



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:51 PM UTC

PDB ID : 1ADB / pdb_00001adb
Title : CRYSTALLOGRAPHIC STUDIES OF ISOSTERIC NAD ANALOGUES
BOUND TO ALCOHOL DEHYDROGENASE: SPECIFICITY AND SUB-
STRATE BINDING IN TWO TERNARY COMPLEXES
Authors : Li, H.; Hallows, W.A.; Punzi, J.S.; Pankiewicz, K.W.; Watanabe, K.A.; Gold-
stein, B.M.
Deposited on : 1993-12-13
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

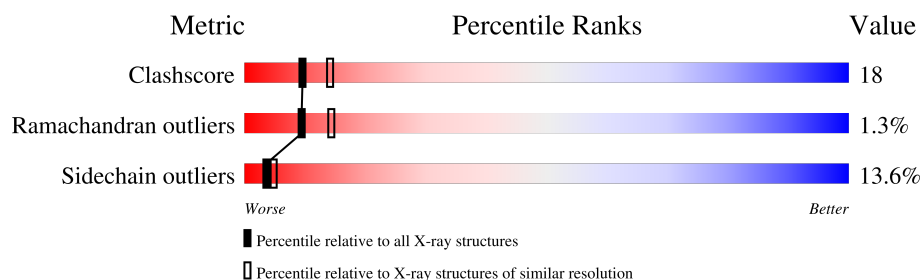
1 Overall quality at a glance

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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	374	
1	B	374	

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
4	EOH	B	378	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7165 atoms, of which 1410 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

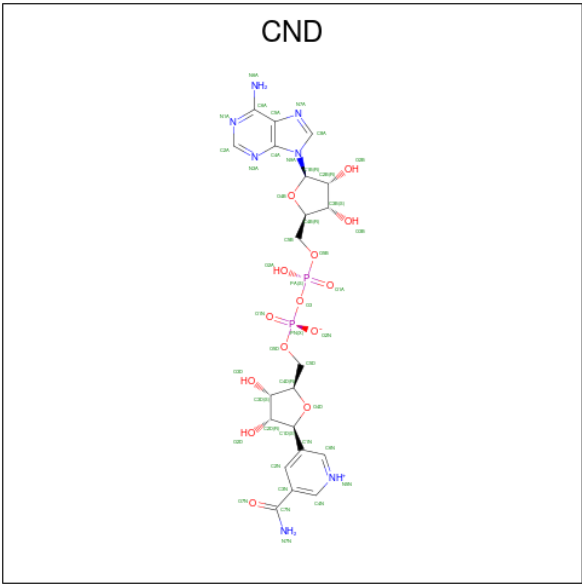
- Molecule 1 is a protein called ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	374	Total	C	H	N	O	S	0	0	0
			3391	1769	607	472	520	23			
1	B	374	Total	C	H	N	O	S	0	0	0
			3392	1769	607	472	521	23			

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

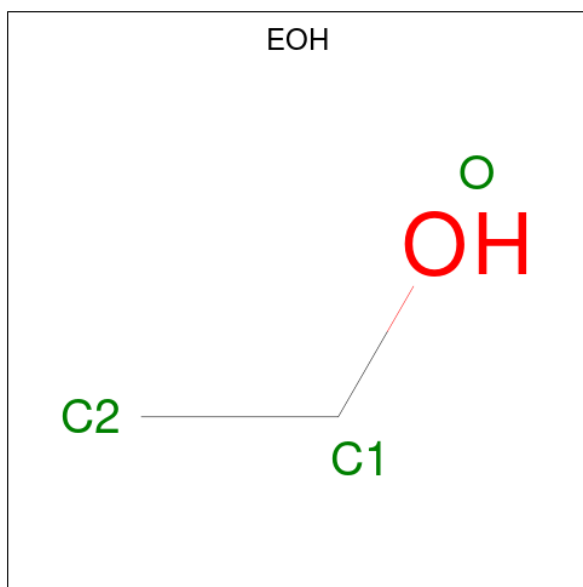
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 5-BETA-D-RIBOFURANOSYLNICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: CND) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			52	21	8	7	14	2		
3	B	1	Total	C	H	N	O	P	0	0
			52	21	8	7	14	2		

- Molecule 4 is ETHANOL (CCD ID: EOH) (formula: C₂H₆O).



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

- Molecule 5 is water.

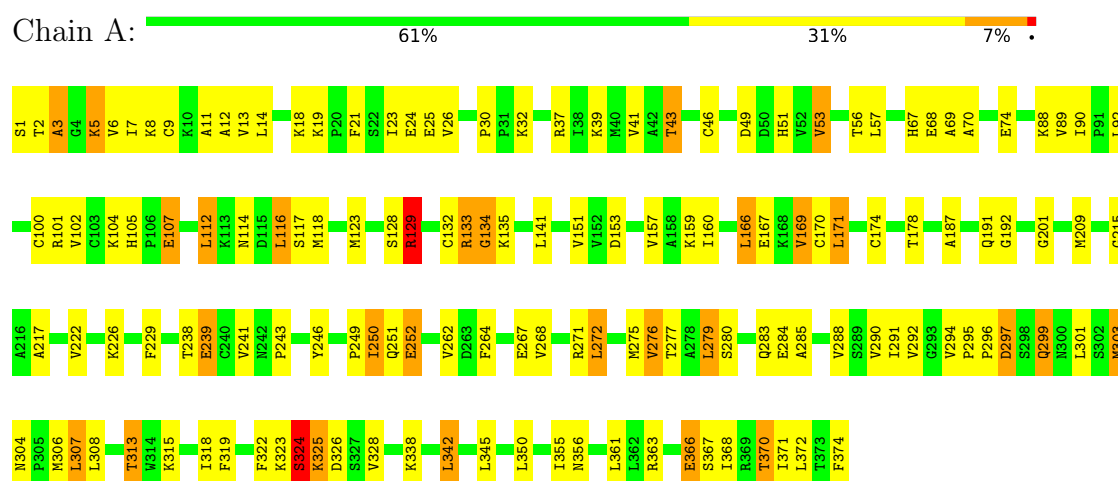
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	50	Total	H	O	0	0
			150	100	50		
5	B	38	Total	H	O	0	0
			114	76	38		

3 Residue-property plots

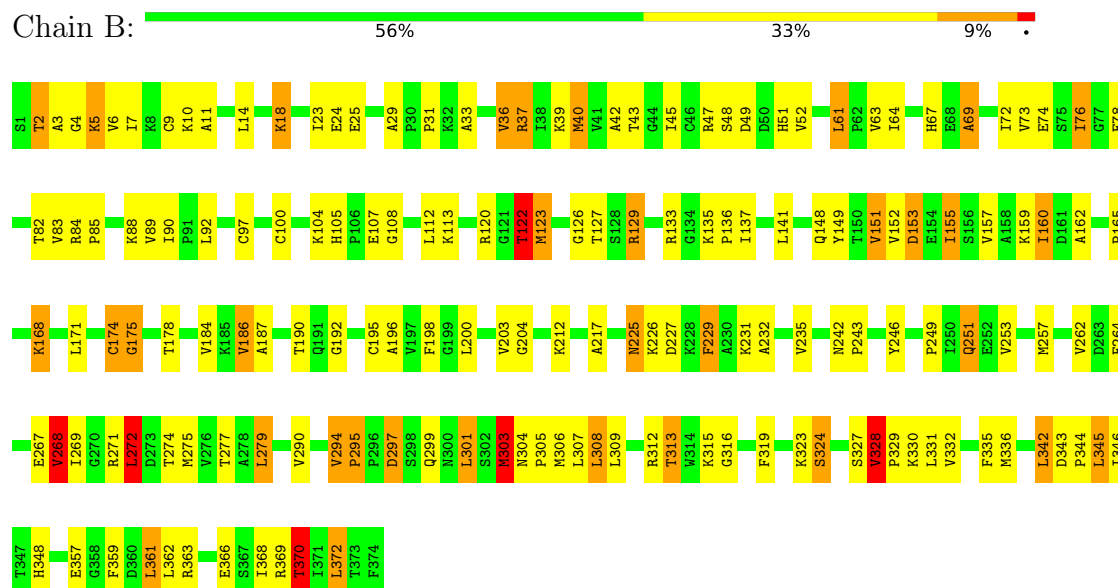
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: ALCOHOL DEHYDROGENASE



• Molecule 1: ALCOHOL DEHYDROGENASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.10Å 44.70Å 93.50Å 103.30° 87.90° 70.40°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7165	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.70	1/2836 (0.0%)	1.12	17/3834 (0.4%)
1	B	0.68	2/2837 (0.1%)	1.17	25/3834 (0.7%)
All	All	0.69	3/5673 (0.1%)	1.14	42/7668 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	MET	SD-CE	-6.91	1.62	1.79
1	B	370	THR	CA-CB	6.00	1.62	1.53
1	B	303	MET	SD-CE	-5.07	1.66	1.79

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	MET	N-CA-C	-8.89	97.36	110.52
1	B	327	SER	N-CA-C	8.67	122.36	111.69
1	B	186	VAL	N-CA-C	7.95	119.66	111.00
1	B	120	ARG	N-CA-C	-7.72	103.99	113.41
1	A	284	GLU	N-CA-C	7.55	119.51	111.28
1	B	294	VAL	N-CA-C	6.94	113.87	107.56
1	B	126	GLY	N-CA-C	-6.82	105.23	115.32
1	A	324	SER	N-CA-C	6.42	124.47	110.80
1	A	166	LEU	N-CA-C	6.30	119.81	111.75
1	B	246	TYR	N-CA-C	6.25	119.89	109.95
1	A	325	LYS	N-CA-C	6.24	118.09	111.28
1	A	229	PHE	N-CA-C	6.15	118.52	111.02
1	A	322	PHE	N-CA-C	6.10	118.58	109.25
1	B	29	ALA	CA-C-N	6.10	124.11	119.66
1	B	29	ALA	C-N-CA	6.10	124.11	119.66
1	B	272	LEU	N-CA-C	6.10	118.71	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	PRO	CA-C-N	5.99	126.30	119.83
1	B	295	PRO	C-N-CA	5.99	126.30	119.83
1	B	229	PHE	N-CA-C	5.97	119.39	111.75
1	A	366	GLU	N-CA-C	5.90	120.27	112.25
1	B	328	VAL	N-CA-CB	5.88	114.21	110.50
1	A	201	GLY	N-CA-C	-5.88	104.69	112.81
1	A	297	ASP	N-CA-C	5.87	123.31	110.80
1	A	252	GLU	N-CA-C	-5.86	104.80	111.07
1	A	368	ILE	N-CA-C	-5.78	97.31	109.34
1	B	122	THR	N-CA-C	5.74	117.33	109.18
1	B	323	LYS	N-CA-C	-5.73	100.89	109.15
1	A	105	HIS	CA-C-N	5.67	126.92	119.84
1	A	105	HIS	C-N-CA	5.67	126.92	119.84
1	A	49	ASP	N-CA-C	-5.61	105.31	111.82
1	A	370	THR	N-CA-C	-5.56	100.12	109.07
1	B	346	ILE	N-CA-C	5.48	115.15	107.37
1	A	88	LYS	N-CA-C	-5.41	101.71	110.32
1	B	49	ASP	N-CA-C	-5.40	105.47	111.36
1	B	268	VAL	CB-CA-C	5.37	120.10	111.29
1	A	323	LYS	N-CA-C	-5.29	101.54	109.15
1	B	184	VAL	N-CA-C	5.23	115.44	110.53
1	B	297	ASP	N-CA-C	5.21	121.89	110.80
1	B	69	ALA	N-CA-C	5.13	115.83	108.74
1	B	82	THR	N-CA-C	5.13	119.59	113.23
1	B	251	GLN	N-CA-C	-5.04	105.69	111.14
1	B	324	SER	N-CA-C	5.03	121.52	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	2784	607	2848	96	0
1	B	2785	607	2848	113	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
3	A	44	8	25	1	0
3	B	44	8	25	1	0
4	A	3	2	6	1	0
4	B	3	2	6	2	0
5	A	50	100	0	6	0
5	B	38	76	0	1	0
All	All	5755	1410	5758	203	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 18.

All (203) 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:B:76:ILE:HD11	1:B:83:VAL:HG23	1.48	0.95
1:A:43:THR:HG23	1:A:69:ALA:HB2	1.49	0.93
1:B:129:ARG:HG2	1:B:151:VAL:HG11	1.55	0.89
1:B:165:PRO:HD2	1:B:336:MET:HE1	1.58	0.85
1:A:251:GLN:HG3	1:A:277:THR:HG23	1.61	0.82
1:A:178:THR:HG22	1:A:319:PHE:HA	1.63	0.80
1:A:301:LEU:HD11	1:B:303:MET:HE2	1.64	0.80
1:B:153:ASP:HB3	1:B:155:ILE:HG22	1.63	0.80
1:B:178:THR:HG22	1:B:319:PHE:HA	1.64	0.79
1:B:313:THR:HG22	5:B:412:HOH:O	1.84	0.75
1:B:160:ILE:HD11	1:B:328:VAL:HG23	1.70	0.74
1:A:92:LEU:HD13	1:A:324:SER:HB3	1.69	0.74
1:B:251:GLN:HG3	1:B:277:THR:HG23	1.73	0.71
1:B:105:HIS:HD2	1:B:107:GLU:H	1.40	0.70
1:A:272:LEU:HD21	1:A:299:GLN:HB3	1.75	0.69
1:B:160:ILE:HG12	1:B:332:VAL:HG21	1.75	0.68
1:B:203:VAL:HG23	1:B:268:VAL:HG23	1.75	0.68
1:A:56:THR:HG23	1:A:296:PRO:HA	1.74	0.67
1:B:335:PHE:HD2	1:B:336:MET:HE2	1.60	0.67
1:A:114:ASN:HD22	1:A:116:LEU:H	1.41	0.67
1:B:100:CYS:O	1:B:104:LYS:HG2	1.94	0.67
1:A:291:ILE:HG22	1:A:315:LYS:O	1.94	0.67
1:A:275:MET:SD	1:A:291:ILE:HD12	2.35	0.66
1:B:348:HIS:HB2	1:B:370:THR:HB	1.78	0.66
1:B:40:MET:HA	1:B:40:MET:HE3	1.76	0.65
1:A:174:CYS:O	1:A:178:THR:HG23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:VAL:HG21	1:B:157:VAL:HG22	1.78	0.65
1:A:90:ILE:HD11	1:A:169:VAL:HG13	1.79	0.65
1:B:294:VAL:HG21	4:B:378:EOH:H23	1.79	0.64
1:B:165:PRO:CD	1:B:336:MET:HE1	2.28	0.64
1:A:169:VAL:HA	5:A:384:HOH:O	1.96	0.64
1:A:249:PRO:HB2	1:A:252:GLU:HG3	1.79	0.64
1:B:89:VAL:CG2	1:B:157:VAL:HG22	2.27	0.63
1:B:47:ARG:HD3	3:B:377:CND:O1A	1.99	0.63
1:A:114:ASN:ND2	1:A:116:LEU:H	1.96	0.63
1:B:7:ILE:HG13	1:B:37:ARG:NH2	2.13	0.63
1:A:361:LEU:HB3	1:A:367:SER:OG	1.98	0.63
1:B:105:HIS:CD2	1:B:107:GLU:H	2.18	0.61
1:A:283:GLN:HE22	1:A:285:ALA:H	1.49	0.61
1:B:129:ARG:HG2	1:B:151:VAL:CG1	2.31	0.60
1:A:283:GLN:NE2	1:A:285:ALA:H	1.98	0.60
1:A:68:GLU:HB3	1:A:174:CYS:HB3	1.84	0.60
1:A:8:LYS:HZ3	1:A:25:GLU:HG2	1.68	0.59
1:A:338:LYS:HA	5:A:420:HOH:O	2.02	0.59
1:B:203:VAL:HG23	1:B:268:VAL:CG2	2.32	0.59
1:A:157:VAL:O	1:A:325:LYS:HE3	2.03	0.58
1:B:97:CYS:HB3	1:B:113:LYS:HG3	1.84	0.58
1:A:275:MET:SD	1:A:291:ILE:CD1	2.93	0.57
1:A:5:LYS:HA	1:A:30:PRO:HG3	1.86	0.57
1:B:225:ASN:HD21	1:B:227:ASP:HB2	1.69	0.57
1:A:21:PHE:H	1:A:356:ASN:HD21	1.53	0.57
1:B:160:ILE:CG1	1:B:332:VAL:HG21	2.35	0.56
1:A:2:THR:O	1:A:3:ALA:HB2	2.06	0.56
1:A:153:ASP:HB3	5:A:403:HOH:O	2.06	0.56
1:A:187:ALA:HB2	1:A:290:VAL:HG21	1.87	0.56
1:B:253:VAL:O	1:B:257:MET:HG3	2.05	0.56
1:A:222:VAL:HG22	1:A:241:VAL:CG1	2.35	0.56
1:A:102:VAL:HG23	1:A:112:LEU:HD22	1.88	0.55
1:A:251:GLN:CG	1:A:277:THR:HG23	2.35	0.55
1:A:51:HIS:HB3	1:A:57:LEU:HB2	1.88	0.55
1:A:178:THR:HG22	1:A:319:PHE:HD1	1.71	0.55
1:A:12:ALA:HB1	1:A:21:PHE:HB3	1.88	0.55
1:A:271:ARG:O	1:A:275:MET:HG3	2.07	0.54
1:A:170:CYS:SG	1:A:371:ILE:HD12	2.48	0.54
1:A:37:ARG:HG3	1:A:151:VAL:HG22	1.90	0.54
1:B:9:CYS:HB2	1:B:148:GLN:OE1	2.07	0.54
1:B:39:LYS:HG3	1:B:149:TYR:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:HG13	1:A:37:ARG:NH2	2.22	0.54
1:B:64:ILE:HG13	1:B:137:ILE:HG21	1.89	0.54
1:A:32:LYS:HG3	1:A:129:ARG:HH12	1.73	0.54
1:B:242:ASN:C	1:B:242:ASN:HD22	2.15	0.54
1:A:191:GLN:HG2	1:A:215:GLY:HA3	1.89	0.54
1:A:292:VAL:O	3:A:377:CND:H2N	2.09	0.53
1:B:11:ALA:O	1:B:23:ILE:HA	2.08	0.53
1:B:18:LYS:NZ	1:B:18:LYS:HB3	2.24	0.53
1:A:160:ILE:HD12	1:A:169:VAL:HG11	1.90	0.53
1:A:299:GLN:O	1:B:304:ASN:ND2	2.42	0.52
1:A:8:LYS:NZ	1:A:25:GLU:HG2	2.24	0.52
1:B:249:PRO:HB3	1:B:251:GLN:HE22	1.75	0.52
1:B:31:PRO:HG3	1:B:37:ARG:HB2	1.91	0.52
1:A:209:MET:HE3	1:A:345:LEU:HD21	1.92	0.52
1:B:200:LEU:HD13	1:B:232:ALA:HB2	1.92	0.51
1:B:2:THR:O	1:B:3:ALA:HB2	2.11	0.51
1:B:63:VAL:HG22	1:B:64:ILE:N	2.25	0.51
1:A:178:THR:HG22	1:A:319:PHE:CD1	2.46	0.51
1:A:285:ALA:HB1	5:A:390:HOH:O	2.10	0.51
1:B:198:PHE:O	1:B:268:VAL:HG13	2.10	0.51
1:A:107:GLU:HG2	1:A:107:GLU:O	2.10	0.50
1:A:272:LEU:O	1:A:276:VAL:HG23	2.10	0.50
1:B:343:ASP:HB2	1:B:344:PRO:HD3	1.92	0.50
1:B:357:GLU:O	1:B:361:LEU:HD22	2.11	0.50
1:B:97:CYS:HA	1:B:155:ILE:HG13	1.93	0.50
1:B:308:LEU:HD12	1:B:312:ARG:O	2.12	0.50
1:B:33:ALA:HA	1:B:78:GLU:O	2.12	0.50
1:A:275:MET:HE1	1:A:295:PRO:HB3	1.93	0.50
1:B:203:VAL:CG2	1:B:268:VAL:HG23	2.41	0.50
1:A:313:THR:HB	1:B:315:LYS:HG2	1.94	0.49
1:B:225:ASN:ND2	1:B:227:ASP:HB2	2.27	0.49
1:B:9:CYS:O	1:B:25:GLU:HA	2.11	0.49
1:B:359:PHE:HB3	1:B:363:ARG:NH2	2.28	0.49
1:A:23:ILE:HD11	1:A:355:ILE:CG2	2.42	0.49
1:B:10:LYS:HA	1:B:24:GLU:O	2.13	0.49
1:B:88:LYS:HD2	1:B:162:ALA:HA	1.95	0.49
1:A:192:GLY:HA2	1:A:217:ALA:HB2	1.94	0.49
1:A:32:LYS:HG3	1:A:129:ARG:NH1	2.28	0.48
1:A:39:LYS:HE2	5:A:396:HOH:O	2.13	0.48
1:B:31:PRO:CG	1:B:37:ARG:HB2	2.43	0.48
1:B:43:THR:HG23	1:B:69:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ALA:HB2	1:B:262:VAL:HG21	1.94	0.48
1:A:350:LEU:HD13	1:A:370:THR:HG23	1.95	0.48
1:A:2:THR:HG22	1:A:3:ALA:H	1.80	0.47
1:B:272:LEU:HG	1:B:301:LEU:HB3	1.96	0.47
1:B:10:LYS:O	1:B:148:GLN:HG3	2.15	0.47
1:B:303:MET:HE1	1:B:305:PRO:HA	1.97	0.47
1:A:238:THR:HG22	1:A:239:GLU:OE1	2.14	0.47
1:A:267:GLU:HG3	1:A:275:MET:HA	1.96	0.47
1:B:39:LYS:HG3	1:B:149:TYR:CZ	2.49	0.47
1:B:5:LYS:HG3	1:B:6:VAL:H	1.80	0.47
1:B:279:LEU:HD23	1:B:312:ARG:HD2	1.97	0.47
1:A:46:CYS:HB3	1:A:67:HIS:CE1	2.50	0.46
1:B:92:LEU:HD13	1:B:324:SER:HB2	1.97	0.46
1:A:301:LEU:CD1	1:B:303:MET:HE2	2.41	0.46
1:A:222:VAL:HG22	1:A:241:VAL:HG13	1.98	0.46
1:B:73:VAL:HG11	1:B:76:ILE:HD13	1.98	0.46
1:A:116:LEU:HG	1:A:141:LEU:CD2	2.46	0.46
1:A:283:GLN:HE22	1:A:285:ALA:HB3	1.80	0.46
1:B:5:LYS:HE3	1:B:5:LYS:HA	1.99	0.45
1:B:48:SER:HA	1:B:51:HIS:CD2	2.51	0.45
1:A:9:CYS:O	1:A:25:GLU:HA	2.16	0.45
1:A:315:LYS:HG2	1:B:313:THR:HB	1.98	0.45
1:B:187:ALA:HB2	1:B:290:VAL:HG21	1.98	0.45
1:B:324:SER:O	1:B:328:VAL:HG13	2.15	0.45
1:A:308:LEU:O	1:B:316:GLY:HA3	2.16	0.45
1:B:36:VAL:O	1:B:151:VAL:HA	2.15	0.45
1:A:114:ASN:HD21	1:A:117:SER:H	1.65	0.45
1:A:68:GLU:HB3	1:A:174:CYS:CB	2.47	0.45
1:A:303:MET:HG2	1:A:304:ASN:N	2.31	0.45
1:A:100:CYS:O	1:A:104:LYS:HG2	2.17	0.45
1:B:204:GLY:HA2	1:B:268:VAL:HG21	1.99	0.45
1:B:335:PHE:CD1	1:B:342:LEU:HD22	2.52	0.45
1:B:294:VAL:CG2	4:B:378:EOH:H23	2.47	0.44
1:B:242:ASN:HD22	1:B:243:PRO:N	2.15	0.44
1:B:268:VAL:CG2	1:B:268:VAL:O	2.66	0.44
1:A:241:VAL:HG23	1:A:246:TYR:CE1	2.53	0.44
1:B:45:ILE:HG23	1:B:359:PHE:CZ	2.52	0.44
1:B:174:CYS:SG	1:B:175:GLY:N	2.89	0.44
1:B:267:GLU:HG3	1:B:275:MET:HA	1.99	0.44
1:B:105:HIS:CD2	1:B:108:GLY:H	2.35	0.44
1:B:89:VAL:HG22	1:B:90:ILE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:LYS:HG3	1:B:368:ILE:CD1	2.47	0.44
1:A:5:LYS:HD2	1:A:30:PRO:HG3	2.00	0.44
1:A:361:LEU:HD23	1:A:361:LEU:HA	1.90	0.44
1:B:229:PHE:CD1	1:B:229:PHE:N	2.85	0.44
1:A:57:LEU:HD23	1:A:294:VAL:HG11	2.00	0.43
1:B:307:LEU:HD23	1:B:312:ARG:NH2	2.32	0.43
1:A:128:SER:OG	1:A:129:ARG:N	2.51	0.43
1:B:40:MET:HE2	1:B:69:ALA:HB1	2.00	0.43
1:B:135:LYS:HA	1:B:136:PRO:HD3	1.78	0.43
1:A:116:LEU:HD11	4:A:378:EOH:H21	1.99	0.43
1:B:61:LEU:HD12	1:B:63:VAL:HG12	2.00	0.43
1:A:101:ARG:HA	1:A:101:ARG:HD2	1.79	0.43
1:A:6:VAL:N	1:A:30:PRO:HD3	2.34	0.43
1:B:335:PHE:CD2	1:B:336:MET:HE2	2.48	0.43
1:A:24:GLU:OE1	1:A:132:CYS:SG	2.77	0.43
1:A:226:LYS:HE2	1:A:226:LYS:HB3	1.90	0.43
1:A:32:LYS:CG	1:A:129:ARG:HH12	2.32	0.42
1:B:48:SER:HB2	1:B:67:HIS:HE1	1.84	0.42
1:B:231:LYS:O	1:B:235:VAL:HG22	2.18	0.42
1:B:294:VAL:HA	1:B:295:PRO:HD2	1.95	0.42
1:B:331:LEU:HA	1:B:331:LEU:HD23	1.83	0.42
1:B:192:GLY:HA2	1:B:217:ALA:HB2	2.01	0.42
1:A:18:LYS:O	1:A:19:LYS:HD2	2.19	0.42
1:A:342:LEU:CD2	5:A:384:HOH:O	2.67	0.42
1:B:37:ARG:HG2	1:B:74:GLU:OE1	2.20	0.42
1:B:272:LEU:HD21	1:B:299:GLN:HB3	2.01	0.42
1:B:175:GLY:HA2	1:B:203:VAL:HG12	2.00	0.42
1:A:53:VAL:HG21	1:A:363:ARG:NH2	2.34	0.42
1:A:264:PHE:HA	1:A:288:VAL:O	2.19	0.42
1:A:5:LYS:C	1:A:30:PRO:HD3	2.45	0.42
1:A:70:ALA:HB1	1:A:166:LEU:HD22	2.01	0.42
1:B:123:MET:HE1	1:B:152:VAL:HA	2.01	0.42
1:A:89:VAL:HG12	1:A:159:LYS:HA	2.01	0.42
1:B:345:LEU:O	1:B:369:ARG:HB2	2.19	0.42
1:A:132:CYS:O	1:A:134:GLY:N	2.54	0.41
1:B:122:THR:HG22	1:B:127:THR:C	2.44	0.41
1:B:165:PRO:HG2	1:B:168:LYS:HB2	2.02	0.41
1:A:279:LEU:HD13	1:A:307:LEU:HD23	2.02	0.41
1:B:301:LEU:C	1:B:301:LEU:HD12	2.46	0.41
1:B:304:ASN:HD22	1:B:304:ASN:HA	1.74	0.41
1:A:41:VAL:C	1:A:374:PHE:HD2	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:SER:O	1:B:52:VAL:HG23	2.21	0.41
1:B:269:ILE:HG21	1:B:271:ARG:HD2	2.02	0.41
1:A:243:PRO:HG3	1:A:250:ILE:HG13	2.03	0.41
1:B:5:LYS:HG3	1:B:6:VAL:N	2.35	0.41
1:A:171:LEU:HD12	1:A:171:LEU:HA	1.91	0.41
1:B:204:GLY:CA	1:B:268:VAL:HG21	2.51	0.41
1:B:195:CYS:HA	1:B:264:PHE:O	2.21	0.40
1:B:268:VAL:O	1:B:268:VAL:HG22	2.21	0.40
1:B:42:ALA:HA	1:B:372:LEU:O	2.22	0.40
1:A:11:ALA:O	1:A:23:ILE:HA	2.22	0.40
1:A:37:ARG:HD3	1:A:74:GLU:OE1	2.22	0.40
1:B:63:VAL:CG2	1:B:64:ILE:N	2.85	0.40
1:B:328:VAL:N	1:B:329:PRO:HD2	2.36	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	372/374 (100%)	331 (89%)	36 (10%)	5 (1%)	9	14
1	B	372/374 (100%)	325 (87%)	42 (11%)	5 (1%)	9	14
All	All	744/748 (100%)	656 (88%)	78 (10%)	10 (1%)	9	14

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	ASP
1	B	174	CYS
1	B	297	ASP
1	B	2	THR
1	B	175	GLY

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Mol	Chain	Res	Type
1	A	3	ALA
1	A	133	ARG
1	A	129	ARG
1	B	4	GLY
1	A	134	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	308/308 (100%)	271 (88%)	37 (12%)	5	7
1	B	308/308 (100%)	261 (85%)	47 (15%)	3	3
All	All	616/616 (100%)	532 (86%)	84 (14%)	3	5

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	5	LYS
1	A	13	VAL
1	A	14	LEU
1	A	26	VAL
1	A	43	THR
1	A	53	VAL
1	A	107	GLU
1	A	112	LEU
1	A	116	LEU
1	A	118	MET
1	A	129	ARG
1	A	133	ARG
1	A	135	LYS
1	A	167	GLU
1	A	169	VAL
1	A	171	LEU
1	A	239	GLU

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Mol	Chain	Res	Type
1	A	250	ILE
1	A	262	VAL
1	A	268	VAL
1	A	272	LEU
1	A	276	VAL
1	A	279	LEU
1	A	280	SER
1	A	299	GLN
1	A	303	MET
1	A	306	MET
1	A	307	LEU
1	A	313	THR
1	A	318	ILE
1	A	324	SER
1	A	326	ASP
1	A	328	VAL
1	A	342	LEU
1	A	366	GLU
1	A	372	LEU
1	B	5	LYS
1	B	14	LEU
1	B	18	LYS
1	B	36	VAL
1	B	37	ARG
1	B	40	MET
1	B	61	LEU
1	B	72	ILE
1	B	76	ILE
1	B	84	ARG
1	B	85	PRO
1	B	112	LEU
1	B	122	THR
1	B	129	ARG
1	B	133	ARG
1	B	141	LEU
1	B	151	VAL
1	B	153	ASP
1	B	155	ILE
1	B	159	LYS
1	B	160	ILE
1	B	168	LYS
1	B	171	LEU

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Mol	Chain	Res	Type
1	B	186	VAL
1	B	190	THR
1	B	212	LYS
1	B	225	ASN
1	B	226	LYS
1	B	268	VAL
1	B	272	LEU
1	B	274	THR
1	B	279	LEU
1	B	301	LEU
1	B	303	MET
1	B	306	MET
1	B	308	LEU
1	B	309	LEU
1	B	313	THR
1	B	328	VAL
1	B	330	LYS
1	B	342	LEU
1	B	345	LEU
1	B	361	LEU
1	B	362	LEU
1	B	366	GLU
1	B	370	THR
1	B	372	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	114	ASN
1	A	124	GLN
1	A	148	GLN
1	A	191	GLN
1	A	244	GLN
1	A	283	GLN
1	A	356	ASN
1	B	105	HIS
1	B	138	HIS
1	B	225	ASN
1	B	242	ASN
1	B	251	GLN
1	B	259	ASN

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Mol	Chain	Res	Type
1	B	304	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	EOH	B	378	-	2,2,2	0.70	0	1,1,1	0.28	0
3	CND	B	377	2	48,48,48	2.03	6 (12%)	64,73,73	1.99	14 (21%)
3	CND	A	377	2	48,48,48	1.72	6 (12%)	64,73,73	2.21	17 (26%)
4	EOH	A	378	-	2,2,2	0.60	0	1,1,1	0.39	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
3	CND	B	377	2	-	5/28/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CND	A	377	2	-	10/28/62/62	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	377	CND	C6N-N5N	10.74	1.42	1.31
3	A	377	CND	C6N-N5N	8.14	1.39	1.31
3	B	377	CND	PA-O3	4.53	1.64	1.59
3	A	377	CND	C5A-N7A	-3.38	1.32	1.39
3	B	377	CND	C4N-C3N	3.37	1.42	1.37
3	A	377	CND	PN-O3	-3.12	1.56	1.59
3	A	377	CND	C2N-C3N	-2.87	1.37	1.43
3	B	377	CND	C5A-N7A	-2.76	1.34	1.39
3	A	377	CND	C4A-N9A	-2.67	1.32	1.37
3	A	377	CND	C1D-C1N	-2.47	1.46	1.49
3	B	377	CND	C4A-N9A	-2.42	1.32	1.37
3	B	377	CND	C3N-C7N	2.28	1.56	1.49

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	377	CND	C5A-C4A-N3A	-6.57	117.67	126.72
3	B	377	CND	N3A-C4A-N9A	6.42	138.08	127.17
3	B	377	CND	C5A-C4A-N3A	-6.16	118.24	126.72
3	A	377	CND	N3A-C4A-N9A	5.95	137.28	127.17
3	A	377	CND	C6A-C5A-C4A	5.21	124.29	117.18
3	A	377	CND	C3D-C2D-C1D	-4.93	95.87	101.69
3	A	377	CND	C6A-C5A-N7A	-4.85	122.74	132.09
3	B	377	CND	C6A-C5A-N7A	-4.39	123.62	132.09
3	B	377	CND	O3-PA-O1A	-4.31	97.74	110.70
3	B	377	CND	N3A-C2A-N1A	-4.31	122.06	128.58
3	A	377	CND	C1N-C6N-N5N	-4.27	117.87	125.13
3	B	377	CND	C6A-C5A-C4A	3.68	122.20	117.18
3	A	377	CND	C2N-C1N-C6N	3.53	123.43	118.55
3	A	377	CND	O2D-C2D-C1D	3.48	119.47	111.21
3	A	377	CND	C2D-C1D-C1N	3.43	119.74	114.30
3	B	377	CND	C4A-C5A-N7A	3.14	114.17	110.58
3	A	377	CND	N3A-C2A-N1A	-2.92	124.16	128.58
3	B	377	CND	C2A-N3A-C4A	2.91	118.94	111.83
3	B	377	CND	C4A-N9A-C8A	2.84	108.72	105.74
3	A	377	CND	C2A-N3A-C4A	2.72	118.48	111.83
3	B	377	CND	N6A-C6A-N1A	2.66	124.31	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	377	CND	O2A-PA-O1A	2.40	123.63	112.44
3	A	377	CND	O2N-PN-O3	2.36	113.64	107.27
3	A	377	CND	N6A-C6A-N1A	2.29	123.48	118.38
3	B	377	CND	C5B-C4B-C3B	-2.28	107.02	115.21
3	A	377	CND	O4B-C1B-N9A	2.23	112.38	108.09
3	A	377	CND	O2N-PN-O1N	2.19	122.65	112.44
3	B	377	CND	O4D-C4D-C5D	-2.16	102.42	109.33
3	A	377	CND	C4A-C5A-N7A	2.09	112.97	110.58
3	B	377	CND	C3D-C2D-C1D	-2.03	99.29	101.69
3	A	377	CND	O3-PN-O1N	-2.00	104.68	110.70

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	377	CND	C5B-O5B-PA-O1A
3	A	377	CND	C5B-O5B-PA-O3
3	A	377	CND	C2D-C1D-C1N-C2N
3	B	377	CND	C5B-O5B-PA-O1A
3	B	377	CND	C2D-C1D-C1N-C2N
3	A	377	CND	O4B-C4B-C5B-O5B
3	A	377	CND	C3B-C4B-C5B-O5B
3	A	377	CND	C2N-C3N-C7N-O7N
3	A	377	CND	C2B-C1B-N9A-C8A
3	A	377	CND	C5B-O5B-PA-O2A
3	B	377	CND	C2N-C3N-C7N-O7N
3	A	377	CND	O4D-C1D-C1N-C2N
3	B	377	CND	O4D-C1D-C1N-C2N
3	A	377	CND	O4B-C1B-N9A-C8A
3	B	377	CND	O4B-C4B-C5B-O5B

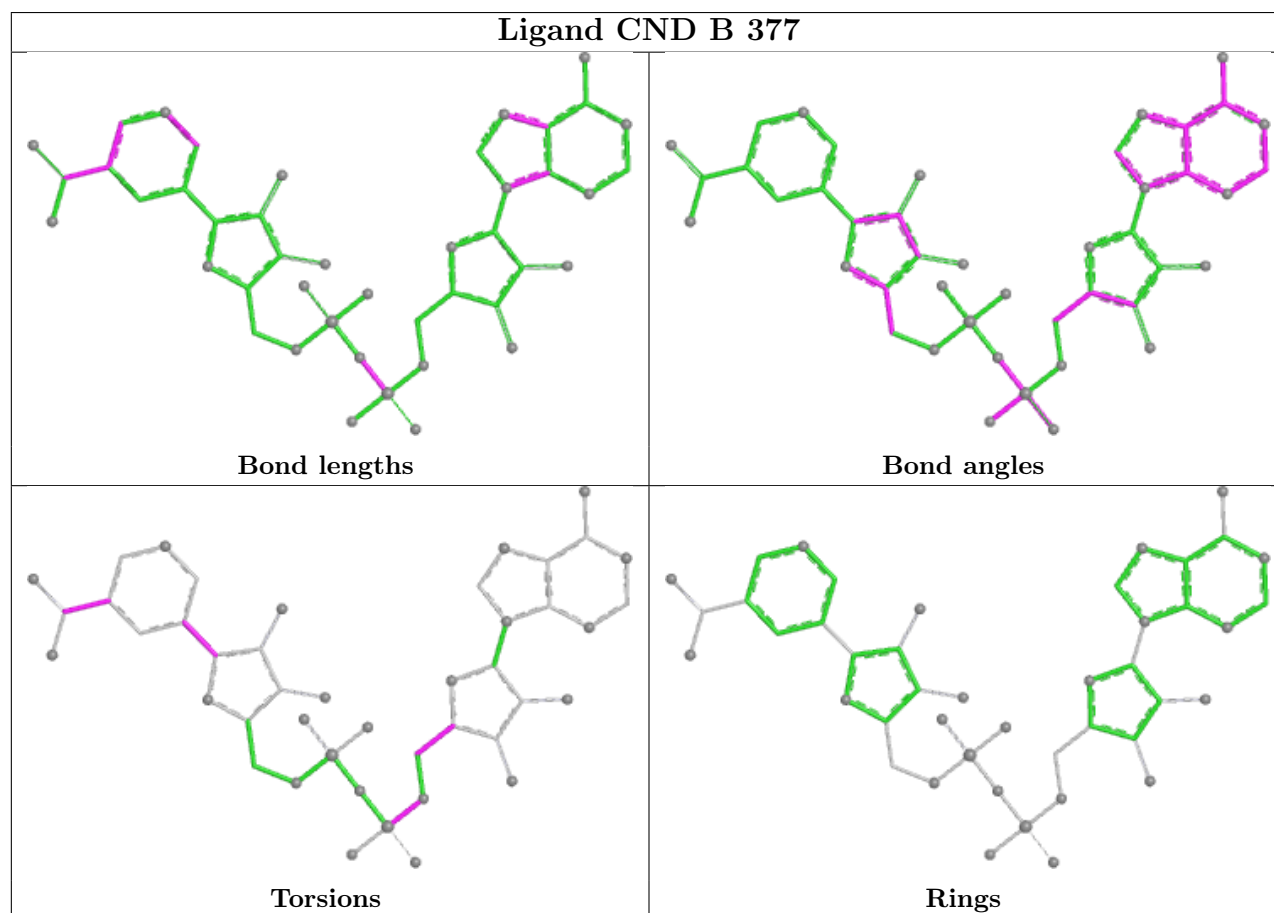
There are no ring outliers.

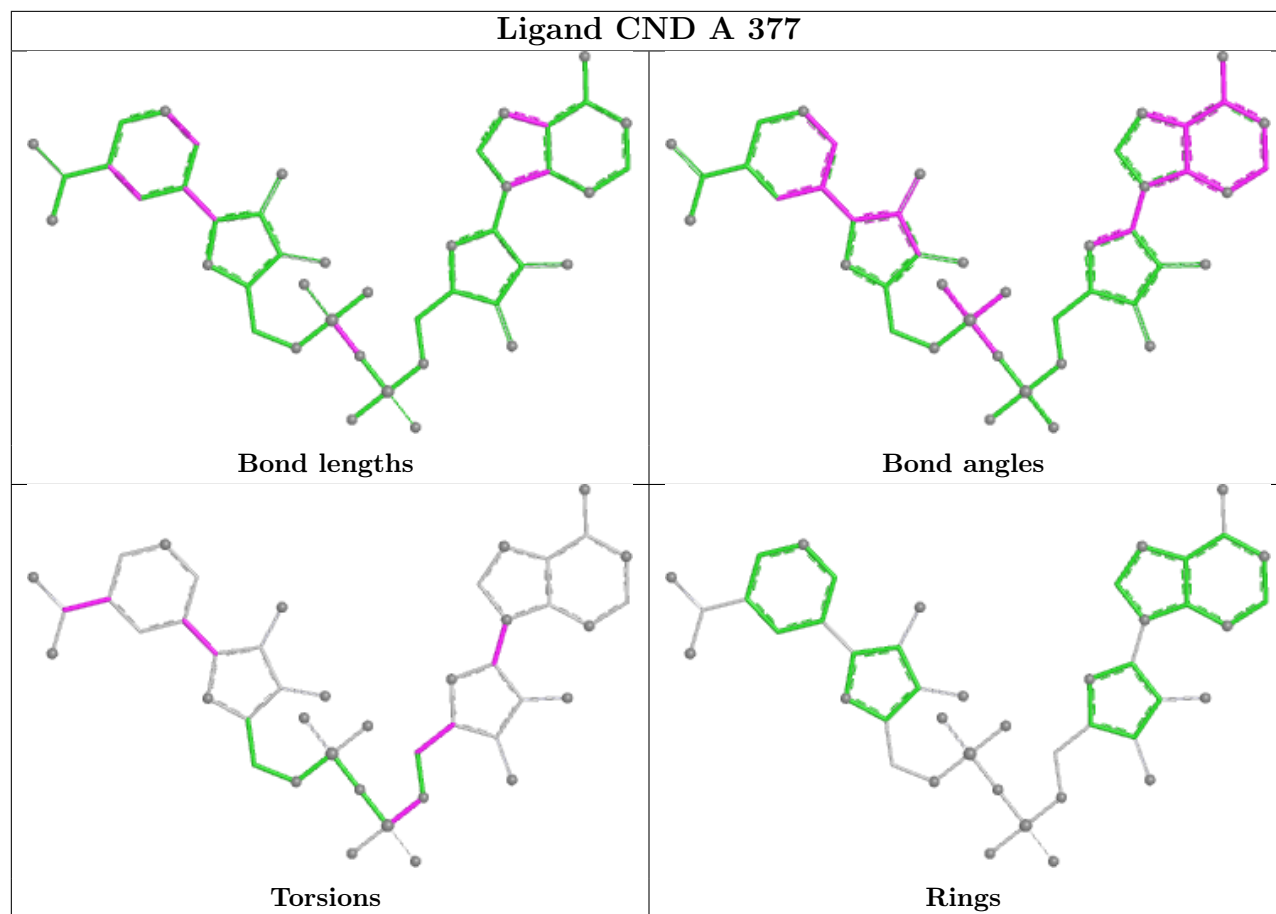
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	378	EOH	2	0
3	B	377	CND	1	0
3	A	377	CND	1	0
4	A	378	EOH	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.