



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:33 PM GMT

PDB ID : 1BDM
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

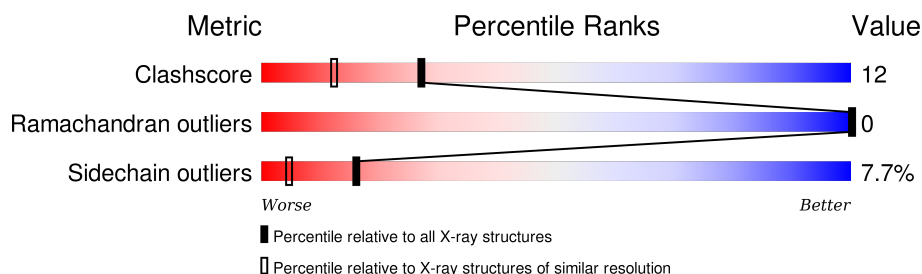
1 Overall quality at a glance

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	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	327	 64% 26% 6% • •
1	B	327	 69% 24% 7%

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.

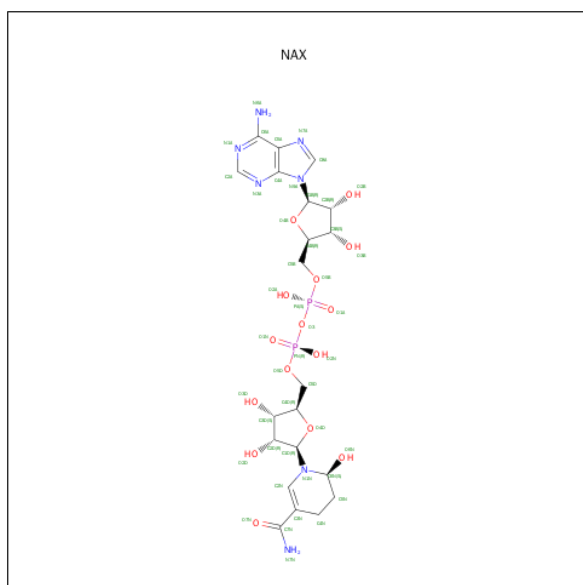
- Molecule 1 is a protein called MALATE DEHYDROGENASE.

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

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 (three-letter code: NAX) (formula: $C_{21}H_{31}N_7O_{15}P_2$).



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.

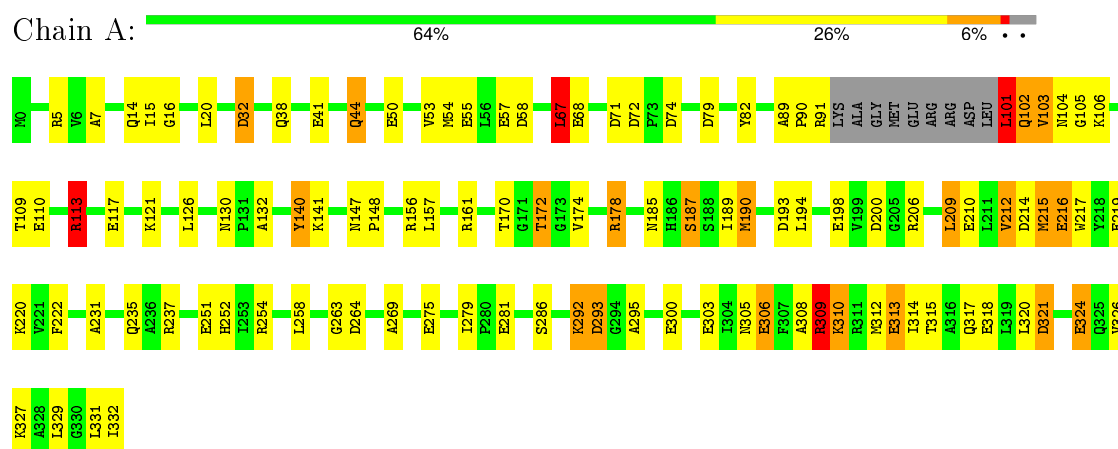
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		
3	B	112	Total	O	0	0
			112	112		

3 Residue-property plots

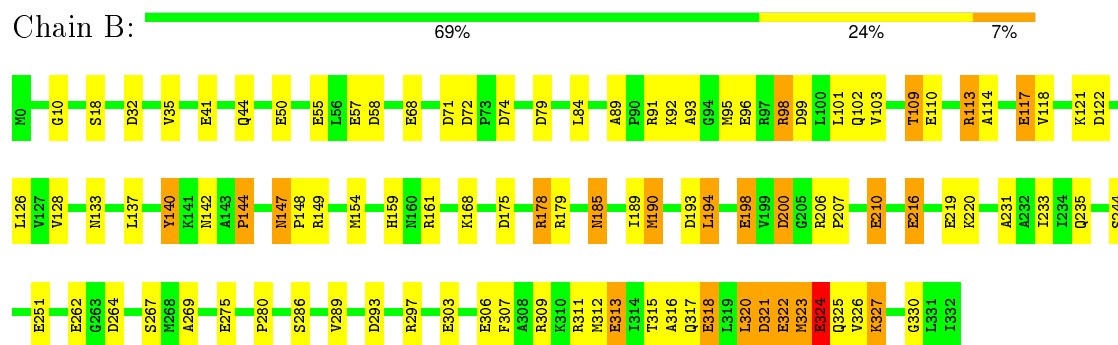
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

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 will therefore be 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	1.03	20/2447 (0.8%)	1.53	39/3316 (1.2%)
1	B	1.05	22/2532 (0.9%)	1.53	36/3428 (1.1%)
All	All	1.04	42/4979 (0.8%)	1.53	75/6744 (1.1%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	68	GLU	CD-OE1	8.01	1.34	1.25
1	A	210	GLU	CD-OE1	7.86	1.34	1.25
1	B	313	GLU	CD-OE1	7.85	1.34	1.25
1	A	110	GLU	CD-OE1	7.63	1.34	1.25
1	A	306	GLU	CD-OE2	7.58	1.33	1.25
1	B	306	GLU	CD-OE1	7.56	1.33	1.25
1	A	198	GLU	CD-OE1	7.54	1.33	1.25
1	A	275	GLU	CD-OE1	7.39	1.33	1.25
1	A	251	GLU	CD-OE1	7.33	1.33	1.25
1	B	210	GLU	CD-OE1	7.33	1.33	1.25
1	B	216	GLU	CD-OE1	7.08	1.33	1.25
1	A	117	GLU	CD-OE2	6.99	1.33	1.25
1	B	262	GLU	CD-OE2	6.99	1.33	1.25
1	A	318	GLU	CD-OE1	6.95	1.33	1.25
1	B	96	GLU	CD-OE1	6.92	1.33	1.25
1	A	324	GLU	CD-OE2	6.92	1.33	1.25
1	B	117	GLU	CD-OE2	6.76	1.33	1.25
1	B	324	GLU	CD-OE1	6.69	1.33	1.25
1	B	55	GLU	CD-OE1	6.44	1.32	1.25
1	B	41	GLU	CD-OE2	6.43	1.32	1.25
1	B	57	GLU	CD-OE2	-6.39	1.18	1.25
1	B	318	GLU	CD-OE2	6.35	1.32	1.25
1	A	313	GLU	CD-OE2	6.35	1.32	1.25
1	A	281	GLU	CD-OE1	6.33	1.32	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	110	GLU	CD-OE1	6.31	1.32	1.25
1	B	322	GLU	CD-OE2	6.22	1.32	1.25
1	A	50	GLU	CD-OE1	6.21	1.32	1.25
1	B	50	GLU	CD-OE2	6.15	1.32	1.25
1	A	55	GLU	CD-OE1	6.11	1.32	1.25
1	A	68	GLU	CD-OE1	6.04	1.32	1.25
1	A	219	GLU	CD-OE1	5.94	1.32	1.25
1	B	219	GLU	CD-OE2	5.86	1.32	1.25
1	B	303	GLU	CD-OE2	5.83	1.32	1.25
1	A	300	GLU	CD-OE2	5.78	1.32	1.25
1	B	251	GLU	CD-OE2	-5.75	1.19	1.25
1	A	41	GLU	CD-OE2	5.69	1.31	1.25
1	B	57	GLU	CD-OE1	5.68	1.31	1.25
1	A	216	GLU	CD-OE2	5.66	1.31	1.25
1	A	303	GLU	CD-OE2	5.55	1.31	1.25
1	A	57	GLU	CD-OE1	-5.47	1.19	1.25
1	B	275	GLU	CD-OE1	5.37	1.31	1.25
1	B	198	GLU	CD-OE1	5.11	1.31	1.25

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	ARG	NE-CZ-NH2	11.17	125.89	120.30
1	A	74	ASP	CB-CG-OD1	-10.06	109.24	118.30
1	A	215	MET	CG-SD-CE	-9.52	84.97	100.20
1	B	149	ARG	NE-CZ-NH1	-9.11	115.74	120.30
1	A	200	ASP	CB-CG-OD1	-8.89	110.30	118.30
1	B	193	ASP	CB-CG-OD1	8.82	126.24	118.30
1	A	193	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	B	74	ASP	CB-CG-OD2	8.24	125.72	118.30
1	B	178	ARG	CD-NE-CZ	8.07	134.90	123.60
1	A	5	ARG	NE-CZ-NH2	8.05	124.33	120.30
1	A	74	ASP	CB-CG-OD2	7.98	125.48	118.30
1	B	71	ASP	CB-CG-OD1	7.87	125.38	118.30
1	A	193	ASP	CB-CG-OD1	7.69	125.22	118.30
1	B	193	ASP	CB-CG-OD2	-7.64	111.43	118.30
1	B	323	MET	CG-SD-CE	-7.62	88.00	100.20
1	A	293	ASP	CB-CG-OD1	7.58	125.12	118.30
1	B	71	ASP	CB-CG-OD2	-7.57	111.49	118.30
1	A	220	LYS	CA-CB-CG	-7.56	96.77	113.40
1	B	178	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	B	96	GLU	N-CA-CB	-7.38	97.32	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	ASP	CB-CG-OD1	-7.25	111.78	118.30
1	A	156	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	B	200	ASP	CB-CG-OD1	-7.14	111.88	118.30
1	B	74	ASP	CB-CG-OD1	-7.10	111.91	118.30
1	A	206	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	B	72	ASP	CB-CG-OD2	7.00	124.60	118.30
1	A	71	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	B	161	ARG	NE-CZ-NH1	-6.93	116.84	120.30
1	A	67	LEU	CB-CA-C	-6.83	97.22	110.20
1	A	264	ASP	CB-CG-OD1	6.83	124.44	118.30
1	B	161	ARG	NE-CZ-NH2	6.69	123.64	120.30
1	A	72	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	B	264	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	264	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	A	214	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	A	237	ARG	NE-CZ-NH1	-6.51	117.04	120.30
1	A	214	ASP	CB-CG-OD1	6.40	124.06	118.30
1	B	35	VAL	CG1-CB-CG2	-6.32	100.78	110.90
1	A	58	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	B	179	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	A	58	ASP	CB-CG-OD1	6.15	123.84	118.30
1	A	324	GLU	N-CA-CB	-5.99	99.82	110.60
1	A	113	ARG	N-CA-CB	5.96	121.33	110.60
1	A	237	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	A	102	GLN	N-CA-CB	5.84	121.12	110.60
1	B	144	PRO	C-N-CA	-5.76	110.21	122.30
1	B	297	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	A	309	ARG	N-CA-CB	5.66	120.79	110.60
1	A	295	ALA	CB-CA-C	5.64	118.56	110.10
1	A	321	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	306	GLU	CB-CA-C	5.61	121.61	110.40
1	B	99	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	A	293	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	B	140	TYR	CA-CB-CG	5.48	123.81	113.40
1	B	293	ASP	CB-CG-OD1	5.44	123.20	118.30
1	A	140	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	B	72	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	B	32	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	185	ASN	CA-CB-CG	-5.34	101.64	113.40
1	B	113	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	A	79	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	71	ASP	CB-CG-OD1	5.31	123.08	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	ASP	CB-CG-OD1	-5.27	113.55	118.30
1	A	32	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	72	ASP	N-CA-CB	-5.25	101.15	110.60
1	B	244	SER	N-CA-CB	5.17	118.25	110.50
1	A	101	LEU	N-CA-CB	5.15	120.70	110.40
1	A	200	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	79	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	175	ASP	CB-CG-OD1	5.11	122.89	118.30
1	B	58	ASP	CB-CG-OD1	5.05	122.85	118.30
1	B	321	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	82	TYR	CB-CG-CD1	-5.04	117.98	121.00
1	B	109	THR	CA-CB-CG2	-5.02	105.37	112.40
1	B	321	ASP	CB-CG-OD1	-5.01	113.79	118.30

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	62	0
1	B	2494	0	2524	59	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	120	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 12.

All (120) 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

Continued on next page...

Continued from previous page...

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: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: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:44:GLN:HA	1:A:44:GLN:NE2	2.07	0.68
1:A:90:PRO:C	1:A:91:ARG:N	2.48	0.67
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:321:ASP:O	1:A:324:GLU:HB3	1.97	0.64
1:B:189:ILE:HD11	1:B:318:GLU:CD	2.18	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:216:GLU:O	1:B:220:LYS:HG2	2.00	0.61
1:B:126:LEU:HD11	1:B:154:MET:HB2	1.81	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: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:102:GLN:NE2	1:A:329:LEU:HD13	2.21	0.56
1:B:231:ALA:O	1:B:235:GLN:HG3	2.05	0.56
1:A:252:HIS:HD2	3:A:792:HOH:O	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LYS:HD3	1:B:95:MET:HB2	1.88	0.56
1:B:309:ARG:O	1:B:313:GLU:HG3	2.06	0.55
1:A:258:LEU:HD23	1:A:258:LEU:N	2.22	0.55
1:B:190:MET:HE3	3:B:909:HOH:O	2.06	0.55
1:A:89:ALA:N	1:A:104:ASN:HD21	1.90	0.54
1:B:142:ASN:C	1:B:144:PRO:HD3	2.28	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:A:292:LYS:NZ	1:A:293:ASP:OD2	2.24	0.53
1:B:269:ALA:HA	1:B:286:SER:HA	1.91	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: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:44:GLN:HG2	3:A:841:HOH:O	2.13	0.48
1:B:317:GLN:HE21	1:B:321:ASP:CG	2.17	0.48
1:A:15:ILE:HD11	2:A:334:NAX:H6N	1.95	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:B:206:ARG:HD2	1:B:210:GLU:OE1	2.14	0.47
1:A:130:ASN:HA	1:A:132:ALA:N	2.29	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

Continued on next page...

Continued from previous page...

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:HA	1:A:313:GLU:OE1	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:B:159:HIS:HD2	1:B:267:SER:OG	2.01	0.43
1:A:231:ALA:O	1:A:235:GLN:HG3	2.18	0.43
1:B:98:ARG:CZ	1:B:98:ARG:HB2	2.48	0.43
1:B:98:ARG:NH1	1:B:98:ARG:CB	2.81	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: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:A:101:LEU:HD12	1:A:101:LEU:HA	1.65	0.43
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:320:LEU:HA	1:A:320:LEU:HD23	1.81	0.42
1:A:209:LEU:HD12	1:A:212:VAL:HG12	2.00	0.42
1:B:98:ARG:HH11	1:B:98:ARG:HB3	1.82	0.42
1:A:209:LEU:HA	1:A:209:LEU:HD12	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: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: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:332:ILE:HG13	1:A:332:ILE:O	2.14	0.41
1:A:215:MET:O	1:A:215:MET:HG3	2.20	0.41
1:B:109:THR:O	1:B:113:ARG:HG2	2.21	0.41
1:B:194:LEU:HA	1:B:194:LEU:HD12	1.88	0.41
1:A:217:TRP:CH2	1:A:222:PHE:CD1	3.09	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

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	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

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%)	219 (90%)	24 (10%)	10	2
1	B	251/252 (100%)	237 (94%)	14 (6%)	26	10
All	All	494/504 (98%)	456 (92%)	38 (8%)	16	5

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	67	LEU
1	A	101	LEU
1	A	103	VAL
1	A	106	LYS
1	A	113	ARG
1	A	121	LYS
1	A	140	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	172	THR
1	A	174	VAL
1	A	178	ARG
1	A	187	SER
1	A	190	MET
1	A	194	LEU
1	A	209	LEU
1	A	212	VAL
1	A	216	GLU
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	98	ARG
1	B	101	LEU
1	B	102	GLN
1	B	121	LYS
1	B	140	TYR
1	B	147	ASN
1	B	190	MET
1	B	194	LEU
1	B	200	ASP
1	B	289	VAL
1	B	320	LEU
1	B	324	GLU
1	B	327	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) 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	165	GLN
1	A	196	HIS
1	A	252	HIS
1	A	273	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	334	-	38,49,49	0.90	2 (5%)	42,75,75	1.63	6 (14%)
2	NAX	B	334	-	38,49,49	1.06	2 (5%)	42,75,75	1.46	5 (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	A	334	-	-	0/25/75/75	0/5/5/5
2	NAX	B	334	-	-	0/25/75/75	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	334	NAX	C2N-C3N	2.06	1.39	1.34
2	B	334	NAX	C2N-C3N	2.97	1.42	1.34
2	A	334	NAX	O6N-C6N	3.36	1.46	1.41
2	B	334	NAX	O6N-C6N	3.74	1.47	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	334	NAX	C4B-O4B-C1B	-5.13	104.08	109.72
2	A	334	NAX	O2N-PN-O3	-4.70	83.77	105.09
2	B	334	NAX	N3A-C2A-N1A	-3.89	125.91	128.89
2	B	334	NAX	O4D-C1D-C2D	-3.07	99.47	106.58
2	A	334	NAX	O4D-C1D-C2D	-2.94	99.76	106.58
2	B	334	NAX	C4B-O4B-C1B	-2.65	106.81	109.72
2	A	334	NAX	C1B-N9A-C4A	-2.43	123.28	126.94
2	A	334	NAX	C2B-C1B-N9A	-2.34	110.72	114.29
2	A	334	NAX	O3D-C3D-C2D	-2.26	104.49	111.83
2	B	334	NAX	O6N-C6N-C5N	2.19	114.17	109.92
2	B	334	NAX	C4A-C5A-N7A	4.10	113.25	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	334	NAX	3	0
2	B	334	NAX	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.