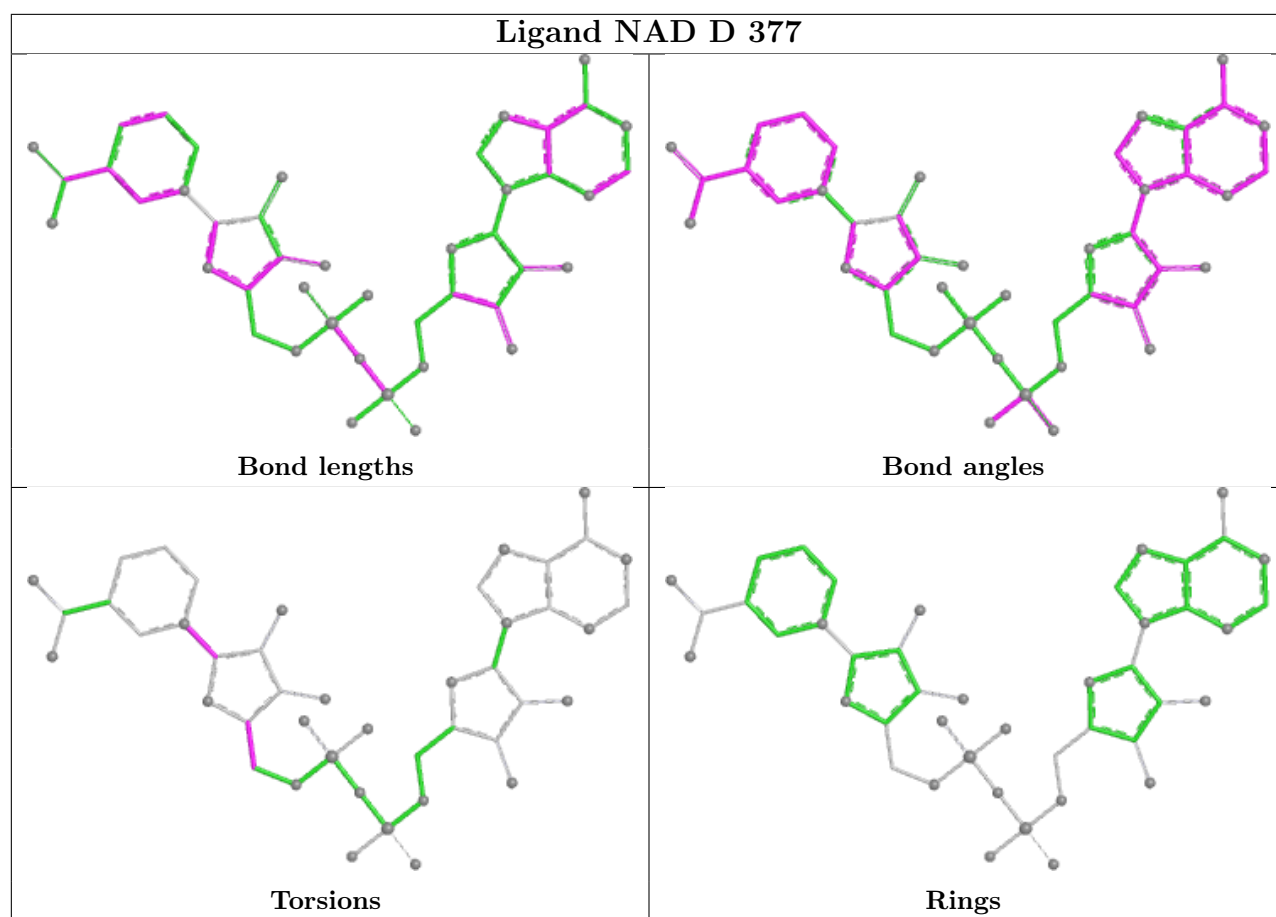
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-0.24	0 100 100	17, 26, 38, 46	0
1	B	374/374 (100%)	-0.23	2 (0%) 87 85	17, 25, 38, 46	0
1	C	374/374 (100%)	0.09	9 (2%) 59 55	17, 26, 38, 46	0
1	D	374/374 (100%)	0.01	5 (1%) 75 71	17, 26, 38, 47	0
All	All	1496/1496 (100%)	-0.09	16 (1%) 78 75	17, 26, 38, 47	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	255	THR	3.0
1	C	341	ALA	3.0
1	D	336	MET	2.7
1	C	191	GLN	2.6
1	C	33	ALA	2.4
1	D	334	ASP	2.3
1	C	333	ALA	2.2
1	B	78	GLU	2.2
1	C	332	VAL	2.1
1	D	161	ASP	2.1
1	D	34	HIS	2.1
1	C	214	ALA	2.1
1	D	335	PHE	2.1
1	C	337	ALA	2.0
1	B	98	GLY	2.0
1	C	336	MET	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

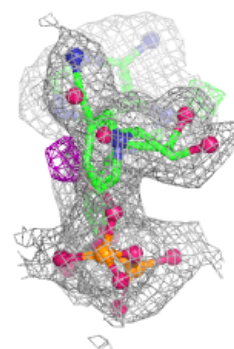
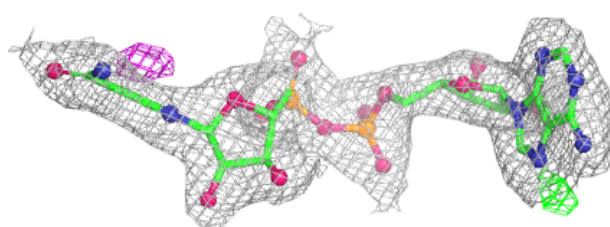
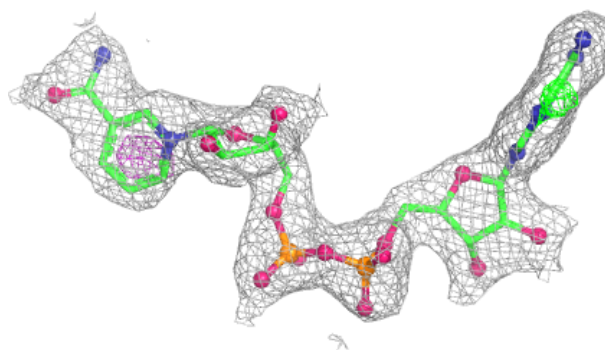
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CXF	C	378	9/9	0.89	0.08	23,26,27,27	0
4	CXF	B	378	9/9	0.91	0.08	23,26,27,27	0
4	CXF	A	378	9/9	0.91	0.08	23,25,27,27	0
4	CXF	D	378	9/9	0.93	0.07	24,26,27,27	0
3	NAD	A	377	44/44	0.95	0.07	14,21,27,28	0
3	NAD	C	377	44/44	0.95	0.07	13,21,27,28	0
3	NAD	B	377	44/44	0.96	0.07	14,21,27,28	0
3	NAD	D	377	44/44	0.97	0.06	13,21,27,28	0
2	ZN	C	375	1/1	0.99	0.03	18,18,18,18	0
2	ZN	D	376	1/1	0.99	0.06	24,24,24,24	0
2	ZN	A	376	1/1	0.99	0.02	23,23,23,23	0
2	ZN	B	375	1/1	0.99	0.02	13,13,13,13	0
2	ZN	B	376	1/1	0.99	0.03	22,22,22,22	0
2	ZN	A	375	1/1	1.00	0.02	13,13,13,13	0
2	ZN	C	376	1/1	1.00	0.04	26,26,26,26	0
2	ZN	D	375	1/1	1.00	0.03	17,17,17,17	0

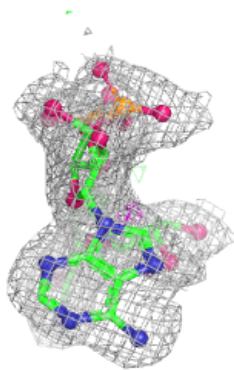
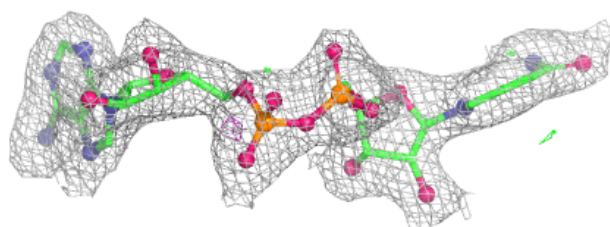
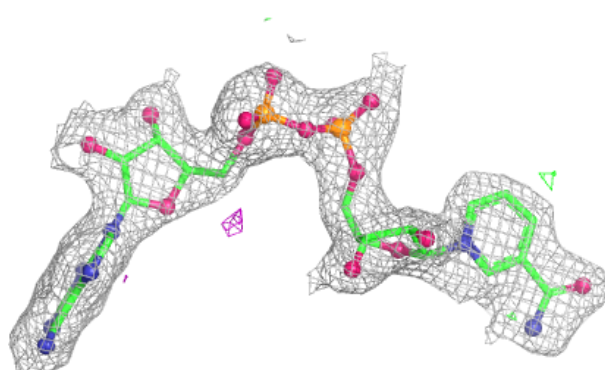
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD 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)

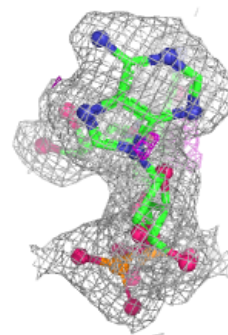
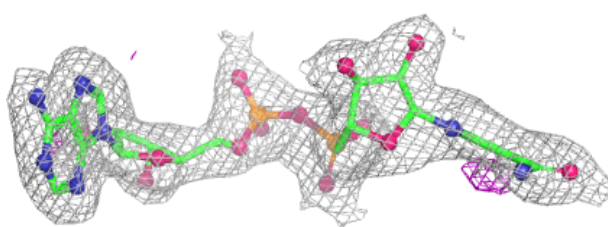
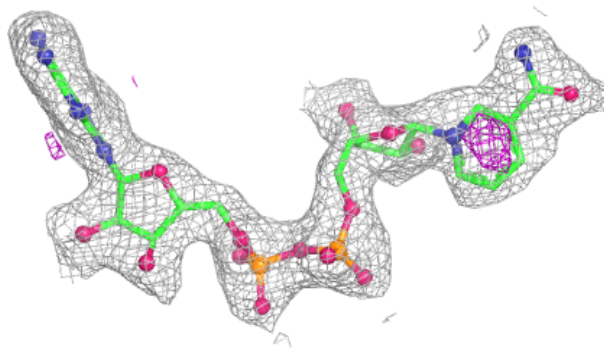
**Electron density around NAD C 377:**

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

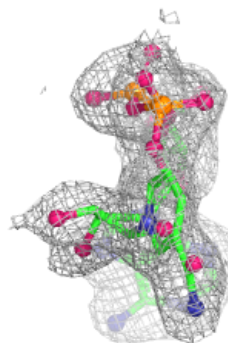
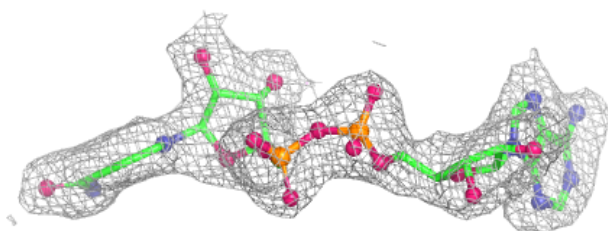
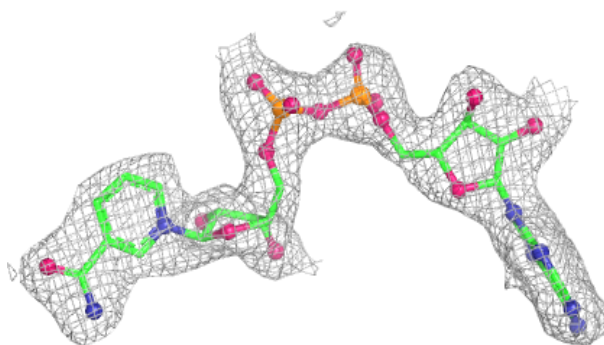


Electron density around NAD B 377:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.