



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 5, 2018 – 12:28 PM EDT

PDB ID : 2X0R
Title : R207S, R292S Mutant of Malate Dehydrogenase from the Halophilic Archeon Haloarcula marismortui (HoloForm)
Authors : Irimia, A.; Ebel, C.; Vellieux, F.M.D.; Richard, S.B.; Cosenza, L.W.; Zaccai, G.; Madern, D.
Deposited on : 2009-12-17
Resolution : 2.92 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031172
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

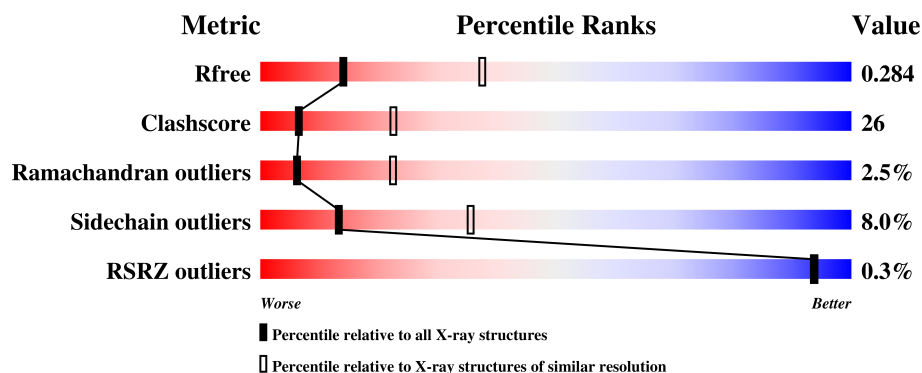
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	1983 (2.94-2.90)
Clashscore	122126	2200 (2.94-2.90)
Ramachandran outliers	120053	2150 (2.94-2.90)
Sidechain outliers	120020	2152 (2.94-2.90)
RSRZ outliers	108989	1928 (2.94-2.90)

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.

Mol	Chain	Length	Quality of chain
1	A	304	<div> <div></div> <div>56%38%6%</div> </div>
1	B	304	<div> <div>%</div> <div>56%40%. .</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	1004	-	-	X	-
3	CL	B	1005	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4824 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.

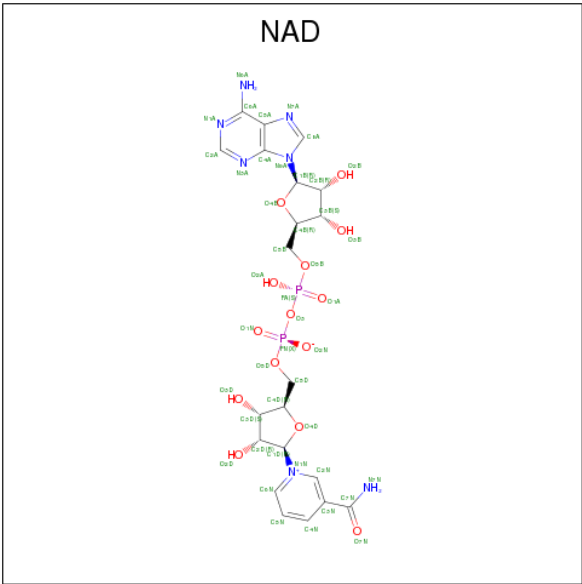
- Molecule 1 is a protein called MALATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	1	0
			2302	1415	391	492	4			
1	B	303	Total	C	N	O	S	0	2	0
			2305	1418	388	494	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	SER	ARG	engineered mutation	UNP Q07841
A	292	SER	ARG	engineered mutation	UNP Q07841
B	207	SER	ARG	engineered mutation	UNP Q07841
B	292	SER	ARG	engineered mutation	UNP Q07841

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cl	0	0
			2	2		
3	A	2	Total	Cl	0	0
			2	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	Na	0	0
			4	4		
4	A	1	Total	Na	0	0
			1	1		

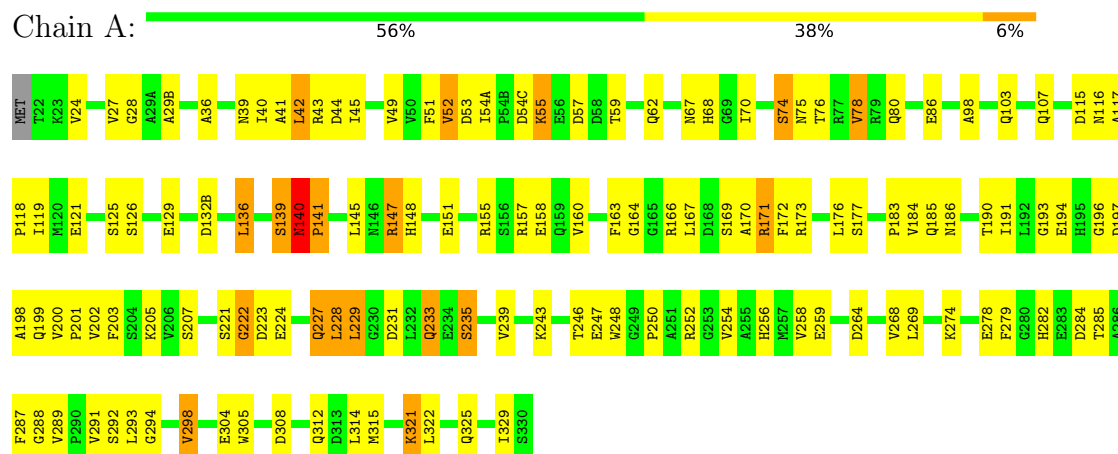
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	48	Total	O	0	0
			48	48		
5	B	72	Total	O	0	0
			72	72		

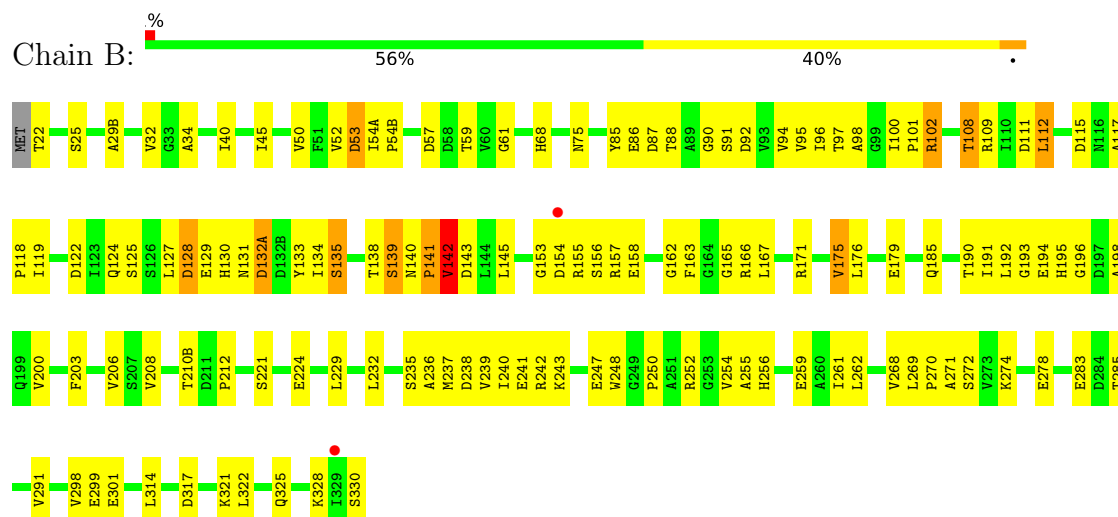
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: MALATE DEHYDROGENASE



• Molecule 1: MALATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	115.36Å 125.91Å 125.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.50 – 2.92 44.50 – 2.92	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.50-2.92) 98.3 (44.50-2.92)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.90Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.184 , 0.286 0.182 , 0.284	Depositor DCC
R_{free} test set	966 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4824	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, NAD, CL

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	0.40	0/2339	0.58	0/3177
1	B	0.40	0/2345	0.61	0/3185
All	All	0.40	0/4684	0.59	0/6362

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	ASN	Peptide
1	B	140	ASN	Peptide

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	2302	0	2161	116	0
1	B	2305	0	2163	126	0
2	A	44	0	26	1	0
2	B	44	0	25	6	0
3	A	2	0	0	3	0
3	B	2	0	0	3	0
4	A	1	0	0	0	0
4	B	4	0	0	0	0
5	A	48	0	0	7	0
5	B	72	0	0	5	0
All	All	4824	0	4375	232	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 26.

All (232) 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:287:PHE:HE1	1:A:315:MET:HE3	1.28	0.99
1:A:36:ALA:O	1:A:40:ILE:HG13	1.66	0.96
1:A:205:LYS:HE3	1:A:305:TRP:HB3	1.53	0.90
1:A:44:ASP:HB2	1:A:74:SER:HB2	1.54	0.90
1:B:247:GLU:O	1:B:250:PRO:HD2	1.73	0.87
1:B:208:VAL:O	1:B:210(B):THR:HB	1.76	0.84
1:B:108:THR:HG23	1:B:111:ASP:HB2	1.62	0.81
1:A:287:PHE:CE1	1:A:315:MET:HE3	2.15	0.79
1:A:193:GLY:HA2	1:A:287:PHE:CD1	2.18	0.78
1:A:274:LYS:HD2	1:A:285:THR:O	1.83	0.78
1:A:252:ARG:NH1	3:A:1004:CL:CL	2.53	0.77
1:A:103:GLN:O	1:A:107:GLN:HB2	1.85	0.75
1:B:91:SER:H	1:B:131:ASN:HD21	1.34	0.75
1:B:237[B]:MET:HG3	1:B:241:GLU:HG3	1.69	0.74
1:A:116:ASN:HB3	1:A:145:LEU:HD21	1.71	0.72
1:B:194:GLU:HG3	1:B:322:LEU:HD11	1.71	0.72
1:B:53:ASP:HB2	1:B:59:THR:HG21	1.70	0.72
1:B:124:GLN:O	1:B:128:ASP:HB2	1.90	0.71
1:B:250:PRO:O	1:B:254:VAL:HG23	1.90	0.71
1:A:140:ASN:O	1:A:145:LEU:HD22	1.92	0.69
1:A:75:ASN:ND2	1:B:185:GLN:HG3	2.07	0.69
1:A:68:HIS:CE1	1:B:171:ARG:HD3	2.28	0.69
1:A:254:VAL:O	1:A:258:VAL:HG23	1.93	0.69
1:A:126:SER:O	1:A:129:GLU:HG2	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ASP:O	1:A:312:GLN:HB2	1.94	0.67
1:B:29(B):ALA:HB2	1:B:59:THR:HG23	1.77	0.67
1:B:119:ILE:O	1:B:122:ASP:HB3	1.95	0.66
1:B:291:VAL:HG13	1:B:298:VAL:HG13	1.77	0.66
1:B:102:ARG:NH1	2:B:608:NAD:O2D	2.30	0.65
1:A:62:GLN:OE1	1:B:243:LYS:HE3	1.97	0.65
1:B:156:SER:HB2	1:B:158:GLU:OE2	1.98	0.64
1:A:140:ASN:HB3	1:A:141:PRO:CD	2.27	0.64
1:A:155:ARG:HH12	1:A:160:VAL:HG22	1.63	0.64
1:B:25:SER:HB2	1:B:94:VAL:HG13	1.79	0.64
1:B:32:VAL:HG23	1:B:97:THR:HB	1.79	0.64
1:A:67:ASN:OD1	1:A:78:VAL:HG13	1.98	0.63
1:A:98:ALA:O	1:A:139:SER:HB3	1.99	0.62
1:A:42:LEU:HD13	1:A:43[B]:ARG:NH2	2.15	0.61
1:B:142:VAL:HG21	1:B:195:HIS:HD2	1.65	0.61
1:B:203:PHE:HA	1:B:206:VAL:HG23	1.83	0.61
1:A:264:ASP:HA	1:A:294:GLY:HA2	1.84	0.60
1:B:193:GLY:HA3	1:B:200:VAL:HG23	1.82	0.60
1:B:98:ALA:O	1:B:139:SER:HB3	2.02	0.59
1:A:259:GLU:OE1	3:A:1004:CL:CL	2.57	0.59
1:A:117:ALA:HB3	1:A:118:PRO:HD3	1.83	0.59
1:A:194:GLU:HG2	5:A:2025:HOH:O	2.03	0.59
1:A:171:ARG:HD3	1:B:68:HIS:CE1	2.38	0.59
1:B:96:ILE:HD12	1:B:96:ILE:N	2.17	0.59
1:A:288:GLY:HA3	5:A:2024:HOH:O	2.03	0.58
1:B:321:LYS:O	1:B:325:GLN:HB2	2.04	0.58
1:A:157:ARG:HG2	5:A:2040:HOH:O	2.04	0.58
1:A:201:PRO:HG2	1:A:229:LEU:HD11	1.86	0.58
1:B:165:GLY:HA3	1:B:270:PRO:HB2	1.86	0.57
1:A:147:ARG:HD2	1:A:274:LYS:HD3	1.86	0.57
1:B:32:VAL:CG2	1:B:97:THR:HB	2.34	0.57
1:A:243:LYS:HB2	1:B:61:GLY:HA3	1.87	0.57
1:B:256:HIS:CD2	1:B:269:LEU:HD11	2.40	0.57
1:B:94:VAL:HG11	1:B:127:LEU:HD11	1.85	0.57
1:B:221:SER:HB3	1:B:224:GLU:CG	2.35	0.57
1:B:271:ALA:HB3	1:B:291:VAL:HG21	1.85	0.57
2:B:608:NAD:H3D	5:B:2019:HOH:O	2.04	0.57
1:A:115:ASP:O	1:A:118:PRO:HD2	2.05	0.56
1:A:158:GLU:HA	1:A:298:VAL:CG1	2.36	0.56
1:B:142:VAL:CG2	1:B:195:HIS:HD2	2.19	0.56
1:A:155:ARG:NH1	1:A:160:VAL:HG22	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLU:HA	1:A:298:VAL:HG13	1.87	0.55
1:B:22:THR:HG22	1:B:92:ASP:OD2	2.06	0.55
1:A:41:ALA:HB1	1:A:70:ILE:HD13	1.88	0.55
1:A:329:ILE:HG13	1:A:329:ILE:O	2.06	0.55
1:B:45:ILE:HD12	1:B:262:LEU:HD12	1.89	0.55
1:A:158:GLU:CB	1:A:298:VAL:HG13	2.36	0.54
1:A:171:ARG:HD3	1:B:68:HIS:ND1	2.23	0.54
1:B:142:VAL:HG21	1:B:195:HIS:CD2	2.41	0.54
1:A:158:GLU:CA	1:A:298:VAL:HG13	2.37	0.54
1:B:237[B]:MET:HG3	1:B:241:GLU:CG	2.34	0.53
1:A:193:GLY:HA2	1:A:287:PHE:HD1	1.69	0.53
1:A:247:GLU:O	1:A:250:PRO:HD2	2.08	0.53
1:A:172:PHE:HB2	1:A:191:ILE:HD11	1.91	0.52
1:A:269:LEU:HD12	1:A:293:LEU:HD12	1.90	0.52
1:A:116:ASN:O	1:A:119:ILE:HB	2.09	0.52
1:B:171:ARG:O	1:B:175:VAL:HG22	2.10	0.52
1:B:100:ILE:HG23	1:B:101:PRO:HD2	1.92	0.52
1:B:133:TYR:O	1:B:155:ARG:NH1	2.43	0.52
1:A:147:ARG:O	1:A:151:GLU:HG2	2.10	0.52
1:B:85:TYR:HA	1:B:88:THR:HG23	1.92	0.51
1:A:202:VAL:O	1:A:202:VAL:HG12	2.09	0.51
2:B:608:NAD:O5D	2:B:608:NAD:H2D	2.09	0.51
1:B:127:LEU:HD23	1:B:133:TYR:CE2	2.45	0.51
1:B:141:PRO:CD	1:B:145:LEU:HD12	2.41	0.51
1:B:179:GLU:O	1:B:179:GLU:HG2	2.09	0.51
1:A:201:PRO:HB2	1:A:203:PHE:CE2	2.45	0.51
1:A:54(A):ILE:HG22	1:A:54(C):ASP:H	1.76	0.51
1:B:138:THR:O	1:B:139:SER:C	2.49	0.51
1:A:246:THR:HB	2:A:607:NAD:H5N	1.93	0.50
1:A:221:SER:O	1:A:224:GLU:N	2.44	0.50
1:A:199:GLN:OE1	5:A:2027:HOH:O	2.20	0.50
1:B:221:SER:HB3	1:B:224:GLU:HG3	1.93	0.50
1:A:252:ARG:NH2	3:A:1004:CL:CL	2.81	0.49
1:A:75:ASN:HD21	1:B:185:GLN:HG3	1.75	0.49
1:B:50:VAL:HG21	1:B:87:ASP:O	2.11	0.49
1:B:141:PRO:HD2	1:B:145:LEU:HD12	1.93	0.49
1:A:243:LYS:HB2	1:B:61:GLY:CA	2.43	0.49
1:A:268:VAL:HA	1:A:291:VAL:O	2.12	0.49
1:B:117:ALA:N	1:B:118:PRO:CD	2.76	0.49
1:B:235:SER:O	1:B:238:ASP:HB2	2.11	0.49
1:A:136:LEU:CD1	1:A:163:PHE:HB2	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:PHE:HB3	1:A:59:THR:CG2	2.43	0.49
1:B:115:ASP:O	1:B:118:PRO:HD2	2.13	0.49
1:A:28:GLY:HA2	1:A:53:ASP:OD2	2.14	0.48
1:A:53:ASP:OD1	1:A:55:LYS:HG3	2.13	0.48
1:A:68:HIS:ND1	1:B:171:ARG:NH1	2.51	0.48
1:B:45:ILE:CD1	1:B:262:LEU:HD12	2.44	0.48
1:A:116:ASN:CB	1:A:145:LEU:HD21	2.40	0.48
1:A:233:GLN:HG2	5:A:2032:HOH:O	2.13	0.48
1:A:205:LYS:HD2	1:A:305:TRP:CE3	2.48	0.48
1:B:141:PRO:HD2	1:B:145:LEU:HG	1.96	0.48
1:B:158:GLU:HB2	1:B:298:VAL:HB	1.95	0.48
1:B:122:ASP:O	1:B:125:SER:HB3	2.14	0.48
1:B:195:HIS:O	1:B:195:HIS:CG	2.67	0.48
1:A:117:ALA:HB1	1:A:148:HIS:CD2	2.49	0.48
1:A:42:LEU:HD13	1:A:43[B]:ARG:CZ	2.44	0.48
1:B:40:ILE:HG12	1:B:255:ALA:HA	1.95	0.48
1:B:203:PHE:HA	1:B:206:VAL:CG2	2.43	0.47
1:A:29(B):ALA:HB3	1:A:53:ASP:CG	2.34	0.47
1:B:32:VAL:HG22	2:B:608:NAD:O2N	2.14	0.47
1:A:51:PHE:HB3	1:A:59:THR:HG23	1.95	0.47
1:B:254:VAL:O	1:B:255:ALA:C	2.52	0.47
1:B:268:VAL:HA	1:B:291:VAL:O	2.15	0.47
1:B:52:VAL:HG12	1:B:53:ASP:N	2.30	0.47
1:A:140:ASN:HB3	1:A:141:PRO:HD3	1.94	0.46
1:A:177:SER:HB3	1:A:184:VAL:HA	1.96	0.46
1:A:287:PHE:CE1	1:A:315:MET:CE	2.92	0.46
1:B:96:ILE:CD1	1:B:96:ILE:N	2.78	0.46
1:A:228:LEU:O	1:A:231:ASP:HB2	2.16	0.46
1:B:141:PRO:HD2	1:B:145:LEU:CD1	2.45	0.46
1:A:291:VAL:CG1	1:A:298:VAL:HB	2.46	0.46
1:B:252:ARG:O	1:B:255:ALA:HB3	2.16	0.46
1:A:190:THR:HG22	1:A:191:ILE:N	2.31	0.46
1:A:169:SER:O	1:A:173:ARG:HG3	2.16	0.46
1:B:166:ARG:NH2	5:B:2037:HOH:O	2.37	0.46
1:A:221:SER:O	1:A:223:ASP:N	2.49	0.46
1:A:59:THR:O	1:A:62:GLN:HB2	2.15	0.46
1:A:243:LYS:HB2	1:B:61:GLY:C	2.35	0.46
1:A:68:HIS:CE1	1:B:171:ARG:HH11	2.30	0.46
1:A:282:HIS:HE1	5:A:2043:HOH:O	1.98	0.45
1:B:138:THR:HB	2:B:608:NAD:C2N	2.46	0.45
1:A:279:PHE:CZ	1:A:304:GLU:HA	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:VAL:O	1:B:200:VAL:HG12	2.15	0.45
1:A:121:GLU:O	1:A:125:SER:HB2	2.16	0.45
1:A:235:SER:OG	1:B:68:HIS:NE2	2.47	0.45
1:B:157:ARG:NH1	1:B:274:LYS:O	2.41	0.45
1:B:252:ARG:NH1	3:B:1005:CL:CL	2.87	0.45
1:A:256:HIS:CD2	1:A:256:HIS:O	2.69	0.45
1:B:133:TYR:N	1:B:133:TYR:CD1	2.84	0.45
1:A:203:PHE:HZ	1:A:229:LEU:HD13	1.82	0.45
1:B:175:VAL:HG11	1:B:232:LEU:HA	1.99	0.45
1:B:158:GLU:H	1:B:158:GLU:CD	2.21	0.44
1:B:194:GLU:C	1:B:196:GLY:H	2.20	0.44
1:A:196:GLY:N	5:A:2025:HOH:O	2.49	0.44
1:A:45:ILE:HG21	1:A:259:GLU:HG3	1.99	0.44
1:A:41:ALA:HA	1:A:76:THR:HG21	1.98	0.44
1:A:43[B]:ARG:HD3	1:A:43[B]:ARG:HA	1.63	0.44
1:B:167:LEU:HD12	1:B:167:LEU:O	2.16	0.44
1:B:86:GLU:CD	1:B:86:GLU:H	2.20	0.44
1:A:193:GLY:C	1:A:287:PHE:HB2	2.37	0.44
1:A:205:LYS:HD2	1:A:305:TRP:HE3	1.82	0.44
1:B:153:GLY:HA3	5:B:2024:HOH:O	2.17	0.44
1:A:183:PRO:HG2	1:A:186:ASN:ND2	2.33	0.44
1:A:278:GLU:CD	1:A:278:GLU:H	2.21	0.44
1:A:321:LYS:HE3	1:A:325:GLN:HE21	1.82	0.44
1:B:109:ARG:HH11	1:B:141:PRO:HA	1.82	0.44
1:B:95:VAL:HG12	1:B:97:THR:HG23	1.98	0.44
1:B:236:ALA:O	1:B:240:ILE:HD12	2.17	0.44
1:B:247:GLU:HB3	1:B:248:TRP:H	1.67	0.44
1:B:145:LEU:HA	1:B:145:LEU:HD23	1.64	0.44
1:B:210(B):THR:O	1:B:212:PRO:HD3	2.18	0.44
1:A:200:VAL:HG22	1:A:314:LEU:HB3	1.99	0.44
1:B:135:SER:HB3	1:B:155:ARG:HH12	1.83	0.44
1:B:158:GLU:O	1:B:298:VAL:HG23	2.18	0.44
1:A:248:TRP:HA	1:A:248:TRP:HE3	1.83	0.44
1:B:194:GLU:HG3	1:B:322:LEU:HD21	1.98	0.43
1:B:134:ILE:HD13	1:B:261:ILE:CG2	2.48	0.43
1:A:248:TRP:CE3	1:A:248:TRP:HA	2.54	0.43
1:A:305:TRP:CD1	1:A:305:TRP:N	2.85	0.43
1:A:279:PHE:CG	1:A:315:MET:HE1	2.53	0.43
1:B:299:GLU:HA	1:B:299:GLU:OE2	2.18	0.43
1:B:314:LEU:O	1:B:317:ASP:HB2	2.18	0.43
1:A:185:GLN:HB2	1:B:75:ASN:OD1	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:VAL:O	1:A:291:VAL:HG23	2.19	0.43
1:B:259:GLU:OE1	3:B:1005:CL:CL	2.73	0.43
1:B:54(A):ILE:O	1:B:54(A):ILE:HD12	2.18	0.43
1:A:167:LEU:HD12	1:A:167:LEU:O	2.18	0.43
1:B:221:SER:HB3	1:B:224:GLU:CD	2.39	0.43
1:A:221:SER:O	1:A:222:GLY:C	2.57	0.43
1:B:132(A):ASP:OD1	1:B:132(A):ASP:N	2.51	0.42
1:B:141:PRO:HD2	1:B:145:LEU:CG	2.49	0.42
1:B:194:GLU:CG	1:B:322:LEU:HD11	2.45	0.42
1:B:229:LEU:HA	1:B:229:LEU:HD23	1.82	0.42
1:A:239:VAL:O	1:A:243:LYS:HB3	2.18	0.42
1:B:135:SER:CB	1:B:155:ARG:HH22	2.32	0.42
1:B:247:GLU:C	1:B:250:PRO:HD2	2.39	0.42
1:B:190:THR:CG2	1:B:191:ILE:N	2.82	0.42
1:A:166:ARG:NH1	1:A:170:ALA:HB2	2.35	0.42
1:A:167:LEU:HD22	1:A:250:PRO:HG3	2.00	0.42
1:A:49:VAL:O	1:A:78:VAL:HA	2.20	0.42
1:B:238:ASP:OD1	1:B:242:ARG:NH1	2.52	0.42
1:A:194:GLU:OE1	1:A:198:ALA:N	2.48	0.42
1:A:27:VAL:HA	1:A:52:VAL:HG13	2.01	0.42
1:B:128:ASP:C	1:B:130:HIS:H	2.22	0.42
1:B:176:LEU:HA	1:B:176:LEU:HD23	1.92	0.42
1:A:172:PHE:O	1:A:176:LEU:HD12	2.19	0.42
1:B:206:VAL:O	1:B:212:PRO:HD2	2.20	0.42
1:B:274:LYS:HD2	1:B:285:THR:O	2.21	0.41
2:B:608:NAD:O5D	2:B:608:NAD:C2D	2.67	0.41
1:B:328:LYS:N	1:B:328:LYS:HD2	2.35	0.41
1:B:91:SER:H	1:B:131:ASN:ND2	2.08	0.41
1:A:291:VAL:HG13	1:A:298:VAL:HB	2.02	0.41
1:B:90:GLY:HA2	5:B:2029:HOH:O	2.21	0.41
1:A:229:LEU:HA	1:A:229:LEU:HD12	1.89	0.41
1:B:112:LEU:O	1:B:115:ASP:HB2	2.20	0.41
1:B:141:PRO:CD	1:B:145:LEU:CD1	2.98	0.41
1:B:162:GLY:HA3	1:B:272:SER:HB3	2.02	0.41
1:B:256:HIS:HA	3:B:1005:CL:CL	2.57	0.41
1:A:205:LYS:CE	1:A:305:TRP:HB3	2.37	0.41
1:B:238:ASP:HA	1:B:242:ARG:HH11	1.86	0.41
1:A:24:VAL:O	1:A:49:VAL:HA	2.20	0.41
1:B:102:ARG:HD3	1:B:102:ARG:HA	1.79	0.41
1:B:278:GLU:H	1:B:278:GLU:CD	2.24	0.41
1:A:284:ASP:O	1:A:284:ASP:OD1	2.39	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ASP:HB2	5:B:2033:HOH:O	2.21	0.40
1:B:142:VAL:HG11	1:B:163:PHE:O	2.22	0.40
1:B:127:LEU:HD23	1:B:133:TYR:CZ	2.56	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	302/304 (99%)	266 (88%)	30 (10%)	6 (2%)	8	29
1	B	303/304 (100%)	254 (84%)	40 (13%)	9 (3%)	5	18
All	All	605/608 (100%)	520 (86%)	70 (12%)	15 (2%)	6	22

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	141	PRO
1	B	102	ARG
1	B	141	PRO
1	B	142	VAL
1	A	222	GLY
1	B	139	SER
1	B	198	ALA
1	A	164	GLY
1	A	227	GLN
1	A	321	LYS
1	B	34	ALA
1	B	129	GLU
1	B	54(B)	PRO
1	B	239	VAL

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	245/245 (100%)	220 (90%)	25 (10%)	8	24
1	B	246/245 (100%)	231 (94%)	15 (6%)	20	50
All	All	491/490 (100%)	451 (92%)	40 (8%)	13	35

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	42	LEU
1	A	52	VAL
1	A	55	LYS
1	A	57	ASP
1	A	74	SER
1	A	78	VAL
1	A	80	GLN
1	A	86	GLU
1	A	132(B)	ASP
1	A	136	LEU
1	A	139	SER
1	A	140	ASN
1	A	147	ARG
1	A	171	ARG
1	A	197	ASP
1	A	207	SER
1	A	227	GLN
1	A	228	LEU
1	A	229	LEU
1	A	233	GLN
1	A	235	SER
1	A	292	SER
1	A	298	VAL
1	A	322	LEU
1	B	53	ASP
1	B	57	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	108	THR
1	B	112	LEU
1	B	128	ASP
1	B	132(A)	ASP
1	B	135	SER
1	B	142	VAL
1	B	154	ASP
1	B	175	VAL
1	B	192	LEU
1	B	283	GLU
1	B	301[A]	GLU
1	B	301[B]	GLU
1	B	330	SER

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

Mol	Chain	Res	Type
1	A	62	GLN
1	A	159	GLN
1	A	199	GLN
1	A	233	GLN
1	A	282	HIS
1	B	103	GLN
1	B	131	ASN
1	B	199	GLN
1	B	282	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 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
2	NAD	A	607	-	40,48,48	1.87	10 (25%)	44,73,73	1.50	6 (13%)
2	NAD	B	608	-	40,48,48	1.93	10 (25%)	44,73,73	1.57	7 (15%)

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	NAD	A	607	-	-	0/22/62/62	0/5/5/5
2	NAD	B	608	-	-	0/22/62/62	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	607	NAD	O4D-C4D	-3.16	1.37	1.45
2	B	608	NAD	C2B-C3B	-3.13	1.45	1.53
2	B	608	NAD	O4D-C4D	-2.87	1.38	1.45
2	B	608	NAD	O4B-C1B	-2.72	1.37	1.41
2	B	608	NAD	O2D-C2D	-2.66	1.36	1.43
2	A	607	NAD	C2B-C3B	-2.65	1.46	1.53
2	B	608	NAD	O3D-C3D	-2.43	1.37	1.43
2	A	607	NAD	O3D-C3D	-2.36	1.37	1.43
2	B	608	NAD	C2D-C3D	-2.28	1.47	1.53
2	A	607	NAD	O2B-C2B	-2.28	1.37	1.43
2	A	607	NAD	O2D-C2D	-2.27	1.37	1.43
2	B	608	NAD	C8A-N9A	-2.10	1.34	1.36
2	A	607	NAD	C2D-C3D	-2.03	1.48	1.53
2	A	607	NAD	C2A-N3A	2.11	1.35	1.32
2	B	608	NAD	C6A-N6A	2.50	1.44	1.34
2	A	607	NAD	C6A-N6A	2.56	1.44	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	607	NAD	O4D-C1D	5.29	1.48	1.41
2	B	608	NAD	O4D-C1D	5.32	1.48	1.41
2	B	608	NAD	C7N-N7N	5.69	1.44	1.33
2	A	607	NAD	C7N-N7N	6.01	1.44	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	607	NAD	N3A-C2A-N1A	-6.69	123.14	128.86
2	B	608	NAD	N3A-C2A-N1A	-6.59	123.22	128.86
2	B	608	NAD	C4B-O4B-C1B	-3.62	106.05	109.83
2	B	608	NAD	C4A-C5A-N7A	-2.63	106.87	109.41
2	A	607	NAD	C4B-O4B-C1B	-2.19	107.54	109.83
2	A	607	NAD	C4A-C5A-N7A	-2.17	107.31	109.41
2	B	608	NAD	C5D-C4D-C3D	-2.12	107.30	115.29
2	A	607	NAD	O5B-PA-O1A	2.19	117.63	109.07
2	B	608	NAD	O5B-PA-O1A	2.20	117.66	109.07
2	B	608	NAD	O5B-C5B-C4B	2.37	117.25	109.00
2	A	607	NAD	O5B-C5B-C4B	2.62	118.11	109.00
2	B	608	NAD	O2A-PA-O5B	2.74	120.46	107.75
2	A	607	NAD	O2A-PA-O5B	2.79	120.71	107.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	607	NAD	1	0
2	B	608	NAD	6	0

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](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	303/304 (99%)	-0.48	0 100 100	17, 40, 70, 87	0
1	B	303/304 (99%)	-0.34	2 (0%) 87 87	11, 39, 74, 142	0
All	All	606/608 (99%)	-0.41	2 (0%) 93 94	11, 39, 72, 142	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	329	ILE	2.9
1	B	154	ASP	2.6

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NA	B	1009	1/1	0.94	0.30	44,44,44,44	0
3	CL	B	1005	1/1	0.94	0.20	100,100,100,100	0
4	NA	B	1010	1/1	0.95	0.30	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NA	B	1006	1/1	0.96	0.14	41,41,41,41	0
2	NAD	A	607	44/44	0.97	0.13	9,25,58,83	6
4	NA	A	1007	1/1	0.97	0.24	63,63,63,63	0
3	CL	A	1004	1/1	0.97	0.22	107,107,107,107	0
2	NAD	B	608	44/44	0.97	0.12	12,29,48,141	3
3	CL	B	1002	1/1	0.98	0.13	61,61,61,61	0
3	CL	A	1001	1/1	0.98	0.09	30,30,30,30	0
4	NA	B	1008	1/1	0.99	0.12	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.