



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:22 PM UTC

PDB ID : 1BDM / pdb_00001bdm
Title : THE STRUCTURE AT 1.8 ANGSTROMS RESOLUTION OF A SINGLE SITE MUTANT (T189I) OF MALATE DEHYDROGENASE FROM THERMUS FLAVUS WITH INCREASED ENZYMATIC ACTIVITY
Authors : Kelly, C.A.; Birktoft, J.J.
Deposited on : 1993-02-16
Resolution : 1.80 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

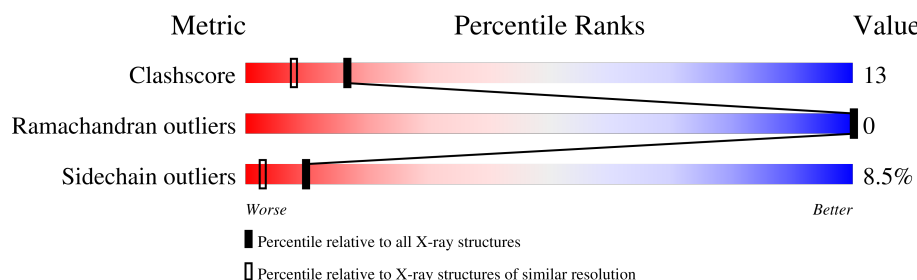
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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	327	 65% 27% 5% • •
1	B	327	 72% 23% 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5197 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.

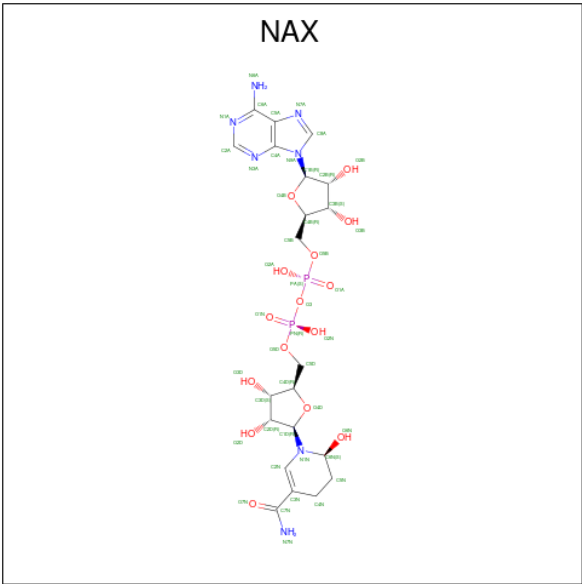
- Molecule 1 is a protein called MALATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	318	2411	1530	417	452	12	0	1	1
1	B	327	2494	1579	436	466	13	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ASP	LYS	conflict	UNP P10584
A	189	ILE	THR	conflict	UNP P10584
B	74	ASP	LYS	conflict	UNP P10584
B	189	ILE	THR	conflict	UNP P10584

- Molecule 2 is BETA-6-HYDROXY-1,4,5,6-TETRHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAX) (formula: C₂₁H₃₁N₇O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			45	21	7	15	2		
2	B	1	Total	C	N	O	P	0	0
			45	21	7	15	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		
3	B	112	Total	O	0	0
			112	112		

3 Residue-property plots

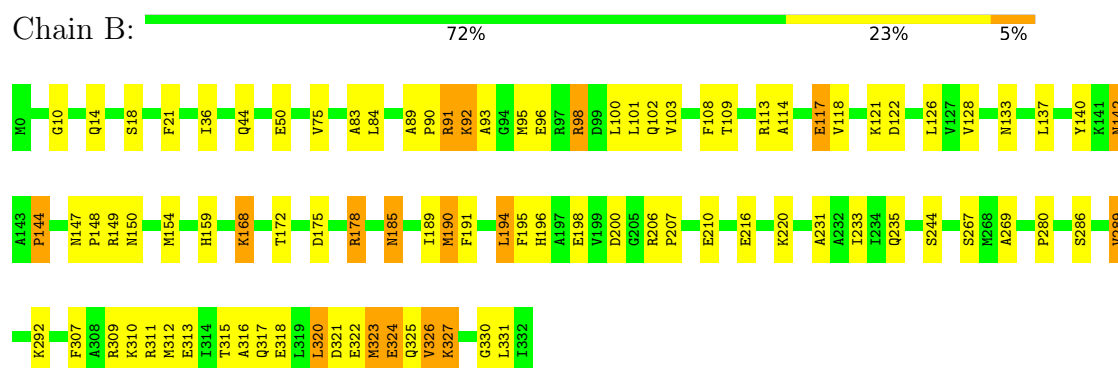
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: MALATE DEHYDROGENASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.75Å 88.64Å 118.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5197	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: NAX

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.17	1/2447 (0.0%)	1.79	38/3316 (1.1%)
1	B	1.23	1/2532 (0.0%)	1.82	34/3428 (1.0%)
All	All	1.20	2/4979 (0.0%)	1.81	72/6744 (1.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	ILE	CA-CB	-6.29	1.50	1.54
1	B	191	PHE	C-O	-5.42	1.20	1.25

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	ASN	CA-CB-CG	-10.96	101.64	112.60
1	B	144	PRO	CA-C-N	-9.54	110.21	123.08
1	B	144	PRO	C-N-CA	-9.54	110.21	123.08
1	B	96	GLU	N-CA-CB	-9.53	97.32	110.38
1	A	220	LYS	CA-CB-CG	-8.66	96.77	114.10
1	A	113	ARG	N-CA-CB	7.76	121.33	110.07
1	A	102	GLN	N-CA-CB	7.62	121.12	110.07
1	B	178	ARG	CD-NE-CZ	7.50	134.90	124.40
1	B	149	ARG	NE-CZ-NH2	7.43	125.89	119.20
1	A	67	LEU	CB-CA-C	-7.40	97.22	109.80
1	A	309	ARG	N-CA-CB	7.26	120.79	110.12
1	A	215	MET	CG-SD-CE	-7.24	84.97	100.90
1	B	195	PHE	CA-CB-CG	-7.16	106.64	113.80
1	A	21	PHE	CA-CB-CG	-7.10	106.70	113.80
1	B	21	PHE	CA-CB-CG	-7.06	106.74	113.80
1	A	142	ASN	CA-CB-CG	-6.84	105.75	112.60
1	B	75	VAL	CB-CA-C	-6.80	103.37	111.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	GLU	N-CA-CB	-6.58	99.82	109.82
1	B	331	LEU	CA-C-O	6.54	126.92	119.27
1	A	196	HIS	CA-CB-CG	-6.53	107.27	113.80
1	B	150	ASN	CA-CB-CG	-6.47	106.13	112.60
1	B	142	ASN	CA-CB-CG	-6.39	106.21	112.60
1	A	306	GLU	CB-CA-C	6.33	121.61	110.85
1	B	100	LEU	CA-C-N	6.23	128.62	120.28
1	B	100	LEU	C-N-CA	6.23	128.62	120.28
1	B	196	HIS	CA-CB-CG	-6.19	107.61	113.80
1	B	168	LYS	CB-CA-C	-6.17	101.19	110.88
1	A	72	ASP	CB-CA-C	-6.14	103.36	110.17
1	B	172	THR	CA-CB-OG1	-6.09	100.46	109.60
1	A	101	LEU	N-CA-CB	6.00	120.70	110.50
1	A	143	ALA	O-C-N	5.99	126.74	121.17
1	B	117	GLU	CA-C-N	-5.99	115.49	122.14
1	B	117	GLU	C-N-CA	-5.99	115.49	122.14
1	A	323	MET	CA-C-N	5.93	129.04	120.79
1	A	323	MET	C-N-CA	5.93	129.04	120.79
1	B	200	ASP	CB-CA-C	-5.90	103.35	111.73
1	A	294	GLY	CA-C-N	-5.87	113.60	122.81
1	A	294	GLY	C-N-CA	-5.87	113.60	122.81
1	B	323	MET	CG-SD-CE	-5.86	88.00	100.90
1	A	79	ASP	CA-CB-CG	-5.80	106.80	112.60
1	B	149	ARG	NE-CZ-NH1	-5.76	115.74	121.50
1	A	5	ARG	NE-CZ-NH2	5.69	124.33	119.20
1	A	154	MET	N-CA-C	5.69	118.01	108.96
1	B	96	GLU	CB-CG-CD	-5.66	102.98	112.60
1	A	271	PRO	N-CA-CB	5.63	107.80	103.30
1	B	91	ARG	N-CA-CB	5.60	119.30	110.23
1	A	220	LYS	CB-CG-CD	5.59	124.17	111.30
1	A	253	ILE	N-CA-CB	5.55	117.04	110.55
1	A	193	ASP	N-CA-C	5.53	117.31	108.41
1	B	108	PHE	CA-CB-CG	-5.53	108.27	113.80
1	A	77	PHE	CA-CB-CG	5.51	119.31	113.80
1	B	140	TYR	CA-CB-CG	5.51	123.81	113.90
1	B	90	PRO	CB-CA-C	-5.44	103.82	110.95
1	A	309	ARG	N-CA-C	5.43	117.20	111.28
1	B	289	VAL	N-CA-CB	-5.41	101.80	111.92
1	B	14	GLN	CB-CG-CD	-5.33	103.53	112.60
1	A	188	SER	CA-C-N	-5.32	114.16	122.56
1	A	188	SER	C-N-CA	-5.32	114.16	122.56
1	A	139	ALA	CA-C-N	-5.30	113.23	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ALA	C-N-CA	-5.30	113.23	120.44
1	A	73	PRO	N-CA-CB	5.29	109.22	103.30
1	A	220	LYS	CG-CD-CE	-5.27	99.19	111.30
1	B	36	ILE	N-CA-C	-5.26	100.80	108.17
1	A	297	ARG	N-CA-CB	-5.17	101.88	111.13
1	A	51	GLY	CA-C-N	5.16	127.75	120.42
1	A	51	GLY	C-N-CA	5.16	127.75	120.42
1	B	175	ASP	CA-CB-CG	-5.15	107.45	112.60
1	B	50	GLU	CB-CG-CD	-5.15	103.85	112.60
1	B	244	SER	N-CA-CB	5.14	118.25	110.28
1	B	96	GLU	N-CA-C	5.09	116.68	110.41
1	A	132	ALA	N-CA-C	5.03	117.15	111.11
1	A	240	SER	CA-CB-OG	-5.02	101.06	111.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2411	0	2433	67	0
1	B	2494	0	2524	62	0
2	A	45	0	29	3	0
2	B	45	0	29	2	0
3	A	90	0	0	5	0
3	B	112	0	0	4	0
All	All	5197	0	5015	128	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 13.

All (128) 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:89:ALA:H	1:A:104:ASN:HD21	1.06	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:PRO:HG2	1:B:320:LEU:HD21	1.55	0.88
1:A:44:GLN:HA	1:A:44:GLN:HE21	1.40	0.86
1:A:89:ALA:HB2	1:A:103:VAL:HG22	1.60	0.84
1:A:89:ALA:H	1:A:104:ASN:ND2	1.75	0.84
1:A:102:GLN:HE22	1:A:329:LEU:CD2	1.91	0.83
1:B:92:LYS:HG2	1:B:93:ALA:N	1.95	0.82
1:A:105:GLY:O	1:A:109:THR:HG23	1.79	0.81
1:A:326:VAL:HG13	1:A:331:LEU:HB2	1.63	0.80
1:B:117:GLU:HG3	1:B:118:VAL:HG13	1.67	0.77
1:B:137:LEU:HD21	1:B:323:MET:HG3	1.68	0.74
1:B:92:LYS:O	1:B:95:MET:HB3	1.88	0.74
1:A:102:GLN:HE22	1:A:329:LEU:HD22	1.52	0.73
1:A:185:ASN:O	1:A:190:MET:HB3	1.88	0.73
1:A:170:THR:OG1	1:A:172:THR:HG23	1.89	0.73
1:A:90:PRO:C	1:A:91:ARG:N	2.48	0.72
1:B:92:LYS:HB3	1:B:95:MET:SD	2.30	0.71
1:B:89:ALA:HB2	1:B:103:VAL:HG12	1.73	0.70
1:B:44:GLN:HG2	3:B:847:HOH:O	1.91	0.70
1:B:189:ILE:HD11	1:B:318:GLU:CD	2.18	0.69
1:B:324:GLU:HG2	1:B:325:GLN:N	2.06	0.68
1:B:133:ASN:ND2	1:B:185:ASN:HB3	2.09	0.68
1:B:185:ASN:O	1:B:190:MET:HB3	1.94	0.68
1:A:305:ASN:O	1:A:309:ARG:HG2	1.94	0.67
1:A:109:THR:O	1:A:113:ARG:HG3	1.97	0.65
1:B:317:GLN:NE2	1:B:321:ASP:OD1	2.30	0.65
1:B:178:ARG:NH2	1:B:198:GLU:OE1	2.29	0.65
1:A:44:GLN:HA	1:A:44:GLN:NE2	2.07	0.65
1:A:321:ASP:O	1:A:324:GLU:HB3	1.97	0.64
1:B:312:MET:O	1:B:315:THR:HG22	1.97	0.64
1:B:216:GLU:HG2	1:B:220:LYS:NZ	2.13	0.63
1:A:89:ALA:CB	1:A:103:VAL:HG22	2.29	0.62
1:B:126:LEU:HD11	1:B:154:MET:HB2	1.81	0.61
1:B:216:GLU:O	1:B:220:LYS:HG2	2.00	0.61
1:A:147:ASN:OD1	1:A:148:PRO:HD2	2.00	0.61
1:B:84:LEU:N	1:B:84:LEU:HD12	2.18	0.59
1:B:142:ASN:C	1:B:144:PRO:HD3	2.28	0.59
1:A:209:LEU:CD1	1:A:212:VAL:HG12	2.33	0.58
1:A:269:ALA:HA	1:A:286:SER:HA	1.85	0.58
1:A:189:ILE:HD11	3:A:921:HOH:O	2.03	0.58
1:A:190:MET:HE1	1:A:226:VAL:HG12	1.87	0.57
1:A:102:GLN:NE2	1:A:329:LEU:HD13	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:HIS:HD2	3:A:792:HOH:O	1.88	0.56
1:B:231:ALA:O	1:B:235:GLN:HG3	2.05	0.56
1:B:92:LYS:HD3	1:B:95:MET:HB2	1.88	0.56
1:A:258:LEU:N	1:A:258:LEU:HD23	2.22	0.55
1:B:309:ARG:O	1:B:313:GLU:HG3	2.06	0.55
1:A:89:ALA:N	1:A:104:ASN:HD21	1.90	0.54
1:A:310:LYS:O	1:A:314:ILE:HG13	2.07	0.54
1:B:216:GLU:HG2	1:B:220:LYS:HZ2	1.73	0.54
1:B:159:HIS:HE1	3:B:779:HOH:O	1.92	0.53
1:B:269:ALA:HA	1:B:286:SER:HA	1.91	0.53
1:B:317:GLN:HE21	1:B:321:ASP:CG	2.17	0.53
1:A:102:GLN:NE2	1:A:329:LEU:HD22	2.20	0.52
1:A:178:ARG:HH12	1:A:263:GLY:HA3	1.72	0.52
1:A:126:LEU:HD13	1:A:252:HIS:CE1	2.45	0.52
1:B:92:LYS:HE2	1:B:93:ALA:O	2.10	0.52
1:A:292:LYS:NZ	1:A:293:ASP:OD2	2.24	0.52
1:B:185:ASN:OD1	1:B:185:ASN:N	2.41	0.52
1:B:207:PRO:HB2	1:B:210:GLU:HG3	1.92	0.52
1:B:206:ARG:HG3	1:B:207:PRO:HD2	1.92	0.52
1:B:92:LYS:HG2	1:B:93:ALA:H	1.73	0.50
1:B:114:ALA:O	1:B:118:VAL:HG22	2.11	0.50
1:B:327:LYS:O	1:B:330:GLY:N	2.43	0.49
1:A:15:ILE:HD11	2:A:334:NAX:H6N	1.95	0.48
1:A:44:GLN:HG2	3:A:841:HOH:O	2.13	0.48
3:A:858:HOH:O	1:B:168:LYS:HE2	2.14	0.48
1:B:98:ARG:NH1	1:B:98:ARG:HB3	2.29	0.47
1:A:89:ALA:HB2	1:A:103:VAL:CG2	2.37	0.47
1:A:130:ASN:HA	1:A:132:ALA:N	2.29	0.47
1:B:206:ARG:HD2	1:B:210:GLU:OE1	2.14	0.47
1:A:102:GLN:NE2	1:A:329:LEU:CD1	2.78	0.47
1:A:254:ARG:HD3	3:A:883:HOH:O	2.15	0.47
1:A:14:GLN:NE2	2:A:334:NAX:O2A	2.38	0.47
1:A:53:VAL:HG13	1:A:67:LEU:HD13	1.97	0.46
1:B:128:VAL:O	2:B:334:NAX:H2N	2.16	0.46
1:A:312:MET:O	1:A:315:THR:HG22	2.15	0.46
1:B:18:SER:O	3:B:850:HOH:O	2.21	0.46
1:B:307:PHE:CZ	1:B:311:ARG:NE	2.83	0.46
1:B:216:GLU:CG	1:B:220:LYS:NZ	2.79	0.46
1:A:44:GLN:HE21	1:A:44:GLN:CA	2.21	0.45
1:B:89:ALA:HB2	1:B:103:VAL:CG1	2.43	0.45
1:A:14:GLN:HE21	2:A:334:NAX:PA	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:GLY:HA2	2:B:334:NAX:H1B	1.99	0.45
1:A:157:LEU:O	1:A:161:ARG:HG3	2.17	0.44
1:B:316:ALA:O	1:B:320:LEU:HD22	2.16	0.44
1:A:313:GLU:OE1	1:A:313:GLU:HA	2.17	0.44
1:B:122:ASP:OD1	1:B:122:ASP:N	2.43	0.44
1:B:142:ASN:O	1:B:144:PRO:HD3	2.18	0.43
1:A:231:ALA:O	1:A:235:GLN:HG3	2.18	0.43
1:B:159:HIS:HD2	1:B:267:SER:OG	2.01	0.43
1:A:307:PHE:CD1	1:A:307:PHE:C	2.97	0.43
1:B:98:ARG:NH1	1:B:98:ARG:CB	2.81	0.43
1:B:98:ARG:CZ	1:B:98:ARG:HB2	2.48	0.43
1:A:170:THR:O	1:A:172:THR:HG22	2.18	0.43
1:A:187:SER:OG	1:A:189:ILE:HG13	2.18	0.43
1:A:257:ALA:C	1:A:258:LEU:HD23	2.42	0.43
1:A:101:LEU:HA	1:A:101:LEU:HD12	1.65	0.43
1:A:102:GLN:HE22	1:A:329:LEU:HD21	1.79	0.43
1:B:206:ARG:HG3	1:B:207:PRO:CD	2.49	0.43
1:B:83:ALA:C	1:B:84:LEU:HD12	2.44	0.42
1:B:323:MET:HE2	1:B:323:MET:HB3	1.67	0.42
1:A:308:ALA:O	1:A:312:MET:HG3	2.19	0.42
1:A:89:ALA:CB	1:A:103:VAL:CG2	2.96	0.42
1:A:326:VAL:HG12	1:A:332:ILE:HG12	2.00	0.42
1:A:142:ASN:C	1:A:144:PRO:HD3	2.44	0.42
1:A:320:LEU:HD23	1:A:320:LEU:HA	1.81	0.42
1:A:209:LEU:HD12	1:A:212:VAL:HG12	2.00	0.42
1:B:98:ARG:HB3	1:B:98:ARG:HH11	1.82	0.42
1:A:209:LEU:HD12	1:A:209:LEU:HA	1.70	0.42
1:B:206:ARG:HG3	1:B:207:PRO:N	2.35	0.42
1:B:89:ALA:CB	1:B:103:VAL:CG1	2.98	0.41
1:B:147:ASN:HD22	1:B:148:PRO:HD2	1.85	0.41
1:A:102:GLN:HE22	1:A:329:LEU:CD1	2.33	0.41
1:B:92:LYS:C	1:B:95:MET:HB3	2.45	0.41
1:A:16:GLY:O	1:A:20:LEU:HG	2.20	0.41
1:A:32:ASP:OD1	1:A:32:ASP:N	2.48	0.41
1:A:46:MET:HE3	1:A:46:MET:HB3	1.88	0.41
1:A:54:MET:HB3	1:B:233:ILE:HD11	2.02	0.41
1:A:141:LYS:HG2	1:A:332:ILE:HB	2.02	0.41
1:A:215:MET:O	1:A:215:MET:HG3	2.20	0.41
1:A:332:ILE:O	1:A:332:ILE:HG13	2.14	0.41
1:B:190:MET:HE3	3:B:909:HOH:O	2.20	0.41
1:A:217:TRP:CH2	1:A:222:PHE:CD1	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:THR:O	1:B:113:ARG:HG2	2.21	0.41
1:B:194:LEU:HD12	1:B:194:LEU:HA	1.88	0.41
1:B:322:GLU:O	1:B:326:VAL:HG13	2.21	0.40
1:A:7:ALA:HA	1:A:38:GLN:O	2.22	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	314/327 (96%)	309 (98%)	5 (2%)	0	100	100
1	B	326/327 (100%)	324 (99%)	2 (1%)	0	100	100
All	All	640/654 (98%)	633 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	243/252 (96%)	216 (89%)	27 (11%)	6	1
1	B	251/252 (100%)	236 (94%)	15 (6%)	17	7
All	All	494/504 (98%)	452 (92%)	42 (8%)	10	3

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	44	GLN
1	A	47	LYS
1	A	67	LEU
1	A	101	LEU
1	A	103	VAL
1	A	106	LYS
1	A	113	ARG
1	A	118	VAL
1	A	121	LYS
1	A	140	TYR
1	A	172	THR
1	A	174	VAL
1	A	178	ARG
1	A	187	SER
1	A	194	LEU
1	A	209	LEU
1	A	212	VAL
1	A	216	GLU
1	A	273	GLN
1	A	279	ILE
1	A	292	LYS
1	A	306	GLU
1	A	309	ARG
1	A	310	LYS
1	A	317	GLN
1	A	327	LYS
1	B	91	ARG
1	B	92	LYS
1	B	98	ARG
1	B	101	LEU
1	B	102	GLN
1	B	121	LYS
1	B	190	MET
1	B	194	LEU
1	B	289	VAL
1	B	292	LYS
1	B	310	LYS
1	B	320	LEU
1	B	324	GLU
1	B	326	VAL
1	B	327	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	102	GLN
1	A	104	ASN
1	A	111	GLN
1	A	196	HIS
1	A	252	HIS
1	A	273	GLN
1	A	325	GLN
1	B	102	GLN
1	B	147	ASN
1	B	159	HIS
1	B	273	GLN
1	B	317	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](#)

2 ligands are modelled in this entry.

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
2	NAX	B	334	-	47,49,49	1.55	5 (10%)	62,75,75	1.27	6 (9%)
2	NAX	A	334	-	47,49,49	1.45	4 (8%)	62,75,75	1.60	7 (11%)

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
2	NAX	B	334	-	-	4/29/75/75	0/5/5/5
2	NAX	A	334	-	-	5/29/75/75	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	334	NAX	PA-O3	-7.26	1.51	1.59
2	A	334	NAX	PA-O3	-5.13	1.54	1.59
2	A	334	NAX	PN-O3	4.58	1.64	1.59
2	A	334	NAX	C4A-N9A	4.32	1.46	1.37
2	B	334	NAX	C4A-N9A	3.77	1.45	1.37
2	B	334	NAX	O6N-C6N	3.71	1.47	1.41
2	A	334	NAX	O6N-C6N	3.34	1.46	1.41
2	B	334	NAX	C2N-C3N	2.47	1.42	1.35
2	B	334	NAX	PN-O3	2.10	1.61	1.59

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	334	NAX	O2N-PN-O3	-8.69	83.77	107.27
2	B	334	NAX	O4D-C1D-C2D	-3.34	99.47	106.62
2	A	334	NAX	O4D-C1D-C2D	-3.20	99.76	106.62
2	B	334	NAX	C5A-C4A-N9A	-2.91	102.64	105.81
2	A	334	NAX	O7N-C7N-C3N	-2.66	115.88	120.90
2	B	334	NAX	O4B-C1B-C2B	-2.65	100.94	106.62
2	A	334	NAX	C4B-O4B-C1B	-2.44	104.08	109.47
2	B	334	NAX	O7N-C7N-C3N	-2.37	116.42	120.90
2	B	334	NAX	C4A-C5A-N7A	2.34	113.25	110.58
2	A	334	NAX	O2N-PN-O1N	2.30	123.13	112.44
2	A	334	NAX	O3D-C3D-C2D	-2.29	104.49	111.82
2	A	334	NAX	O3-PN-O1N	2.27	117.54	110.70
2	B	334	NAX	O3-PA-O1A	-2.17	104.19	110.70

There are no chirality outliers.

All (9) torsion outliers are listed below:

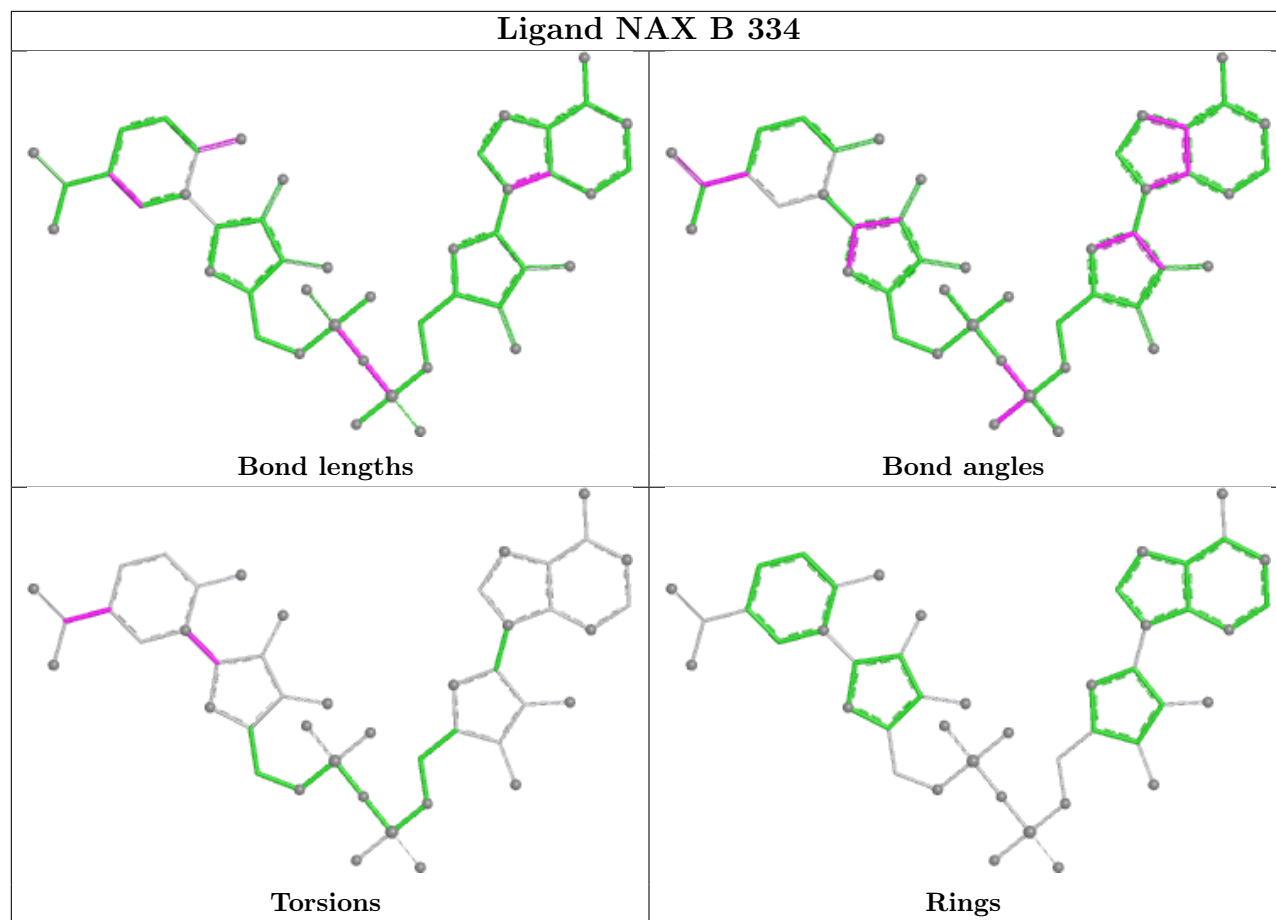
Mol	Chain	Res	Type	Atoms
2	A	334	NAX	PN-O3-PA-O1A
2	B	334	NAX	O4D-C1D-N1N-C2N
2	A	334	NAX	O4D-C1D-N1N-C2N
2	B	334	NAX	C2N-C3N-C7N-N7N
2	B	334	NAX	C2D-C1D-N1N-C2N
2	A	334	NAX	C2D-C1D-N1N-C2N
2	A	334	NAX	C2D-C1D-N1N-C6N
2	B	334	NAX	C2D-C1D-N1N-C6N
2	A	334	NAX	PN-O3-PA-O2A

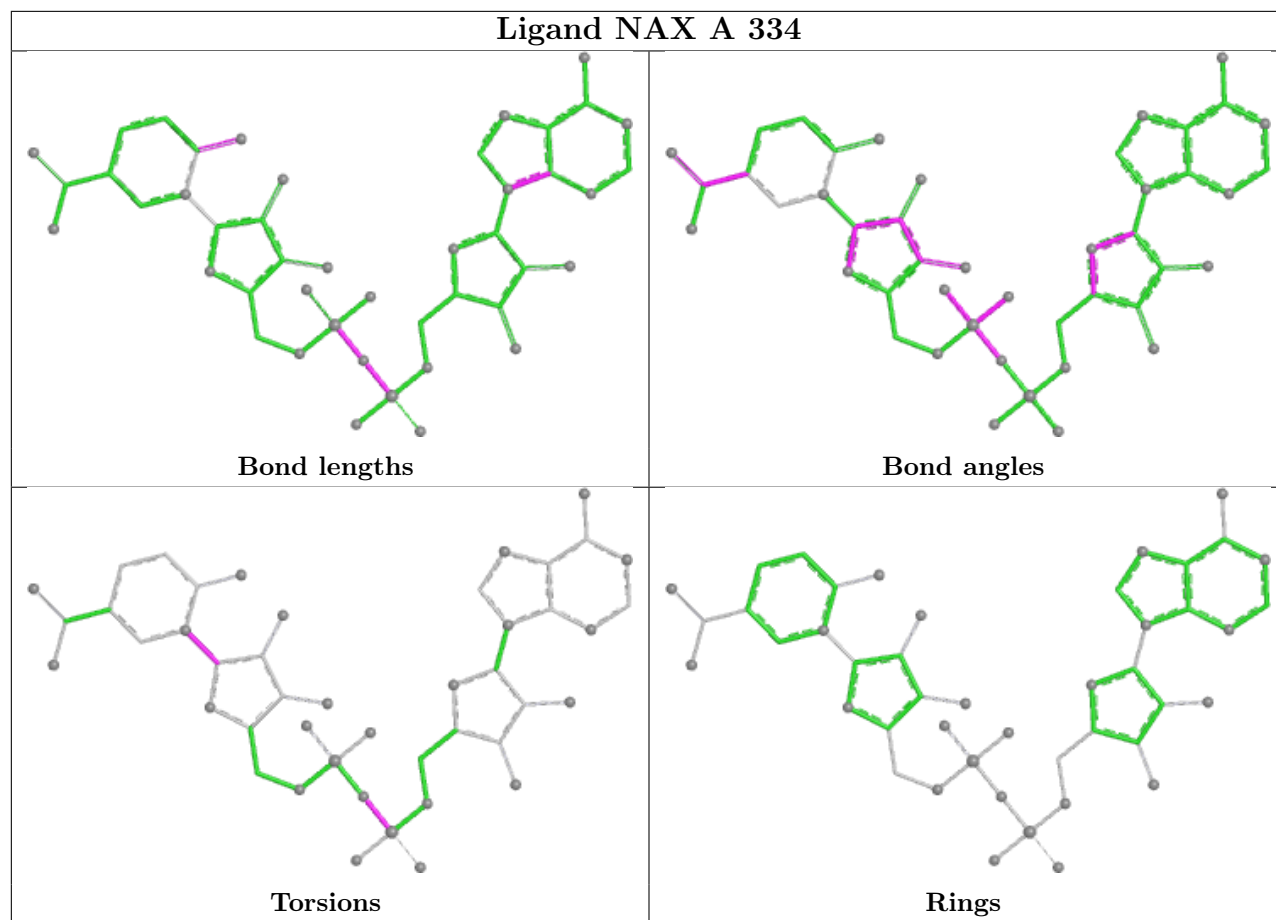
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	334	NAX	2	0
2	A	334	NAX	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	90:PRO	C	91:ARG	N	2.48

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.