



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:57 PM UTC

PDB ID : 1AGN / pdb_00001agn
Title : X-RAY STRUCTURE OF HUMAN SIGMA ALCOHOL DEHYDROGE-
NASE
Authors : Hurley, T.D.; Xie, P.
Deposited on : 1996-06-04
Resolution : 3.00 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

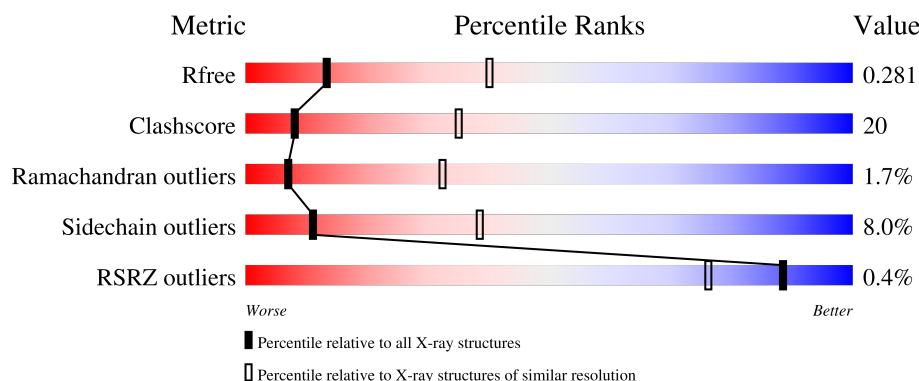
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	373	
1	B	373	
1	C	373	
1	D	373	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	A	502	-	-	X	-
3	ACT	D	378	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11397 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 HUMAN SIGMA ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2789	1772	468	526	23			
1	B	373	Total	C	N	O	S	0	0	0
			2789	1772	468	526	23			
1	C	373	Total	C	N	O	S	0	0	0
			2789	1772	468	526	23			
1	D	373	Total	C	N	O	S	0	0	0
			2789	1772	468	526	23			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	5	Total	Zn	0	0
			5	5		
2	C	3	Total	Zn	0	0
			3	3		
2	D	5	Total	Zn	0	0
			5	5		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

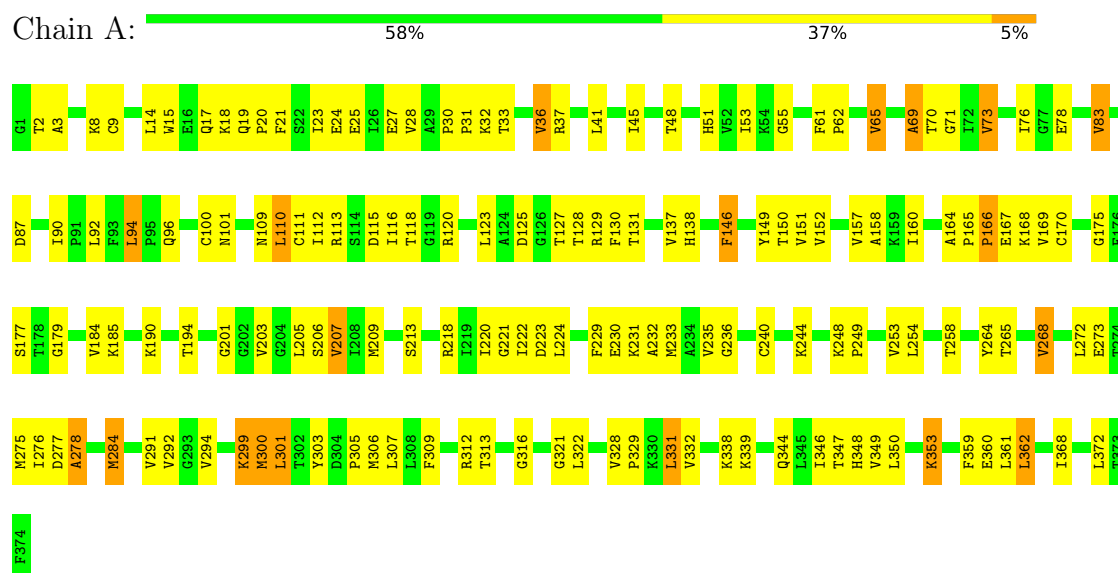
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	4	Total	O	0	0
			4	4		
5	C	1	Total	O	0	0
			1	1		
5	D	3	Total	O	0	0
			3	3		

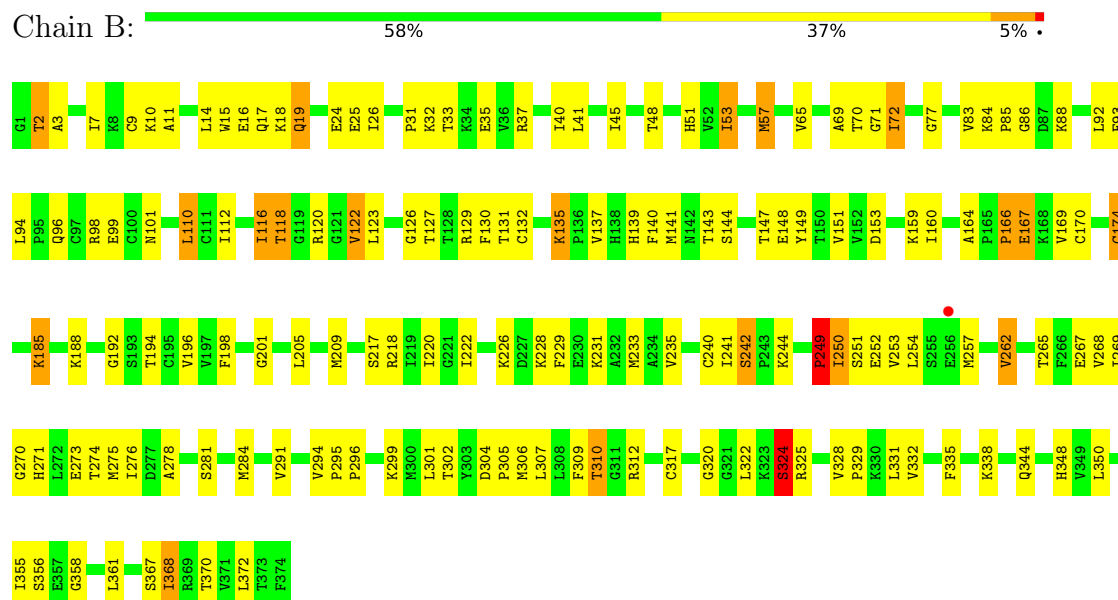
3 Residue-property plots

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.

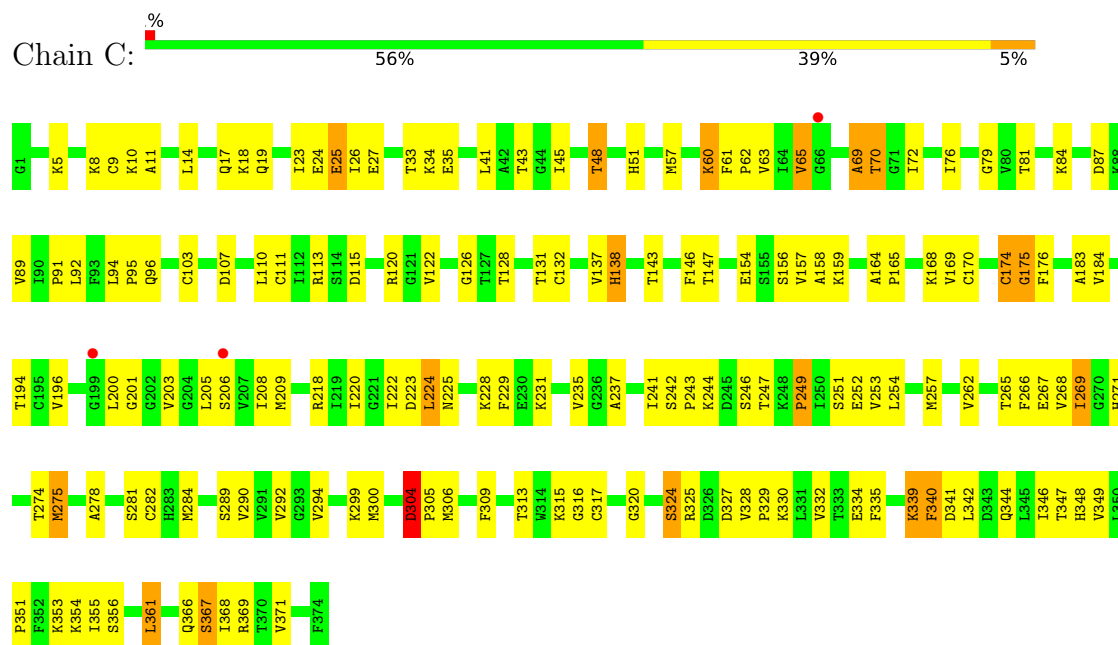
• Molecule 1: HUMAN SIGMA ALCOHOL DEHYDROGENASE



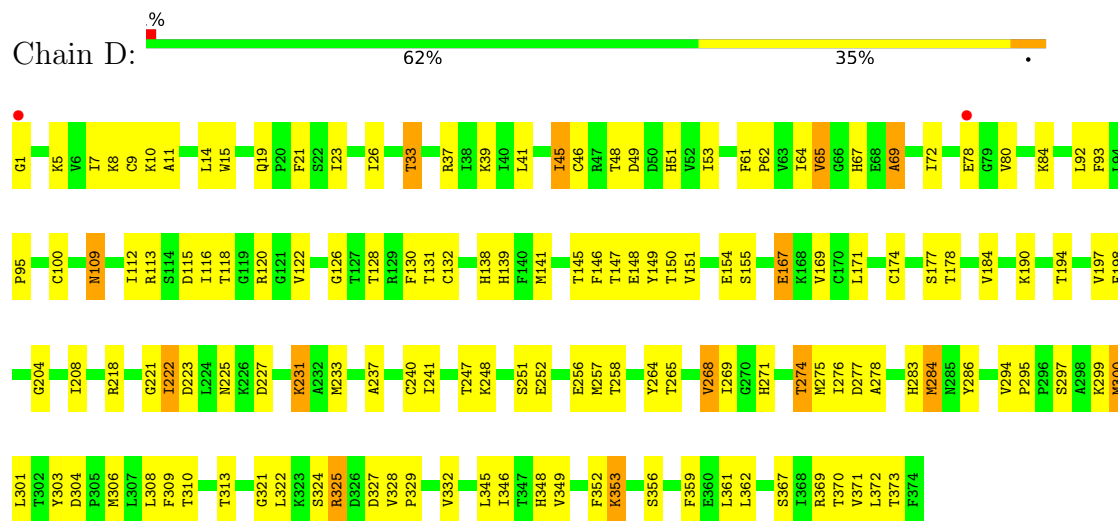
• Molecule 1: HUMAN SIGMA ALCOHOL DEHYDROGENASE



• Molecule 1: HUMAN SIGMA ALCOHOL DEHYDROGENASE



• Molecule 1: HUMAN SIGMA 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	86.30Å 94.65Å 121.66Å 90.00° 100.03° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00 8.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.00) 84.4 (8.00-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.01Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.225 , 0.305 0.207 , 0.281	Depositor DCC
R_{free} test set	2410 reflections (6.96%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 66.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11397	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.55	0/2840	1.00	9/3839 (0.2%)
1	B	0.59	0/2840	1.00	6/3839 (0.2%)
1	C	0.54	0/2840	1.00	10/3839 (0.3%)
1	D	0.61	1/2840 (0.0%)	1.05	7/3839 (0.2%)
All	All	0.57	1/11360 (0.0%)	1.01	32/15356 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	300	MET	SD-CE	5.21	1.92	1.79

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	69	ALA	N-CA-C	7.97	120.10	108.86
1	D	184	VAL	N-CA-C	7.91	118.71	110.72
1	C	45	ILE	N-CA-C	7.07	113.78	106.21
1	C	184	VAL	N-CA-C	7.07	117.18	110.53
1	C	304	ASP	CB-CA-C	7.02	119.48	109.38
1	D	327	ASP	N-CA-C	6.25	119.03	111.40
1	C	69	ALA	N-CA-C	5.96	117.30	108.60
1	B	350	LEU	CA-C-N	-5.82	113.97	119.85
1	B	350	LEU	C-N-CA	-5.82	113.97	119.85
1	C	327	ASP	N-CA-C	5.73	117.60	111.36
1	A	278	ALA	N-CA-C	-5.72	104.66	111.69
1	C	138	HIS	N-CA-C	5.68	119.17	110.20
1	A	69	ALA	N-CA-C	5.67	115.73	108.24
1	A	275	MET	N-CA-C	-5.66	105.19	111.36
1	B	135	LYS	N-CA-C	5.65	116.81	109.64
1	D	248	LYS	CA-C-N	5.61	126.85	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	248	LYS	C-N-CA	5.61	126.85	119.84
1	A	94	LEU	CA-C-N	5.53	126.30	120.11
1	A	94	LEU	C-N-CA	5.53	126.30	120.11
1	C	304	ASP	CA-C-N	5.46	125.29	119.28
1	C	304	ASP	C-N-CA	5.46	125.29	119.28
1	A	184	VAL	N-CA-C	5.40	116.13	110.62
1	B	69	ALA	N-CA-C	5.38	115.23	108.45
1	D	138	HIS	N-CA-C	5.33	117.56	110.53
1	C	25	GLU	N-CA-C	-5.20	101.49	109.76
1	A	303	TYR	N-CA-C	5.16	117.25	109.41
1	D	325	ARG	N-CA-C	5.14	117.62	111.71
1	B	250	ILE	N-CA-C	5.07	116.39	110.62
1	C	247	THR	N-CA-C	-5.05	107.29	113.50
1	A	146	PHE	N-CA-C	-5.04	104.56	111.81
1	A	313	THR	N-CA-C	-5.03	101.03	109.24
1	B	324	SER	N-CA-C	5.01	121.46	110.80

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	2789	0	2858	116	0
1	B	2789	0	2858	114	0
1	C	2789	0	2858	120	0
1	D	2789	0	2858	112	0
2	A	3	0	0	0	0
2	B	5	0	0	0	0
2	C	3	0	0	0	0
2	D	5	0	0	0	0
3	A	12	0	9	3	0
3	B	16	0	12	0	0
3	C	4	0	3	1	0
3	D	8	0	6	3	0
4	A	44	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	44	0	26	2	0
4	C	44	0	26	3	0
4	D	44	0	26	9	0
5	A	1	0	0	0	0
5	B	4	0	0	0	0
5	C	1	0	0	0	0
5	D	3	0	0	0	0
All	All	11397	0	11566	448	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 20.

All (448) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:ASP:HB2	1:D:300:MET:HE1	1.10	1.09
1:D:348:HIS:HB2	1:D:370:THR:HG23	1.46	0.96
1:C:304:ASP:HB2	1:D:300:MET:CE	1.96	0.95
1:C:205:LEU:HD11	1:C:368:ILE:HD13	1.46	0.95
1:D:178:THR:HG21	4:D:377:NAD:C4N	1.97	0.93
1:D:46:CYS:HA	1:D:369:ARG:NH1	1.88	0.88
1:C:164:ALA:HB1	1:C:169:VAL:HG11	1.56	0.87
1:D:26:ILE:HG22	1:D:132:CYS:HB2	1.55	0.86
1:C:304:ASP:CB	1:D:300:MET:HE1	2.02	0.84
1:A:70:THR:HG22	1:A:170:CYS:HB3	1.59	0.84
1:A:306:MET:HE2	1:B:295:PRO:HG2	1.60	0.83
1:D:49:ASP:OD1	1:D:67:HIS:CE1	2.34	0.81
1:D:241:ILE:CD1	1:D:257:MET:HE1	2.11	0.81
1:D:276:ILE:HD12	1:D:303:TYR:HB2	1.64	0.80
1:C:122:VAL:HG12	1:C:128:THR:HG23	1.63	0.80
1:D:92:LEU:HD13	1:D:324:SER:HB2	1.64	0.80
1:D:14:LEU:HG	1:D:61:PHE:HE1	1.47	0.78
1:C:194:THR:HG22	1:C:218:ARG:HB2	1.65	0.77
1:C:300:MET:HE1	1:D:304:ASP:HB2	1.66	0.77
1:C:353:LYS:H	1:C:353:LYS:HD2	1.49	0.77
1:C:10:LYS:HD2	1:C:23:ILE:HG22	1.68	0.76
1:A:130:PHE:HB2	1:A:137:VAL:HG23	1.69	0.74
1:A:348:HIS:ND1	1:A:361:LEU:HD13	2.02	0.74
1:B:122:VAL:HG11	1:B:126:GLY:HA2	1.69	0.73
1:C:249:PRO:HB2	1:C:252:GLU:HG3	1.69	0.73
1:D:197:VAL:HG21	1:D:208:ILE:HD13	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:PHE:HB2	1:A:137:VAL:CG2	2.20	0.72
1:B:11:ALA:HB2	1:B:147:THR:HG23	1.73	0.71
1:A:294:VAL:HG22	1:B:309:PHE:CZ	2.26	0.71
1:D:122:VAL:HG12	1:D:128:THR:HG23	1.72	0.70
1:A:164:ALA:HB1	1:A:169:VAL:HG11	1.74	0.69
1:D:194:THR:HG23	1:D:218:ARG:HB3	1.75	0.69
1:B:32:LYS:HD2	1:B:129:ARG:NH2	2.07	0.69
1:D:46:CYS:HA	1:D:369:ARG:HH12	1.55	0.68
1:C:11:ALA:HB3	1:C:26:ILE:HD13	1.75	0.68
1:A:100:CYS:HB2	1:A:112:ILE:HG23	1.74	0.68
1:A:224:LEU:HD21	1:A:244:LYS:HE3	1.75	0.67
1:C:23:ILE:HD12	1:C:23:ILE:H	1.58	0.67
1:D:155:SER:HA	1:D:325:ARG:HH11	1.60	0.67
1:B:276:ILE:HD11	1:B:301:LEU:HD11	1.76	0.67
1:A:231:LYS:HD2	1:A:344:GLN:HG3	1.75	0.67
1:D:252:GLU:O	1:D:256:GLU:HG3	1.95	0.66
1:C:348:HIS:CD2	1:C:361:LEU:HD13	2.30	0.66
1:D:128:THR:HG22	1:D:139:HIS:HD2	1.59	0.66
1:C:231:LYS:HG2	1:C:368:ILE:CD1	2.26	0.66
1:A:231:LYS:HG2	1:A:368:ILE:CD1	2.25	0.66
1:C:76:ILE:HD13	1:C:84:LYS:HA	1.78	0.66
1:D:348:HIS:CB	1:D:370:THR:HG23	2.24	0.66
1:A:94:LEU:HD11	1:A:110:LEU:HA	1.78	0.66
1:D:49:ASP:OD1	1:D:67:HIS:ND1	2.30	0.65
1:C:267:GLU:HG3	1:C:275:MET:HA	1.77	0.65
1:C:218:ARG:HH21	1:C:220:ILE:HD11	1.61	0.65
1:A:19:GLN:HG2	1:A:20:PRO:HD2	1.77	0.65
1:D:155:SER:HA	1:D:325:ARG:NH1	2.11	0.64
1:C:69:ALA:O	1:C:91:PRO:HD2	1.98	0.64
1:B:271:HIS:O	1:B:275:MET:HG3	1.98	0.64
1:A:307:LEU:O	1:A:312:ARG:HD2	1.97	0.64
1:D:100:CYS:HB2	1:D:112:ILE:HG13	1.80	0.63
1:D:223:ASP:OD1	4:D:377:NAD:H1B	1.98	0.63
1:B:304:ASP:OD1	1:B:306:MET:HB2	1.98	0.63
1:A:32:LYS:HD2	1:A:129:ARG:NH2	2.14	0.63
1:A:307:LEU:HD22	1:A:312:ARG:HH12	1.64	0.63
1:D:241:ILE:HD12	1:D:257:MET:HE1	1.81	0.62
1:A:27:GLU:HB2	1:A:131:THR:HB	1.81	0.62
1:B:88:LYS:HG2	1:B:160:ILE:HD11	1.81	0.62
1:D:198:PHE:HD2	1:D:274:THR:HG22	1.65	0.61
1:D:15:TRP:CH2	1:D:132:CYS:SG	2.91	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:LYS:HD3	1:D:149:TYR:CZ	2.36	0.61
1:C:353:LYS:HD2	1:C:353:LYS:N	2.13	0.61
1:B:271:HIS:HB2	1:B:274:THR:OG1	2.01	0.61
1:C:341:ASP:O	1:C:344:GLN:HG2	2.00	0.61
1:D:231:LYS:HE3	1:D:231:LYS:HA	1.82	0.61
1:D:11:ALA:HB2	1:D:147:THR:HG23	1.82	0.61
1:C:309:PHE:CZ	1:D:294:VAL:HG22	2.35	0.61
1:D:269:ILE:HD12	1:D:274:THR:HG21	1.82	0.61
1:B:33:THR:O	1:B:35:GLU:HG3	2.01	0.60
1:D:41:LEU:HD11	1:D:72:ILE:HG13	1.82	0.60
1:C:251:SER:HA	1:C:281:SER:HB3	1.83	0.60
1:C:334:GLU:O	1:C:339:LYS:HB2	2.01	0.60
1:A:123:LEU:HD12	1:A:127:THR:O	2.02	0.60
1:A:128:THR:HG21	1:A:138:HIS:HA	1.84	0.60
1:D:128:THR:HG22	1:D:139:HIS:CD2	2.36	0.60
1:C:341:ASP:HB3	1:C:344:GLN:NE2	2.17	0.60
1:A:31:PRO:HD3	1:A:37:ARG:HB2	1.84	0.60
1:A:359:PHE:O	1:A:362:LEU:HB3	2.02	0.59
1:A:17:GLN:OE1	1:A:55:GLY:HA2	2.03	0.59
1:C:65:VAL:HG23	1:C:146:PHE:CD2	2.37	0.59
1:C:94:LEU:HD11	1:C:110:LEU:HD12	1.85	0.59
1:B:262:VAL:HG11	1:B:281:SER:O	2.02	0.59
1:C:165:PRO:HG3	1:C:168:LYS:HD2	1.84	0.59
1:A:272:LEU:HD11	1:A:299:LYS:HB3	1.83	0.59
1:B:129:ARG:HG3	1:B:151:VAL:HB	1.83	0.59
1:C:154:GLU:O	1:C:157:VAL:HG12	2.03	0.59
1:C:317:CYS:SG	1:C:320:GLY:HA2	2.43	0.59
1:B:118:THR:HG23	1:B:120:ARG:HG3	1.83	0.59
1:C:17:GLN:HG2	1:C:18:LYS:HG3	1.85	0.58
1:A:17:GLN:HB2	1:A:61:PHE:HE2	1.67	0.58
1:C:165:PRO:HG2	1:C:168:LYS:HB2	1.86	0.58
1:C:115:ASP:OD1	1:C:120:ARG:HB2	2.04	0.58
1:A:17:GLN:HB2	1:A:61:PHE:CE2	2.38	0.58
1:A:353:LYS:H	1:A:353:LYS:CD	2.17	0.58
1:B:70:THR:HG22	1:B:170:CYS:HB3	1.86	0.58
1:C:96:GLN:HB2	1:C:324:SER:OG	2.04	0.58
1:D:178:THR:HG21	4:D:377:NAD:H4N	1.84	0.58
1:D:190:LYS:HG2	1:D:264:TYR:OH	2.02	0.57
1:C:224:LEU:HD12	1:C:243:PRO:HD2	1.84	0.57
1:D:169:VAL:HG21	1:D:332:VAL:HG13	1.86	0.57
1:D:115:ASP:HA	1:D:120:ARG:NH2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:GLU:CD	1:D:167:GLU:H	2.12	0.57
1:C:48:THR:HG22	1:C:57:MET:SD	2.45	0.57
1:A:9:CYS:O	1:A:25:GLU:HA	2.03	0.57
1:D:348:HIS:CE1	1:D:367:SER:HB3	2.41	0.56
1:B:31:PRO:HD3	1:B:37:ARG:HB2	1.86	0.56
1:B:41:LEU:HG	1:B:71:GLY:HA2	1.87	0.56
1:C:24:GLU:OE1	1:C:132:CYS:SG	2.61	0.56
1:D:23:ILE:HD12	1:D:352:PHE:CE2	2.40	0.56
1:A:360:GLU:CB	3:A:502:ACT:H3	2.35	0.56
1:B:96:GLN:HE21	1:B:98:ARG:HG2	1.68	0.56
1:A:344:GLN:HA	1:A:344:GLN:OE1	2.05	0.56
1:B:196:VAL:HG12	1:B:220:ILE:HB	1.88	0.56
1:A:301:LEU:HB2	1:B:305:PRO:HG3	1.87	0.56
1:D:65:VAL:HG23	1:D:146:PHE:CD2	2.41	0.56
1:D:122:VAL:HG21	1:D:126:GLY:HA2	1.88	0.56
1:B:348:HIS:CD2	1:B:361:LEU:HD13	2.41	0.55
1:A:185:LYS:HE2	1:A:321:GLY:O	2.06	0.55
1:B:284:MET:HA	1:B:312:ARG:NE	2.22	0.55
1:B:332:VAL:O	1:B:335:PHE:HB3	2.06	0.55
1:C:222:ILE:HD11	1:C:254:LEU:HD11	1.89	0.55
1:A:76:ILE:HG21	1:A:83:VAL:O	2.06	0.55
1:B:147:THR:HG22	1:B:149:TYR:H	1.71	0.55
1:C:351:PRO:HD2	1:C:354:LYS:HD2	1.87	0.55
1:D:328:VAL:HB	1:D:329:PRO:HD3	1.87	0.55
1:D:353:LYS:H	1:D:353:LYS:HD3	1.71	0.55
1:B:15:TRP:HZ2	1:B:132:CYS:HG	1.47	0.55
1:A:152:VAL:CG2	1:A:157:VAL:HG23	2.37	0.55
1:B:122:VAL:HG22	1:B:127:THR:C	2.31	0.55
1:B:348:HIS:CE1	1:B:367:SER:HB3	2.42	0.55
1:C:9:CYS:O	1:C:25:GLU:HA	2.07	0.55
1:D:37:ARG:HG3	1:D:151:VAL:HG22	1.89	0.55
1:D:178:THR:CG2	4:D:377:NAD:H4N	2.37	0.55
1:A:265:THR:HG21	1:A:278:ALA:O	2.07	0.54
1:B:164:ALA:HB1	1:B:169:VAL:HG11	1.88	0.54
1:D:48:THR:HA	1:D:51:HIS:CD2	2.43	0.54
1:A:41:LEU:HG	1:A:71:GLY:HA2	1.88	0.54
1:C:200:LEU:HD12	1:C:223:ASP:HB2	1.90	0.54
1:D:276:ILE:HD12	1:D:303:TYR:CB	2.37	0.54
1:A:73:VAL:HG23	1:A:87:ASP:O	2.08	0.54
1:B:167:GLU:H	1:B:167:GLU:CD	2.15	0.54
1:D:21:PHE:CZ	1:D:53:ILE:HD11	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:THR:HA	1:D:277:ASP:HB2	1.90	0.54
3:A:378:ACT:OXT	4:A:377:NAD:C3N	2.56	0.54
1:B:209:MET:HG3	1:B:235:VAL:HG13	1.88	0.54
1:B:122:VAL:CG1	1:B:126:GLY:HA2	2.37	0.54
1:B:14:LEU:HD21	1:B:53:ILE:HG22	1.88	0.54
1:C:347:THR:HG21	1:C:367:SER:CB	2.37	0.54
1:C:347:THR:HG21	1:C:367:SER:HB2	1.90	0.53
1:B:116:ILE:HD13	1:B:116:ILE:H	1.73	0.53
1:B:265:THR:HG21	1:B:278:ALA:O	2.07	0.53
1:B:284:MET:O	1:B:310:THR:HB	2.08	0.53
1:C:92:LEU:O	1:C:156:SER:HB3	2.08	0.53
1:D:348:HIS:ND1	1:D:367:SER:HB3	2.23	0.53
1:C:174:CYS:SG	4:C:377:NAD:H5N	2.48	0.53
4:D:377:NAD:H6N	4:D:377:NAD:H51N	1.90	0.53
1:D:271:HIS:HB2	1:D:274:THR:OG1	2.08	0.53
1:C:41:LEU:HD11	1:C:72:ILE:HD11	1.91	0.53
1:C:292:VAL:O	4:C:377:NAD:H2N	2.08	0.53
1:C:265:THR:HG21	1:C:278:ALA:O	2.09	0.53
1:D:9:CYS:HB2	1:D:148:GLU:OE2	2.09	0.53
1:D:15:TRP:HH2	1:D:132:CYS:SG	2.32	0.53
1:D:297:SER:O	1:D:299:LYS:HG2	2.08	0.53
1:B:222:ILE:HD11	1:B:250:ILE:HD11	1.90	0.53
1:C:290:VAL:HG22	1:C:315:LYS:HG3	1.91	0.53
1:D:100:CYS:CB	1:D:112:ILE:HG13	2.39	0.53
1:C:334:GLU:HB2	1:C:340:PHE:CE1	2.44	0.52
1:B:253:VAL:HG12	1:B:257:MET:HE3	1.92	0.52
1:D:178:THR:CG2	4:D:377:NAD:C4N	2.79	0.52
1:D:45:ILE:HD11	1:D:372:LEU:HD11	1.91	0.52
1:A:125:ASP:HB3	1:A:127:THR:OG1	2.10	0.52
1:C:334:GLU:HB2	1:C:340:PHE:HE1	1.74	0.52
1:A:21:PHE:CZ	1:A:53:ILE:HD11	2.45	0.52
1:B:201:GLY:O	1:B:205:LEU:HG	2.08	0.52
1:A:349:VAL:O	1:A:350:LEU:HD23	2.09	0.52
1:B:275:MET:HE2	1:B:291:VAL:HG13	1.91	0.52
1:C:79:GLY:O	1:C:81:THR:HG23	2.09	0.52
1:A:23:ILE:N	1:A:23:ILE:HD12	2.25	0.51
1:D:348:HIS:CE1	1:D:361:LEU:HD13	2.46	0.51
1:A:249:PRO:O	1:A:253:VAL:HG23	2.09	0.51
1:A:300:MET:CE	1:B:304:ASP:HB2	2.40	0.51
3:C:378:ACT:H3	1:D:309:PHE:CZ	2.45	0.51
1:C:349:VAL:HA	1:C:371:VAL:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:CYS:SG	4:B:377:NAD:H5N	2.50	0.51
1:B:296:PRO:HB2	1:B:299:LYS:HD3	1.93	0.51
1:B:198:PHE:O	1:B:269:ILE:HG13	2.11	0.51
1:B:222:ILE:CD1	1:B:250:ILE:HD11	2.41	0.51
1:C:33:THR:O	1:C:35:GLU:HG3	2.10	0.51
1:C:165:PRO:CG	1:C:168:LYS:HD2	2.41	0.51
1:D:204:GLY:O	1:D:208:ILE:HG12	2.11	0.51
1:B:70:THR:HG21	1:B:166:PRO:HA	1.93	0.51
1:C:332:VAL:O	1:C:335:PHE:HB3	2.11	0.51
1:D:198:PHE:O	1:D:268:VAL:HG23	2.10	0.51
1:C:60:LYS:O	1:C:63:VAL:HB	2.10	0.51
1:C:205:LEU:CD1	1:C:368:ILE:HD13	2.30	0.51
1:D:225:ASN:OD1	1:D:227:ASP:HB2	2.11	0.50
1:C:92:LEU:CD1	1:C:325:ARG:HG2	2.41	0.50
1:C:231:LYS:HG2	1:C:368:ILE:HD12	1.92	0.50
1:A:48:THR:O	1:A:51:HIS:HB2	2.12	0.50
1:B:275:MET:HE2	1:B:291:VAL:CG1	2.41	0.50
1:D:241:ILE:CD1	1:D:257:MET:CE	2.88	0.50
1:B:94:LEU:HD11	1:B:110:LEU:HA	1.93	0.50
1:C:94:LEU:HD11	1:C:110:LEU:HA	1.94	0.50
1:C:305:PRO:HG3	1:D:301:LEU:HB2	1.93	0.50
1:C:330:LYS:O	1:C:334:GLU:HG2	2.11	0.50
1:C:95:PRO:HG3	1:C:113:ARG:HB2	1.94	0.50
1:A:112:ILE:HD12	1:A:112:ILE:C	2.37	0.50
1:A:305:PRO:HG3	1:B:301:LEU:HB2	1.92	0.50
1:C:89:VAL:HG12	1:C:159:LYS:HA	1.93	0.50
1:B:17:GLN:HG3	1:B:18:LYS:HG2	1.94	0.50
1:D:80:VAL:HG13	1:D:154:GLU:HG3	1.93	0.50
1:C:94:LEU:CD1	1:C:110:LEU:HD12	2.42	0.49
1:A:111:CYS:SG	1:A:112:ILE:N	2.85	0.49
1:A:194:THR:HG21	1:A:258:THR:HG21	1.93	0.49
1:A:231:LYS:HG2	1:A:368:ILE:HD11	1.92	0.49
1:B:209:MET:HG3	1:B:235:VAL:CG1	2.43	0.49
1:C:271:HIS:HB2	1:C:274:THR:OG1	2.12	0.49
1:A:45:ILE:HD11	1:A:372:LEU:HD21	1.94	0.49
1:C:347:THR:HG22	1:C:369:ARG:H	1.77	0.49
1:D:221:GLY:O	1:D:240:CYS:HA	2.13	0.49
1:A:128:THR:CG2	1:A:138:HIS:HA	2.41	0.49
3:D:378:ACT:O	4:D:377:NAD:C3N	2.61	0.49
1:D:241:ILE:HD11	1:D:257:MET:SD	2.53	0.48
1:A:175:GLY:HA2	1:A:203:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ILE:HD11	1:A:254:LEU:HD11	1.95	0.48
1:B:130:PHE:HB2	1:B:137:VAL:HB	1.93	0.48
1:B:269:ILE:HD13	4:B:377:NAD:C4A	2.42	0.48
1:D:178:THR:OG1	4:D:377:NAD:H4N	2.14	0.48
1:B:140:PHE:CZ	1:B:141:MET:HE2	2.47	0.48
1:B:143:THR:O	1:B:144:SER:HB2	2.12	0.48
1:A:276:ILE:HG12	1:A:301:LEU:HD21	1.94	0.48
1:B:307:LEU:HD22	1:B:312:ARG:NH1	2.29	0.48
1:C:304:ASP:OD1	1:C:306:MET:HB2	2.13	0.48
1:B:26:ILE:HG22	1:B:132:CYS:HB2	1.96	0.48
1:A:201:GLY:O	1:A:205:LEU:HG	2.14	0.48
1:B:32:LYS:O	1:B:77:GLY:HA3	2.13	0.48
1:C:361:LEU:HB3	1:C:367:SER:OG	2.13	0.48
1:A:33:THR:HG22	1:A:78:GLU:HB2	1.96	0.48
1:D:328:VAL:O	1:D:332:VAL:HG23	2.13	0.48
1:A:284:MET:HA	1:A:312:ARG:NE	2.29	0.48
1:A:300:MET:HE1	1:B:304:ASP:HB2	1.96	0.47
1:A:328:VAL:HB	1:A:329:PRO:HD3	1.96	0.47
1:A:164:ALA:O	1:A:166:PRO:HD3	2.14	0.47
1:A:218:ARG:HH21	1:A:220:ILE:HD11	1.79	0.47
1:B:233:MET:HB2	1:B:233:MET:HE2	1.82	0.47
1:C:300:MET:HE1	1:D:304:ASP:CB	2.40	0.47
1:B:267:GLU:HG3	1:B:275:MET:HA	1.97	0.47
1:A:62:PRO:HG2	1:A:137:VAL:HA	1.97	0.47
1:A:291:VAL:HG13	1:A:316:GLY:HA2	1.97	0.47
1:C:175:GLY:HA2	1:C:203:VAL:HG22	1.97	0.47
1:A:8:LYS:NZ	1:A:25:GLU:HB3	2.30	0.46
1:B:328:VAL:HB	1:B:329:PRO:HD3	1.96	0.46
1:B:355:ILE:HG23	1:B:356:SER:N	2.29	0.46
1:C:335:PHE:CE1	1:C:342:LEU:HG	2.50	0.46
1:B:17:GLN:C	1:B:19:GLN:H	2.24	0.46
1:C:299:LYS:C	1:C:300:MET:HE2	2.40	0.46
1:C:347:THR:HG21	1:C:368:ILE:H	1.80	0.46
1:D:353:LYS:HD3	1:D:353:LYS:N	2.30	0.46
1:A:62:PRO:CG	1:A:137:VAL:HG12	2.46	0.46
1:D:130:PHE:HZ	1:D:150:THR:OG1	1.98	0.46
1:A:276:ILE:HD11	1:A:301:LEU:HD22	1.97	0.46
1:B:241:ILE:HG22	1:B:242:SER:N	2.31	0.46
1:D:15:TRP:CZ2	1:D:132:CYS:SG	3.00	0.46
1:D:95:PRO:HB2	1:D:113:ARG:HB2	1.98	0.46
1:D:1:GLY:O	1:D:5:LYS:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:PRO:HB2	1:C:143:THR:HG22	1.97	0.46
1:B:48:THR:HG21	1:B:141:MET:HE1	1.97	0.46
1:B:229:PHE:N	1:B:229:PHE:CD1	2.84	0.46
1:B:240:CYS:O	1:B:241:ILE:HD13	2.16	0.46
1:B:32:LYS:HD2	1:B:129:ARG:HH22	1.81	0.46
1:D:346:ILE:HG23	1:D:371:VAL:HG23	1.98	0.46
1:B:355:ILE:HG23	1:B:356:SER:H	1.80	0.45
1:D:353:LYS:H	1:D:353:LYS:CD	2.25	0.45
1:A:100:CYS:SG	1:A:111:CYS:HA	2.56	0.45
1:C:201:GLY:O	1:C:205:LEU:HG	2.16	0.45
1:C:306:MET:HE2	1:D:295:PRO:HD2	1.99	0.45
1:D:7:ILE:HG13	1:D:37:ARG:NH1	2.31	0.45
1:A:30:PRO:HA	1:A:37:ARG:NH1	2.32	0.45
1:B:307:LEU:HD22	1:B:312:ARG:HH12	1.80	0.45
1:C:92:LEU:HD11	1:C:158:ALA:HB2	1.98	0.45
1:A:92:LEU:HD11	1:A:158:ALA:HB2	1.97	0.45
1:C:43:THR:CB	1:C:69:ALA:HB2	2.47	0.45
1:B:48:THR:O	1:B:51:HIS:HB2	2.17	0.45
1:C:128:THR:HG21	1:C:138:HIS:HA	1.98	0.45
1:B:205:LEU:HD12	1:B:368:ILE:HG21	1.98	0.45
1:B:276:ILE:CD1	1:B:301:LEU:HD11	2.45	0.45
1:C:92:LEU:HD13	1:C:324:SER:HB2	1.98	0.45
1:D:359:PHE:O	1:D:362:LEU:HB3	2.16	0.45
1:C:208:ILE:HD13	1:C:237:ALA:HB2	1.98	0.45
1:C:231:LYS:HD2	1:C:344:GLN:O	2.16	0.45
1:B:93:PHE:HB2	1:B:141:MET:HB3	1.99	0.45
1:B:355:ILE:O	1:B:358:GLY:N	2.49	0.45
1:A:268:VAL:HG13	1:A:292:VAL:HB	1.99	0.45
1:A:205:LEU:HD22	1:A:232:ALA:HA	1.98	0.45
1:C:51:HIS:HB3	1:C:57:MET:HB2	1.99	0.45
1:C:92:LEU:CD2	1:C:328:VAL:HG21	2.47	0.45
1:C:103:CYS:SG	1:C:111:CYS:HB2	2.57	0.45
1:A:78:GLU:N	1:A:78:GLU:OE1	2.50	0.44
1:C:335:PHE:CD1	1:C:342:LEU:HG	2.52	0.44
1:D:33:THR:HG23	1:D:78:GLU:HB2	1.99	0.44
1:B:2:THR:CG2	1:B:7:ILE:HG12	2.47	0.44
1:C:222:ILE:CD1	1:C:254:LEU:HD11	2.47	0.44
1:C:316:GLY:HA3	1:D:308:LEU:O	2.18	0.44
1:D:233:MET:HG2	1:D:237:ALA:O	2.18	0.44
1:D:345:LEU:HD12	1:D:345:LEU:N	2.33	0.44
1:B:10:LYS:HA	1:B:24:GLU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:VAL:HG12	1:B:159:LYS:HB2	1.99	0.44
1:B:229:PHE:N	1:B:229:PHE:HD1	2.14	0.44
1:C:61:PHE:HA	1:C:62:PRO:C	2.41	0.44
1:A:209:MET:HG2	1:A:235:VAL:HG13	2.00	0.44
1:A:221:GLY:O	1:A:240:CYS:HA	2.16	0.44
1:A:223:ASP:OD1	4:A:377:NAD:H1B	2.17	0.44
1:C:268:VAL:C	1:C:269:ILE:HG13	2.43	0.44
1:D:177:SER:HB3	1:D:322:LEU:HD12	1.99	0.44
1:D:283:HIS:CD2	1:D:286:TYR:CZ	3.05	0.44
1:A:353:LYS:CD	1:A:353:LYS:N	2.80	0.44
1:C:265:THR:CG2	1:C:289:SER:HA	2.47	0.44
1:C:241:ILE:HG12	1:C:242:SER:N	2.32	0.44
1:A:309:PHE:CZ	1:B:294:VAL:HG22	2.53	0.44
1:B:122:VAL:HG22	1:B:127:THR:O	2.18	0.44
1:B:229:PHE:CD2	1:B:240:CYS:HB2	2.53	0.44
1:A:115:ASP:OD2	1:A:120:ARG:HB3	2.18	0.44
1:C:25:GLU:C	1:C:26:ILE:HD12	2.42	0.44
1:C:183:ALA:HA	1:C:266:PHE:CZ	2.52	0.44
1:B:147:THR:HG22	1:B:148:GLU:N	2.33	0.43
1:D:265:THR:HG21	1:D:278:ALA:O	2.18	0.43
1:B:270:GLY:O	1:B:296:PRO:HD3	2.18	0.43
1:C:361:LEU:HD23	1:C:366:GLN:HB2	2.00	0.43
1:D:109:ASN:ND2	1:D:321:GLY:HA2	2.33	0.43
1:A:276:ILE:CG1	1:A:301:LEU:HD21	2.48	0.43
1:A:360:GLU:HB3	3:A:502:ACT:H3	2.00	0.43
1:C:346:ILE:HG23	1:C:371:VAL:HG23	2.00	0.43
1:D:294:VAL:HG21	3:D:378:ACT:H3	2.01	0.43
3:D:501:ACT:H2	4:D:377:NAD:H62A	1.82	0.43
1:A:18:LYS:N	1:A:53:ILE:O	2.48	0.43
1:B:45:ILE:HD11	1:B:372:LEU:HD11	1.99	0.43
1:A:152:VAL:HG23	1:A:157:VAL:HG23	1.99	0.43
1:A:164:ALA:HA	1:A:165:PRO:HD2	1.90	0.43
1:A:328:VAL:O	1:A:332:VAL:HG23	2.18	0.43
1:C:10:LYS:HA	1:C:24:GLU:O	2.19	0.43
1:A:110:LEU:HD11	1:A:116:ILE:CD1	2.48	0.43
1:C:328:VAL:N	1:C:329:PRO:HD2	2.33	0.43
1:A:14:LEU:HD11	1:A:19:GLN:O	2.18	0.43
1:A:347:THR:O	1:A:348:HIS:CD2	2.72	0.43
1:B:185:LYS:O	1:B:188:LYS:HG3	2.19	0.43
1:B:226:LYS:HA	1:B:229:PHE:CE1	2.53	0.43
1:C:253:VAL:O	1:C:257:MET:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:ILE:HG22	1:D:8:LYS:N	2.33	0.43
1:A:179:GLY:HA2	1:A:207:VAL:HG12	2.01	0.43
1:A:229:PHE:N	1:A:229:PHE:CD1	2.86	0.43
1:A:291:VAL:CG1	1:A:316:GLY:HA2	2.49	0.43
1:B:244:LYS:HA	1:B:244:LYS:HD3	1.64	0.43
1:A:116:ILE:HG22	1:A:116:ILE:O	2.19	0.43
1:B:317:CYS:SG	1:B:320:GLY:HA2	2.59	0.43
1:D:349:VAL:HA	1:D:371:VAL:O	2.19	0.43
1:B:51:HIS:HB3	1:B:57:MET:HB2	2.01	0.43
1:A:100:CYS:HB2	1:A:112:ILE:CG2	2.44	0.42
1:A:123:LEU:HD11	1:A:129:ARG:HG2	2.00	0.42
1:A:231:LYS:HE2	1:A:344:GLN:OE1	2.19	0.42
1:A:19:GLN:HG2	1:A:20:PRO:CD	2.45	0.42
1:B:231:LYS:O	1:B:235:VAL:HG23	2.20	0.42
1:C:205:LEU:O	1:C:209:MET:HG3	2.20	0.42
1:C:347:THR:CG2	1:C:368:ILE:H	2.32	0.42
1:D:65:VAL:HG23	1:D:146:PHE:HD2	1.85	0.42
1:B:140:PHE:O	1:B:141:MET:C	2.61	0.42
1:B:192:GLY:HA2	1:B:217:SER:OG	2.19	0.42
1:D:171:LEU:HD11	1:D:346:ILE:HG12	2.01	0.42
1:D:361:LEU:HD23	1:D:361:LEU:HA	1.92	0.42
1:B:122:VAL:HG13	1:B:123:LEU:O	2.19	0.42
1:B:348:HIS:HB2	1:B:370:THR:HG23	2.00	0.42
1:C:92:LEU:HD22	1:C:328:VAL:HG21	2.02	0.42
1:B:72:ILE:HG13	1:B:86:GLY:O	2.20	0.42
1:A:36:VAL:O	1:A:151:VAL:HA	2.19	0.42
1:B:122:VAL:HG13	1:B:123:LEU:N	2.35	0.42
1:C:225:ASN:HD22	1:C:228:LYS:HE3	1.83	0.42
1:B:9:CYS:O	1:B:25:GLU:HA	2.18	0.42
1:D:69:ALA:HB3	1:D:145:THR:HG21	2.02	0.42
1:A:17:GLN:CD	1:A:55:GLY:HA2	2.44	0.42
1:D:198:PHE:HA	1:D:222:ILE:HG13	2.02	0.42
1:D:301:LEU:HD23	1:D:301:LEU:C	2.44	0.42
1:A:331:LEU:HD12	1:A:331:LEU:HA	1.85	0.42
1:B:26:ILE:HD11	1:B:147:THR:CG2	2.50	0.42
1:C:43:THR:OG1	1:C:69:ALA:HB2	2.20	0.42
1:D:218:ARG:HH11	1:D:258:THR:HG22	1.83	0.42
1:A:179:GLY:HA3	1:A:206:SER:HB2	2.01	0.41
1:A:353:LYS:H	1:A:353:LYS:HD2	1.82	0.41
1:B:307:LEU:CD2	1:B:312:ARG:HH12	2.33	0.41
1:A:8:LYS:HZ2	1:A:25:GLU:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:SER:HB3	1:A:322:LEU:HD12	2.02	0.41
1:B:15:TRP:CZ2	1:B:132:CYS:SG	3.02	0.41
1:D:122:VAL:CG2	1:D:126:GLY:HA2	2.50	0.41
1:A:65:VAL:HG23	1:A:146:PHE:CD2	2.55	0.41
1:A:152:VAL:HG21	1:A:157:VAL:HG23	2.02	0.41
1:A:160:ILE:HD12	1:A:332:VAL:HG11	2.01	0.41
1:D:61:PHE:HA	1:D:62:PRO:C	2.45	0.41
1:A:190:LYS:HG2	1:A:264:TYR:OH	2.20	0.41
1:B:84:LYS:HG3	1:B:85:PRO:HD2	2.01	0.41
1:A:15:TRP:HZ2	1:A:24:GLU:OE1	2.04	0.41
1:A:36:VAL:HG22	1:A:76:ILE:HG22	2.02	0.41
1:A:224:LEU:CD2	1:A:244:LYS:HE3	2.49	0.41
1:C:26:ILE:CG2	1:C:27:GLU:N	2.83	0.41
1:A:28:VAL:HG21	1:A:149:TYR:HB2	2.02	0.41
1:A:110:LEU:HD22	1:B:310:THR:HG22	2.02	0.41
1:A:130:PHE:HE1	1:A:150:THR:HA	1.86	0.41
1:B:194:THR:HA	1:B:218:ARG:O	2.21	0.41
1:B:254:LEU:HD23	1:B:254:LEU:HA	1.90	0.41
1:D:222:ILE:HD12	1:D:222:ILE:C	2.46	0.41
1:D:304:ASP:OD2	1:D:306:MET:HB2	2.21	0.41
1:A:167:GLU:CD	1:A:167:GLU:H	2.28	0.41
1:B:231:LYS:NZ	1:B:344:GLN:O	2.49	0.41
1:B:331:LEU:HD23	1:B:331:LEU:HA	1.91	0.41
1:C:14:LEU:HD11	1:C:19:GLN:O	2.20	0.41
1:C:294:VAL:HG23	4:C:377:NAD:H1D	2.02	0.41
1:D:257:MET:HE3	1:D:257:MET:HB2	1.87	0.41
1:A:129:ARG:HG3	1:A:151:VAL:HB	2.02	0.41
1:B:276:ILE:HD11	1:B:301:LEU:CD1	2.49	0.41
1:C:122:VAL:HG21	1:C:126:GLY:HA2	2.02	0.41
1:C:315:LYS:HE2	1:D:313:THR:OG1	2.21	0.41
1:C:355:ILE:HG23	1:C:356:SER:N	2.36	0.41
1:B:15:TRP:HZ2	1:B:132:CYS:SG	2.40	0.41
1:C:176:PHE:HD1	1:C:206:SER:OG	2.03	0.41
1:A:69:ALA:O	1:A:90:ILE:HG23	2.21	0.40
1:B:10:LYS:O	1:B:148:GLU:HG3	2.21	0.40
1:B:249:PRO:O	1:B:253:VAL:HG23	2.20	0.40
1:C:8:LYS:HA	1:C:26:ILE:O	2.21	0.40
1:C:299:LYS:O	1:C:300:MET:HE2	2.21	0.40
1:D:222:ILE:HA	1:D:241:ILE:O	2.21	0.40
1:D:241:ILE:HD11	1:D:257:MET:CE	2.50	0.40
1:C:70:THR:OG1	1:C:170:CYS:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:ILE:CG1	1:C:242:SER:N	2.85	0.40
1:D:64:ILE:HG21	1:D:147:THR:OG1	2.21	0.40
1:B:92:LEU:HD13	1:B:324:SER:HB3	2.03	0.40
1:B:164:ALA:O	1:B:166:PRO:HD3	2.21	0.40
1:C:33:THR:HG22	1:C:34:LYS:HD3	2.02	0.40
1:C:84:LYS:HG2	1:C:87:ASP:OD2	2.21	0.40
1:D:93:PHE:HB2	1:D:141:MET:HB3	2.04	0.40
1:A:168:LYS:HA	1:A:346:ILE:HD11	2.04	0.40
1:B:139:HIS:N	1:B:139:HIS:CD2	2.89	0.40
1:D:115:ASP:OD1	1:D:120:ARG:HB2	2.21	0.40
1:A:353:LYS:N	1:A:353:LYS:HD2	2.37	0.40
1:C:306:MET:HE1	1:C:309:PHE:CD2	2.56	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	371/373 (100%)	328 (88%)	36 (10%)	7 (2%)	6	30
1	B	371/373 (100%)	332 (90%)	32 (9%)	7 (2%)	6	30
1	C	371/373 (100%)	323 (87%)	41 (11%)	7 (2%)	6	30
1	D	371/373 (100%)	337 (91%)	30 (8%)	4 (1%)	11	43
All	All	1484/1492 (100%)	1320 (89%)	139 (9%)	25 (2%)	7	32

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	B	3	ALA
1	C	324	SER

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Mol	Chain	Res	Type
1	A	3	ALA
1	B	324	SER
1	D	109	ASN
1	B	249	PRO
1	C	175	GLY
1	C	229	PHE
1	C	284	MET
1	A	109	ASN
1	B	110	LEU
1	B	174	CYS
1	D	174	CYS
1	A	110	LEU
1	A	284	MET
1	C	174	CYS
1	D	284	MET
1	B	65	VAL
1	A	166	PRO
1	A	236	GLY
1	C	65	VAL
1	D	65	VAL
1	B	368	ILE
1	C	269	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	312/312 (100%)	288 (92%)	24 (8%)	12	40
1	B	312/312 (100%)	280 (90%)	32 (10%)	7	28
1	C	312/312 (100%)	289 (93%)	23 (7%)	13	42
1	D	312/312 (100%)	291 (93%)	21 (7%)	15	46
All	All	1248/1248 (100%)	1148 (92%)	100 (8%)	11	38

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	36	VAL
1	A	73	VAL
1	A	83	VAL
1	A	96	GLN
1	A	101	ASN
1	A	113	ARG
1	A	118	THR
1	A	207	VAL
1	A	213	SER
1	A	230	GLU
1	A	233	MET
1	A	248	LYS
1	A	268	VAL
1	A	273	GLU
1	A	277	ASP
1	A	299	LYS
1	A	300	MET
1	A	301	LEU
1	A	331	LEU
1	A	338	LYS
1	A	339	LYS
1	A	353	LYS
1	A	362	LEU
1	B	2	THR
1	B	16	GLU
1	B	19	GLN
1	B	40	ILE
1	B	53	ILE
1	B	57	MET
1	B	72	ILE
1	B	99	GLU
1	B	101	ASN
1	B	112	ILE
1	B	116	ILE
1	B	118	THR
1	B	122	VAL
1	B	131	THR
1	B	135	LYS
1	B	153	ASP
1	B	166	PRO
1	B	167	GLU
1	B	185	LYS

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Mol	Chain	Res	Type
1	B	228	LYS
1	B	242	SER
1	B	249	PRO
1	B	251	SER
1	B	252	GLU
1	B	262	VAL
1	B	268	VAL
1	B	273	GLU
1	B	302	THR
1	B	310	THR
1	B	322	LEU
1	B	325	ARG
1	B	338	LYS
1	C	5	LYS
1	C	48	THR
1	C	60	LYS
1	C	70	THR
1	C	107	ASP
1	C	131	THR
1	C	137	VAL
1	C	147	THR
1	C	196	VAL
1	C	224	LEU
1	C	235	VAL
1	C	244	LYS
1	C	246	SER
1	C	249	PRO
1	C	262	VAL
1	C	275	MET
1	C	282	CYS
1	C	304	ASP
1	C	313	THR
1	C	339	LYS
1	C	340	PHE
1	C	361	LEU
1	C	367	SER
1	D	10	LYS
1	D	19	GLN
1	D	33	THR
1	D	45	ILE
1	D	84	LYS
1	D	116	ILE

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Mol	Chain	Res	Type
1	D	118	THR
1	D	131	THR
1	D	167	GLU
1	D	222	ILE
1	D	231	LYS
1	D	247	THR
1	D	251	SER
1	D	268	VAL
1	D	274	THR
1	D	275	MET
1	D	284	MET
1	D	310	THR
1	D	353	LYS
1	D	356	SER
1	D	373	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	142	ASN
1	A	261	ASN
1	B	96	GLN
1	B	260	ASN
1	B	283	HIS
1	C	17	GLN
1	C	51	HIS
1	D	109	ASN
1	D	142	ASN
1	D	261	ASN
1	D	283	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 16 are monoatomic - leaving 14 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	$\# Z > 2$
3	ACT	A	501	-	3,3,3	0.90	0	3,3,3	0.75	0
3	ACT	C	378	-	3,3,3	0.82	0	3,3,3	0.95	0
3	ACT	A	502	-	3,3,3	1.19	0	3,3,3	0.07	0
3	ACT	B	378	2	3,3,3	0.86	0	3,3,3	0.78	0
4	NAD	B	377	2	46,48,48	2.49	10 (21%)	64,73,73	2.11	15 (23%)
4	NAD	D	377	2	46,48,48	2.61	11 (23%)	64,73,73	2.07	17 (26%)
3	ACT	A	378	-	3,3,3	0.94	0	3,3,3	0.58	0
3	ACT	B	501	2	3,3,3	0.93	0	3,3,3	0.59	0
4	NAD	A	377	2	46,48,48	2.19	11 (23%)	64,73,73	1.93	23 (35%)
3	ACT	B	503	2	3,3,3	1.04	0	3,3,3	0.68	0
3	ACT	D	378	-	3,3,3	0.85	0	3,3,3	0.91	0
3	ACT	D	501	-	3,3,3	0.91	0	3,3,3	0.76	0
4	NAD	C	377	2	46,48,48	2.74	11 (23%)	64,73,73	1.72	12 (18%)
3	ACT	B	502	-	3,3,3	0.99	0	3,3,3	0.70	0

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	NAD	B	377	2	-	15/30/62/62	0/5/5/5
4	NAD	A	377	2	-	9/30/62/62	0/5/5/5
4	NAD	D	377	2	-	11/30/62/62	0/5/5/5
4	NAD	C	377	2	-	13/30/62/62	0/5/5/5

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	377	NAD	C3N-C7N	-14.10	1.29	1.50
4	D	377	NAD	C3N-C7N	-12.53	1.31	1.50
4	B	377	NAD	C3N-C7N	-11.02	1.34	1.50
4	A	377	NAD	C3N-C7N	-8.45	1.38	1.50
4	D	377	NAD	O4D-C1D	5.45	1.48	1.40
4	C	377	NAD	PA-O3	-5.30	1.53	1.59
4	A	377	NAD	PN-O3	-5.20	1.53	1.59
4	A	377	NAD	C2N-N1N	-4.82	1.29	1.35
4	B	377	NAD	PN-O3	-4.78	1.54	1.59
4	D	377	NAD	C4N-C3N	-4.71	1.32	1.39
4	D	377	NAD	C5N-C4N	-4.53	1.31	1.38
4	C	377	NAD	C8A-N7A	4.50	1.40	1.31
4	A	377	NAD	C4N-C3N	-4.20	1.33	1.39
4	B	377	NAD	C4N-C3N	-4.20	1.33	1.39
4	A	377	NAD	C8A-N7A	4.16	1.39	1.31
4	C	377	NAD	C4N-C3N	-4.10	1.33	1.39
4	B	377	NAD	C5N-C4N	-4.09	1.31	1.38
4	B	377	NAD	C8A-N7A	3.86	1.39	1.31
4	B	377	NAD	C2A-N1A	3.82	1.40	1.33
4	C	377	NAD	C2A-N3A	3.80	1.40	1.33
4	D	377	NAD	C8A-N7A	3.73	1.38	1.31
4	B	377	NAD	C2A-N3A	3.69	1.40	1.33
4	A	377	NAD	C5N-C4N	-3.50	1.32	1.38
4	C	377	NAD	C2A-N1A	3.43	1.40	1.33
4	B	377	NAD	C4A-N3A	3.21	1.40	1.34
4	C	377	NAD	C5N-C4N	-3.19	1.33	1.38
4	D	377	NAD	C2N-N1N	-3.10	1.31	1.35
4	D	377	NAD	PA-O3	3.04	1.62	1.59
4	B	377	NAD	C2N-C3N	-3.02	1.34	1.39
4	D	377	NAD	C2A-N1A	3.00	1.39	1.33
4	D	377	NAD	C4A-N3A	2.95	1.39	1.34
4	C	377	NAD	PN-O3	-2.84	1.56	1.59
4	D	377	NAD	C2N-C3N	-2.80	1.34	1.39
4	C	377	NAD	C2N-C3N	-2.79	1.34	1.39
4	A	377	NAD	C2A-N1A	2.65	1.38	1.33
4	B	377	NAD	O4D-C1D	-2.63	1.37	1.40
4	A	377	NAD	C6N-N1N	-2.33	1.30	1.35
4	A	377	NAD	C4A-N3A	2.24	1.38	1.34
4	A	377	NAD	C2A-N3A	2.19	1.37	1.33
4	C	377	NAD	C2N-N1N	-2.14	1.32	1.35
4	A	377	NAD	C2N-C3N	-2.07	1.35	1.39
4	D	377	NAD	C2A-N3A	2.05	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	377	NAD	C4A-N3A	2.05	1.38	1.34

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	377	NAD	C4D-O4D-C1D	-8.24	102.38	109.92
4	D	377	NAD	O7N-C7N-C3N	-6.48	111.67	119.60
4	D	377	NAD	N3A-C2A-N1A	-5.52	120.23	128.58
4	B	377	NAD	O7N-C7N-N7N	-5.22	115.07	122.62
4	D	377	NAD	C3N-C7N-N7N	4.81	123.67	117.74
4	B	377	NAD	C6N-N1N-C2N	-4.77	117.82	121.88
4	C	377	NAD	C5A-C4A-N9A	4.45	110.66	105.81
4	C	377	NAD	C6N-N1N-C2N	-4.35	118.17	121.88
4	B	377	NAD	O5B-C5B-C4B	-4.33	94.24	108.99
4	B	377	NAD	C3N-C7N-N7N	4.29	123.02	117.74
4	A	377	NAD	O2N-PN-O3	3.98	118.04	107.27
4	C	377	NAD	O2N-PN-O3	3.97	118.00	107.27
4	D	377	NAD	C2N-C3N-C4N	3.90	122.79	118.26
4	D	377	NAD	O2N-PN-O3	3.89	117.79	107.27
4	B	377	NAD	N3A-C2A-N1A	-3.88	122.70	128.58
4	A	377	NAD	C3N-C7N-N7N	3.87	122.50	117.74
4	A	377	NAD	N3A-C2A-N1A	-3.84	122.76	128.58
4	B	377	NAD	C5A-C4A-N9A	3.80	109.95	105.81
4	D	377	NAD	C3B-C2B-C1B	-3.78	94.32	101.46
4	A	377	NAD	C4A-N9A-C8A	-3.69	101.86	105.74
4	A	377	NAD	O4B-C1B-C2B	-3.67	98.76	106.62
4	C	377	NAD	C2N-C3N-C4N	3.65	122.50	118.26
4	B	377	NAD	C6N-N1N-C1D	3.46	126.53	119.73
4	D	377	NAD	C6N-N1N-C2N	-3.45	118.94	121.88
4	C	377	NAD	N3A-C2A-N1A	-3.44	123.37	128.58
4	A	377	NAD	C5A-N7A-C8A	-3.32	98.23	103.45
4	D	377	NAD	O2N-PN-O1N	-3.29	97.14	112.44
4	A	377	NAD	C6A-C5A-N7A	-3.24	125.84	132.09
4	A	377	NAD	C5A-C4A-N9A	3.14	109.23	105.81
4	D	377	NAD	O5D-C5D-C4D	3.09	119.53	108.99
4	B	377	NAD	C5A-C4A-N3A	-3.07	122.49	126.72
4	A	377	NAD	C4A-C5A-N7A	3.03	114.04	110.58
4	A	377	NAD	O3-PA-O1A	-2.98	101.73	110.70
4	C	377	NAD	C4A-N9A-C8A	-2.97	102.62	105.74
4	D	377	NAD	C6A-C5A-N7A	-2.94	126.43	132.09
4	A	377	NAD	N6A-C6A-N1A	2.94	124.92	118.38
4	D	377	NAD	N6A-C6A-N1A	2.92	124.89	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	377	NAD	C5A-C6A-N6A	-2.88	116.15	123.29
4	A	377	NAD	O7N-C7N-N7N	-2.80	118.57	122.62
4	C	377	NAD	O4B-C1B-C2B	-2.80	100.63	106.62
4	A	377	NAD	O5B-C5B-C4B	-2.74	99.65	108.99
4	B	377	NAD	O2N-PN-O3	2.69	114.54	107.27
4	D	377	NAD	C4N-C3N-C7N	-2.68	113.77	121.06
4	A	377	NAD	C6N-N1N-C1D	2.66	124.95	119.73
4	D	377	NAD	O2N-PN-O5D	2.65	119.58	107.57
4	A	377	NAD	C2B-C1B-N9A	2.62	119.81	113.30
4	C	377	NAD	C2B-C3B-C4B	-2.59	97.60	102.61
4	A	377	NAD	C1B-N9A-C8A	2.57	132.80	127.09
4	D	377	NAD	C6A-C5A-C4A	2.55	120.66	117.18
4	B	377	NAD	C6A-C5A-C4A	2.52	120.62	117.18
4	A	377	NAD	O2A-PA-O3	2.51	114.06	107.27
4	A	377	NAD	C2B-C3B-C4B	-2.47	97.84	102.61
4	C	377	NAD	C6A-C5A-C4A	2.44	120.50	117.18
4	B	377	NAD	C4A-N9A-C8A	-2.43	103.19	105.74
4	C	377	NAD	C2D-C3D-C4D	-2.39	98.00	102.61
4	D	377	NAD	C2A-N1A-C6A	2.37	122.62	118.73
4	B	377	NAD	O4B-C4B-C3B	2.36	109.84	105.15
4	B	377	NAD	O2A-PA-O1A	-2.34	101.56	112.44
4	C	377	NAD	C4N-C3N-C7N	-2.28	114.85	121.06
4	A	377	NAD	O5D-C5D-C4D	2.28	116.74	108.99
4	C	377	NAD	C1B-N9A-C8A	2.26	132.11	127.09
4	D	377	NAD	C5A-C4A-N3A	-2.22	123.66	126.72
4	A	377	NAD	O5D-PN-O1N	-2.14	100.47	108.94
4	A	377	NAD	C2N-N1N-C1D	-2.08	114.53	119.13
4	B	377	NAD	C2B-C3B-C4B	-2.07	98.61	102.61
4	A	377	NAD	C5A-C4A-N3A	-2.06	123.87	126.72
4	D	377	NAD	C4A-C5A-N7A	2.04	112.91	110.58

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	377	NAD	O4D-C1D-N1N-C6N
4	A	377	NAD	C2D-C1D-N1N-C2N
4	B	377	NAD	C5B-O5B-PA-O1A
4	B	377	NAD	C5B-O5B-PA-O2A
4	B	377	NAD	C5B-O5B-PA-O3
4	B	377	NAD	C5D-O5D-PN-O3
4	B	377	NAD	C5D-O5D-PN-O2N

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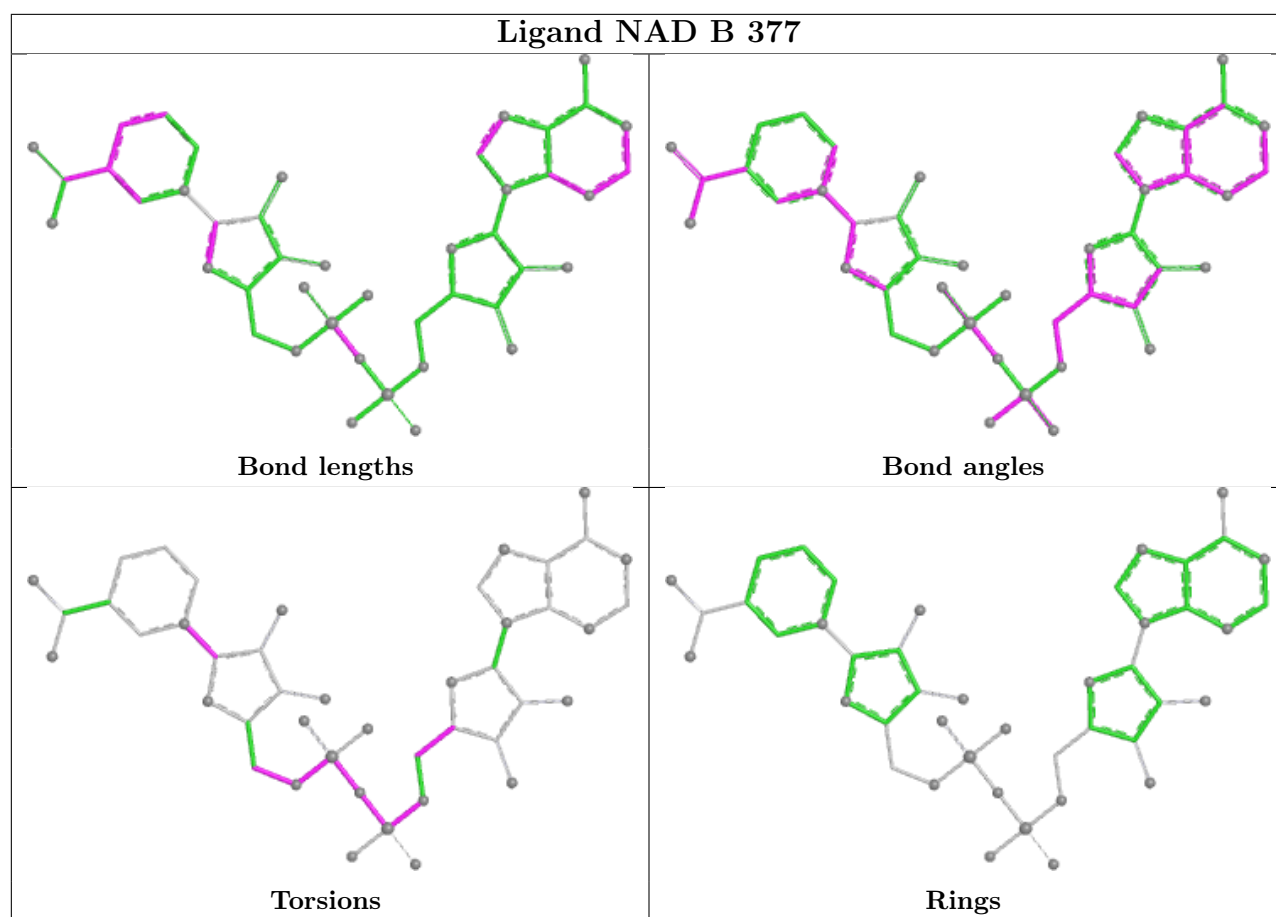
Mol	Chain	Res	Type	Atoms
4	C	377	NAD	C5B-O5B-PA-O1A
4	C	377	NAD	C5B-O5B-PA-O2A
4	C	377	NAD	C5B-O5B-PA-O3
4	C	377	NAD	C3B-C4B-C5B-O5B
4	C	377	NAD	O4D-C1D-N1N-C2N
4	C	377	NAD	O4D-C1D-N1N-C6N
4	C	377	NAD	C2D-C1D-N1N-C2N
4	C	377	NAD	C2D-C1D-N1N-C6N
4	D	377	NAD	C5B-O5B-PA-O1A
4	D	377	NAD	C5B-O5B-PA-O2A
4	D	377	NAD	C5B-O5B-PA-O3
4	D	377	NAD	PN-O3-PA-O5B
4	D	377	NAD	O4D-C1D-N1N-C2N
4	D	377	NAD	O4D-C1D-N1N-C6N
4	D	377	NAD	C2D-C1D-N1N-C2N
4	A	377	NAD	O4D-C4D-C5D-O5D
4	C	377	NAD	O4D-C4D-C5D-O5D
4	B	377	NAD	O4B-C4B-C5B-O5B
4	C	377	NAD	O4B-C4B-C5B-O5B
4	B	377	NAD	C3B-C4B-C5B-O5B
4	C	377	NAD	C3D-C4D-C5D-O5D
4	A	377	NAD	C3D-C4D-C5D-O5D
4	B	377	NAD	PN-O3-PA-O5B
4	B	377	NAD	PA-O3-PN-O5D
4	B	377	NAD	C5D-O5D-PN-O1N
4	D	377	NAD	C5D-O5D-PN-O1N
4	B	377	NAD	C2D-C1D-N1N-C2N
4	D	377	NAD	O4B-C4B-C5B-O5B
4	A	377	NAD	O4D-C1D-N1N-C2N
4	B	377	NAD	O4D-C1D-N1N-C2N
4	A	377	NAD	O4B-C4B-C5B-O5B
4	B	377	NAD	C4D-C5D-O5D-PN
4	D	377	NAD	C3B-C4B-C5B-O5B
4	A	377	NAD	PA-O3-PN-O2N
4	B	377	NAD	PN-O3-PA-O2A
4	C	377	NAD	PA-O3-PN-O1N
4	C	377	NAD	PA-O3-PN-O2N
4	A	377	NAD	C3B-C4B-C5B-O5B
4	A	377	NAD	PA-O3-PN-O1N
4	B	377	NAD	PN-O3-PA-O1A
4	D	377	NAD	PN-O3-PA-O2A

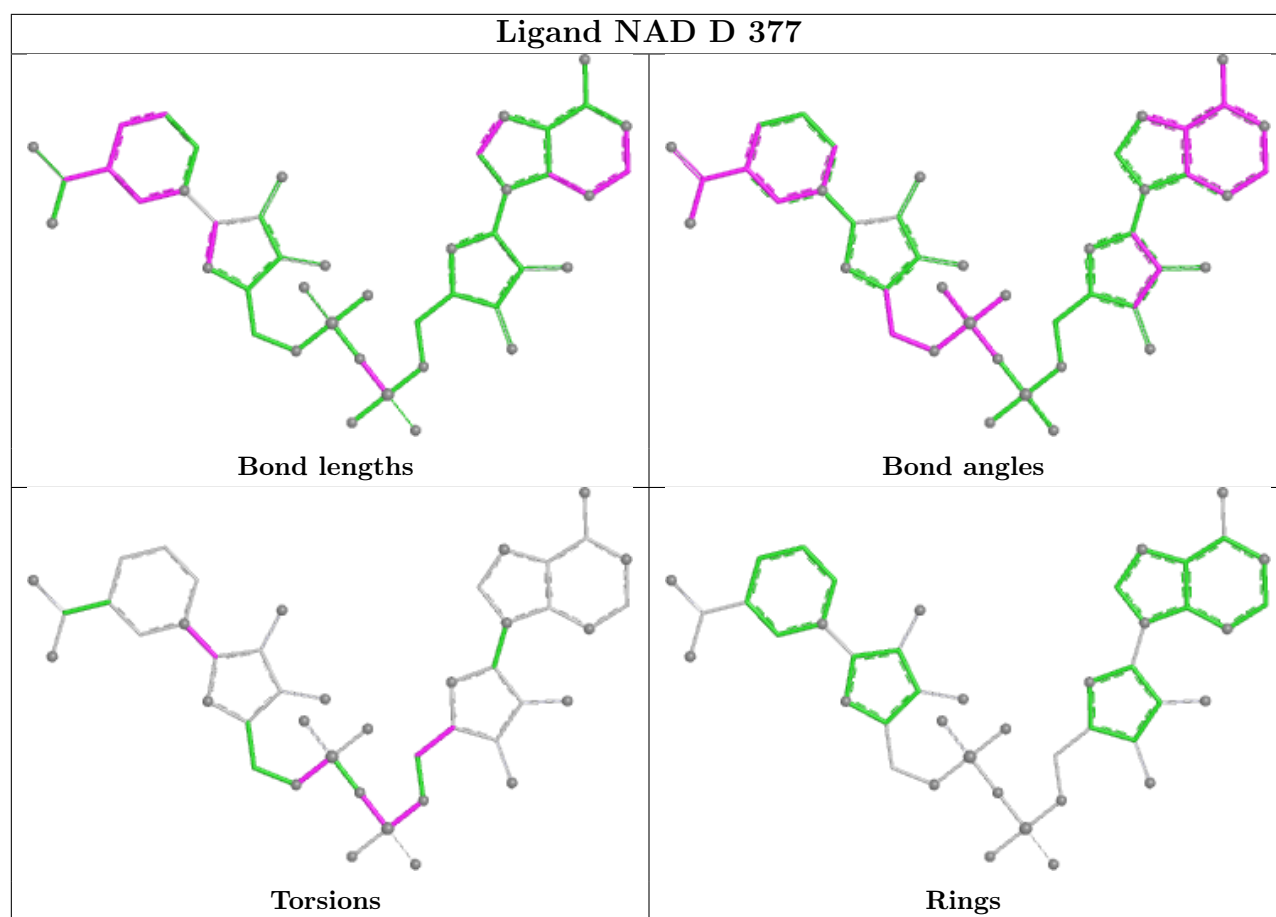
There are no ring outliers.

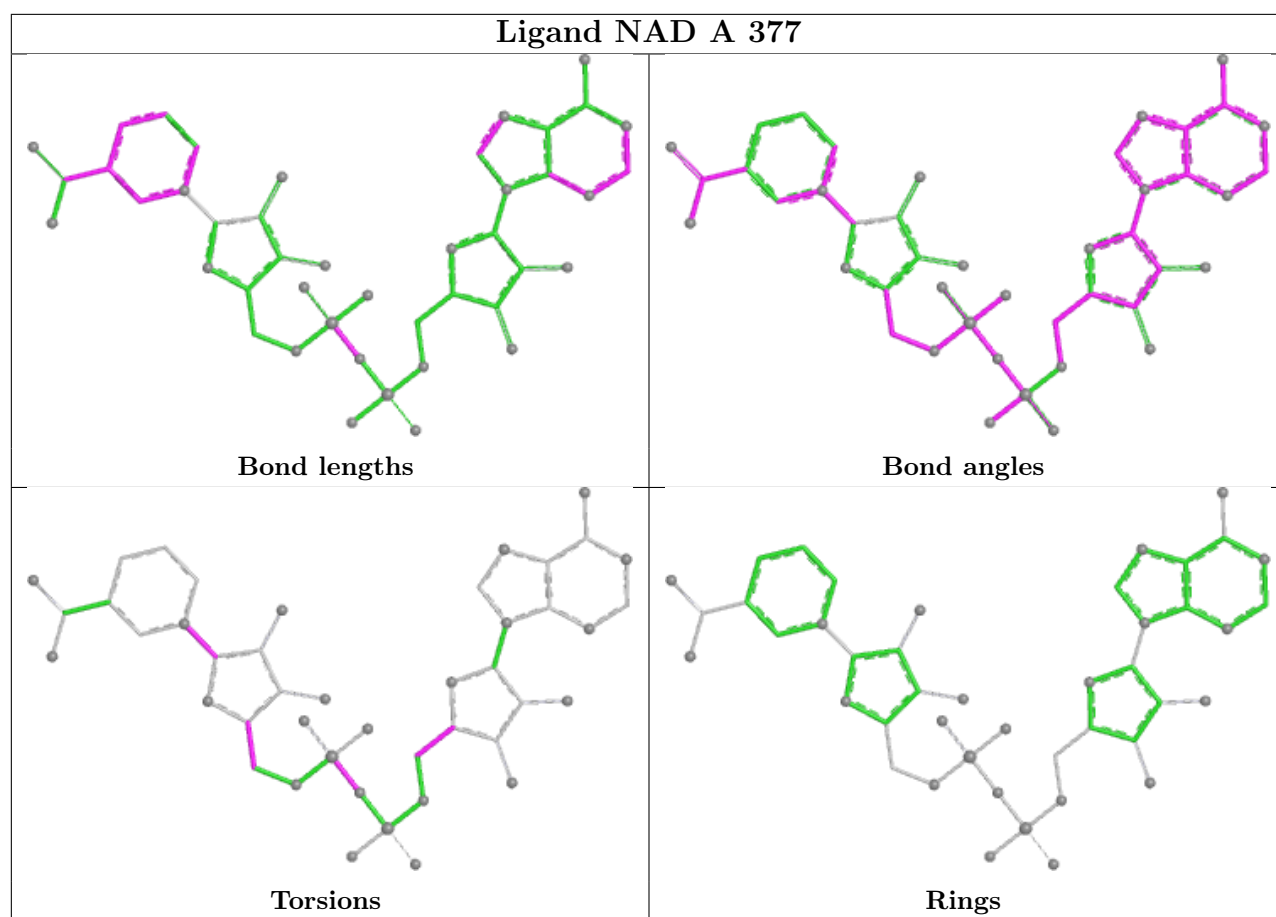
9 monomers are involved in 20 short contacts:

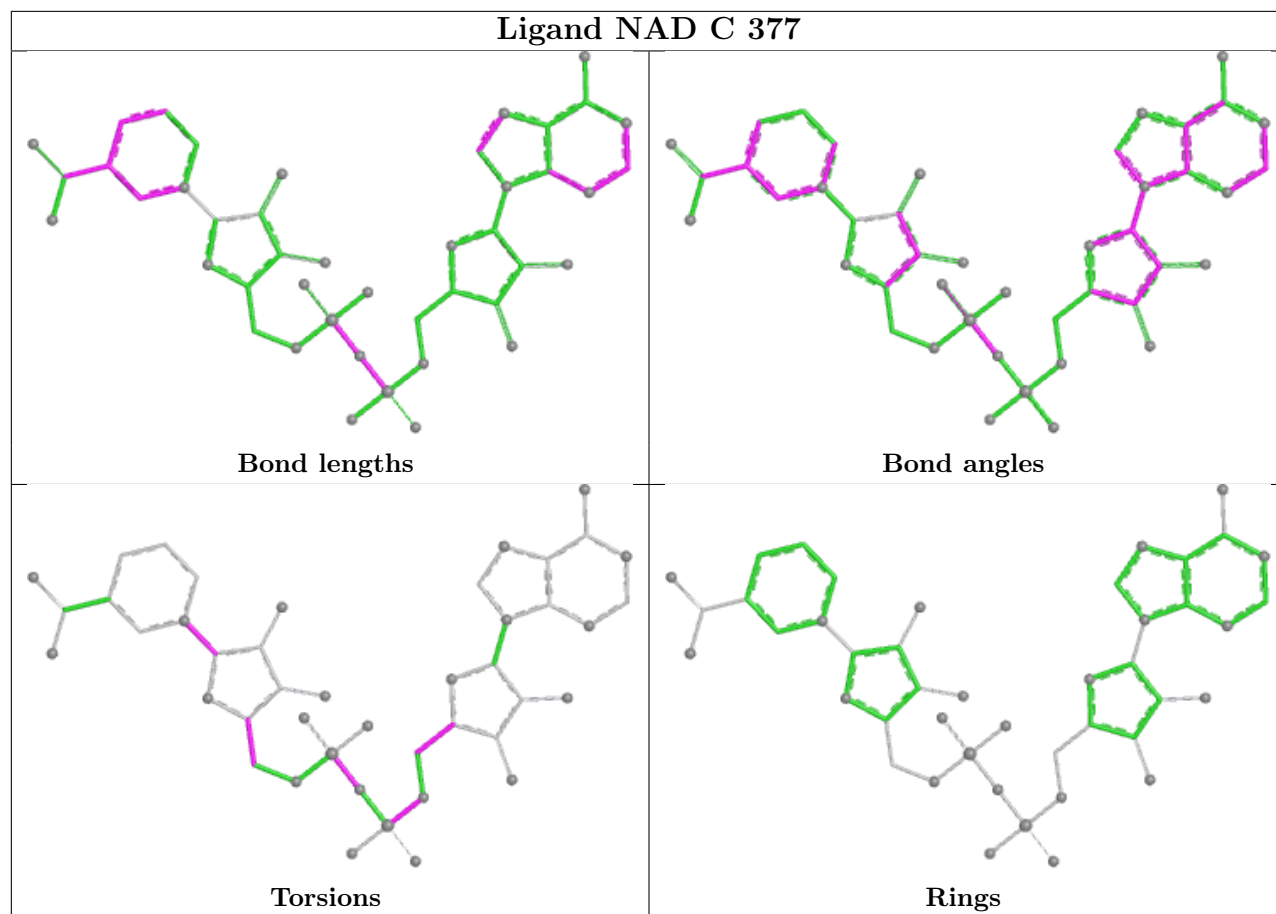
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	378	ACT	1	0
3	A	502	ACT	2	0
4	B	377	NAD	2	0
4	D	377	NAD	9	0
3	A	378	ACT	1	0
4	A	377	NAD	2	0
3	D	378	ACT	2	0
3	D	501	ACT	1	0
4	C	377	NAD	3	0

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	373/373 (100%)	-0.22	0 100 100	20, 20, 20, 20	0
1	B	373/373 (100%)	-0.30	1 (0%) 90 79	15, 15, 15, 15	0
1	C	373/373 (100%)	-0.08	3 (0%) 82 64	26, 26, 26, 26	0
1	D	373/373 (100%)	-0.35	2 (0%) 87 72	15, 15, 15, 15	0
All	All	1492/1492 (100%)	-0.24	6 (0%) 88 76	15, 15, 26, 26	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	206	SER	3.3
1	D	78	GLU	2.5
1	C	66	GLY	2.5
1	C	199	GLY	2.1
1	B	256	GLU	2.0
1	D	1	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

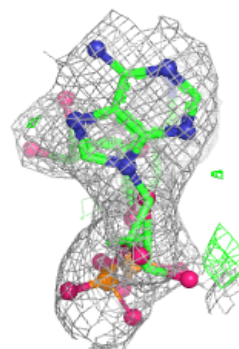
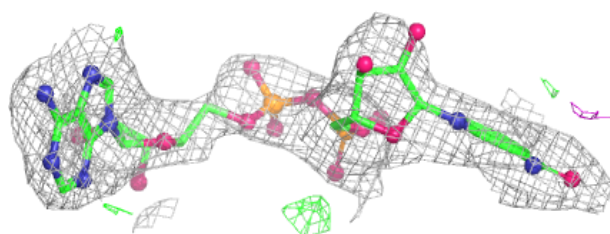
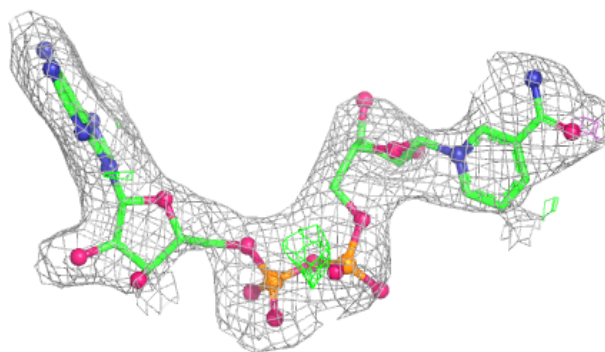
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	C	401	1/1	0.28	0.07	15,15,15,15	1
3	ACT	A	502	4/4	0.43	0.25	19,19,19,19	0
2	ZN	D	401	1/1	0.75	0.03	24,24,24,24	0
3	ACT	C	378	4/4	0.77	0.25	25,25,25,25	0
2	ZN	D	375	1/1	0.82	0.03	14,14,14,14	0
3	ACT	A	378	4/4	0.90	0.09	19,19,19,19	0
3	ACT	D	378	4/4	0.90	0.08	14,14,14,14	0
2	ZN	D	402	1/1	0.91	0.06	27,27,27,27	0
3	ACT	D	501	4/4	0.91	0.08	14,14,14,14	0
2	ZN	B	376	1/1	0.92	0.03	15,15,15,15	0
4	NAD	C	377	44/44	0.92	0.10	25,25,25,25	0
3	ACT	A	501	4/4	0.93	0.11	19,19,19,19	0
3	ACT	B	378	4/4	0.93	0.09	15,15,15,15	0
3	ACT	B	503	4/4	0.94	0.07	15,15,15,15	0
3	ACT	B	502	4/4	0.94	0.08	15,15,15,15	0
4	NAD	B	377	44/44	0.94	0.09	15,15,15,15	0
2	ZN	D	403	1/1	0.94	0.04	17,17,17,17	1
2	ZN	D	376	1/1	0.95	0.05	14,14,14,14	0
4	NAD	A	377	44/44	0.96	0.09	19,19,19,19	0
3	ACT	B	501	4/4	0.96	0.06	15,15,15,15	0
2	ZN	B	401	1/1	0.96	0.05	23,23,23,23	0
4	NAD	D	377	44/44	0.96	0.07	14,14,14,14	0
2	ZN	A	376	1/1	0.97	0.05	19,19,19,19	0
2	ZN	C	375	1/1	0.97	0.01	25,25,25,25	0
2	ZN	A	375	1/1	0.98	0.06	19,19,19,19	0
2	ZN	A	401	1/1	0.98	0.11	15,15,15,15	0
2	ZN	B	403	1/1	0.98	0.05	24,24,24,24	0
2	ZN	B	375	1/1	0.98	0.01	15,15,15,15	0
2	ZN	C	376	1/1	0.98	0.02	25,25,25,25	0
2	ZN	B	402	1/1	0.99	0.02	19,19,19,19	0

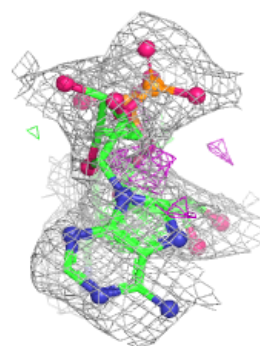
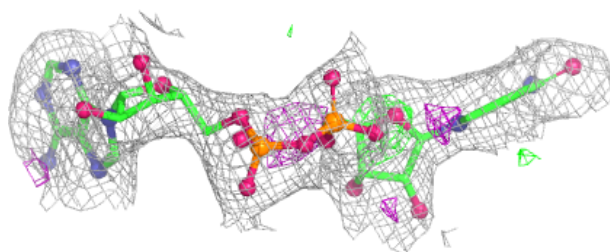
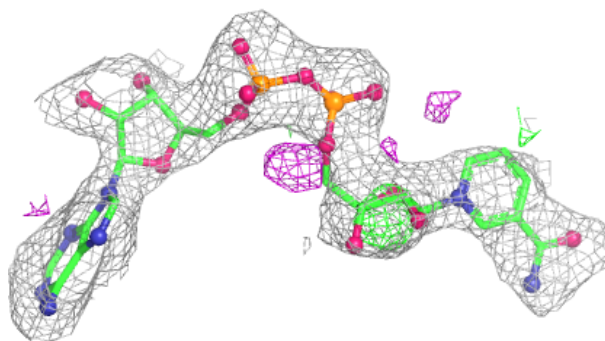
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD C 377:

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

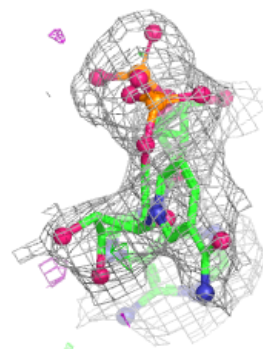
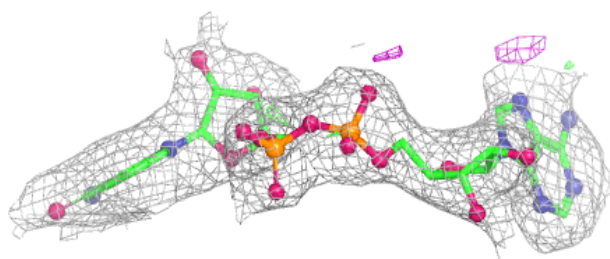
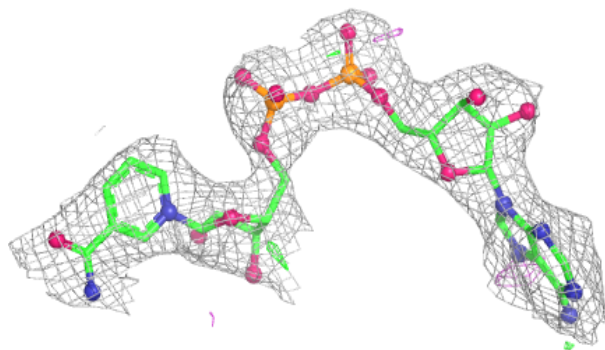
**Electron density around NAD B 377:**

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

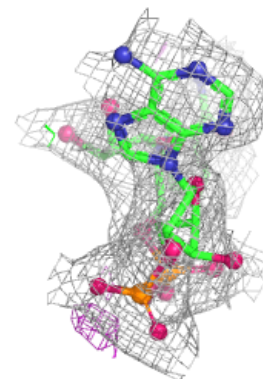
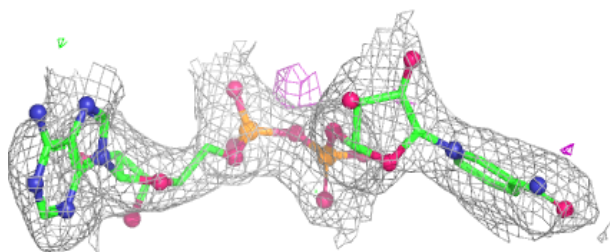
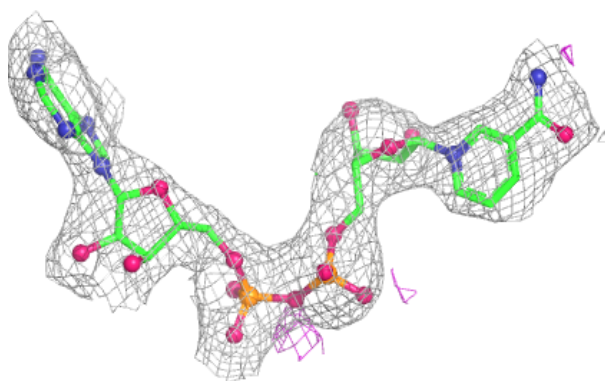


Electron density around NAD A 377:

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

**Electron density around NAD 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.