



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:37 PM UTC

PDB ID : 1D1T / pdb_00001d1t
Title : MUTANT OF HUMAN SIGMA ALCOHOL DEHYDROGENASE WITH
LEUCINE AT POSITION 141
Authors : Xie, P.T.; Hurley, T.D.
Deposited on : 1999-09-21
Resolution : 2.40 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

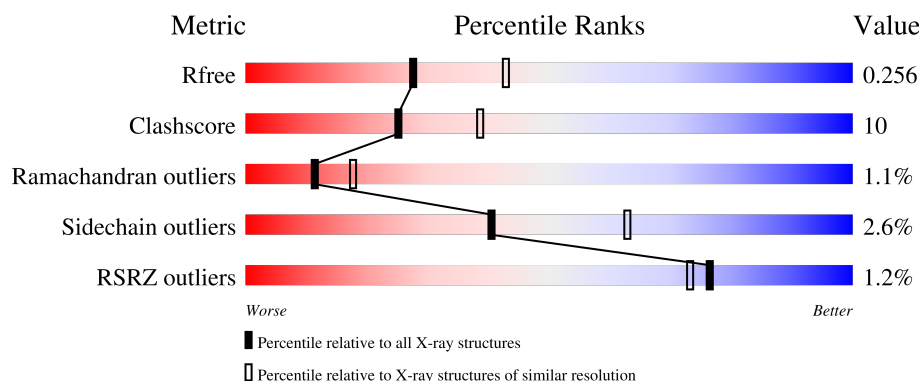
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	79% 19% .
1	B	373	76% 21% .
1	C	373	4% 74% 25% .
1	D	373	77% 21% .

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	501	-	-	X	-
3	ACT	A	502	-	-	-	X
3	ACT	A	513	-	-	-	X
3	ACT	D	509	-	-	X	-
3	ACT	D	514	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11799 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 CLASS IV SIGMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2789	1773	468	526	22			
1	B	373	Total	C	N	O	S	0	0	0
			2789	1773	468	526	22			
1	C	373	Total	C	N	O	S	0	0	0
			2789	1773	468	526	22			
1	D	373	Total	C	N	O	S	0	0	0
			2789	1773	468	526	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	LEU	MET	engineered mutation	UNP P40394
B	141	LEU	MET	engineered mutation	UNP P40394
C	141	LEU	MET	engineered mutation	UNP P40394
D	141	LEU	MET	engineered mutation	UNP P40394

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

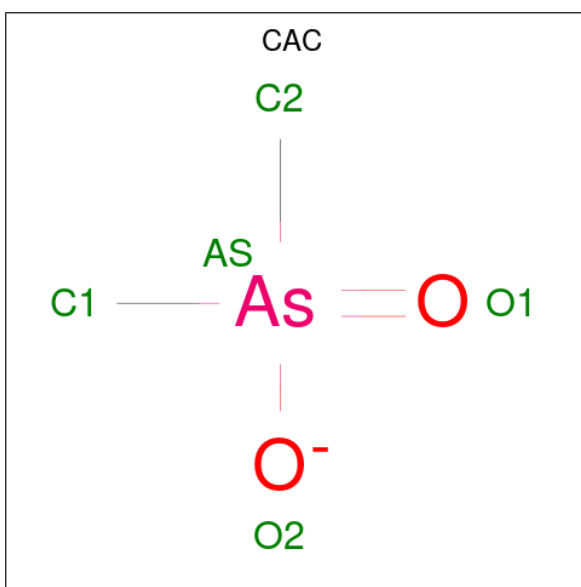
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Zn	0	0
			6	6		
2	B	5	Total	Zn	0	0
			5	5		
2	C	3	Total	Zn	0	0
			3	3		
2	D	5	Total	Zn	0	0
			5	5		

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



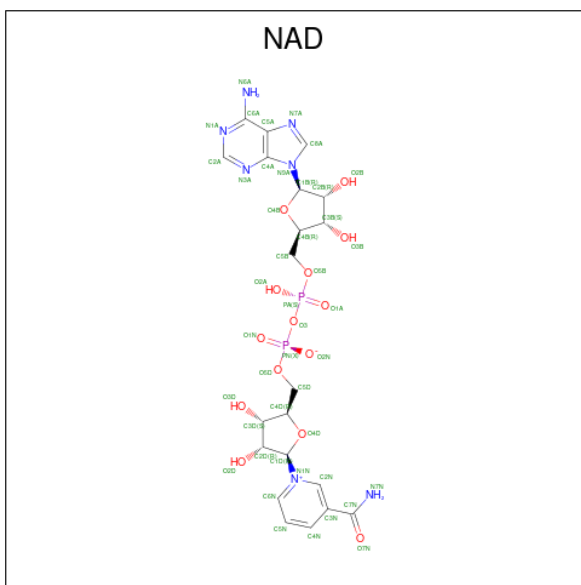
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total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

- Molecule 4 is CACODYLATE ION (CCD ID: CAC') (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

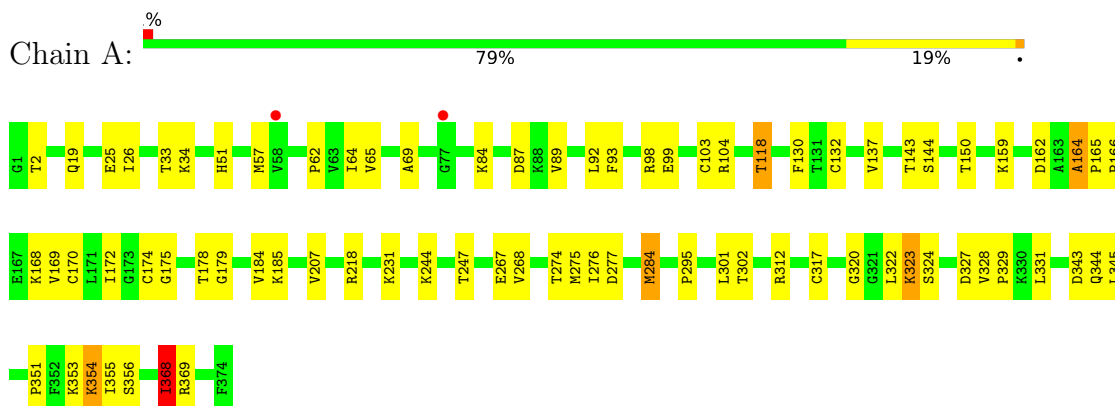
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	79	Total O 79 79	0	0
6	B	126	Total O 126 126	0	0
6	C	45	Total O 45 45	0	0
6	D	121	Total O 121 121	0	0

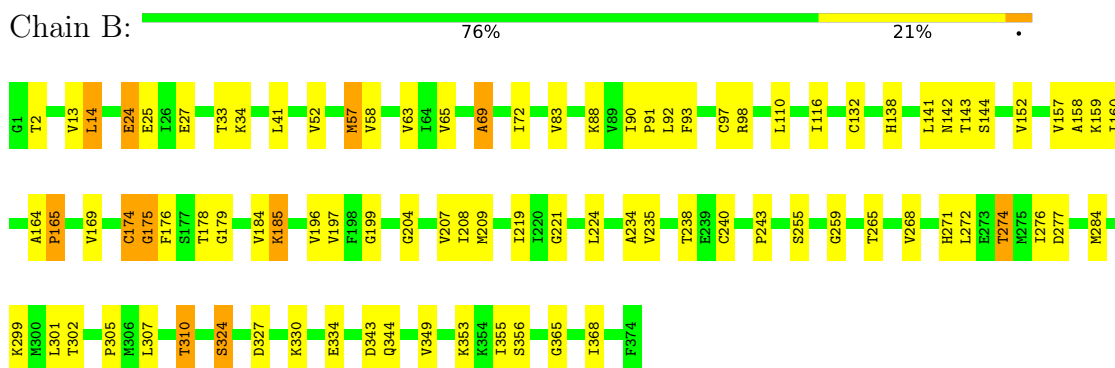
3 Residue-property plots

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.

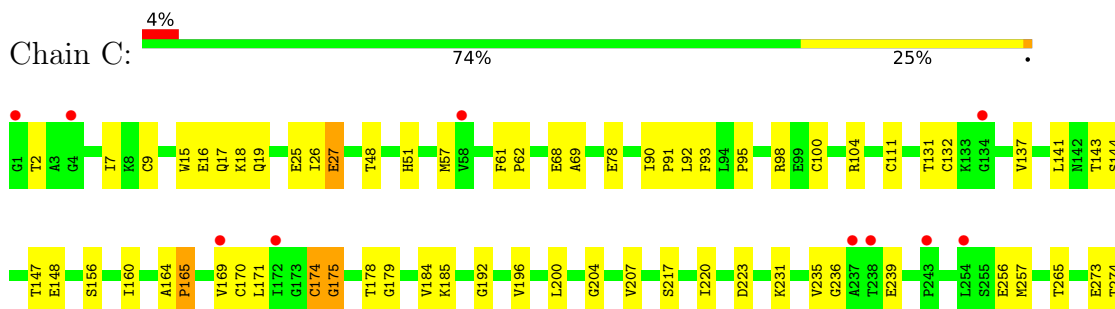
• Molecule 1: ALCOHOL DEHYDROGENASE CLASS IV SIGMA CHAIN

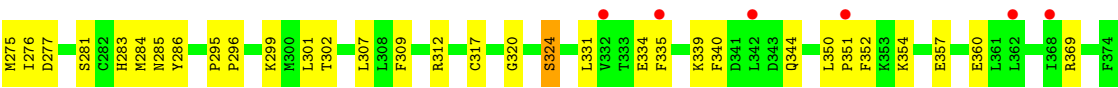


• Molecule 1: ALCOHOL DEHYDROGENASE CLASS IV SIGMA CHAIN

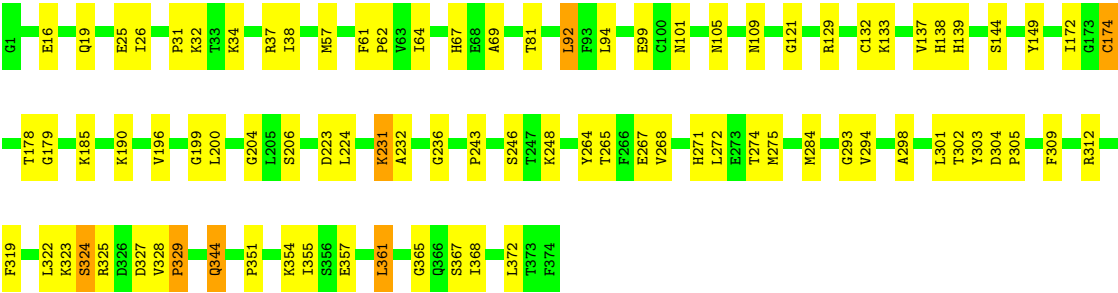
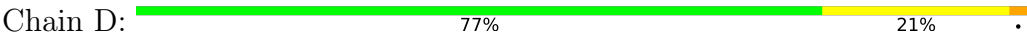


• Molecule 1: ALCOHOL DEHYDROGENASE CLASS IV SIGMA CHAIN





● Molecule 1: ALCOHOL DEHYDROGENASE CLASS IV SIGMA CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.90Å 90.50Å 119.80Å 90.00° 99.30° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	77.0 (50.00-2.40) 90.8 (50.00-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.216 , 0.274 0.205 , 0.256	Depositor DCC
R_{free} test set	4522 reflections (7.04%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11799	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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: CAC, 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	0.56	1/2840 (0.0%)	0.98	8/3840 (0.2%)
1	B	0.63	0/2840	1.02	11/3840 (0.3%)
1	C	0.52	0/2840	0.97	7/3840 (0.2%)
1	D	0.62	0/2840	0.99	12/3840 (0.3%)
All	All	0.58	1/11360 (0.0%)	0.99	38/15360 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	MET	SD-CE	-5.16	1.66	1.79

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	368	ILE	N-CA-C	-7.20	94.36	109.34
1	C	184	VAL	N-CA-C	7.03	117.75	110.36
1	C	25	GLU	N-CA-C	-6.87	97.70	108.90
1	A	327	ASP	N-CA-C	6.78	120.03	111.69
1	D	25	GLU	N-CA-C	-6.67	97.86	108.73
1	A	184	VAL	N-CA-C	6.51	117.29	110.72
1	D	327	ASP	N-CA-C	6.42	119.58	111.69
1	B	324	SER	N-CA-C	6.25	124.11	110.80
1	D	236	GLY	N-CA-C	6.16	123.16	114.85
1	B	349	VAL	N-CA-C	-6.11	98.83	107.75
1	B	165	PRO	CA-C-N	6.02	125.50	119.24
1	B	165	PRO	C-N-CA	6.02	125.50	119.24
1	D	304	ASP	CA-C-N	5.94	126.09	119.32
1	D	304	ASP	C-N-CA	5.94	126.09	119.32
1	B	69	ALA	N-CA-C	5.89	118.02	109.07
1	A	368	ILE	N-CA-C	-5.88	97.11	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	THR	N-CA-C	-5.79	106.55	113.97
1	D	323	LYS	N-CA-C	-5.74	97.08	107.75
1	D	298	ALA	N-CA-C	5.70	119.29	111.54
1	C	165	PRO	CA-C-N	5.66	126.92	119.84
1	C	165	PRO	C-N-CA	5.66	126.92	119.84
1	D	324	SER	N-CA-C	5.66	120.65	111.37
1	C	281	SER	N-CA-C	5.57	119.80	112.89
1	B	14	LEU	N-CA-C	-5.44	99.55	108.41
1	A	323	LYS	N-CA-C	-5.42	97.78	107.98
1	A	118	THR	N-CA-C	5.42	120.05	113.38
1	A	164	ALA	CA-C-N	5.28	125.82	120.38
1	A	164	ALA	C-N-CA	5.28	125.82	120.38
1	C	275	MET	N-CA-C	-5.26	105.21	111.69
1	B	327	ASP	N-CA-C	5.26	118.86	112.23
1	D	69	ALA	N-CA-C	5.25	116.26	108.60
1	B	25	GLU	N-CA-C	-5.20	100.70	108.96
1	B	307	LEU	N-CA-C	-5.16	105.66	111.28
1	D	293	GLY	CA-C-N	-5.15	119.09	122.60
1	D	293	GLY	C-N-CA	-5.15	119.09	122.60
1	D	92	LEU	N-CA-C	5.13	116.88	108.52
1	A	25	GLU	N-CA-C	-5.11	100.92	109.24
1	C	185	LYS	N-CA-C	5.10	119.78	113.50

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	2860	51	0
1	B	2789	0	2860	64	0
1	C	2789	0	2860	63	0
1	D	2789	0	2860	56	0
2	A	6	0	0	0	0
2	B	5	0	0	0	0
2	C	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	5	0	0	0	0
3	A	16	0	12	2	0
3	B	8	0	6	1	0
3	C	8	0	6	1	0
3	D	20	0	15	3	0
4	A	5	0	0	0	0
4	B	20	0	0	1	0
5	A	44	0	26	2	0
5	B	44	0	26	2	0
5	C	44	0	26	2	0
5	D	44	0	26	4	0
6	A	79	0	0	5	0
6	B	126	0	0	4	0
6	C	45	0	0	2	0
6	D	121	0	0	10	0
All	All	11799	0	11583	224	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 (224) 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:284:MET:HE1	1:B:116:ILE:CD1	2.07	0.85
1:D:92:LEU:HD13	1:D:324:SER:HB2	1.64	0.78
1:C:307:LEU:O	1:C:312:ARG:HD2	1.82	0.78
1:D:351:PRO:HD2	1:D:354:LYS:HD2	1.64	0.77
1:D:344:GLN:HB2	6:D:882:HOH:O	1.85	0.77
1:C:204:GLY:O	1:C:207:VAL:HG12	1.84	0.76
1:A:276:ILE:HD11	1:A:301:LEU:HD11	1.65	0.76
1:B:90:ILE:HG13	1:B:160:ILE:HD13	1.68	0.74
1:C:301:LEU:HB2	1:D:305:PRO:HG3	1.70	0.74
1:B:179:GLY:O	1:B:207:VAL:HA	1.90	0.71
1:C:26:ILE:HG22	1:C:132:CYS:HB2	1.73	0.70
1:B:24:GLU:HG2	1:B:132:CYS:SG	2.32	0.70
1:C:295:PRO:HG3	6:D:716:HOH:O	1.92	0.68
1:B:58:VAL:HA	6:B:928:HOH:O	1.93	0.68
1:B:184:VAL:HG12	1:B:185:LYS:HE2	1.75	0.68
1:D:231:LYS:HE2	1:D:344:GLN:NE2	2.10	0.66
3:A:501:ACT:H1	6:A:912:HOH:O	1.96	0.66
1:B:92:LEU:HD13	1:B:324:SER:HB3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:LYS:HE2	1:D:344:GLN:HE21	1.59	0.66
1:B:24:GLU:HG3	6:B:896:HOH:O	1.95	0.65
1:A:345:LEU:O	1:A:369:ARG:HB2	1.96	0.65
1:B:353:LYS:H	1:B:353:LYS:HD2	1.61	0.65
1:C:178:THR:HG21	5:C:3377:NAD:C4N	2.27	0.64
1:C:301:LEU:HD12	1:C:302:THR:H	1.62	0.64
1:B:69:ALA:O	1:B:91:PRO:HD2	1.97	0.64
1:B:41:LEU:HD11	1:B:72:ILE:HG12	1.78	0.64
1:B:208:ILE:HG23	1:B:219:ILE:HG21	1.78	0.63
1:B:276:ILE:HD11	1:B:301:LEU:HD11	1.81	0.62
1:B:224:LEU:HD23	1:B:243:PRO:HD2	1.81	0.62
1:D:92:LEU:HA	6:D:778:HOH:O	1.98	0.62
1:C:48:THR:HG22	1:C:57:MET:HE2	1.82	0.61
1:C:92:LEU:HD13	1:C:324:SER:HB2	1.82	0.61
1:A:62:PRO:HG2	1:A:137:VAL:HA	1.82	0.61
1:B:164:ALA:HB1	1:B:169:VAL:HG11	1.81	0.61
1:C:301:LEU:HD12	1:C:302:THR:N	2.16	0.61
1:C:27:GLU:HG2	1:C:131:THR:HB	1.82	0.60
1:D:185:LYS:HD2	1:D:322:LEU:HD23	1.83	0.60
1:B:33:THR:HG22	1:B:34:LYS:HG3	1.82	0.60
1:D:271:HIS:HB2	1:D:274:THR:OG1	2.02	0.60
1:D:309:PHE:HB2	6:D:716:HOH:O	2.00	0.60
1:D:361:LEU:HB3	1:D:367:SER:HB2	1.83	0.59
1:B:92:LEU:HD11	1:B:158:ALA:HB2	1.84	0.59
1:D:64:ILE:HA	6:D:688:HOH:O	2.02	0.59
1:D:272:LEU:HB3	1:D:301:LEU:HD13	1.84	0.59
1:D:174:CYS:SG	5:D:4377:NAD:H5N	2.44	0.58
1:B:143:THR:O	1:B:144:SER:HB2	2.02	0.58
1:D:196:VAL:HB	1:D:265:THR:HG22	1.84	0.58
1:C:231:LYS:O	1:C:235:VAL:HG23	2.02	0.58
1:C:95:PRO:HG2	1:C:111:CYS:HB3	1.86	0.57
1:A:172:ILE:HG22	1:A:172:ILE:O	2.02	0.57
1:B:271:HIS:HB2	1:B:274:THR:OG1	2.03	0.57
1:D:272:LEU:HG	6:D:824:HOH:O	2.04	0.57
1:C:301:LEU:O	1:D:302:THR:HA	2.05	0.57
1:D:328:VAL:HB	1:D:329:PRO:HD3	1.86	0.57
1:D:64:ILE:HG13	1:D:137:VAL:HG11	1.86	0.57
1:C:17:GLN:HG2	1:C:18:LYS:HG3	1.87	0.57
1:B:365:GLY:HA2	6:B:755:HOH:O	2.06	0.56
1:C:164:ALA:HB1	1:C:169:VAL:HG11	1.86	0.56
1:D:224:LEU:HD23	1:D:243:PRO:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:THR:O	1:A:144:SER:HB2	2.06	0.56
1:B:152:VAL:HG21	1:B:157:VAL:HG22	1.87	0.56
1:B:234:ALA:HA	1:D:81:THR:HG21	1.87	0.55
1:C:91:PRO:HB2	1:C:143:THR:HG22	1.88	0.55
1:C:143:THR:O	1:C:144:SER:HB2	2.07	0.55
1:A:284:MET:HE2	1:B:110:LEU:CD2	2.37	0.55
1:B:93:PHE:HB2	1:B:141:LEU:HB3	1.89	0.55
1:C:283:HIS:HD2	1:C:286:TYR:H	1.55	0.55
1:B:152:VAL:CG2	1:B:157:VAL:HG22	2.37	0.54
1:B:209:MET:HG3	1:B:235:VAL:HG13	1.89	0.54
1:A:317:CYS:SG	1:A:320:GLY:HA2	2.47	0.54
1:C:48:THR:CG2	1:C:57:MET:HE2	2.37	0.54
1:B:178:THR:HG21	5:B:2377:NAD:C4N	2.39	0.53
1:C:174:CYS:SG	1:C:175:GLY:N	2.82	0.53
1:B:176:PHE:HE2	1:B:209:MET:HE2	1.74	0.53
1:C:283:HIS:CD2	1:C:285:ASN:H	2.27	0.53
1:D:16:GLU:HB3	1:D:19:GLN:OE1	2.09	0.53
1:D:32:LYS:HD2	1:D:129:ARG:NH2	2.23	0.53
1:A:164:ALA:HB1	1:A:169:VAL:HG11	1.91	0.52
1:A:178:THR:HG21	5:A:1377:NAD:C4N	2.40	0.52
1:C:192:GLY:HA2	1:C:217:SER:OG	2.10	0.52
1:D:185:LYS:HD2	1:D:322:LEU:CD2	2.39	0.52
1:A:33:THR:HG22	1:A:34:LYS:HG3	1.90	0.52
1:A:93:PHE:CE2	3:A:501:ACT:H3	2.44	0.52
1:D:31:PRO:HD3	1:D:37:ARG:HB2	1.93	0.51
1:D:303:TYR:O	1:D:305:PRO:HD3	2.11	0.51
1:C:15:TRP:O	1:C:16:GLU:HG2	2.11	0.51
1:B:199:GLY:O	1:B:204:GLY:HA3	2.11	0.50
1:C:92:LEU:HA	6:C:950:HOH:O	2.11	0.50
1:B:276:ILE:HD11	1:B:301:LEU:CD1	2.42	0.50
1:D:267:GLU:HG3	1:D:275:MET:HA	1.93	0.50
1:B:63:VAL:HG23	1:B:138:HIS:O	2.11	0.50
1:C:174:CYS:SG	5:C:3377:NAD:H5N	2.51	0.50
1:D:34:LYS:NZ	3:D:509:ACT:H3	2.27	0.49
1:A:164:ALA:O	1:A:166:PRO:HD3	2.12	0.49
1:C:200:LEU:HD12	1:C:223:ASP:HB2	1.94	0.49
4:B:992:CAC:AS	4:B:993:CAC:O2	2.91	0.49
1:A:275:MET:HE1	1:A:295:PRO:HB3	1.94	0.49
1:B:72:ILE:HD13	1:B:88:LYS:HA	1.94	0.49
1:B:209:MET:HG3	1:B:235:VAL:CG1	2.43	0.49
1:A:284:MET:HE2	1:B:110:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:VAL:HG22	1:B:57:MET:HG2	1.94	0.48
1:B:284:MET:CE	1:B:310:THR:HG21	2.43	0.48
1:C:296:PRO:HG2	1:C:299:LYS:HG3	1.94	0.48
1:D:34:LYS:HD3	3:D:509:ACT:H1	1.94	0.48
1:A:301:LEU:HD12	1:A:302:THR:N	2.29	0.48
1:B:301:LEU:HD12	1:B:302:THR:N	2.29	0.48
1:C:231:LYS:NZ	1:C:344:GLN:HE21	2.11	0.48
1:A:351:PRO:HG2	1:A:354:LYS:HD2	1.95	0.48
1:C:354:LYS:HE2	1:C:357:GLU:HB2	1.95	0.48
1:D:26:ILE:HG22	1:D:132:CYS:HB2	1.95	0.48
1:A:132:CYS:HA	6:A:741:HOH:O	2.14	0.48
1:A:284:MET:HE1	1:B:116:ILE:HD11	1.93	0.47
1:B:93:PHE:CE2	3:B:506:ACT:H2	2.49	0.47
1:D:199:GLY:O	1:D:204:GLY:HA3	2.14	0.47
1:A:89:VAL:HG12	1:A:159:LYS:HA	1.95	0.47
1:A:276:ILE:CD1	1:A:301:LEU:HD11	2.41	0.47
1:C:98:ARG:HG2	1:C:98:ARG:HH21	1.79	0.47
1:B:197:VAL:HG21	1:B:208:ILE:HG12	1.94	0.47
1:B:330:LYS:O	1:B:334:GLU:HG3	2.14	0.47
1:D:357:GLU:O	1:D:361:LEU:HD22	2.13	0.47
1:B:274:THR:HA	1:B:277:ASP:HB2	1.97	0.47
1:C:276:ILE:HD11	1:C:301:LEU:HD11	1.96	0.47
1:A:179:GLY:O	1:A:207:VAL:HA	2.14	0.47
1:D:178:THR:HG21	5:D:4377:NAD:C4N	2.44	0.47
1:C:51:HIS:HB3	1:C:57:MET:HB2	1.97	0.47
1:A:69:ALA:HA	1:A:170:CYS:HB2	1.97	0.47
1:B:343:ASP:HB3	1:D:99:GLU:HG2	1.97	0.47
1:C:93:PHE:CZ	3:C:505:ACT:H3	2.50	0.47
1:C:331:LEU:O	1:C:340:PHE:HZ	1.98	0.47
1:A:284:MET:HE1	1:B:116:ILE:HD13	1.94	0.46
1:B:272:LEU:HD11	1:B:299:LYS:HB3	1.97	0.46
1:C:273:GLU:H	1:C:273:GLU:CD	2.23	0.46
1:B:174:CYS:SG	5:B:2377:NAD:H5N	2.55	0.46
1:D:101:ASN:O	1:D:105:ASN:HB2	2.16	0.46
1:C:2:THR:HB	1:C:7:ILE:HD11	1.98	0.46
1:D:38:ILE:O	1:D:149:TYR:HA	2.15	0.46
1:A:162:ASP:N	6:A:887:HOH:O	2.49	0.46
1:C:68:GLU:OE1	1:C:171:LEU:HD23	2.15	0.46
1:C:171:LEU:HD22	1:C:369:ARG:HG3	1.97	0.46
1:D:94:LEU:HD22	1:D:319:PHE:HB3	1.98	0.46
1:A:231:LYS:HD2	1:A:344:GLN:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:SER:O	1:B:259:GLY:N	2.50	0.45
1:C:100:CYS:HB2	6:C:849:HOH:O	2.16	0.45
1:A:301:LEU:HB2	1:B:305:PRO:HG3	1.98	0.45
1:A:62:PRO:CG	1:A:137:VAL:HG12	2.47	0.45
1:B:174:CYS:SG	1:B:175:GLY:N	2.89	0.45
1:D:272:LEU:HB3	1:D:301:LEU:CD1	2.46	0.45
1:A:328:VAL:HB	1:A:329:PRO:HD3	1.98	0.45
1:A:84:LYS:O	1:A:87:ASP:HB2	2.18	0.44
1:B:90:ILE:CG1	1:B:160:ILE:HD13	2.43	0.44
1:C:274:THR:HA	1:C:277:ASP:HB2	1.98	0.44
1:D:61:PHE:HA	1:D:62:PRO:C	2.42	0.44
1:D:190:LYS:HG3	1:D:264:TYR:OH	2.16	0.44
1:B:221:GLY:O	1:B:240:CYS:HA	2.17	0.44
1:C:334:GLU:O	1:C:339:LYS:HB2	2.16	0.44
1:D:284:MET:HE2	6:D:715:HOH:O	2.18	0.44
1:D:223:ASP:OD1	5:D:4377:NAD:H1B	2.17	0.44
1:C:69:ALA:HA	1:C:170:CYS:HB2	1.99	0.44
1:B:83:VAL:HG12	1:B:159:LYS:HB2	1.98	0.44
1:B:209:MET:CG	1:B:235:VAL:HG13	2.48	0.44
1:C:301:LEU:CB	1:D:305:PRO:HG3	2.42	0.44
1:D:138:HIS:CE1	6:D:867:HOH:O	2.71	0.44
1:A:164:ALA:HA	1:A:165:PRO:HD3	1.79	0.44
1:A:323:LYS:HG2	6:A:914:HOH:O	2.17	0.43
1:A:64:ILE:HA	6:A:884:HOH:O	2.17	0.43
1:A:98:ARG:HA	1:A:103:CYS:HB3	1.99	0.43
1:A:26:ILE:HG22	1:A:132:CYS:HB2	2.00	0.43
1:B:353:LYS:HD2	1:B:353:LYS:N	2.31	0.43
1:A:99:GLU:O	1:A:104:ARG:NH2	2.51	0.43
1:A:301:LEU:HD12	1:A:302:THR:H	1.84	0.43
1:C:90:ILE:HG13	1:C:160:ILE:HD13	2.00	0.43
1:D:365:GLY:HA2	6:D:860:HOH:O	2.18	0.43
1:C:48:THR:O	1:C:51:HIS:HB2	2.18	0.43
1:D:34:LYS:HZ1	3:D:509:ACT:H3	1.84	0.43
1:D:246:SER:OG	1:D:248:LYS:HG2	2.18	0.43
1:A:51:HIS:HE1	5:A:1377:NAD:O2D	2.01	0.43
1:A:276:ILE:HD11	1:A:301:LEU:CD1	2.40	0.43
1:B:93:PHE:HA	1:B:141:LEU:O	2.18	0.43
1:B:355:ILE:HG23	1:B:356:SER:N	2.34	0.43
1:C:95:PRO:HB3	1:C:156:SER:OG	2.19	0.42
1:B:196:VAL:HB	1:B:265:THR:HG22	2.01	0.42
1:A:353:LYS:HE2	1:A:353:LYS:HB2	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:ILE:HD13	1:C:257:MET:HE2	2.00	0.42
1:C:171:LEU:CD2	1:C:369:ARG:HG3	2.49	0.42
1:C:309:PHE:CZ	1:D:294:VAL:HG22	2.54	0.42
1:A:185:LYS:HD2	1:A:322:LEU:CD2	2.49	0.42
1:B:164:ALA:HA	1:B:165:PRO:HD2	1.95	0.42
1:C:196:VAL:HB	1:C:265:THR:HG22	2.01	0.42
1:C:220:ILE:HG12	1:C:239:GLU:HG3	2.01	0.42
1:B:13:VAL:HG12	1:B:14:LEU:N	2.34	0.42
1:B:97:CYS:O	1:B:98:ARG:HB2	2.19	0.42
1:A:274:THR:HA	1:A:277:ASP:HB2	2.02	0.42
1:B:276:ILE:CG1	1:B:301:LEU:HD11	2.50	0.42
1:C:352:PHE:CD2	1:C:352:PHE:C	2.97	0.42
1:C:317:CYS:SG	1:C:320:GLY:HA2	2.59	0.41
1:A:267:GLU:HG3	1:A:275:MET:HA	2.01	0.41
1:A:168:LYS:HE2	1:A:343:ASP:OD2	2.21	0.41
1:C:9:CYS:HB2	1:C:148:GLU:HB2	2.03	0.41
1:D:16:GLU:HB3	1:D:19:GLN:CD	2.46	0.41
1:A:92:LEU:HD22	1:A:324:SER:HB2	2.03	0.41
1:A:284:MET:HA	1:A:312:ARG:CZ	2.50	0.41
1:D:200:LEU:HD13	1:D:232:ALA:HB2	2.03	0.41
1:A:130:PHE:HZ	1:A:150:THR:OG1	2.03	0.41
1:C:16:GLU:HB2	1:C:19:GLN:OE1	2.21	0.41
1:C:61:PHE:HA	1:C:62:PRO:C	2.46	0.41
1:D:284:MET:HG2	6:D:714:HOH:O	2.20	0.41
1:A:331:LEU:HD23	1:A:331:LEU:HA	1.70	0.41
1:A:355:ILE:HG23	1:A:356:SER:N	2.36	0.41
1:B:41:LEU:HD11	1:B:72:ILE:CG1	2.48	0.41
1:B:141:LEU:O	1:B:142:ASN:HB2	2.21	0.41
1:B:142:ASN:ND2	6:B:933:HOH:O	2.49	0.41
1:C:93:PHE:HA	1:C:141:LEU:O	2.21	0.41
1:C:164:ALA:HA	1:C:165:PRO:HD2	1.88	0.41
1:C:179:GLY:O	1:C:207:VAL:HA	2.20	0.41
1:C:335:PHE:HB2	1:C:340:PHE:CE2	2.56	0.41
1:D:284:MET:HA	1:D:312:ARG:CZ	2.52	0.40
1:A:172:ILE:O	1:A:172:ILE:CG2	2.67	0.40
1:C:62:PRO:HG2	1:C:137:VAL:HA	2.03	0.40
1:C:350:LEU:HB3	1:C:351:PRO:HD2	2.04	0.40
1:D:121:GLY:HA2	1:D:139:HIS:O	2.22	0.40
1:A:368:ILE:HG22	1:A:369:ARG:N	2.36	0.40
1:D:179:GLY:HA3	1:D:206:SER:HB2	2.02	0.40
1:D:294:VAL:HG23	5:D:4377:NAD:H1D	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:ILE:HG13	1:D:372:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	371/373 (100%)	340 (92%)	27 (7%)	4 (1%)	11	18
1	B	371/373 (100%)	343 (92%)	25 (7%)	3 (1%)	16	25
1	C	371/373 (100%)	335 (90%)	31 (8%)	5 (1%)	9	14
1	D	371/373 (100%)	344 (93%)	22 (6%)	5 (1%)	9	14
All	All	1484/1492 (100%)	1362 (92%)	105 (7%)	17 (1%)	11	18

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	174	CYS
1	B	175	GLY
1	C	174	CYS
1	C	324	SER
1	D	109	ASN
1	D	174	CYS
1	A	174	CYS
1	A	65	VAL
1	A	175	GLY
1	C	284	MET
1	D	144	SER
1	A	368	ILE
1	B	65	VAL
1	C	175	GLY

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Mol	Chain	Res	Type
1	D	67	HIS
1	D	368	ILE
1	C	236	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	312/312 (100%)	303 (97%)	9 (3%)	37	60
1	B	312/312 (100%)	303 (97%)	9 (3%)	37	60
1	C	312/312 (100%)	306 (98%)	6 (2%)	50	71
1	D	312/312 (100%)	303 (97%)	9 (3%)	37	60
All	All	1248/1248 (100%)	1215 (97%)	33 (3%)	40	63

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	19	GLN
1	A	57	MET
1	A	118	THR
1	A	218	ARG
1	A	244	LYS
1	A	247	THR
1	A	268	VAL
1	A	354	LYS
1	B	2	THR
1	B	24	GLU
1	B	27	GLU
1	B	57	MET
1	B	185	LYS
1	B	268	VAL
1	B	274	THR
1	B	310	THR
1	B	344	GLN

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Mol	Chain	Res	Type
1	C	27	GLU
1	C	78	GLU
1	C	104	ARG
1	C	147	THR
1	C	256	GLU
1	C	360	GLU
1	D	57	MET
1	D	133	LYS
1	D	172	ILE
1	D	231	LYS
1	D	268	VAL
1	D	325	ARG
1	D	329	PRO
1	D	344	GLN
1	D	361	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	142	ASN
1	A	225	ASN
1	A	261	ASN
1	A	344	GLN
1	A	348	HIS
1	B	344	GLN
1	B	366	GLN
1	C	19	GLN
1	C	283	HIS
1	C	344	GLN
1	C	366	GLN
1	D	17	GLN
1	D	19	GLN
1	D	344	GLN
1	D	366	GLN

5.3.3 RNA ⓘ

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 41 ligands modelled in this entry, 19 are monoatomic - leaving 22 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	D	512	-	3,3,3	0.94	0	3,3,3	0.47	0
3	ACT	C	510	2	3,3,3	0.92	0	3,3,3	0.89	0
4	CAC	A	994	-	2,4,4	1.36	0	4,6,6	1.83	1 (25%)
3	ACT	A	513	2	3,3,3	0.44	0	3,3,3	0.51	0
4	CAC	B	991	2	2,4,4	1.98	1 (50%)	4,6,6	2.00	2 (50%)
5	NAD	A	1377	2	46,48,48	2.27	10 (21%)	64,73,73	2.00	15 (23%)
3	ACT	B	507	2	3,3,3	0.93	0	3,3,3	0.64	0
3	ACT	C	505	2	3,3,3	0.76	0	3,3,3	0.92	0
5	NAD	D	4377	2	46,48,48	2.19	8 (17%)	64,73,73	1.95	15 (23%)
4	CAC	B	992	2	2,4,4	1.21	0	4,6,6	1.66	2 (50%)
3	ACT	D	508	-	3,3,3	0.87	0	3,3,3	0.75	0
3	ACT	A	502	2	3,3,3	1.20	0	3,3,3	0.91	0
3	ACT	D	509	2	3,3,3	0.86	0	3,3,3	0.72	0
4	CAC	B	995	-	2,4,4	1.39	0	4,6,6	1.51	1 (25%)
3	ACT	A	501	2	3,3,3	0.68	0	3,3,3	1.05	0
3	ACT	B	506	2	3,3,3	0.97	0	3,3,3	0.52	0
3	ACT	A	504	2	3,3,3	0.86	0	3,3,3	1.01	0
5	NAD	B	2377	2	46,48,48	2.05	9 (19%)	64,73,73	1.95	14 (21%)
4	CAC	B	993	2	2,4,4	1.24	0	4,6,6	2.41	2 (50%)
3	ACT	D	514	2	3,3,3	0.94	0	3,3,3	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAD	C	3377	2	46,48,48	2.15	10 (21%)	64,73,73	1.80	13 (20%)
3	ACT	D	511	2	3,3,3	0.81	0	3,3,3	1.06	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
5	NAD	A	1377	2	-	9/30/62/62	0/5/5/5
5	NAD	B	2377	2	-	8/30/62/62	0/5/5/5
5	NAD	C	3377	2	-	13/30/62/62	0/5/5/5
5	NAD	D	4377	2	-	8/30/62/62	0/5/5/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	4377	NAD	C3N-C7N	-10.29	1.35	1.50
5	C	3377	NAD	C3N-C7N	-8.33	1.38	1.50
5	B	2377	NAD	C3N-C7N	-7.72	1.39	1.50
5	A	1377	NAD	C3N-C7N	-7.57	1.39	1.50
5	A	1377	NAD	PA-O3	-6.87	1.52	1.59
5	A	1377	NAD	PN-O3	-5.30	1.53	1.59
5	C	3377	NAD	PA-O3	-5.22	1.53	1.59
5	B	2377	NAD	C2A-N3A	5.12	1.43	1.33
5	C	3377	NAD	PN-O3	-5.10	1.54	1.59
5	B	2377	NAD	C2A-N1A	5.07	1.42	1.33
5	A	1377	NAD	C8A-N7A	4.52	1.40	1.31
5	D	4377	NAD	O4D-C1D	4.51	1.46	1.40
5	C	3377	NAD	C8A-N7A	4.35	1.40	1.31
5	B	2377	NAD	C8A-N7A	4.27	1.39	1.31
5	D	4377	NAD	C8A-N7A	4.19	1.39	1.31
5	D	4377	NAD	C2A-N1A	3.74	1.40	1.33
5	A	1377	NAD	C2A-N1A	3.67	1.40	1.33
5	C	3377	NAD	C2A-N1A	3.66	1.40	1.33
5	D	4377	NAD	C2N-C3N	-3.52	1.33	1.39
5	A	1377	NAD	C2A-N3A	3.35	1.39	1.33
5	C	3377	NAD	C2A-N3A	3.35	1.39	1.33
5	B	2377	NAD	C2N-C3N	-3.31	1.33	1.39
5	B	2377	NAD	C4A-N3A	3.19	1.40	1.34
5	A	1377	NAD	C2N-N1N	-3.01	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1377	NAD	O5D-C5D	2.91	1.55	1.44
5	B	2377	NAD	PN-O3	-2.82	1.56	1.59
5	A	1377	NAD	C2N-C3N	-2.72	1.34	1.39
5	B	2377	NAD	C5A-N7A	-2.64	1.34	1.39
5	C	3377	NAD	C4A-N3A	2.62	1.39	1.34
5	D	4377	NAD	C4N-C3N	-2.62	1.35	1.39
5	C	3377	NAD	C2N-C3N	-2.56	1.34	1.39
5	D	4377	NAD	C2A-N3A	2.49	1.38	1.33
5	A	1377	NAD	C4A-N3A	2.38	1.38	1.34
5	D	4377	NAD	C4A-N3A	2.33	1.38	1.34
4	B	991	CAC	AS-C1	2.30	1.95	1.90
5	C	3377	NAD	O4D-C1D	2.23	1.43	1.40
5	C	3377	NAD	C1B-N9A	-2.12	1.40	1.46
5	B	2377	NAD	C6A-N1A	2.06	1.41	1.35

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	4377	NAD	O7N-C7N-N7N	-8.39	110.49	122.62
5	B	2377	NAD	O7N-C7N-N7N	-8.38	110.51	122.62
5	A	1377	NAD	O7N-C7N-N7N	-7.52	111.75	122.62
5	C	3377	NAD	O7N-C7N-N7N	-7.28	112.10	122.62
5	A	1377	NAD	N3A-C2A-N1A	-4.95	121.08	128.58
5	A	1377	NAD	O7N-C7N-C3N	4.69	125.33	119.60
5	D	4377	NAD	O2N-PN-O3	4.57	119.62	107.27
5	D	4377	NAD	N3A-C2A-N1A	-4.48	121.80	128.58
5	A	1377	NAD	C5A-C4A-N9A	4.30	110.50	105.81
5	A	1377	NAD	O2N-PN-O3	4.04	118.18	107.27
5	B	2377	NAD	C6A-C5A-N7A	-4.03	124.33	132.09
4	B	993	CAC	O1-AS-C2	-3.96	106.58	111.50
5	B	2377	NAD	O2N-PN-O3	3.88	117.76	107.27
5	D	4377	NAD	C5A-C4A-N9A	3.80	109.95	105.81
5	C	3377	NAD	N3A-C2A-N1A	-3.69	123.00	128.58
5	D	4377	NAD	O2A-PA-O3	3.65	117.14	107.27
5	B	2377	NAD	N6A-C6A-N1A	3.60	126.39	118.38
5	C	3377	NAD	O7N-C7N-C3N	3.55	123.94	119.60
5	B	2377	NAD	C5A-C6A-N6A	-3.52	114.57	123.29
5	A	1377	NAD	O4B-C4B-C3B	3.48	112.07	105.15
5	C	3377	NAD	O4B-C4B-C3B	3.41	111.93	105.15
5	D	4377	NAD	C3N-C7N-N7N	3.37	121.89	117.74
5	B	2377	NAD	C6A-C5A-C4A	3.37	121.77	117.18
4	B	991	CAC	O1-AS-C2	-3.34	107.35	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	3377	NAD	C5A-C4A-N9A	3.32	109.42	105.81
5	C	3377	NAD	C2B-C3B-C4B	-3.27	96.29	102.61
5	B	2377	NAD	N3A-C2A-N1A	-3.24	123.67	128.58
5	C	3377	NAD	O2A-PA-O3	3.20	115.92	107.27
5	B	2377	NAD	O5B-C5B-C4B	-3.14	98.30	108.99
4	A	994	CAC	O1-AS-C2	-2.99	107.78	111.50
5	C	3377	NAD	O5B-C5B-C4B	-2.92	99.06	108.99
5	D	4377	NAD	O4B-C4B-C3B	2.91	110.93	105.15
5	A	1377	NAD	C6A-C5A-N7A	-2.86	126.57	132.09
5	B	2377	NAD	C4A-C5A-N7A	2.83	113.82	110.58
5	A	1377	NAD	C6N-N1N-C2N	-2.82	119.48	121.88
5	B	2377	NAD	C2B-C3B-C4B	-2.80	97.20	102.61
5	B	2377	NAD	O4B-C4B-C3B	2.78	110.68	105.15
5	B	2377	NAD	O2A-PA-O3	2.73	114.66	107.27
5	A	1377	NAD	O5B-C5B-C4B	-2.70	99.79	108.99
5	A	1377	NAD	C3N-C7N-N7N	-2.66	114.46	117.74
5	D	4377	NAD	C6N-N1N-C1D	2.62	124.86	119.73
5	B	2377	NAD	C6N-N1N-C2N	-2.61	119.65	121.88
5	D	4377	NAD	O5B-C5B-C4B	-2.57	100.23	108.99
4	B	992	CAC	O1-AS-C2	-2.55	108.32	111.50
5	D	4377	NAD	O5B-PA-O1A	2.53	118.98	108.94
5	A	1377	NAD	C6N-N1N-C1D	2.53	124.69	119.73
5	C	3377	NAD	C6A-C5A-C4A	2.51	120.60	117.18
5	D	4377	NAD	O5D-C5D-C4D	2.50	117.51	108.99
5	C	3377	NAD	O3-PN-O1N	2.43	118.00	110.70
4	B	993	CAC	O2-AS-C1	2.41	111.67	105.84
5	D	4377	NAD	C5A-C4A-N3A	-2.37	123.45	126.72
5	C	3377	NAD	C6N-N1N-C1D	2.35	124.34	119.73
5	A	1377	NAD	C2B-C3B-C4B	-2.34	98.08	102.61
5	D	4377	NAD	C4A-N9A-C8A	-2.31	103.31	105.74
5	C	3377	NAD	C3N-C7N-N7N	2.29	120.55	117.74
4	B	995	CAC	O2-AS-C1	2.26	111.32	105.84
5	D	4377	NAD	C2N-N1N-C1D	-2.26	114.15	119.13
5	D	4377	NAD	C6A-C5A-C4A	2.24	120.24	117.18
5	A	1377	NAD	N3A-C4A-N9A	-2.16	123.49	127.17
5	B	2377	NAD	O7N-C7N-C3N	2.11	122.18	119.60
5	A	1377	NAD	C4B-O4B-C1B	-2.11	104.82	109.47
4	B	992	CAC	O2-AS-C1	2.10	110.93	105.84
5	A	1377	NAD	C5A-C4A-N3A	-2.07	123.86	126.72
4	B	991	CAC	O2-AS-C1	2.06	110.82	105.84
5	C	3377	NAD	O2N-PN-O3	2.05	112.82	107.27

There are no chirality outliers.

All (38) torsion outliers are listed below:

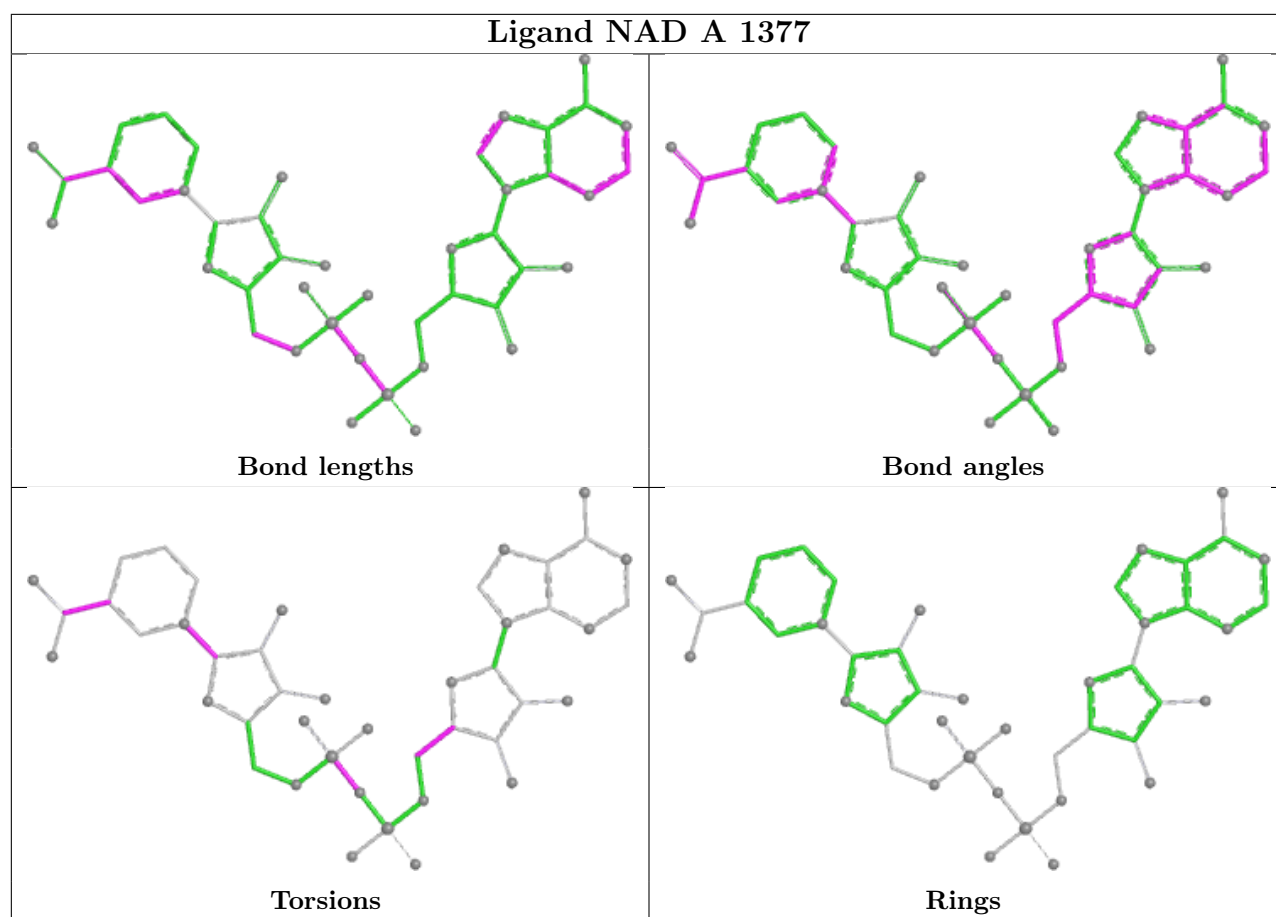
Mol	Chain	Res	Type	Atoms
5	A	1377	NAD	O4D-C1D-N1N-C2N
5	A	1377	NAD	O4D-C1D-N1N-C6N
5	A	1377	NAD	C2D-C1D-N1N-C2N
5	B	2377	NAD	O4D-C1D-N1N-C2N
5	B	2377	NAD	O4D-C1D-N1N-C6N
5	B	2377	NAD	C2D-C1D-N1N-C2N
5	B	2377	NAD	C2D-C1D-N1N-C6N
5	C	3377	NAD	C5B-O5B-PA-O1A
5	C	3377	NAD	C5B-O5B-PA-O3
5	C	3377	NAD	C5D-O5D-PN-O2N
5	C	3377	NAD	O4D-C1D-N1N-C2N
5	C	3377	NAD	O4D-C1D-N1N-C6N
5	C	3377	NAD	C2D-C1D-N1N-C2N
5	C	3377	NAD	C2D-C1D-N1N-C6N
5	D	4377	NAD	O4D-C1D-N1N-C2N
5	D	4377	NAD	O4D-C1D-N1N-C6N
5	D	4377	NAD	C2D-C1D-N1N-C2N
5	D	4377	NAD	C2D-C1D-N1N-C6N
5	C	3377	NAD	O4D-C4D-C5D-O5D
5	C	3377	NAD	O4B-C4B-C5B-O5B
5	C	3377	NAD	C3B-C4B-C5B-O5B
5	B	2377	NAD	O4B-C4B-C5B-O5B
5	C	3377	NAD	C3D-C4D-C5D-O5D
5	B	2377	NAD	C3B-C4B-C5B-O5B
5	A	1377	NAD	O4B-C4B-C5B-O5B
5	D	4377	NAD	C4N-C3N-C7N-N7N
5	D	4377	NAD	O4B-C4B-C5B-O5B
5	D	4377	NAD	C2N-C3N-C7N-N7N
5	B	2377	NAD	C5B-O5B-PA-O2A
5	C	3377	NAD	C5B-O5B-PA-O2A
5	C	3377	NAD	C5D-O5D-PN-O3
5	A	1377	NAD	PA-O3-PN-O2N
5	A	1377	NAD	C2D-C1D-N1N-C6N
5	A	1377	NAD	C3B-C4B-C5B-O5B
5	B	2377	NAD	O4D-C4D-C5D-O5D
5	A	1377	NAD	C4N-C3N-C7N-N7N
5	D	4377	NAD	C2B-C1B-N9A-C8A
5	A	1377	NAD	PA-O3-PN-O1N

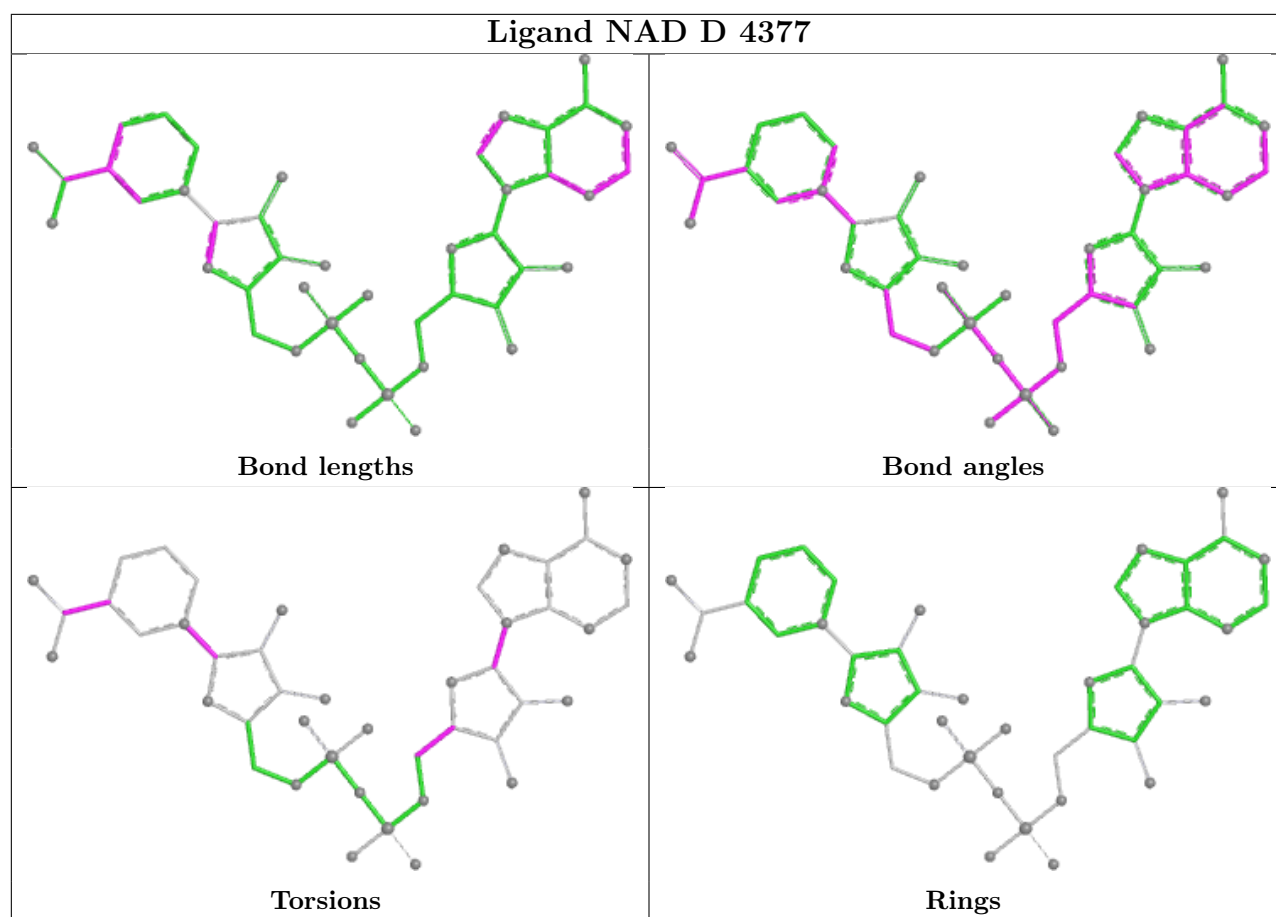
There are no ring outliers.

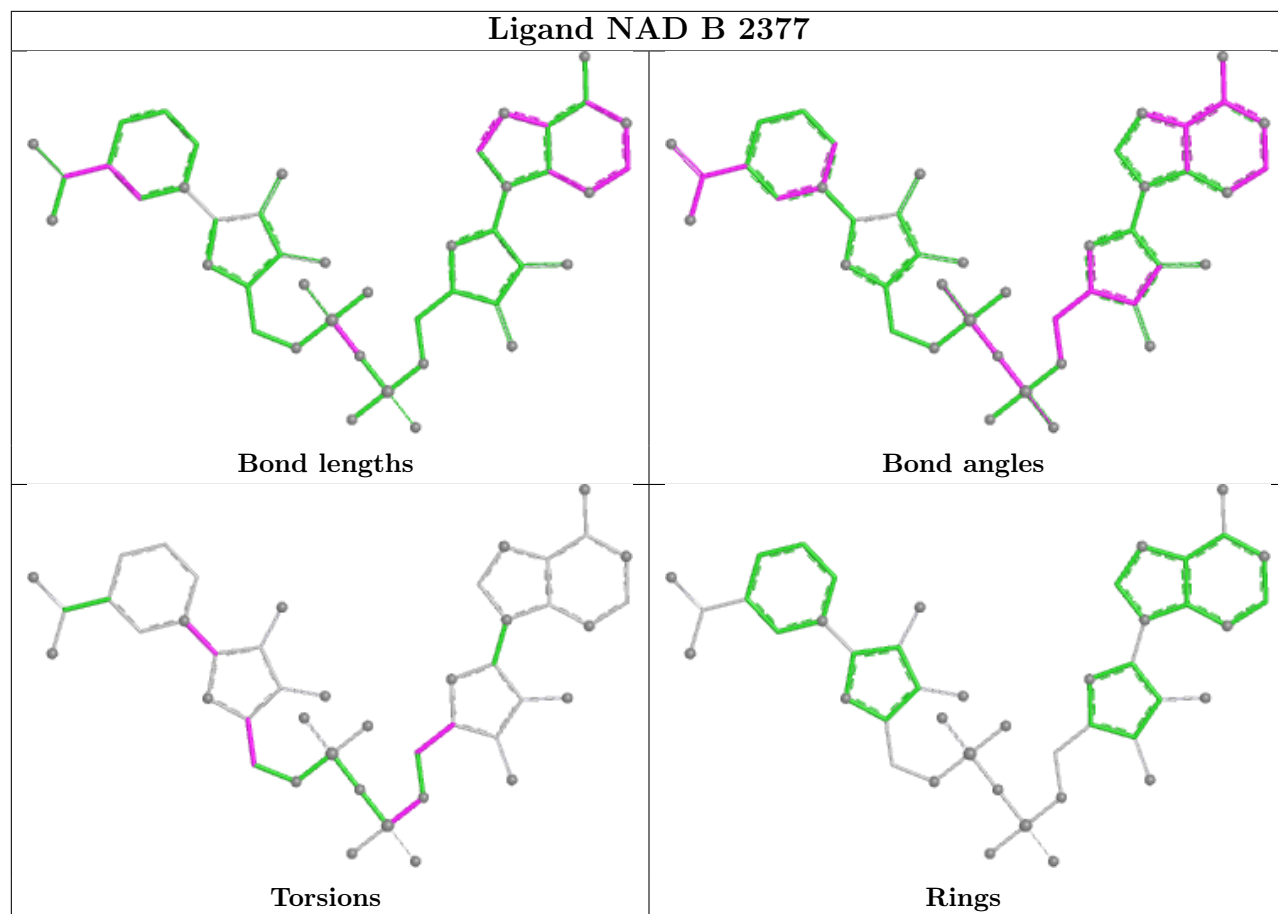
10 monomers are involved in 18 short contacts:

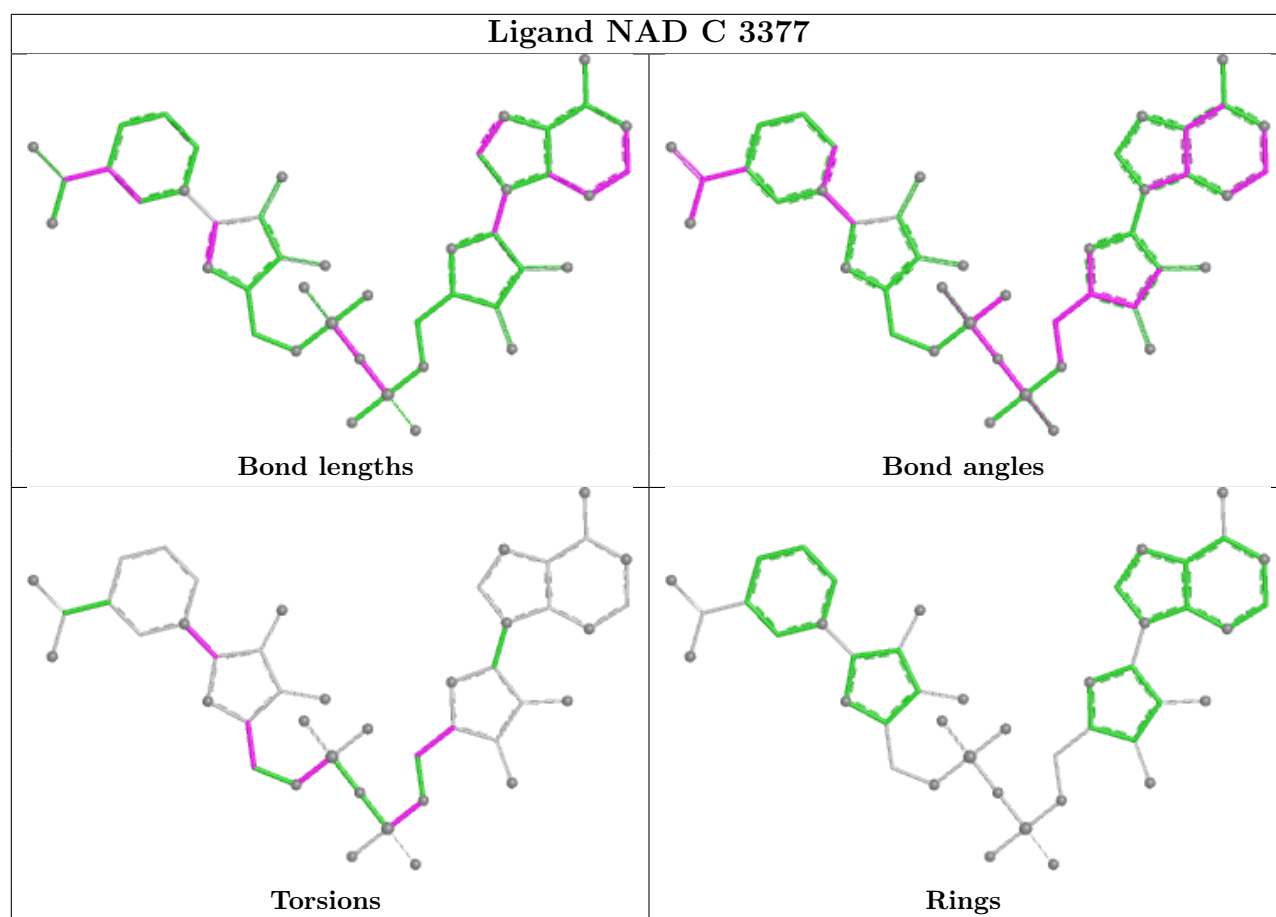
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1377	NAD	2	0
3	C	505	ACT	1	0
5	D	4377	NAD	4	0
4	B	992	CAC	1	0
3	D	509	ACT	3	0
3	A	501	ACT	2	0
3	B	506	ACT	1	0
5	B	2377	NAD	2	0
4	B	993	CAC	1	0
5	C	3377	NAD	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	373/373 (100%)	0.09	2 (0%) 87 85	16, 40, 58, 65	0
1	B	373/373 (100%)	-0.14	0 100 100	12, 33, 49, 62	0
1	C	373/373 (100%)	0.78	16 (4%) 40 36	22, 52, 67, 74	0
1	D	373/373 (100%)	-0.31	0 100 100	16, 30, 46, 57	0
All	All	1492/1492 (100%)	0.11	18 (1%) 76 73	12, 38, 62, 74	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	362	LEU	3.0
1	C	4	GLY	2.9
1	C	1	GLY	2.8
1	A	58	VAL	2.8
1	C	237	ALA	2.7
1	C	368	ILE	2.4
1	C	254	LEU	2.4
1	A	77	GLY	2.4
1	C	332	VAL	2.4
1	C	243	PRO	2.3
1	C	342	LEU	2.3
1	C	172	ILE	2.2
1	C	58	VAL	2.2
1	C	134	GLY	2.2
1	C	169	VAL	2.1
1	C	351	PRO	2.1
1	C	335	PHE	2.0
1	C	238	THR	2.0

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

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

6.3 Carbohydrates ⓘ

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.

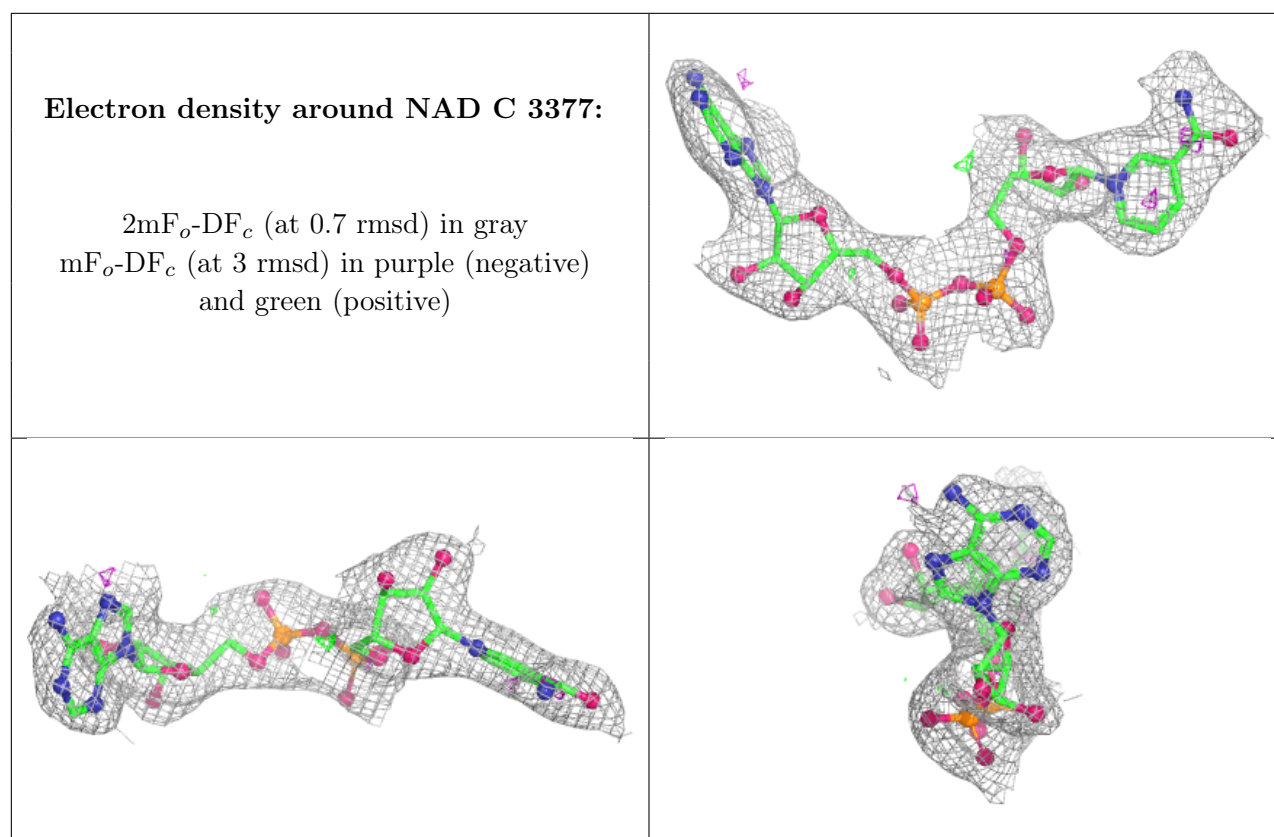
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ACT	D	514	4/4	0.61	0.52	49,52,53,54	4
3	ACT	A	513	4/4	0.67	0.47	52,52,53,54	4
3	ACT	A	502	4/4	0.79	0.41	50,51,51,51	4
2	ZN	D	410	1/1	0.87	0.21	47,47,47,47	1
3	ACT	C	510	4/4	0.88	0.11	33,33,34,34	0
3	ACT	B	506	4/4	0.89	0.15	12,26,27,37	0
4	CAC	A	994	5/5	0.90	0.16	69,70,71,73	0
4	CAC	B	995	5/5	0.90	0.32	74,74,76,77	0
3	ACT	D	508	4/4	0.92	0.10	23,25,26,31	0
5	NAD	C	3377	44/44	0.92	0.09	19,49,55,60	0
3	ACT	D	509	4/4	0.93	0.12	16,18,20,20	0
3	ACT	D	512	4/4	0.93	0.19	32,35,38,39	0
3	ACT	B	507	4/4	0.93	0.10	23,24,25,29	0
3	ACT	A	501	4/4	0.95	0.10	37,39,40,41	0
2	ZN	A	402	1/1	0.95	0.19	50,50,50,50	1
3	ACT	A	504	4/4	0.95	0.09	15,18,19,19	0
3	ACT	C	505	4/4	0.95	0.14	33,34,35,41	0
2	ZN	D	411	1/1	0.96	0.05	48,48,48,48	0
5	NAD	A	1377	44/44	0.96	0.07	23,30,35,38	0
5	NAD	B	2377	44/44	0.96	0.07	14,25,35,39	0
2	ZN	B	405	1/1	0.96	0.06	51,51,51,51	0
2	ZN	C	407	1/1	0.97	0.04	63,63,63,63	0
2	ZN	A	401	1/1	0.97	0.06	48,48,48,48	0
4	CAC	B	992	5/5	0.97	0.09	49,52,55,57	0
4	CAC	B	993	5/5	0.97	0.10	47,49,51,55	0
5	NAD	D	4377	44/44	0.97	0.07	21,29,35,37	0
2	ZN	B	376	1/1	0.98	0.03	28,28,28,28	0

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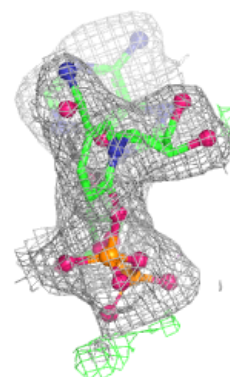
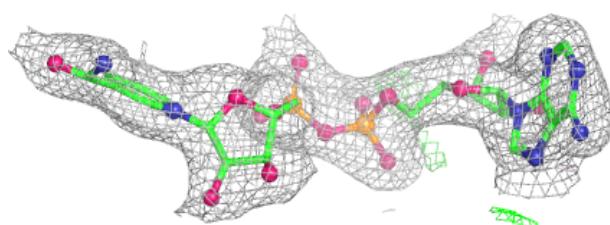
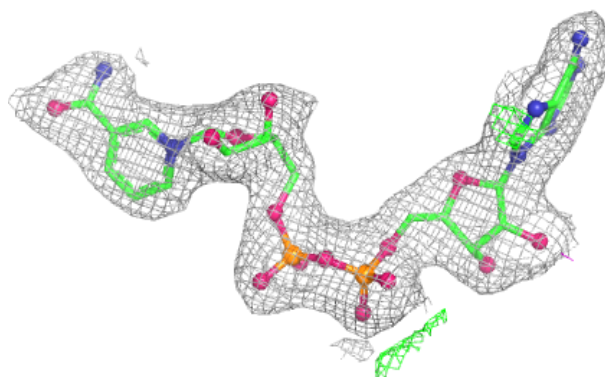
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CAC	B	991	5/5	0.98	0.07	17,32,35,38	0
2	ZN	B	404	1/1	0.98	0.03	31,31,31,31	0
2	ZN	A	375	1/1	0.98	0.04	49,49,49,49	0
2	ZN	B	406	1/1	0.98	0.05	42,42,42,42	0
2	ZN	C	376	1/1	0.98	0.03	46,46,46,46	0
3	ACT	D	511	4/4	0.98	0.08	26,29,32,32	0
2	ZN	A	408	1/1	0.98	0.03	47,47,47,47	0
2	ZN	D	409	1/1	0.98	0.10	48,48,48,48	0
2	ZN	A	403	1/1	0.99	0.05	49,49,49,49	0
2	ZN	A	376	1/1	0.99	0.02	35,35,35,35	0
2	ZN	B	375	1/1	0.99	0.04	28,28,28,28	0
2	ZN	D	375	1/1	0.99	0.03	30,30,30,30	0
2	ZN	D	376	1/1	0.99	0.04	29,29,29,29	0
2	ZN	C	375	1/1	1.00	0.02	43,43,43,43	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.

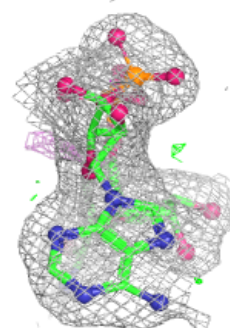
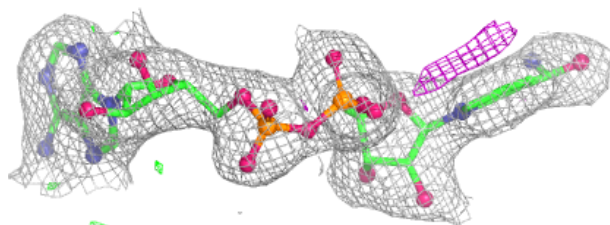
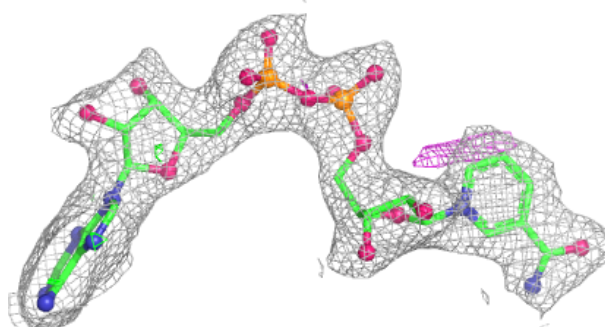


Electron density around NAD A 1377:

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

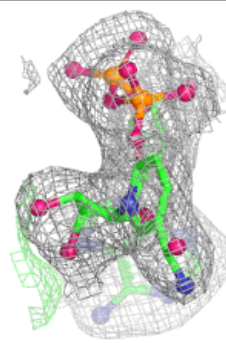
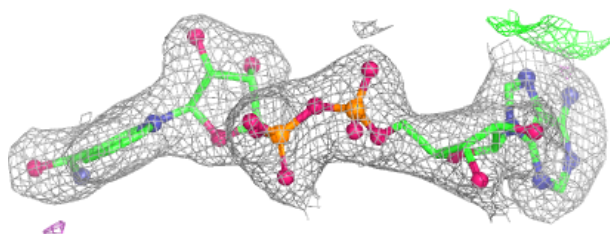
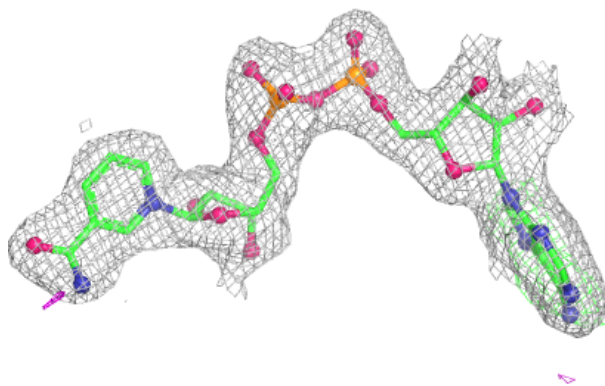
**Electron density around NAD B 2377:**

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



Electron density around NAD D 4377:

$2mF_o-DF_c$ (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.