



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:16 AM UTC

PDB ID : 1ADC / pdb_00001adc
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 : 2.70 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

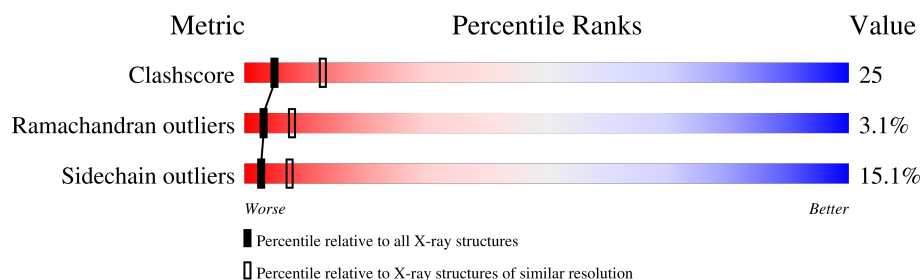
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	51% 37% 11%
1	B	374	47% 40% 11%

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	A	378	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7009 atoms, of which 1306 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.

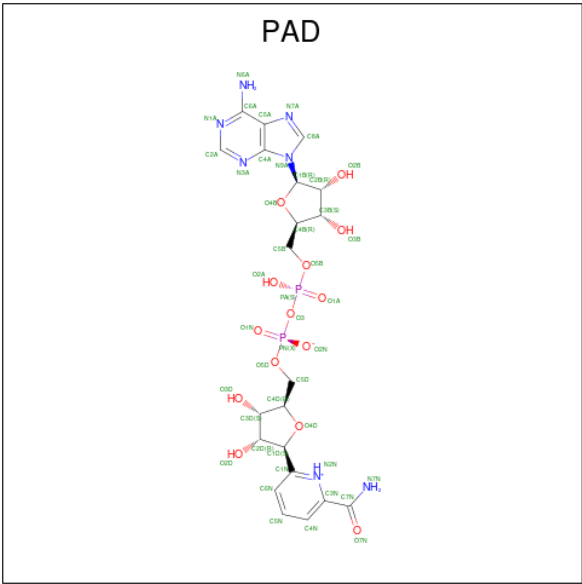
- Molecule 1 is a protein called ALCOHOL DEHYDROGENASE.

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).

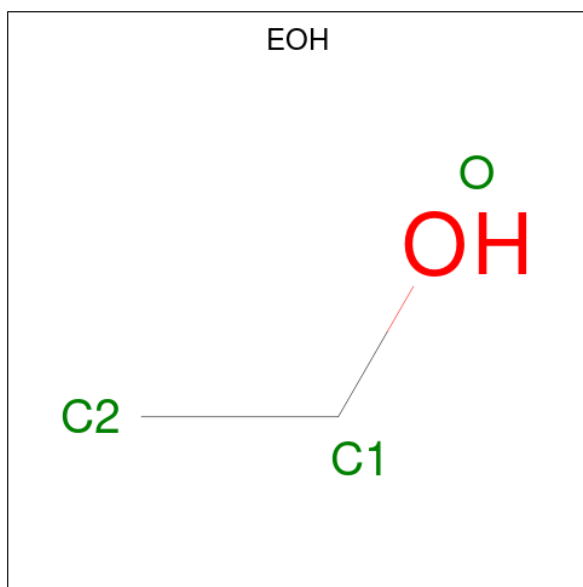
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 5-BETA-D-RIBOFURANOSYLPICOLINAMIDE ADENINE-DINUCLEOTIDE (CCD ID: PAD) (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: C_2H_6O).



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.

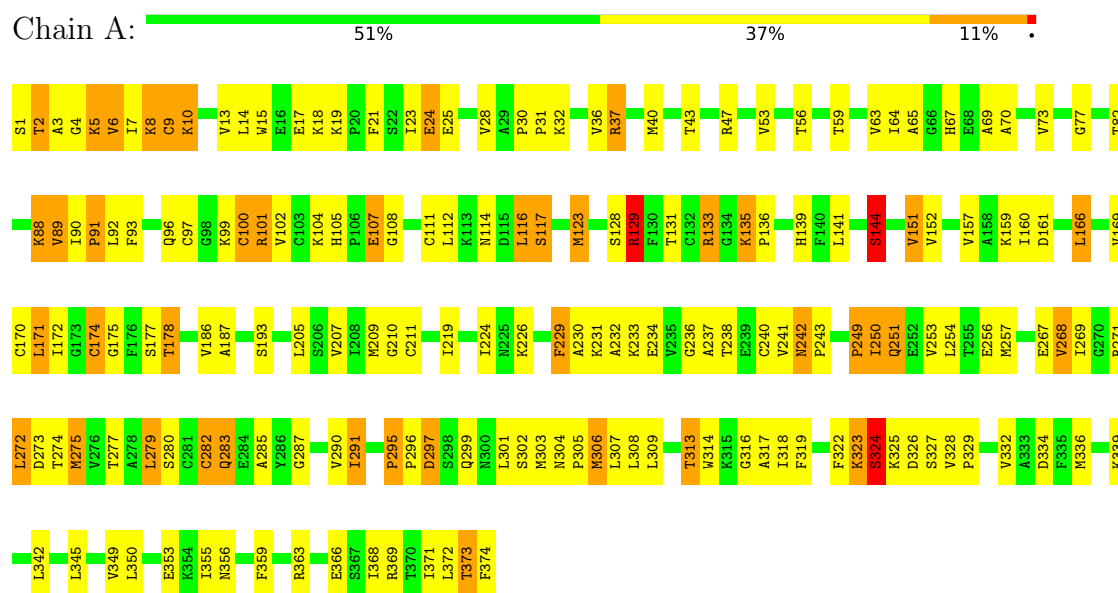
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	28	Total	H	O	0	0
			84	56	28		
5	B	8	Total	H	O	0	0
			24	16	8		

3 Residue-property plots

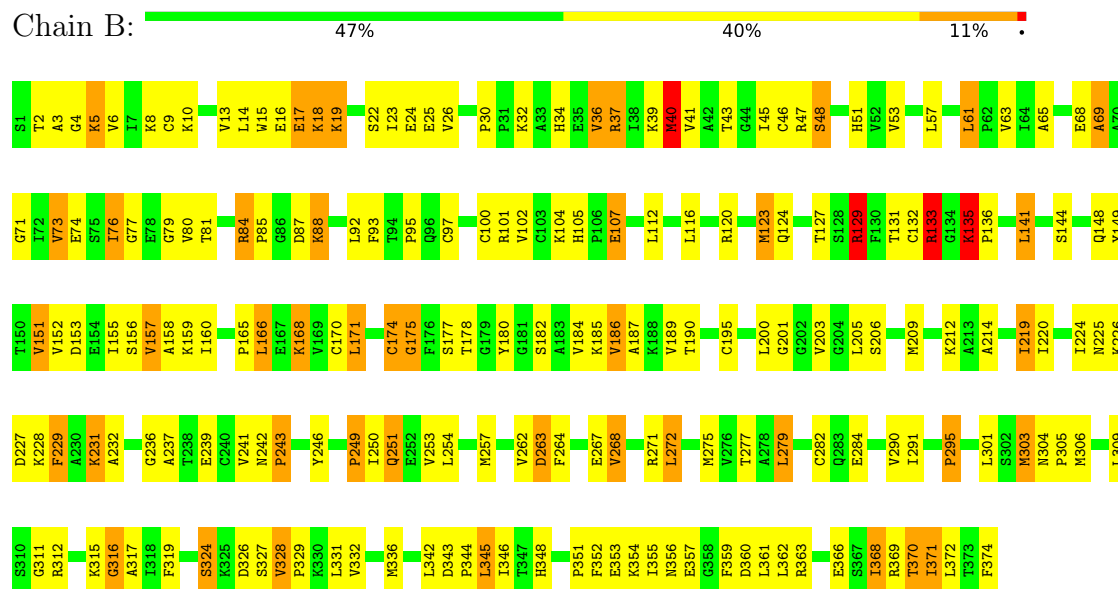
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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	51.90Å 44.80Å 93.00Å 103.10° 87.80° 70.40°	Depositor
Resolution (Å)	(Not available) – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7009	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, PAD, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.71	0/2836	1.17	28/3834 (0.7%)
1	B	0.70	0/2837	1.20	23/3834 (0.6%)
All	All	0.71	0/5673	1.18	51/7668 (0.7%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	PHE	N-CA-C	8.57	120.24	111.07
1	A	133	ARG	N-CA-C	-8.36	94.70	108.67
1	A	24	GLU	N-CA-C	7.43	117.81	108.45
1	B	135	LYS	CA-C-N	6.92	127.46	119.99
1	B	135	LYS	C-N-CA	6.92	127.46	119.99
1	A	295	PRO	N-CA-C	6.90	119.12	110.70
1	B	120	ARG	N-CA-C	-6.58	104.90	113.12
1	B	316	GLY	N-CA-C	-6.49	101.30	110.96
1	B	371	ILE	N-CA-C	6.20	117.34	107.98
1	B	229	PHE	N-CA-C	6.17	118.80	111.33
1	A	193	SER	N-CA-C	6.14	118.25	110.33
1	A	89	VAL	N-CA-C	6.12	116.00	108.53
1	B	3	ALA	N-CA-C	5.98	116.31	107.88
1	B	133	ARG	N-CA-C	-5.96	98.11	110.80
1	A	82	THR	N-CA-C	5.91	120.51	113.12
1	A	135	LYS	CA-C-N	5.86	125.81	119.78
1	A	135	LYS	C-N-CA	5.86	125.81	119.78
1	A	123	MET	N-CA-C	-5.86	101.52	109.95
1	A	9	CYS	N-CA-C	5.83	115.94	108.24
1	A	324	SER	N-CA-C	5.68	122.89	110.80
1	B	327	SER	N-CA-C	5.63	117.28	111.03
1	B	69	ALA	N-CA-C	5.61	115.79	107.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	371	ILE	CB-CA-C	-5.58	105.21	111.23
1	A	242	ASN	CA-C-N	5.57	126.81	119.84
1	A	242	ASN	C-N-CA	5.57	126.81	119.84
1	A	73	VAL	N-CA-C	5.56	116.77	108.54
1	A	63	VAL	N-CA-C	5.53	116.33	108.42
1	A	88	LYS	N-CA-C	-5.53	100.97	109.76
1	B	123	MET	N-CA-C	-5.50	101.86	110.17
1	B	328	VAL	N-CA-CB	5.49	114.20	110.52
1	A	37	ARG	N-CA-C	-5.43	100.86	109.76
1	B	168	LYS	N-CA-C	-5.38	104.76	112.13
1	A	91	PRO	N-CA-C	-5.36	103.72	111.22
1	B	34	HIS	N-CA-C	5.25	119.64	113.23
1	A	100	CYS	N-CA-C	5.25	117.46	110.53
1	B	40	MET	N-CA-C	5.24	116.69	109.15
1	B	135	LYS	N-CA-C	5.22	117.86	110.24
1	A	207	VAL	N-CA-C	-5.21	105.46	110.72
1	B	295	PRO	CA-C-N	5.16	126.29	119.84
1	B	295	PRO	C-N-CA	5.16	126.29	119.84
1	A	59	THR	N-CA-C	-5.13	100.15	108.82
1	B	4	GLY	N-CA-C	-5.12	101.05	113.18
1	A	323	LYS	N-CA-C	-5.10	100.76	108.67
1	B	19	LYS	CA-C-N	-5.09	115.35	120.85
1	B	19	LYS	C-N-CA	-5.09	115.35	120.85
1	B	182	SER	N-CA-C	-5.08	105.66	111.14
1	A	317	ALA	N-CA-C	5.07	116.77	108.76
1	A	67	HIS	CA-C-N	-5.07	116.25	122.84
1	A	67	HIS	C-N-CA	-5.07	116.25	122.84
1	A	135	LYS	N-CA-C	5.02	116.15	109.93
1	A	327	SER	N-CA-C	5.00	117.69	111.24

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	2850	131	0
1	B	2785	607	2848	164	0
2	A	2	0	0	1	0
2	B	2	0	0	0	0
3	A	44	8	26	3	0
3	B	44	8	26	3	0
4	A	3	2	6	2	0
4	B	3	2	5	0	0
5	A	28	56	0	4	0
5	B	8	16	0	0	0
All	All	5703	1306	5761	286	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 25.

All (286) 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:105:HIS:HD2	1:B:107:GLU:H	1.10	0.93
1:B:251:GLN:HG3	1:B:277:THR:HG23	1.50	0.92
1:B:47:ARG:HD3	3:B:377:PAD:O1A	1.71	0.90
1:B:187:ALA:HB2	1:B:290:VAL:HG21	1.56	0.86
1:A:209:MET:HE3	1:A:345:LEU:HD21	1.59	0.84
1:B:224:ILE:HA	1:B:242:ASN:ND2	1.94	0.83
1:B:105:HIS:CD2	1:B:107:GLU:H	1.97	0.82
1:A:114:ASN:HD22	1:A:116:LEU:H	1.28	0.82
1:B:129:ARG:HG2	1:B:151:VAL:HG11	1.61	0.82
1:A:9:CYS:O	1:A:25:GLU:HA	1.79	0.81
1:A:272:LEU:HG	1:A:301:LEU:HB3	1.64	0.80
1:B:165:PRO:HD2	1:B:336:MET:HE1	1.64	0.79
1:B:5:LYS:HE2	1:B:6:VAL:HG23	1.64	0.78
1:B:249:PRO:HB3	1:B:251:GLN:HE22	1.49	0.78
1:A:169:VAL:HG13	1:A:172:ILE:HD12	1.67	0.76
1:B:153:ASP:HB2	1:B:155:ILE:HG22	1.67	0.76
1:B:180:TYR:O	1:B:184:VAL:HG12	1.85	0.75
1:A:92:LEU:HD13	1:A:324:SER:HB3	1.67	0.74
1:A:70:ALA:HB1	1:A:166:LEU:HD22	1.67	0.74
1:A:301:LEU:HD11	1:B:303:MET:HE2	1.70	0.74
1:B:129:ARG:HG2	1:B:151:VAL:CG1	2.18	0.73
1:A:43:THR:HG23	1:A:374:PHE:HE1	1.53	0.72
1:A:5:LYS:HD2	1:A:30:PRO:HG3	1.72	0.71
1:B:40:MET:HE3	1:B:40:MET:HA	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:CYS:O	1:A:104:LYS:HG2	1.91	0.70
1:B:68:GLU:OE2	1:B:171:LEU:HD12	1.91	0.70
1:B:231:LYS:HE3	1:B:344:PRO:O	1.92	0.69
1:A:251:GLN:HG3	1:A:277:THR:HG23	1.74	0.69
1:B:105:HIS:HD2	1:B:107:GLU:N	1.89	0.69
1:A:187:ALA:HB2	1:A:290:VAL:HG21	1.75	0.69
1:B:178:THR:HG21	3:B:377:PAD:H4N	1.73	0.68
1:A:43:THR:HG22	1:A:69:ALA:HB2	1.73	0.68
1:A:64:ILE:O	1:A:144:SER:HB3	1.92	0.68
1:B:160:ILE:HG13	1:B:332:VAL:HG21	1.76	0.68
1:A:5:LYS:NZ	1:A:6:VAL:HG23	2.09	0.67
1:B:351:PRO:HD2	1:B:354:LYS:HD2	1.76	0.67
1:A:229:PHE:HB3	1:A:233:LYS:HZ2	1.58	0.66
1:A:93:PHE:CE2	4:A:378:EOH:H22	2.30	0.66
1:B:97:CYS:HB3	1:B:155:ILE:HD11	1.78	0.66
1:B:5:LYS:HA	1:B:30:PRO:HG3	1.77	0.65
1:B:93:PHE:HB2	1:B:141:LEU:HD23	1.79	0.64
1:A:313:THR:HB	1:B:315:LYS:HG2	1.79	0.64
1:B:203:VAL:HG22	3:B:377:PAD:O2N	1.96	0.64
1:B:263:ASP:HB3	1:B:264:PHE:CD1	2.33	0.64
1:B:359:PHE:O	1:B:363:ARG:HG3	1.97	0.64
1:A:313:THR:HG21	5:A:401:HOH:O	1.98	0.64
1:A:111:CYS:HG	2:A:376:ZN:ZN	1.11	0.63
1:A:253:VAL:HG12	1:A:257:MET:HE3	1.80	0.63
1:A:89:VAL:HG12	1:A:159:LYS:HA	1.82	0.62
1:A:282:CYS:SG	1:A:287:GLY:HA3	2.40	0.62
1:B:36:VAL:O	1:B:151:VAL:HA	1.98	0.62
1:B:250:ILE:HG13	1:B:254:LEU:HD12	1.82	0.61
1:A:178:THR:HG21	3:A:377:PAD:H4N	1.82	0.61
1:A:174:CYS:O	1:A:178:THR:HG23	2.00	0.61
1:B:195:CYS:HA	1:B:264:PHE:O	1.99	0.61
1:B:5:LYS:CA	1:B:30:PRO:HG3	2.31	0.61
1:B:324:SER:O	1:B:328:VAL:HG22	2.00	0.61
1:B:203:VAL:HG23	1:B:268:VAL:CG2	2.31	0.60
1:B:346:ILE:HG12	1:B:371:ILE:HD11	1.83	0.60
1:A:373:THR:HG21	5:A:403:HOH:O	2.02	0.60
1:A:231:LYS:O	1:A:234:GLU:HB3	2.02	0.60
1:B:133:ARG:HD2	1:B:133:ARG:N	2.17	0.60
1:A:43:THR:HG22	1:A:69:ALA:CB	2.32	0.59
1:B:102:VAL:HG23	1:B:112:LEU:HD12	1.84	0.59
1:A:233:LYS:HA	1:A:237:ALA:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:LYS:HA	1:B:24:GLU:O	2.03	0.59
1:A:5:LYS:HA	1:A:30:PRO:HG3	1.85	0.59
1:B:17:GLU:H	1:B:17:GLU:CD	2.10	0.59
1:B:241:VAL:HG13	1:B:246:TYR:CE2	2.37	0.59
1:B:69:ALA:HA	1:B:170:CYS:HB2	1.86	0.58
1:B:328:VAL:HG23	1:B:329:PRO:HD3	1.84	0.58
1:A:283:GLN:HE22	1:A:285:ALA:HB3	1.69	0.58
1:A:250:ILE:HD12	1:A:254:LEU:CD2	2.34	0.58
1:B:225:ASN:HD21	1:B:227:ASP:HB2	1.68	0.58
1:A:269:ILE:HG22	1:A:271:ARG:HG3	1.85	0.57
1:B:132:CYS:O	1:B:133:ARG:HB2	2.04	0.57
1:A:295:PRO:HD2	1:B:309:LEU:CD1	2.34	0.57
1:B:267:GLU:HG3	1:B:275:MET:HA	1.85	0.57
1:A:105:HIS:CE1	1:A:107:GLU:HB3	2.38	0.57
1:B:61:LEU:HD12	1:B:63:VAL:HG12	1.85	0.57
1:B:282:CYS:O	1:B:312:ARG:NH1	2.38	0.57
1:A:295:PRO:HD2	1:B:309:LEU:HD11	1.86	0.57
1:B:348:HIS:HB2	1:B:370:THR:HB	1.87	0.57
1:A:28:VAL:O	1:A:37:ARG:NH2	2.37	0.57
1:B:209:MET:HE3	1:B:345:LEU:HD11	1.86	0.57
1:A:4:GLY:O	1:A:5:LYS:HG2	2.05	0.57
1:B:174:CYS:O	1:B:178:THR:HG23	2.05	0.57
1:B:16:GLU:HB2	1:B:19:LYS:HG3	1.87	0.56
1:B:88:LYS:HG2	1:B:166:LEU:HD11	1.88	0.56
1:B:5:LYS:HA	1:B:30:PRO:CG	2.35	0.56
1:B:45:ILE:HD13	1:B:359:PHE:CD1	2.40	0.56
1:B:76:ILE:HD13	1:B:85:PRO:HG3	1.86	0.56
1:A:170:CYS:SG	1:A:371:ILE:CD1	2.94	0.56
1:A:301:LEU:HD12	1:A:301:LEU:O	2.05	0.56
1:B:152:VAL:HG21	1:B:157:VAL:HG23	1.88	0.56
1:B:225:ASN:HD22	1:B:228:LYS:HG2	1.70	0.56
1:A:229:PHE:HB3	1:A:233:LYS:NZ	2.21	0.55
1:B:5:LYS:C	1:B:30:PRO:HG3	2.32	0.55
1:B:359:PHE:HB3	1:B:363:ARG:HH21	1.72	0.55
1:B:241:VAL:HG13	1:B:246:TYR:HE2	1.71	0.55
5:A:401:HOH:O	1:B:315:LYS:HE2	2.07	0.55
1:A:187:ALA:HB2	1:A:290:VAL:CG2	2.36	0.55
1:A:40:MET:HA	1:A:40:MET:HE2	1.90	0.54
1:B:123:MET:HE1	1:B:151:VAL:O	2.07	0.54
1:A:100:CYS:HB2	1:A:112:LEU:HD23	1.89	0.54
1:B:343:ASP:HB2	1:B:344:PRO:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:VAL:HB	1:A:329:PRO:HD3	1.89	0.53
1:B:187:ALA:HB2	1:B:290:VAL:CG2	2.31	0.53
1:B:206:SER:O	1:B:209:MET:HB2	2.09	0.53
1:A:178:THR:HG22	1:A:319:PHE:HA	1.89	0.53
1:A:31:PRO:HD3	1:A:37:ARG:HB2	1.90	0.53
1:B:102:VAL:HG23	1:B:112:LEU:CD1	2.38	0.53
1:A:308:LEU:O	1:B:316:GLY:HA3	2.09	0.53
1:B:97:CYS:HA	1:B:155:ILE:HG13	1.92	0.52
1:B:219:ILE:HB	1:B:237:ALA:HA	1.91	0.52
1:A:108:GLY:O	1:A:323:LYS:NZ	2.42	0.52
1:B:328:VAL:HG23	1:B:329:PRO:CD	2.39	0.52
1:A:97:CYS:SG	1:A:111:CYS:SG	3.07	0.52
1:A:250:ILE:HD12	1:A:254:LEU:HD21	1.92	0.52
1:B:73:VAL:HG11	1:B:76:ILE:HD11	1.91	0.52
1:A:229:PHE:O	1:A:233:LYS:HG3	2.10	0.52
1:B:32:LYS:O	1:B:77:GLY:HA3	2.10	0.52
1:B:201:GLY:O	1:B:205:LEU:HG	2.10	0.52
1:B:253:VAL:O	1:B:257:MET:HG3	2.09	0.52
1:B:46:CYS:SG	1:B:48:SER:OG	2.68	0.51
1:A:279:LEU:HD13	1:A:307:LEU:HD23	1.92	0.51
1:B:8:LYS:HA	1:B:26:VAL:O	2.10	0.51
1:B:73:VAL:HG11	1:B:76:ILE:CD1	2.40	0.51
1:B:220:ILE:HG21	1:B:254:LEU:HD21	1.93	0.51
1:A:23:ILE:HD11	1:A:355:ILE:HG22	1.93	0.51
1:A:229:PHE:CD1	1:A:240:CYS:HB3	2.46	0.51
1:B:345:LEU:O	1:B:369:ARG:HB2	2.11	0.51
1:A:90:ILE:HD12	1:A:328:VAL:CG1	2.41	0.51
1:A:8:LYS:HZ1	1:A:25:GLU:HG2	1.74	0.51
1:B:43:THR:OG1	1:B:374:PHE:HE2	1.94	0.51
1:A:32:LYS:O	1:A:77:GLY:HA3	2.11	0.50
1:B:301:LEU:C	1:B:301:LEU:HD12	2.36	0.50
1:B:368:ILE:HG22	1:B:369:ARG:N	2.27	0.50
1:B:17:GLU:HB3	1:B:53:VAL:O	2.12	0.50
1:A:328:VAL:O	1:A:332:VAL:HG23	2.11	0.50
1:B:51:HIS:HB3	1:B:57:LEU:HB2	1.94	0.50
1:B:158:ALA:O	1:B:160:ILE:HD13	2.11	0.50
1:A:114:ASN:ND2	1:A:116:LEU:H	2.04	0.50
1:B:5:LYS:HE2	1:B:6:VAL:H	1.77	0.50
1:A:305:PRO:HG2	1:B:295:PRO:HG3	1.94	0.49
1:B:209:MET:HE3	1:B:345:LEU:CD1	2.41	0.49
1:B:73:VAL:HB	1:B:85:PRO:HA	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:PRO:CD	1:B:336:MET:HE1	2.39	0.49
1:A:21:PHE:H	1:A:356:ASN:HD21	1.58	0.49
1:A:271:ARG:HB2	1:A:274:THR:OG1	2.12	0.49
1:B:279:LEU:CD2	1:B:312:ARG:HD2	2.42	0.49
1:A:30:PRO:HA	1:A:37:ARG:NH1	2.28	0.49
1:A:171:LEU:HD11	1:A:369:ARG:HG3	1.94	0.49
1:A:283:GLN:HG3	1:B:101:ARG:NH2	2.28	0.49
1:B:206:SER:HA	1:B:209:MET:HG3	1.94	0.48
1:B:100:CYS:O	1:B:104:LYS:HG2	2.13	0.48
1:B:18:LYS:NZ	1:B:18:LYS:HB3	2.28	0.48
1:B:22:SER:O	1:B:24:GLU:HG3	2.14	0.48
1:B:73:VAL:HG23	1:B:87:ASP:O	2.11	0.48
1:B:272:LEU:O	1:B:275:MET:HB2	2.12	0.48
1:A:230:ALA:O	1:A:234:GLU:HB2	2.14	0.48
1:B:275:MET:HE2	1:B:291:ILE:HG23	1.95	0.48
1:B:361:LEU:HD13	1:B:366:GLU:HG3	1.96	0.48
1:B:268:VAL:HG22	1:B:268:VAL:O	2.14	0.48
1:B:14:LEU:HD12	1:B:61:LEU:HD11	1.96	0.48
1:B:39:LYS:HG3	1:B:149:TYR:CZ	2.49	0.48
1:B:355:ILE:HG23	1:B:356:ASN:H	1.79	0.48
1:A:96:GLN:HG2	1:A:96:GLN:O	2.14	0.47
1:B:224:ILE:HA	1:B:242:ASN:HD21	1.74	0.47
1:B:41:VAL:HG23	1:B:71:GLY:HA2	1.96	0.47
1:B:279:LEU:HD22	1:B:312:ARG:HD2	1.95	0.47
1:B:205:LEU:O	1:B:209:MET:HG3	2.15	0.47
1:A:350:LEU:N	1:A:350:LEU:HD12	2.30	0.47
1:A:8:LYS:NZ	1:A:25:GLU:HG2	2.29	0.47
1:B:37:ARG:HB3	1:B:74:GLU:OE1	2.15	0.47
1:B:153:ASP:CB	1:B:155:ILE:HG22	2.38	0.47
1:A:253:VAL:CG1	1:A:257:MET:HE3	2.42	0.47
1:B:61:LEU:CD1	1:B:63:VAL:HG12	2.45	0.47
1:A:161:ASP:OD2	1:A:336:MET:HE2	2.15	0.47
1:A:269:ILE:CG2	1:A:271:ARG:HG3	2.45	0.47
1:B:5:LYS:O	1:B:37:ARG:NH2	2.48	0.47
1:B:250:ILE:HG13	1:B:254:LEU:CD1	2.45	0.47
1:A:6:VAL:N	1:A:30:PRO:HD3	2.30	0.46
1:A:250:ILE:HG23	1:A:254:LEU:CD2	2.45	0.46
1:A:275:MET:SD	1:A:291:ILE:HD12	2.55	0.46
1:B:37:ARG:HH11	1:B:37:ARG:CG	2.27	0.46
1:A:10:LYS:HA	1:A:24:GLU:O	2.16	0.46
1:A:334:ASP:O	1:A:339:LYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:LYS:HG3	1:B:6:VAL:H	1.81	0.46
1:B:284:GLU:HA	1:B:312:ARG:NH1	2.31	0.46
1:A:88:LYS:HB3	1:A:166:LEU:HD21	1.98	0.46
1:A:250:ILE:HG23	1:A:254:LEU:HD23	1.98	0.46
1:A:302:SER:HA	1:B:301:LEU:O	2.16	0.46
1:A:345:LEU:O	1:A:369:ARG:HB2	2.16	0.46
1:B:351:PRO:O	1:B:352:PHE:C	2.59	0.46
1:B:178:THR:HG22	1:B:319:PHE:HA	1.98	0.46
1:A:13:VAL:HG11	1:A:15:TRP:CE2	2.51	0.45
1:A:135:LYS:HA	1:A:136:PRO:HD3	1.79	0.45
1:A:47:ARG:HB3	3:A:377:PAD:H3D	1.98	0.45
1:A:56:THR:HG23	1:A:296:PRO:HA	1.97	0.45
1:A:18:LYS:O	1:A:19:LYS:HD2	2.17	0.45
1:B:186:VAL:CG2	1:B:187:ALA:N	2.79	0.45
1:B:200:LEU:HD23	1:B:200:LEU:HA	1.78	0.45
1:B:189:VAL:O	1:B:214:ALA:HB1	2.17	0.45
1:B:92:LEU:HD21	1:B:328:VAL:HG21	1.99	0.45
1:A:114:ASN:HD21	1:A:117:SER:H	1.64	0.44
1:A:174:CYS:O	1:A:175:GLY:C	2.60	0.44
1:B:355:ILE:HG23	1:B:356:ASN:N	2.31	0.44
1:A:101:ARG:HD2	1:A:101:ARG:HA	1.75	0.44
1:A:256:GLU:HG3	5:A:395:HOH:O	2.18	0.44
1:B:155:ILE:HG23	1:B:156:SER:OG	2.17	0.44
1:B:357:GLU:O	1:B:361:LEU:HD23	2.18	0.44
1:B:92:LEU:HD13	1:B:324:SER:HB2	1.99	0.44
1:B:37:ARG:NH1	1:B:74:GLU:OE1	2.50	0.44
1:B:135:LYS:HA	1:B:136:PRO:HD3	1.71	0.44
1:A:177:SER:O	1:A:322:PHE:HE2	2.01	0.44
1:B:37:ARG:HG2	1:B:74:GLU:OE1	2.18	0.44
1:B:10:LYS:HB2	1:B:148:GLN:OE1	2.18	0.44
1:B:76:ILE:HG23	1:B:80:VAL:HB	1.99	0.44
1:A:169:VAL:HG12	1:A:169:VAL:O	2.18	0.44
1:B:242:ASN:HD22	1:B:243:PRO:HD2	1.83	0.44
1:B:37:ARG:HH11	1:B:37:ARG:CB	2.31	0.44
1:A:43:THR:HG23	1:A:374:PHE:CE1	2.42	0.43
1:A:92:LEU:HD21	1:A:328:VAL:HG21	2.00	0.43
1:B:45:ILE:HD11	1:B:372:LEU:HD11	1.99	0.43
1:A:349:VAL:HA	1:A:371:ILE:O	2.18	0.43
1:A:93:PHE:CD2	4:A:378:EOH:H22	2.53	0.43
1:A:2:THR:O	1:A:3:ALA:HB2	2.18	0.43
1:A:219:ILE:HD12	1:A:236:GLY:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LEU:HD12	1:A:301:LEU:C	2.43	0.43
1:A:5:LYS:C	1:A:30:PRO:HD3	2.43	0.43
1:A:5:LYS:HZ3	1:A:6:VAL:HG23	1.84	0.43
1:A:316:GLY:O	1:B:311:GLY:HA2	2.19	0.43
1:A:5:LYS:HD2	1:A:5:LYS:HA	1.88	0.43
1:A:160:ILE:HD11	1:A:166:LEU:CD2	2.48	0.43
1:A:350:LEU:O	1:A:372:LEU:HA	2.19	0.43
1:B:177:SER:OG	1:B:331:LEU:HD13	2.19	0.43
1:A:359:PHE:O	1:A:363:ARG:HG3	2.19	0.43
1:B:368:ILE:HG22	1:B:369:ARG:H	1.84	0.43
1:B:212:LYS:O	1:B:212:LYS:HG2	2.19	0.43
1:B:249:PRO:HB3	1:B:251:GLN:NE2	2.25	0.43
1:B:304:ASN:HA	1:B:305:PRO:HD2	1.91	0.43
1:B:262:VAL:HG12	1:B:264:PHE:N	2.34	0.42
1:A:139:HIS:CD2	1:A:139:HIS:N	2.87	0.42
1:A:306:MET:HE2	1:A:309:LEU:HB3	2.01	0.42
1:A:90:ILE:HG22	1:A:91:PRO:O	2.19	0.42
1:A:267:GLU:HG3	1:A:275:MET:HA	2.01	0.42
1:B:61:LEU:HD12	1:B:61:LEU:HA	1.80	0.42
1:B:229:PHE:O	1:B:232:ALA:HB3	2.20	0.42
1:B:186:VAL:HG11	1:B:317:ALA:CB	2.50	0.42
1:B:13:VAL:HG11	1:B:15:TRP:CE2	2.54	0.42
1:A:366:GLU:OE1	1:A:366:GLU:HA	2.19	0.42
1:B:175:GLY:HA2	1:B:203:VAL:HG12	2.02	0.42
1:A:36:VAL:O	1:A:151:VAL:HA	2.19	0.41
1:B:116:LEU:HD12	1:B:116:LEU:O	2.20	0.41
1:B:231:LYS:HD3	1:B:231:LYS:HA	1.88	0.41
1:A:93:PHE:HB2	1:A:141:LEU:HD13	2.02	0.41
1:A:129:ARG:HB2	1:A:139:HIS:CE1	2.56	0.41
1:A:304:ASN:OD1	1:A:306:MET:HB2	2.19	0.41
1:B:262:VAL:HG12	1:B:263:ASP:N	2.35	0.41
1:A:128:SER:O	1:A:129:ARG:NE	2.49	0.41
1:A:268:VAL:HG12	3:A:377:PAD:H51N	2.01	0.41
1:B:9:CYS:O	1:B:25:GLU:HA	2.21	0.41
1:B:275:MET:HE2	1:B:291:ILE:CG2	2.51	0.41
1:A:224:ILE:HA	1:A:242:ASN:ND2	2.35	0.41
1:A:296:PRO:O	1:A:297:ASP:C	2.64	0.41
1:A:102:VAL:HG23	1:A:112:LEU:CD2	2.51	0.41
1:A:205:LEU:HD22	1:A:232:ALA:HA	2.03	0.41
1:A:353:GLU:CD	1:A:353:GLU:H	2.29	0.41
1:B:81:THR:HA	1:B:84:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:GLY:O	1:A:211:CYS:C	2.64	0.41
1:A:279:LEU:HG	1:A:314:TRP:CE2	2.56	0.41
1:B:79:GLY:O	1:B:80:VAL:C	2.63	0.41
1:B:88:LYS:HG2	1:B:166:LEU:HD21	2.03	0.41
1:A:349:VAL:O	1:A:349:VAL:HG12	2.21	0.40
1:B:175:GLY:O	1:B:203:VAL:HG12	2.22	0.40
1:A:92:LEU:CD2	1:A:328:VAL:HG21	2.52	0.40
1:A:152:VAL:HG21	1:A:157:VAL:HB	2.03	0.40
1:A:157:VAL:O	1:A:325:LYS:HE3	2.20	0.40
1:B:76:ILE:HD13	1:B:85:PRO:CG	2.50	0.40
1:B:186:VAL:CG2	1:B:290:VAL:HG11	2.50	0.40
1:B:93:PHE:CB	1:B:141:LEU:HD23	2.49	0.40
1:B:123:MET:HB2	1:B:127:THR:O	2.21	0.40
1:A:7:ILE:HG13	1:A:37:ARG:NH2	2.36	0.40
1:B:224:ILE:HA	1:B:242:ASN:HD22	1.80	0.40
1:B:369:ARG:HD3	1:B:369:ARG:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	372/374 (100%)	325 (87%)	35 (9%)	12 (3%)	3	7
1	B	372/374 (100%)	321 (86%)	40 (11%)	11 (3%)	3	8
All	All	744/748 (100%)	646 (87%)	75 (10%)	23 (3%)	3	8

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	THR
1	A	2	THR

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Mol	Chain	Res	Type
1	A	166	LEU
1	A	174	CYS
1	A	297	ASP
1	A	324	SER
1	B	174	CYS
1	A	144	SER
1	B	65	ALA
1	B	166	LEU
1	A	65	ALA
1	A	368	ILE
1	B	368	ILE
1	B	129	ARG
1	B	144	SER
1	A	129	ARG
1	B	175	GLY
1	B	324	SER
1	A	186	VAL
1	A	6	VAL
1	B	95	PRO
1	A	249	PRO
1	B	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	308/308 (100%)	264 (86%)	44 (14%)	3	8
1	B	308/308 (100%)	259 (84%)	49 (16%)	2	7
All	All	616/616 (100%)	523 (85%)	93 (15%)	3	7

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	5	LYS

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Mol	Chain	Res	Type
1	A	8	LYS
1	A	10	LYS
1	A	14	LEU
1	A	17	GLU
1	A	53	VAL
1	A	99	LYS
1	A	101	ARG
1	A	107	GLU
1	A	116	LEU
1	A	117	SER
1	A	123	MET
1	A	129	ARG
1	A	131	THR
1	A	133	ARG
1	A	144	SER
1	A	151	VAL
1	A	171	LEU
1	A	178	THR
1	A	226	LYS
1	A	238	THR
1	A	241	VAL
1	A	243	PRO
1	A	249	PRO
1	A	250	ILE
1	A	251	GLN
1	A	268	VAL
1	A	272	LEU
1	A	273	ASP
1	A	275	MET
1	A	279	LEU
1	A	280	SER
1	A	282	CYS
1	A	283	GLN
1	A	291	ILE
1	A	299	GLN
1	A	303	MET
1	A	306	MET
1	A	313	THR
1	A	318	ILE
1	A	326	ASP
1	A	342	LEU
1	A	373	THR

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Mol	Chain	Res	Type
1	B	5	LYS
1	B	17	GLU
1	B	18	LYS
1	B	23	ILE
1	B	36	VAL
1	B	37	ARG
1	B	40	MET
1	B	48	SER
1	B	61	LEU
1	B	73	VAL
1	B	76	ILE
1	B	84	ARG
1	B	88	LYS
1	B	107	GLU
1	B	124	GLN
1	B	129	ARG
1	B	131	THR
1	B	133	ARG
1	B	135	LYS
1	B	141	LEU
1	B	151	VAL
1	B	157	VAL
1	B	159	LYS
1	B	168	LYS
1	B	171	LEU
1	B	185	LYS
1	B	186	VAL
1	B	190	THR
1	B	219	ILE
1	B	226	LYS
1	B	231	LYS
1	B	239	GLU
1	B	243	PRO
1	B	249	PRO
1	B	251	GLN
1	B	263	ASP
1	B	268	VAL
1	B	271	ARG
1	B	272	LEU
1	B	279	LEU
1	B	303	MET
1	B	306	MET

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Mol	Chain	Res	Type
1	B	326	ASP
1	B	342	LEU
1	B	345	LEU
1	B	353	GLU
1	B	360	ASP
1	B	362	LEU
1	B	370	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	138	HIS
1	A	259	ASN
1	A	283	GLN
1	B	105	HIS
1	B	138	HIS
1	B	225	ASN
1	B	242	ASN
1	B	251	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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
3	PAD	A	377	-	47,48,48	1.41	6 (12%)	63,73,73	2.20	18 (28%)
4	EOH	B	378	2	2,2,2	1.16	0	1,1,1	0.09	0
4	EOH	A	378	2	2,2,2	0.91	0	1,1,1	0.27	0
3	PAD	B	377	-	47,48,48	1.77	6 (12%)	63,73,73	2.36	21 (33%)

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	PAD	A	377	-	-	3/25/62/62	0/5/5/5
3	PAD	B	377	-	-	5/25/62/62	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	PAD	C1N-N2N	6.94	1.40	1.32
3	B	377	PAD	C3N-C7N	5.78	1.56	1.48
3	A	377	PAD	C1N-N2N	5.33	1.38	1.32
3	A	377	PAD	C5A-N7A	-3.58	1.32	1.39
3	B	377	PAD	C6N-C1N	-3.10	1.37	1.43
3	A	377	PAD	C1D-C1N	-3.08	1.46	1.50
3	A	377	PAD	C3N-C7N	2.93	1.52	1.48
3	B	377	PAD	C5A-N7A	-2.90	1.33	1.39
3	B	377	PAD	C3D-C4D	-2.76	1.46	1.53
3	A	377	PAD	C4A-N9A	-2.14	1.33	1.37
3	A	377	PAD	C6N-C1N	-2.09	1.39	1.43
3	B	377	PAD	C2D-C1D	-2.04	1.51	1.53

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	377	PAD	N3A-C4A-N9A	7.85	140.51	127.17
3	B	377	PAD	C5A-C4A-N3A	-7.74	116.06	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	377	PAD	C5A-C4A-N3A	-6.60	117.63	126.72
3	A	377	PAD	O4D-C1D-C1N	-5.84	101.14	108.92
3	A	377	PAD	N3A-C4A-N9A	5.81	137.05	127.17
3	B	377	PAD	C6A-C5A-C4A	5.27	124.37	117.18
3	B	377	PAD	C6A-C5A-N7A	-5.08	122.29	132.09
3	A	377	PAD	C6A-C5A-N7A	-4.90	122.65	132.09
3	A	377	PAD	C6A-C5A-C4A	4.81	123.75	117.18
3	A	377	PAD	C3N-C7N-N7N	-4.71	111.49	116.28
3	B	377	PAD	O4D-C1D-C2D	-3.57	100.21	105.15
3	B	377	PAD	O4D-C4D-C5D	3.52	120.62	109.33
3	B	377	PAD	N3A-C2A-N1A	-3.49	123.30	128.58
3	B	377	PAD	C2A-N3A-C4A	3.41	120.17	111.83
3	B	377	PAD	N6A-C6A-N1A	3.34	125.81	118.38
3	B	377	PAD	O2N-PN-O3	3.33	116.27	107.27
3	A	377	PAD	O7N-C7N-C3N	3.29	123.41	120.25
3	A	377	PAD	N3A-C2A-N1A	-3.24	123.68	128.58
3	B	377	PAD	C4N-C3N-N2N	-3.17	118.15	122.40
3	B	377	PAD	O5D-C5D-C4D	3.00	119.21	108.99
3	B	377	PAD	C4A-N9A-C8A	2.98	108.86	105.74
3	B	377	PAD	O4D-C1D-C1N	2.95	112.85	108.92
3	A	377	PAD	C2A-N3A-C4A	2.86	118.81	111.83
3	A	377	PAD	O5D-PN-O1N	-2.83	97.72	108.94
3	A	377	PAD	O2N-PN-O3	2.74	114.69	107.27
3	A	377	PAD	C4A-C5A-N7A	2.64	113.60	110.58
3	A	377	PAD	O5B-C5B-C4B	2.49	117.49	108.99
3	B	377	PAD	C3D-C2D-C1D	2.45	104.58	101.69
3	B	377	PAD	C4A-C5A-N7A	2.41	113.33	110.58
3	B	377	PAD	O2A-PA-O1A	2.41	123.64	112.44
3	A	377	PAD	O3-PA-O1A	2.40	117.91	110.70
3	B	377	PAD	N9A-C8A-N7A	-2.32	110.65	113.94
3	B	377	PAD	C5A-C6A-N6A	-2.27	117.66	123.29
3	A	377	PAD	O2B-C2B-C1B	2.24	117.83	110.10
3	B	377	PAD	C4D-O4D-C1D	2.23	114.03	108.44
3	A	377	PAD	N6A-C6A-N1A	2.21	123.30	118.38
3	B	377	PAD	C5A-C4A-N9A	-2.19	103.42	105.81
3	A	377	PAD	C4N-C3N-C7N	2.18	123.20	119.27
3	A	377	PAD	O3D-C3D-C4D	-2.11	105.01	111.08

There are no chirality outliers.

All (8) torsion outliers are listed below:

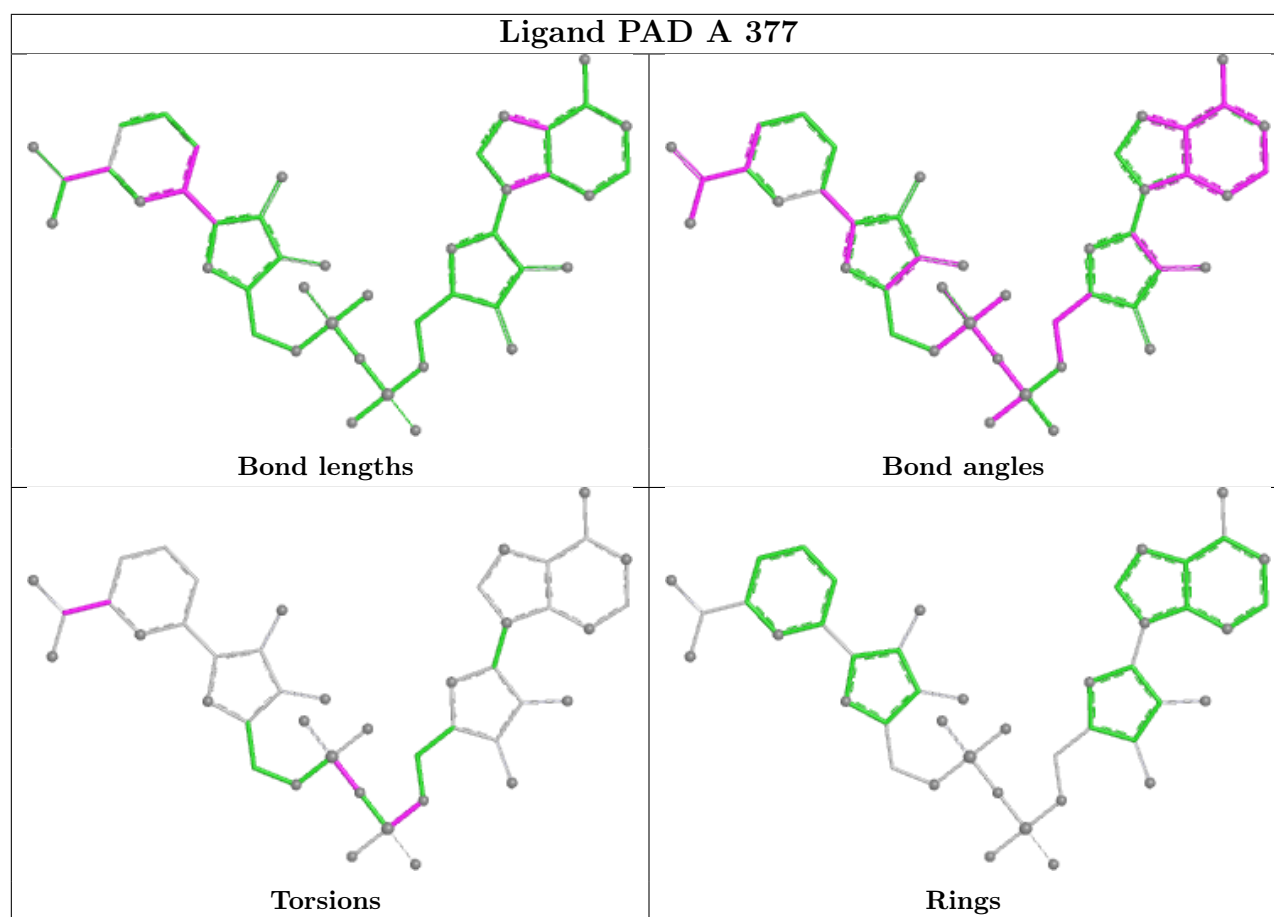
Mol	Chain	Res	Type	Atoms
3	A	377	PAD	C4N-C3N-C7N-N7N
3	B	377	PAD	C5D-O5D-PN-O3
3	B	377	PAD	C5D-O5D-PN-O2N
3	A	377	PAD	C5B-O5B-PA-O3
3	B	377	PAD	C5D-O5D-PN-O1N
3	B	377	PAD	C3B-C4B-C5B-O5B
3	B	377	PAD	O4B-C4B-C5B-O5B
3	A	377	PAD	PA-O3-PN-O1N

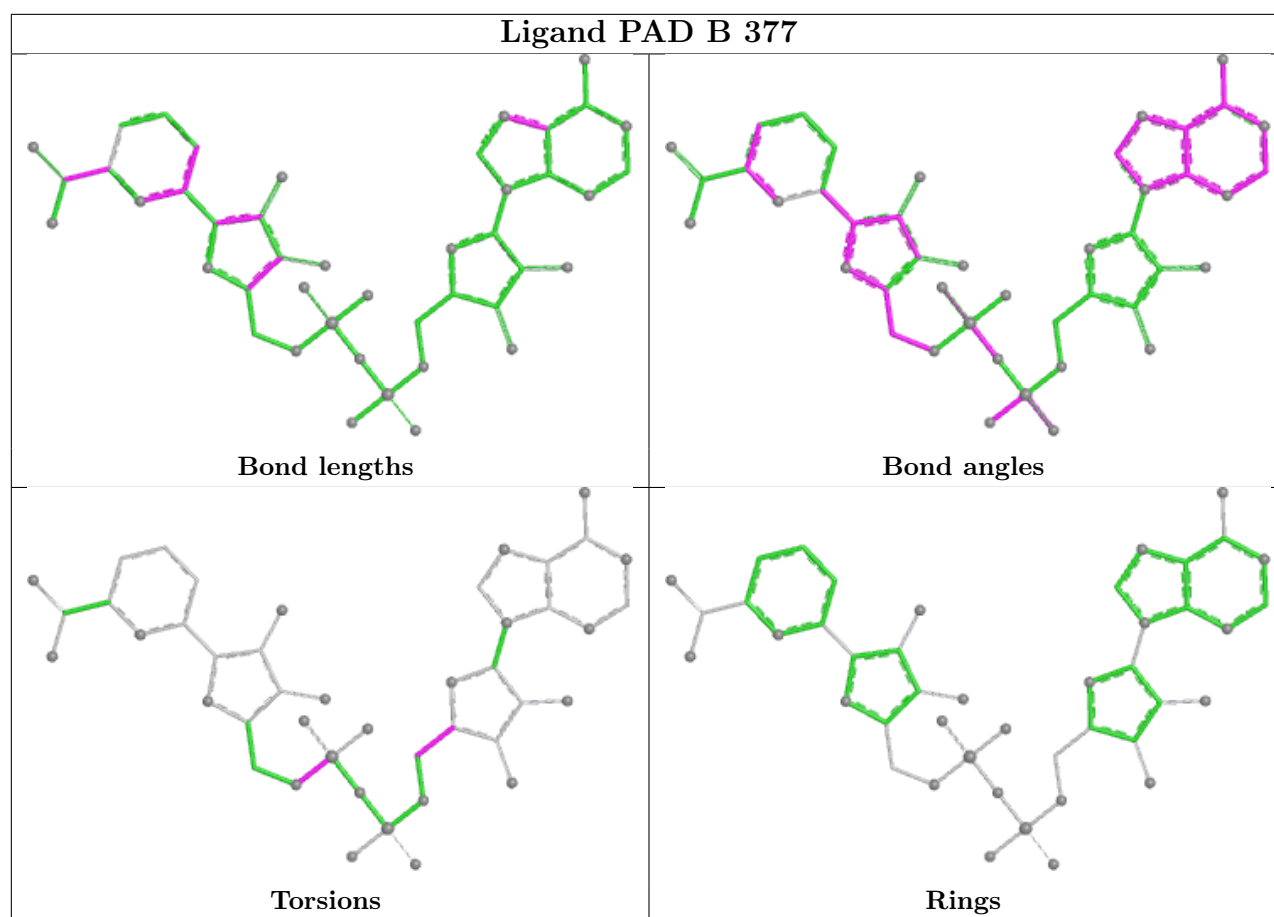
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	377	PAD	3	0
4	A	378	EOH	2	0
3	B	377	PAD	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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.