Full wwPDB X-ray Structure Validation Report (i)

Dec 4, 2023 – 02:02 am GMT

PDB ID	:	2J5R
Title	:	2.25 A resolution structure of the wild type malate dehydrogenase from Haloarcula marismortui after second radiation burn (radiation damage series)
Authors	:	Fioravanti, E.; Vellieux, F.M.D.; Amara, P.; Madern, D.; Weik, M.
Deposited on	:	2006-09-19
Resolution	:	2.25 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 (i) 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 (1)) were used in the production of this report:

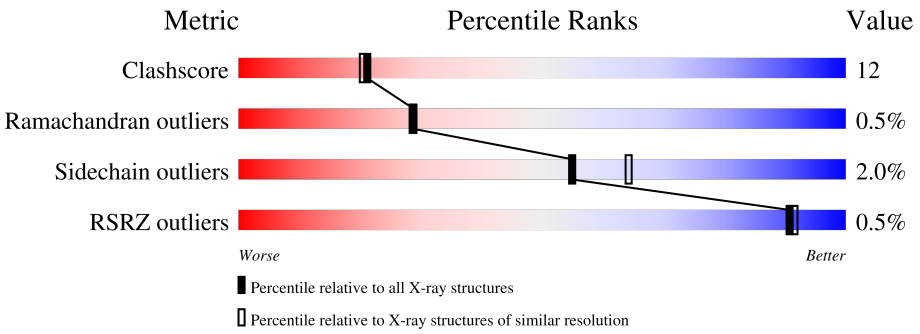
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 <=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	% 75% 24% .
1	B	304	% 74% 23% . .
1	C	304	78% 21% .
1	D	304	% 76% 22% . .

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
2	CL	A	1333	-	-	X	-
2	CL	B	1332	-	-	X	-
2	CL	C	1332	-	-	X	-
2	CL	D	1331	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10082 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	303	2278	1406	391	477	4	0	0	0
1	B	298	2240	1383	383	470	4	0	0	0
1	C	303	2285	1409	393	479	4	0	0	0
1	D	298	2248	1387	383	474	4	0	0	0

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	A	3	3	3	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	1	1	1	0	0

- Molecule 3 is water.

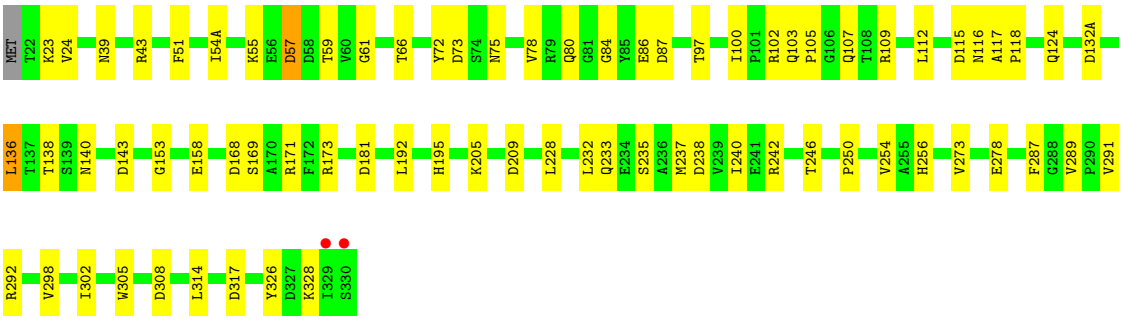
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	265	265	265	0	0
3	B	230	230	230	0	0
3	C	259	259	259	0	0
3	D	269	269	269	0	0

3 Residue-property plots (i)

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 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.

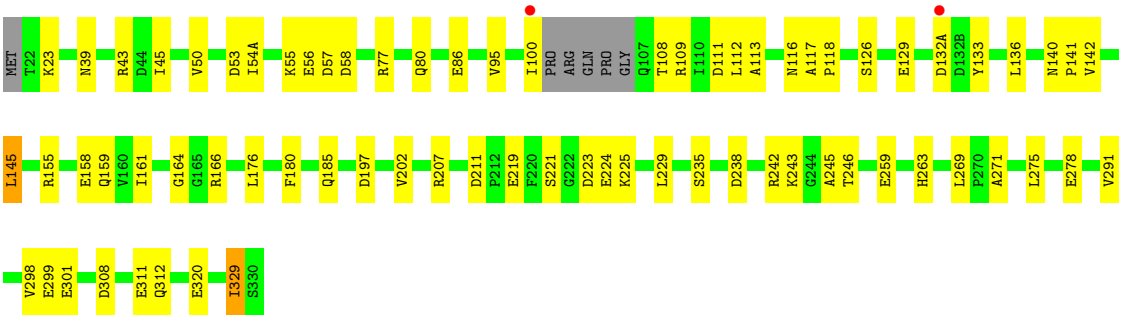
• Molecule 1: MALATE DEHYDROGENASE

Chain A:



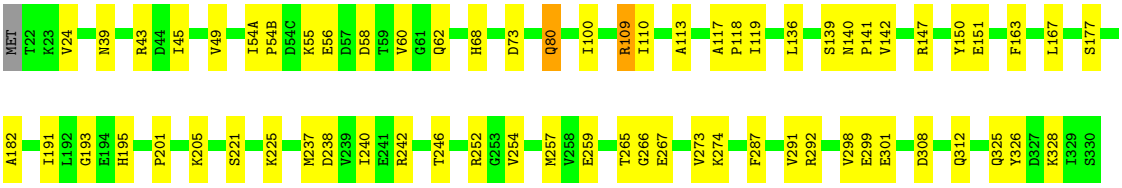
• Molecule 1: MALATE DEHYDROGENASE

Chain B:



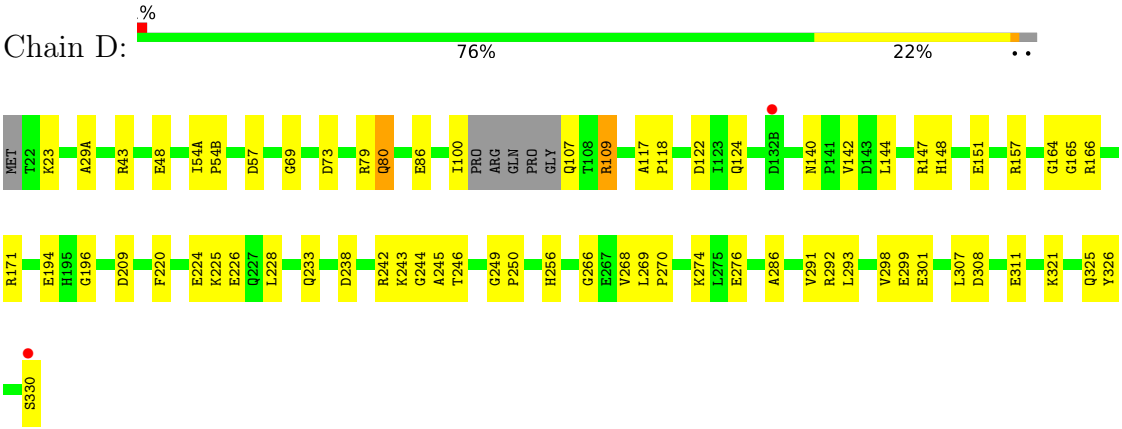
• Molecule 1: MALATE DEHYDROGENASE

Chain C:



• Molecule 1: MALATE DEHYDROGENASE

Chain D:


%
76%
22%
MET T22 K23 A29A R43 E48 I54A P54B D57 G69 D73 R79 Q80 E86 I100 PRO ARG GLN PRO GLY Q107 T108 R109 A117 P118 D122 I123 Q124 D132B N140 P141 V142 D143 L144 R147 H148 E151 R157 G164 G165 R166
R171 E194 H195 G196 D209 F220 E224 K225 E226 Q227 L228 Q233 D238 R242 K243 G244 A245 T246 G249 P250 H256 G266 E267 V268 L269 P270 K274 L275 E276 A286 V291 R292 L293 V298 E299 E301 L307 D308 E311 K321 Q325 Y326
S330

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	127.38Å 114.57Å 124.53Å 90.00° 93.34° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25 19.99 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-2.25) 81.1 (19.99-2.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.26Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.271 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	20.4	Xtriage
Anisotropy	0.701	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 38.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10082	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.52	0/2313	0.68	0/3139
1	B	0.49	0/2274	0.69	0/3087
1	C	0.52	0/2322	0.71	0/3154
1	D	0.50	0/2282	0.71	0/3097
All	All	0.51	0/9191	0.70	0/12477

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	C	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	326	TYR	Sidechain
1	C	326	TYR	Sidechain

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	2278	0	2144	57	0
1	B	2240	0	2106	53	0
1	C	2285	0	2153	52	0
1	D	2248	0	2114	59	0
2	A	3	0	0	2	0
2	B	2	0	0	3	0
2	C	2	0	0	2	0
2	D	1	0	0	2	0
3	A	265	0	0	9	0
3	B	230	0	0	12	0
3	C	259	0	0	6	0
3	D	269	0	0	10	0
All	All	10082	0	8517	213	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 (213) 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:103:GLN:O	1:A:105:PRO:N	1.86	1.08
1:A:140:ASN:HB2	3:A:2118:HOH:O	1.62	0.97
1:C:238:ASP:HA	1:C:242:ARG:HD2	1.56	0.88
1:A:181:ASP:HB2	3:A:2146:HOH:O	1.73	0.87
1:D:86:GLU:CD	1:D:86:GLU:H	1.81	0.82
1:B:308:ASP:OD1	1:B:311:GLU:HG3	1.83	0.79
1:C:45:ILE:HG21	1:C:259:GLU:HG3	1.69	0.75
1:D:291:VAL:HG13	1:D:298:VAL:HG13	1.69	0.74
1:B:320:GLU:HA	3:B:2222:HOH:O	1.87	0.73
1:D:109:ARG:HH21	1:D:109:ARG:CB	2.01	0.73
1:B:100:ILE:HG12	1:B:116:ASN:OD1	1.88	0.72
1:C:39:ASN:O	1:C:43:ARG:HG2	1.88	0.71
1:D:100:ILE:O	1:D:100:ILE:HG13	1.89	0.71
1:A:75:ASN:OD1	1:B:185:GLN:HG3	1.89	0.71
2:A:1333:CL:CL	3:B:2036:HOH:O	2.46	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:GLU:H	1:B:86:GLU:CD	1.95	0.70
1:C:62:GLN:NE2	1:D:243:LYS:HE3	2.06	0.69
2:C:1332:CL:CL	3:D:2056:HOH:O	2.47	0.69
1:D:117:ALA:HB3	1:D:118:PRO:HD3	1.76	0.68
1:B:246:THR:HG21	3:B:2113:HOH:O	1.93	0.68
1:A:140:ASN:HB3	3:A:2122:HOH:O	1.94	0.67
1:A:328:LYS:O	1:A:328:LYS:HD3	1.94	0.67
1:A:205:LYS:HE3	1:A:305:TRP:HB3	1.77	0.66
1:C:140:ASN:HA	1:C:142:VAL:N	2.11	0.66
1:D:109:ARG:HH21	1:D:109:ARG:CG	2.08	0.65
1:A:232:LEU:HD23	3:A:2196:HOH:O	1.96	0.64
1:D:308:ASP:OD1	1:D:311:GLU:HG3	1.98	0.64
1:A:143:ASP:HB2	3:A:2124:HOH:O	1.98	0.63
1:A:100:ILE:HG12	1:A:116:ASN:OD1	1.97	0.63
1:C:62:GLN:CD	1:D:243:LYS:HE3	2.20	0.62
1:D:109:ARG:HH21	1:D:109:ARG:HB3	1.63	0.62
1:D:157:ARG:NE	1:D:276:GLU:OE1	2.34	0.60
1:D:165:GLY:HA3	3:D:2138:HOH:O	2.00	0.60
1:B:95:VAL:HG13	3:B:2093:HOH:O	2.00	0.60
1:B:100:ILE:HG13	1:B:100:ILE:O	2.01	0.59
1:B:166:ARG:NH2	2:B:1332:CL:CL	2.72	0.59
1:D:321:LYS:O	1:D:325:GLN:HG3	2.02	0.59
1:A:86:GLU:H	1:A:86:GLU:CD	2.06	0.59
1:A:256:HIS:ND1	2:A:1333:CL:CL	2.73	0.59
1:D:220:PHE:HB2	1:D:225:LYS:NZ	2.18	0.59
1:A:100:ILE:HD11	1:A:115:ASP:HB3	1.85	0.58
1:B:235:SER:O	1:B:238:ASP:HB2	2.04	0.58
1:D:140:ASN:HA	1:D:142:VAL:N	2.19	0.57
1:B:140:ASN:HA	1:B:142:VAL:N	2.20	0.57
1:C:109:ARG:HD3	3:C:2159:HOH:O	2.03	0.57
1:D:268:VAL:HA	1:D:291:VAL:O	2.05	0.56
1:B:23:LYS:HE3	1:B:50:VAL:HG21	1.88	0.56
1:D:256:HIS:HB2	2:D:1331:CL:CL	2.43	0.56
1:D:270:PRO:HB2	3:D:2138:HOH:O	2.05	0.56
1:A:143:ASP:OD1	1:A:287:PHE:HA	2.06	0.55
1:B:308:ASP:HB2	3:B:2211:HOH:O	2.07	0.55
1:C:177:SER:HB2	1:C:182:ALA:O	2.06	0.55
1:C:100:ILE:HD11	1:C:119:ILE:HD11	1.89	0.55
1:D:242:ARG:HH21	1:D:242:ARG:HG3	1.71	0.55
1:B:100:ILE:HD11	1:B:112:LEU:HD12	1.89	0.54
1:D:242:ARG:HG3	1:D:242:ARG:NH2	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:LEU:O	1:A:317:ASP:HB2	2.08	0.54
1:A:237:MET:CE	1:A:240:ILE:HD12	2.37	0.54
1:B:141:PRO:HB2	3:B:2098:HOH:O	2.07	0.54
1:C:110:ILE:HD11	1:C:325:GLN:OE1	2.07	0.54
1:C:273:VAL:HG21	1:C:298:VAL:HG21	1.89	0.54
1:B:108:THR:OG1	1:B:111:ASP:HB2	2.07	0.53
1:A:273:VAL:HG11	1:A:298:VAL:HG21	1.88	0.53
1:D:144:LEU:HG	3:D:2128:HOH:O	2.09	0.53
1:D:238:ASP:O	1:D:242:ARG:HB2	2.07	0.53
1:D:244:GLY:O	1:D:245:ALA:HB2	2.09	0.53
1:D:326:TYR:O	1:D:330:SER:HB2	2.09	0.52
1:A:103:GLN:O	1:A:103:GLN:CA	2.57	0.52
1:C:110:ILE:HD11	1:C:325:GLN:HG2	1.90	0.52
1:C:291:VAL:HB	1:C:298:VAL:HG13	1.92	0.52
1:D:107:GLN:N	3:D:2085:HOH:O	2.43	0.52
1:B:219:GLU:HB2	3:B:2156:HOH:O	2.08	0.52
1:D:220:PHE:HB2	1:D:225:LYS:HZ1	1.73	0.52
1:A:169:SER:O	1:A:173:ARG:HG3	2.09	0.51
1:C:141:PRO:HB2	3:C:2117:HOH:O	2.10	0.51
1:B:39:ASN:O	1:B:43:ARG:HG2	2.09	0.51
1:B:155:ARG:HB3	1:B:159:GLN:HE21	1.75	0.51
1:C:117:ALA:HB3	1:C:118:PRO:HD3	1.92	0.51
1:B:56:GLU:HA	3:B:2027:HOH:O	2.10	0.51
1:B:141:PRO:O	1:B:145:LEU:HB2	2.11	0.51
1:B:176:LEU:O	1:B:180:PHE:HD1	1.94	0.51
1:B:207:ARG:HG2	3:B:2127:HOH:O	2.10	0.51
1:B:221:SER:OG	1:B:224:GLU:HG3	2.10	0.50
1:A:23:LYS:HG2	1:A:24:VAL:N	2.25	0.50
1:A:102:ARG:HD2	1:A:107:GLN:O	2.11	0.50
1:D:246:THR:HG22	1:D:250:PRO:CD	2.41	0.50
1:A:117:ALA:N	1:A:118:PRO:HD2	2.26	0.50
1:B:299:GLU:O	1:B:301:GLU:HB3	2.10	0.50
1:D:43:ARG:NH1	3:D:2014:HOH:O	2.45	0.50
1:C:43:ARG:NH1	3:C:2012:HOH:O	2.37	0.49
1:A:84:GLY:N	1:A:87:ASP:OD1	2.39	0.49
1:C:252:ARG:HG2	1:D:69:GLY:O	2.13	0.49
1:C:325:GLN:O	1:C:328:LYS:HB2	2.12	0.49
1:A:72:TYR:HB2	2:B:1332:CL:CL	2.49	0.49
1:A:75:ASN:CG	1:B:185:GLN:HG3	2.33	0.49
1:C:136:LEU:HD23	1:C:254:VAL:HG13	1.95	0.49
1:D:166:ARG:HH11	1:D:166:ARG:HG3	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:GLU:O	1:D:228:LEU:HD12	2.13	0.49
1:A:109:ARG:HH11	1:A:109:ARG:HG3	1.78	0.49
1:C:308:ASP:HB2	3:C:2245:HOH:O	2.12	0.49
1:D:291:VAL:HG11	1:D:298:VAL:HG22	1.95	0.49
1:A:238:ASP:O	1:A:242:ARG:HB2	2.13	0.49
1:B:155:ARG:HB3	1:B:159:GLN:NE2	2.28	0.48
1:A:103:GLN:O	1:A:105:PRO:CA	2.60	0.48
1:C:56:GLU:O	1:C:60:VAL:HG23	2.14	0.48
1:B:54(A):ILE:HG12	1:B:55:LYS:HD2	1.96	0.48
1:A:291:VAL:HG12	1:A:302:ILE:HG12	1.94	0.48
1:D:80:GLN:NE2	3:D:2065:HOH:O	2.46	0.48
1:B:269:LEU:O	1:B:291:VAL:HG22	2.14	0.48
1:B:271:ALA:HB3	1:B:291:VAL:HG21	1.96	0.48
1:A:237:MET:HE2	1:A:240:ILE:HD12	1.97	0.47
1:C:73:ASP:OD2	2:D:1331:CL:CL	2.68	0.47
1:C:110:ILE:CD1	1:C:325:GLN:HG2	2.43	0.47
1:B:117:ALA:N	1:B:118:PRO:HD2	2.29	0.47
1:C:110:ILE:HD11	1:C:325:GLN:CD	2.35	0.47
1:D:86:GLU:CD	1:D:86:GLU:N	2.59	0.47
1:A:51:PHE:HB3	1:A:59:THR:CG2	2.44	0.47
1:C:167:LEU:HD12	1:C:167:LEU:O	2.15	0.47
1:D:147:ARG:O	1:D:151:GLU:HG2	2.15	0.47
1:D:166:ARG:HG3	1:D:166:ARG:NH1	2.30	0.47
1:A:171:ARG:HH22	1:A:246:THR:HG21	1.79	0.47
1:C:308:ASP:O	1:C:312:GLN:HG3	2.15	0.46
1:C:237:MET:CE	1:C:240:ILE:HD12	2.45	0.46
1:D:124:GLN:NE2	3:D:2107:HOH:O	2.49	0.46
1:C:195:HIS:O	1:C:195:HIS:CG	2.67	0.46
1:A:153:GLY:HA3	3:A:2104:HOH:O	2.16	0.45
1:B:243:LYS:HE2	1:B:245:ALA:O	2.15	0.45
1:C:265:THR:OG1	1:C:267:GLU:HG3	2.17	0.45
1:B:329:ILE:O	1:B:329:ILE:HG13	2.16	0.45
1:B:23:LYS:HE3	1:B:50:VAL:CG2	2.46	0.45
1:C:273:VAL:CG1	1:C:274:LYS:N	2.80	0.45
1:A:102:ARG:HB2	1:A:112:LEU:HD22	1.99	0.45
1:B:145:LEU:HD12	1:B:145:LEU:HA	1.83	0.45
1:A:205:LYS:CE	1:A:305:TRP:HB3	2.46	0.45
1:B:158:GLU:HB2	1:B:298:VAL:HB	1.99	0.45
1:C:147:ARG:O	1:C:151:GLU:HG2	2.17	0.45
1:A:328:LYS:HD3	1:A:328:LYS:C	2.37	0.45
1:C:299:GLU:O	1:C:301:GLU:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:GLU:O	1:D:301:GLU:HB3	2.18	0.44
1:D:23:LYS:HG3	1:D:48:GLU:HG3	1.99	0.44
1:B:275:LEU:HD22	1:B:278:GLU:HB2	1.99	0.44
1:C:191:ILE:HD13	1:C:201:PRO:HA	2.00	0.44
1:C:139:SER:O	1:C:142:VAL:HA	2.18	0.44
1:A:235:SER:O	1:A:238:ASP:HB2	2.18	0.44
2:C:1332:CL:CL	1:D:73:ASP:OD2	2.73	0.44
1:D:109:ARG:HH21	1:D:109:ARG:HG3	1.80	0.44
1:B:45:ILE:HG22	1:B:263:HIS:NE2	2.33	0.44
1:B:126:SER:O	1:B:129:GLU:HG2	2.17	0.44
1:D:79:ARG:HG2	3:D:2061:HOH:O	2.17	0.44
1:A:66:THR:CG2	1:A:78:VAL:HG21	2.48	0.43
1:A:97:THR:HG22	1:A:138:THR:OG1	2.17	0.43
1:B:113:ALA:HB2	1:B:141:PRO:HG2	1.98	0.43
1:C:54(A):ILE:HG12	1:C:55:LYS:HD2	2.01	0.43
1:C:54(B):PRO:HD2	3:C:2027:HOH:O	2.19	0.43
1:C:193:GLY:HA2	1:C:287:PHE:CD2	2.53	0.43
1:B:140:ASN:HA	1:B:141:PRO:C	2.39	0.43
1:A:168:ASP:CG	1:A:195:HIS:HD1	2.22	0.43
1:C:237:MET:HE1	1:C:240:ILE:HD12	1.99	0.43
1:C:266:GLY:O	1:C:292:ARG:HG3	2.17	0.43
1:D:122:ASP:HB3	3:D:2102:HOH:O	2.17	0.43
1:B:202:VAL:O	1:B:202:VAL:HG12	2.19	0.43
1:C:163:PHE:HD1	1:C:257:MET:SD	2.41	0.43
1:D:291:VAL:CG1	1:D:298:VAL:HG13	2.43	0.43
1:D:166:ARG:HD3	1:D:269:LEU:HD22	2.01	0.43
1:A:209:ASP:OD2	1:D:292:ARG:NH2	2.52	0.43
1:A:100:ILE:HD11	1:A:115:ASP:CB	2.47	0.42
1:A:228:LEU:HG	3:A:2192:HOH:O	2.18	0.42
1:A:308:ASP:OD1	1:A:308:ASP:C	2.57	0.42
1:B:136:LEU:HA	1:B:161:ILE:O	2.18	0.42
1:A:54(A):ILE:HD11	1:A:55:LYS:HE3	2.01	0.42
1:A:124:GLN:HB3	3:A:2103:HOH:O	2.18	0.42
1:C:246:THR:O	1:C:246:THR:HG23	2.19	0.42
1:D:157:ARG:HD2	1:D:274:LYS:O	2.20	0.42
1:D:194:GLU:HG2	1:D:196:GLY:N	2.34	0.42
1:A:61:GLY:HA3	1:B:243:LYS:HB2	2.02	0.42
1:C:325:GLN:HG3	3:C:2253:HOH:O	2.19	0.42
1:C:221:SER:O	1:C:225:LYS:HG3	2.19	0.42
1:A:292:ARG:NH1	1:D:209:ASP:OD2	2.53	0.42
1:B:320:GLU:HG3	3:B:2222:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:GLY:HA2	1:D:293:LEU:O	2.20	0.42
1:C:110:ILE:HD11	1:C:325:GLN:CG	2.49	0.42
1:D:307:LEU:HB3	1:D:311:GLU:HB2	2.02	0.42
1:A:57:ASP:HB2	3:A:2034:HOH:O	2.20	0.41
1:B:211:ASP:OD2	1:C:205:LYS:NZ	2.50	0.41
1:C:68:HIS:CE1	1:D:171:ARG:HG2	2.55	0.41
1:C:113:ALA:HB2	1:C:141:PRO:HG3	2.01	0.41
1:C:273:VAL:HG12	1:C:274:LYS:N	2.35	0.41
1:D:109:ARG:CG	1:D:109:ARG:NH2	2.74	0.41
1:C:24:VAL:O	1:C:49:VAL:HA	2.21	0.41
1:C:150:TYR:CE2	1:C:274:LYS:HG2	2.56	0.41
1:D:54(A):ILE:HB	1:D:54(B):PRO:CD	2.51	0.41
1:B:312:GLN:HG2	3:B:2085:HOH:O	2.21	0.41
1:D:109:ARG:HG3	1:D:109:ARG:NH2	2.36	0.41
1:B:109:ARG:NH2	3:B:2067:HOH:O	2.52	0.41
1:A:73:ASP:OD2	2:B:1332:CL:CL	2.75	0.41
1:A:103:GLN:CA	1:A:105:PRO:N	2.84	0.41
1:A:158:GLU:CD	1:A:158:GLU:H	2.24	0.41
1:B:225:LYS:O	1:B:229:LEU:HG	2.21	0.41
1:D:117:ALA:HB1	1:D:148:HIS:CD2	2.56	0.41
1:A:39:ASN:O	1:A:43:ARG:HG2	2.21	0.41
1:B:238:ASP:O	1:B:242:ARG:HB2	2.21	0.41
1:C:80:GLN:HE21	1:C:80:GLN:HB3	1.64	0.41
1:C:238:ASP:O	1:C:242:ARG:HB2	2.21	0.41
1:D:109:ARG:HB3	1:D:109:ARG:NH2	2.33	0.41
1:A:136:LEU:HA	1:A:136:LEU:HD23	1.78	0.41
1:B:259:GLU:HG3	1:B:263:HIS:CD2	2.56	0.41
1:D:249:GLY:N	1:D:250:PRO:HD2	2.34	0.41
1:D:274:LYS:HA	1:D:286:ALA:HB2	2.03	0.41
1:A:278:GLU:HG2	1:A:302:ILE:HG21	2.03	0.40
1:A:192:LEU:HD22	1:A:289:VAL:HA	2.04	0.40
1:B:77:ARG:HA	1:B:77:ARG:HE	1.86	0.40
1:B:133:TYR:N	1:B:133:TYR:CD1	2.89	0.40
1:A:250:PRO:O	1:A:254:VAL:HG23	2.21	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	299/304 (98%)	286 (96%)	12 (4%)	1 (0%)	41	46
1	B	294/304 (97%)	279 (95%)	12 (4%)	3 (1%)	15	13
1	C	301/304 (99%)	286 (95%)	15 (5%)	0	100	100
1	D	294/304 (97%)	280 (95%)	12 (4%)	2 (1%)	22	21
All	All	1188/1216 (98%)	1131 (95%)	51 (4%)	6 (0%)	29	29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	132(A)	ASP
1	B	164	GLY
1	A	132(A)	ASP
1	D	29(A)	ALA
1	D	164	GLY
1	B	329	ILE

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	237/245 (97%)	233 (98%)	4 (2%)	60	71
1	B	233/245 (95%)	226 (97%)	7 (3%)	41	50
1	C	239/245 (98%)	236 (99%)	3 (1%)	69	79
1	D	235/245 (96%)	230 (98%)	5 (2%)	53	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	944/980 (96%)	925 (98%)	19 (2%)	55 64

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ASP
1	A	80	GLN
1	A	136	LEU
1	A	233	GLN
1	B	53	ASP
1	B	57	ASP
1	B	58	ASP
1	B	80	GLN
1	B	145	LEU
1	B	197	ASP
1	B	223	ASP
1	C	58	ASP
1	C	80	GLN
1	C	109	ARG
1	D	57	ASP
1	D	80	GLN
1	D	109	ARG
1	D	226	GLU
1	D	233	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	199	GLN
1	A	233	GLN
1	A	325	GLN
1	B	80	GLN
1	B	159	GLN
1	B	199	GLN
1	C	80	GLN
1	C	199	GLN
1	C	233	GLN
1	C	325	GLN
1	D	80	GLN
1	D	107	GLN

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Mol	Chain	Res	Type
1	D	233	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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%)	-0.10	2 (0%)	87	88	11, 22, 35, 59	0
1	B	298/304 (98%)	-0.10	2 (0%)	87	88	12, 23, 41, 55	0
1	C	303/304 (99%)	-0.12	0	100	100	9, 21, 33, 47	0
1	D	298/304 (98%)	-0.08	2 (0%)	87	88	11, 23, 37, 57	0
All	All	1202/1216 (98%)	-0.10	6 (0%)	91	91	9, 22, 37, 59	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	SER	3.2
1	D	132(B)	ASP	2.7
1	B	100	ILE	2.4
1	B	132(A)	ASP	2.2
1	A	329	ILE	2.2
1	D	330	SER	2.1

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 monosaccharides 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
2	CL	B	1332	1/1	0.96	0.72	78,78,78,78	0
2	CL	D	1331	1/1	0.96	0.24	52,52,52,52	0
2	CL	A	1331	1/1	0.98	0.09	17,17,17,17	0
2	CL	C	1332	1/1	0.98	0.13	36,36,36,36	0
2	CL	A	1333	1/1	0.98	0.18	43,43,43,43	0
2	CL	C	1331	1/1	0.99	0.10	13,13,13,13	0
2	CL	B	1331	1/1	0.99	0.09	22,22,22,22	0
2	CL	A	1332	1/1	0.99	0.06	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.