Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:26 PM GMT

PDB ID : 3ZH2

Title : Structure of Plasmodium falciparum lactate dehydrogenase in complex with a DNA aptamer

Authors : Cheung, Y.W.; Kwok, J.; Law, A.W.L.; Watt, R.M.; Kotaka, M.; Tanner, J.A.

Deposited on : 2012-12-20

Resolution : 2.10 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:
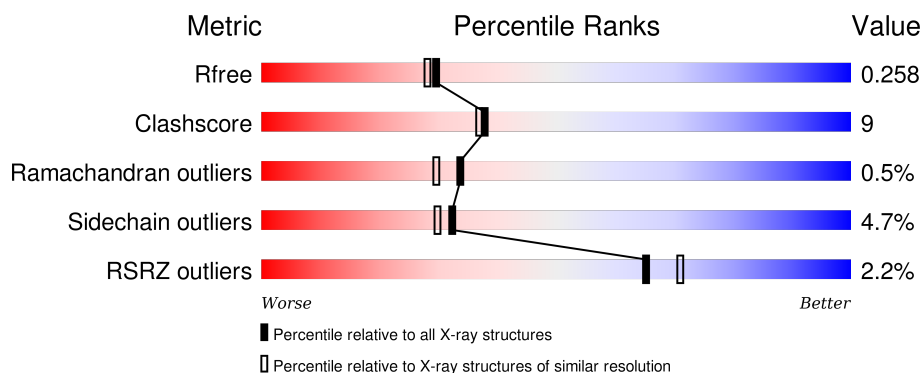
1　Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	Percentile Ranks	Value
Rfree		0.258
Clashscore		9
Ramachandran outliers		0.5%
Sidechain outliers		4.7%
RSRZ outliers		2.2%

Worse — *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 <=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	316	% 83% 13% · ·
1	B	316	2% 75% 20% · · ·
1	C	316	% 85% 13% ·
1	D	316	3% 80% 17% · ·
2	E	35	6% 17% 43% 17% 23%

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Mol	Chain	Length	Quality of chain
2	G	35	

6%

37% 26% 14% 23%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11217 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 L-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2379	1515	406	445	13			
1	B	308	Total	C	N	O	S	0	0	0
			2336	1489	398	436	13			
1	C	315	Total	C	N	O	S	0	0	0
			2380	1516	407	444	13			
1	D	311	Total	C	N	O	S	0	0	0
			2360	1504	402	441	13			

- Molecule 2 is a DNA chain called DNA APTAMER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	27	Total	C	N	O	P	0	0	0
			559	263	109	160	27			
2	G	27	Total	C	N	O	P	0	0	0
			559	263	109	160	27			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	195	Total	O	0	0
			195	195		
3	B	164	Total	O	0	0
			164	164		
3	C	154	Total	O	0	0
			154	154		
3	D	109	Total	O	0	0
			109	109		
3	E	11	Total	O	0	0
			11	11		
3	G	11	Total	O	0	0
			11	11		

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.
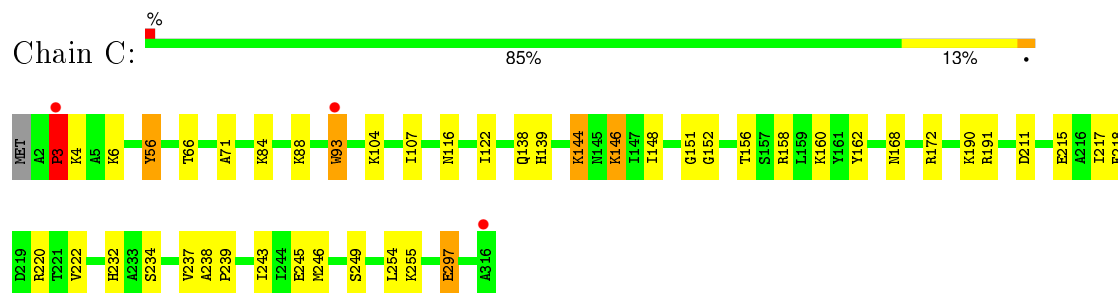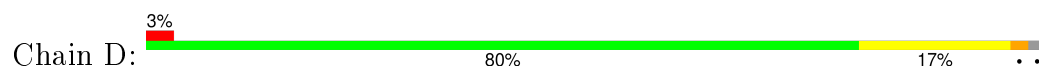
- Molecule 1: L-LACTATE DEHYDROGENASE
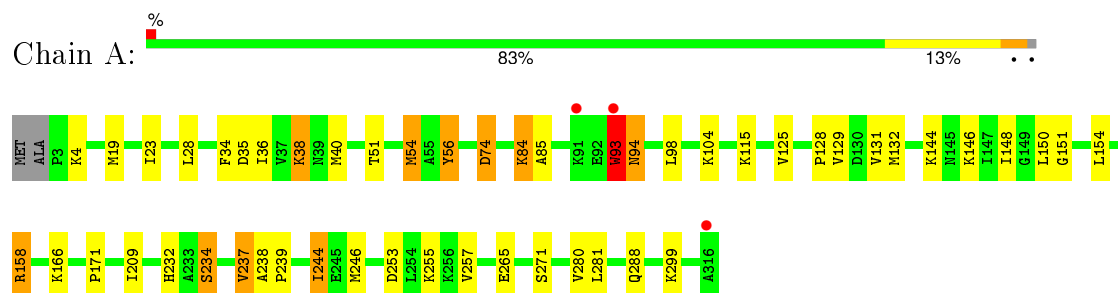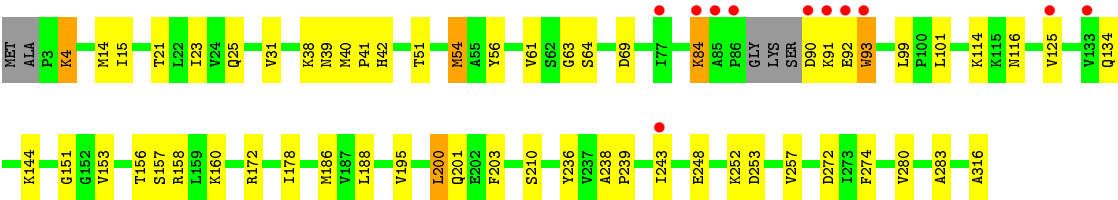

- Molecule 1: L-LACTATE DEHYDROGENASE
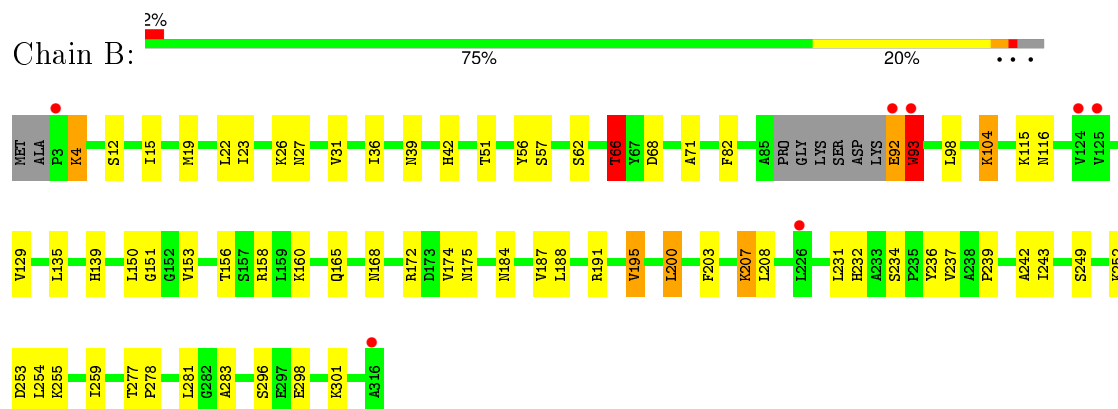
- Molecule 1: L-LACTATE DEHYDROGENASE

- Molecule 1: L-LACTATE DEHYDROGENASE

• Molecule 2: DNA APTAMER
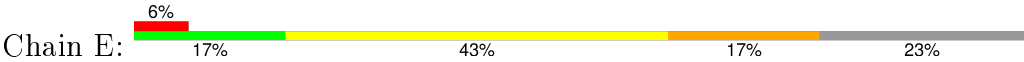
• Molecule 2: DNA APTAMER
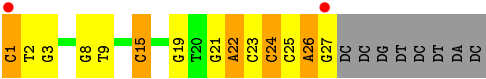
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.46Å 159.49Å 88.66Å 90.00° 102.18° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.51 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-2.10) 97.5 (29.51-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.51 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.206 , 0.257 0.206 , 0.258	Depositor DCC
R_{free} test set	6264 reflections (5.43%)	DCC
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Outliers	1 of 121466 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11217	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	1.05	3/2416 (0.1%)	1.10	4/3270 (0.1%)
1	B	0.99	1/2371 (0.0%)	1.04	4/3209 (0.1%)
1	C	0.95	1/2417 (0.0%)	1.01	5/3273 (0.2%)
1	D	0.93	2/2396 (0.1%)	0.98	4/3243 (0.1%)
2	E	0.63	1/628 (0.2%)	1.17	11/966 (1.1%)
2	G	0.70	1/628 (0.2%)	1.24	12/966 (1.2%)
All	All	0.95	9/10856 (0.1%)	1.06	40/14927 (0.3%)

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	C	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	DC	OP3-P	-10.15	1.49	1.61
2	E	1	DC	OP3-P	-9.73	1.49	1.61
1	D	200	LEU	C-O	6.56	1.35	1.23
1	A	237	VAL	C-O	6.43	1.35	1.23
1	A	93	TRP	CD2-CE2	6.05	1.48	1.41
1	B	93	TRP	CD2-CE2	5.90	1.48	1.41
1	C	93	TRP	CD2-CE2	5.80	1.48	1.41
1	D	93	TRP	CD2-CE2	5.57	1.48	1.41
1	A	244	ILE	C-O	5.10	1.33	1.23

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	4	DG	P-O3'-C3'	10.10	131.82	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	24	DC	P-O3'-C3'	9.62	131.25	119.70
2	G	8	DG	O3'-P-O5'	-8.80	87.27	104.00
1	C	220	ARG	NE-CZ-NH2	-8.35	116.13	120.30
2	G	8	DG	P-O3'-C3'	8.28	129.63	119.70
2	G	23	DC	P-O3'-C3'	8.00	129.30	119.70
2	E	23	DC	O5'-P-OP1	7.60	119.82	110.70
1	B	66	THR	CB-CA-C	-7.40	91.63	111.60
2	E	22	DA	O3'-P-O5'	-7.16	90.39	104.00
1	A	253	ASP	CB-CG-OD1	7.10	124.69	118.30
1	D	158	ARG	NE-CZ-NH1	-7.09	116.76	120.30
2	G	9	DT	P-O3'-C3'	6.97	128.07	119.70
2	G	21	DG	P-O3'-C3'	6.90	127.98	119.70
2	E	11	DG	O5'-P-OP2	-6.84	99.54	105.70
1	A	158	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	D	54	MET	CG-SD-CE	6.61	110.77	100.20
2	E	6	DC	P-O3'-C3'	-6.36	112.07	119.70
2	E	24	DC	P-O3'-C3'	6.35	127.32	119.70
2	G	22	DA	O3'-P-O5'	-6.31	92.00	104.00
1	D	14	MET	CG-SD-CE	-6.21	90.26	100.20
1	A	74	ASP	CB-CG-OD2	6.09	123.78	118.30
2	E	26	DA	P-O3'-C3'	6.04	126.95	119.70
1	C	220	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	B	62	SER	CB-CA-C	-6.00	98.70	110.10
1	A	281	LEU	CA-CB-CG	5.93	128.93	115.30
2	E	1	DC	P-O3'-C3'	5.90	126.78	119.70
1	C	255	LYS	CD-CE-NZ	-5.74	98.49	111.70
2	G	15	DC	P-O3'-C3'	-5.72	112.84	119.70
2	E	9	DT	P-O3'-C3'	5.70	126.54	119.70
1	C	172	ARG	NE-CZ-NH2	-5.66	117.47	120.30
2	E	15	DC	O3'-P-O5'	-5.61	93.33	104.00
2	G	26	DA	P-O3'-C3'	5.47	126.26	119.70
2	G	9	DT	O5'-P-OP1	5.43	117.21	110.70
2	G	22	DA	P-O3'-C3'	5.38	126.16	119.70
2	G	1	DC	O3'-P-O5'	-5.37	93.81	104.00
2	E	21	DG	P-O3'-C3'	5.34	126.11	119.70
1	C	122	ILE	CB-CA-C	-5.31	100.97	111.60
1	D	63	GLY	N-CA-C	-5.28	99.90	113.10
1	B	200	LEU	CB-CG-CD2	5.25	119.92	111.00
1	B	195	VAL	CB-CA-C	-5.04	101.83	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	3	PRO	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	2379	0	2464	44	0
1	B	2336	0	2418	51	0
1	C	2380	0	2464	34	0
1	D	2360	0	2442	32	0
2	E	559	0	302	23	0
2	G	559	0	302	22	0
3	A	195	0	0	15	0
3	B	164	0	0	9	0
3	C	154	0	0	10	0
3	D	109	0	0	2	0
3	E	11	0	0	0	0
3	G	11	0	0	0	0
All	All	11217	0	10392	190	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 9.

All (190) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:LYS:HE2	3:B:2133:HOH:O	1.48	1.12
1:C:168:ASN:HB2	3:C:2092:HOH:O	1.53	1.06
1:A:93:TRP:CH2	3:A:2057:HOH:O	2.13	1.02
2:E:24:DC:H2"	2:E:25:DC:H5"	1.04	1.01
2:E:24:DC:C2'	2:E:25:DC:H5"	1.92	0.98
2:E:25:DC:H2"	2:E:26:DA:C8	2.01	0.96
2:E:6:DC:H2"	2:E:7:DG:H5'	1.48	0.93
2:E:24:DC:H2"	2:E:25:DC:C5'	1.96	0.92
2:G:26:DA:H2"	2:G:27:DG:H5"	1.49	0.92
1:B:252:LYS:CE	3:B:2133:HOH:O	2.12	0.90
1:A:93:TRP:HH2	3:A:2057:HOH:O	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:TRP:CD1	3:A:2059:HOH:O	2.30	0.83
1:D:15:ILE:HG12	1:D:236:TYR:HB2	1.60	0.81
1:B:239:PRO:O	1:B:243:ILE:HD12	1.80	0.81
1:A:232:HIS:HD2	3:A:2148:HOH:O	1.65	0.79
2:E:25:DC:H2"	2:E:26:DA:N7	1.97	0.78
1:A:4:LYS:HD3	3:A:2021:HOH:O	1.84	0.77
1:A:166:LYS:HG2	1:A:209:ILE:HD12	1.68	0.76
2:G:1:DC:H2'	2:G:1:DC:OP2	1.86	0.75
1:B:4:LYS:HD3	3:B:2016:HOH:O	1.87	0.74
2:G:2:DT:H2"	2:G:3:DG:OP2	1.87	0.73
1:B:66:THR:CG2	3:B:2017:HOH:O	2.38	0.71
1:C:152:GLY:O	1:C:156:THR:HG23	1.89	0.71
1:A:74:ASP:OD2	3:A:2001:HOH:O	2.09	0.70
1:C:168:ASN:CB	3:C:2092:HOH:O	2.23	0.70
1:B:153:VAL:HG12	1:B:242:ALA:HB1	1.73	0.70
2:G:1:DC:OP1	2:G:1:DC:H3'	1.92	0.69
1:B:66:THR:HG23	3:B:2017:HOH:O	1.93	0.68
2:E:26:DA:H8	2:E:26:DA:OP2	1.78	0.67
1:B:156:THR:O	1:B:160:LYS:HG3	1.95	0.66
2:G:25:DC:C2'	2:G:26:DA:C8	2.79	0.66
1:B:66:THR:HB	1:B:68:ASP:H	1.61	0.66
1:C:158:ARG:HD3	3:C:2081:HOH:O	1.96	0.66
1:A:93:TRP:CZ3	3:A:2057:HOH:O	2.41	0.65
2:E:2:DT:H2"	2:E:3:DG:C8	2.32	0.65
1:D:156:THR:O	1:D:160:LYS:HG3	1.97	0.64
2:G:25:DC:H2'	2:G:26:DA:C8	2.32	0.64
1:A:237:VAL:HG12	1:B:51:THR:HG21	1.79	0.63
1:D:272:ASP:HB3	3:D:2103:HOH:O	1.98	0.62
1:B:174:VAL:HG22	1:B:195:VAL:HG13	1.83	0.61
1:B:249:SER:HA	1:B:254:LEU:HD12	1.81	0.61
2:E:1:DC:H2'	2:E:2:DT:C6	2.36	0.61
1:A:54:MET:CE	1:B:242:ALA:HB2	2.31	0.60
2:G:15:DC:H6	2:G:15:DC:C5'	2.13	0.60
1:A:232:HIS:HE1	2:E:18:DA:N3	1.99	0.59
1:A:255:LYS:HE3	1:C:168:ASN:OD1	2.02	0.59
1:D:15:ILE:HG12	1:D:236:TYR:CB	2.30	0.59
1:A:54:MET:HE3	1:B:242:ALA:HB2	1.83	0.58
1:C:232:HIS:ND1	3:C:2126:HOH:O	2.32	0.58
1:B:104:LYS:HE2	3:B:2040:HOH:O	2.03	0.58
1:C:234:SER:HB2	2:G:19:DG:OP1	2.02	0.58
1:A:84:LYS:HD2	1:A:85:ALA:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ALA:HB3	1:A:239:PRO:HD3	1.87	0.57
2:E:4:DG:H2"	2:E:5:DG:C8	2.38	0.57
1:D:39:ASN:HA	1:D:42:HIS:HD2	1.70	0.57
1:A:93:TRP:HD1	3:A:2026:HOH:O	1.89	0.56
2:E:6:DC:H2"	2:E:7:DG:C5'	2.29	0.56
1:A:94:ASN:C	1:A:94:ASN:HD22	2.09	0.56
2:G:25:DC:H2'	2:G:26:DA:N7	2.22	0.55
1:C:6:LYS:NZ	1:C:71:ALA:O	2.37	0.55
1:A:128:PRO:HG2	1:A:131:VAL:HB	1.87	0.55
1:A:280:VAL:HB	1:A:288:GLN:HB2	1.89	0.55
2:E:5:DG:OP1	2:E:5:DG:H2'	2.05	0.55
1:A:51:THR:HG21	1:B:237:VAL:HG12	1.88	0.55
2:G:25:DC:H2"	2:G:26:DA:C8	2.40	0.55
1:C:297:GLU:H	1:C:297:GLU:CD	2.10	0.55
2:G:1:DC:H2'	2:G:1:DC:P	2.47	0.54
1:C:218:PHE:O	1:C:222:VAL:HG23	2.07	0.54
1:D:248:GLU:HG3	1:D:252:LYS:HD2	1.90	0.54
1:B:188:LEU:HD12	1:B:188:LEU:H	1.73	0.54
1:C:168:ASN:CG	3:C:2092:HOH:O	2.45	0.53
1:A:93:TRP:HZ2	1:A:98:LEU:CG	2.22	0.53
1:C:245:GLU:OE1	1:D:54:MET:HG3	2.08	0.53
2:E:9:DT:H5'	2:E:10:DA:H5"	1.90	0.52
1:C:190:LYS:NZ	1:C:211:ASP:OD1	2.42	0.52
1:B:158:ARG:N	1:B:158:ARG:HD2	2.24	0.52
1:A:38:LYS:HG2	3:A:2024:HOH:O	2.09	0.52
1:C:238:ALA:N	1:C:239:PRO:CD	2.73	0.52
1:B:255:LYS:HA	1:B:281:LEU:O	2.10	0.52
1:A:93:TRP:CD1	3:A:2026:HOH:O	2.55	0.51
1:C:56:TYR:CE2	1:D:172:ARG:HG2	2.46	0.51
1:D:84:LYS:HE2	2:G:15:DC:C2	2.46	0.51
1:B:277:THR:OG1	1:B:278:PRO:HD2	2.10	0.51
1:C:146:LYS:NZ	3:C:2066:HOH:O	2.44	0.51
1:C:88:LYS:HD3	2:G:22:DA:H3'	1.93	0.50
1:A:144:LYS:HE3	1:A:265:GLU:OE1	2.11	0.50
1:D:156:THR:HB	1:D:160:LYS:HE3	1.93	0.50
2:G:15:DC:H6	2:G:15:DC:O5'	1.95	0.50
1:B:187:VAL:HG22	1:B:301:LYS:HB3	1.94	0.50
2:E:2:DT:C2'	2:E:3:DG:C8	2.95	0.49
3:C:2132:HOH:O	1:D:54:MET:O	2.20	0.49
1:D:23:ILE:HG21	1:D:31:VAL:HG22	1.94	0.49
1:B:39:ASN:HA	1:B:42:HIS:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LYS:HD3	3:A:2090:HOH:O	2.13	0.49
1:D:31:VAL:HB	1:D:61:VAL:HG13	1.94	0.49
1:B:23:ILE:HG21	1:B:31:VAL:HG22	1.94	0.49
1:A:93:TRP:CZ2	1:A:98:LEU:HG	2.48	0.49
2:E:2:DT:H2"	2:E:3:DG:H5'	1.95	0.49
1:A:56:TYR:CE2	1:B:172:ARG:HG2	2.48	0.49
2:G:24:DC:H2"	2:G:25:DC:O5'	2.13	0.48
1:C:3:PRO:HA	1:C:4:LYS:C	2.33	0.48
1:B:66:THR:HG22	3:B:2017:HOH:O	2.07	0.48
1:D:40:MET:N	1:D:41:PRO:HD2	2.28	0.48
1:B:158:ARG:H	1:B:158:ARG:HD2	1.79	0.48
1:D:101:LEU:HD23	1:D:101:LEU:HA	1.67	0.47
1:B:253:ASP:HB2	1:B:283:ALA:HB2	1.97	0.47
1:A:129:VAL:HG11	1:A:150:LEU:O	2.14	0.47
2:G:3:DG:H2'	2:G:3:DG:OP2	2.15	0.47
1:C:3:PRO:CD	3:C:2001:HOH:O	2.61	0.47
2:E:6:DC:C2'	2:E:7:DG:H5'	2.33	0.47
1:C:104:LYS:HB3	1:C:104:LYS:HE3	1.65	0.47
2:G:2:DT:OP2	2:G:2:DT:H6	1.97	0.47
1:D:186:MET:HG3	1:D:188:LEU:CD1	2.45	0.46
1:C:148:ILE:HD12	1:C:246:MET:HE2	1.98	0.46
1:D:195:VAL:HB	1:D:203:PHE:CE1	2.51	0.46
1:B:252:LYS:HE3	3:B:2133:HOH:O	2.00	0.46
1:B:23:ILE:HG21	1:B:31:VAL:CG2	2.45	0.46
1:D:99:LEU:HB3	1:D:316:ALA:HB2	1.98	0.45
1:B:259:ILE:HA	1:B:278:PRO:HA	1.98	0.45
1:A:34:PHE:C	1:A:34:PHE:CD1	2.89	0.45
1:A:93:TRP:HB2	3:A:2026:HOH:O	2.16	0.45
1:D:200:LEU:O	1:D:201:GLN:C	2.54	0.45
1:B:15:ILE:HG12	1:B:236:TYR:CB	2.46	0.45
1:D:134:GLN:HB2	1:D:274:PHE:CD1	2.51	0.45
1:A:104:LYS:HE3	3:A:2067:HOH:O	2.16	0.45
1:B:207:LYS:HB2	1:B:207:LYS:HE3	1.67	0.45
2:G:15:DC:H6	2:G:15:DC:H5"	1.81	0.44
1:A:148:ILE:HD12	1:A:246:MET:HE2	1.99	0.44
1:D:153:VAL:O	1:D:157:SER:HB3	2.17	0.44
1:C:237:VAL:HG12	1:D:51:THR:HG21	1.99	0.44
1:D:178:ILE:CG2	1:D:186:MET:HB2	2.47	0.44
1:B:22:LEU:HA	1:B:22:LEU:HD23	1.74	0.44
1:B:203:PHE:HD2	1:B:208:LEU:HD12	1.83	0.44
1:B:191:ARG:HH21	1:B:298:GLU:CD	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:TRP:HZ2	1:A:98:LEU:HG	1.82	0.44
1:A:125:VAL:O	1:A:125:VAL:HG12	2.18	0.44
1:A:36:ILE:HG12	2:E:9:DT:N3	2.33	0.44
1:B:252:LYS:O	1:B:253:ASP:C	2.56	0.43
1:C:297:GLU:CD	1:C:297:GLU:N	2.71	0.43
1:A:244:ILE:HA	1:A:244:ILE:HD13	1.84	0.43
1:C:144:LYS:H	1:C:144:LYS:HG3	1.37	0.43
1:A:40:MET:C	1:A:40:MET:SD	2.97	0.43
1:A:23:ILE:HG23	1:A:28:LEU:HB2	2.01	0.43
1:B:203:PHE:CD2	1:B:208:LEU:HD12	2.53	0.43
1:C:211:ASP:O	1:C:215:GLU:HG2	2.19	0.43
1:C:156:THR:O	1:C:160:LYS:HG3	2.18	0.43
1:C:71:ALA:HA	1:C:116:ASN:HB3	2.01	0.43
1:B:188:LEU:HD12	1:B:188:LEU:N	2.34	0.43
1:B:231:LEU:O	1:B:232:HIS:HB2	2.18	0.43
1:D:116:ASN:ND2	3:D:2028:HOH:O	2.52	0.43
1:B:71:ALA:HA	1:B:116:ASN:HB3	2.00	0.43
1:B:4:LYS:HE2	1:B:4:LYS:HB2	1.68	0.42
1:A:234:SER:HB2	2:E:19:DG:OP1	2.19	0.42
1:B:153:VAL:CG1	1:B:242:ALA:HB1	2.46	0.42
1:C:217:ILE:HG13	3:C:2117:HOH:O	2.19	0.42
1:B:150:LEU:HD22	1:B:243:ILE:HD11	2.00	0.42
1:C:158:ARG:O	1:C:162:TYR:CD2	2.72	0.42
1:B:191:ARG:HD2	3:B:2095:HOH:O	2.18	0.42
1:C:249:SER:HA	1:C:254:LEU:HB2	2.00	0.42
2:G:26:DA:C2'	2:G:27:DG:H5"	2.34	0.42
1:D:257:VAL:HG22	1:D:280:VAL:HG22	2.01	0.42
1:A:19:MET:O	1:A:23:ILE:HG13	2.19	0.42
1:B:231:LEU:HD23	1:B:231:LEU:HA	1.82	0.42
1:A:132:MET:HE3	3:A:2065:HOH:O	2.20	0.42
1:A:154:LEU:HD11	1:A:158:ARG:CZ	2.50	0.41
2:G:15:DC:C6	2:G:15:DC:H5"	2.56	0.41
1:D:125:VAL:HG21	1:D:243:ILE:CD1	2.50	0.41
1:C:107:ILE:HG13	1:C:139:HIS:CD2	2.54	0.41
1:D:64:SER:HB2	1:D:69:ASP:OD2	2.21	0.41
1:B:160:LYS:HE3	1:B:175:ASN:HA	2.02	0.41
1:B:82:PHE:HB3	1:B:98:LEU:HD22	2.03	0.41
1:D:156:THR:CB	1:D:160:LYS:HE3	2.51	0.41
1:A:257:VAL:HG22	1:A:280:VAL:HG22	2.03	0.41
2:E:5:DG:H2"	2:E:6:DC:O5'	2.21	0.41
1:B:92:GLU:HB3	1:B:93:TRP:H	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:6:DC:C2'	2:E:7:DG:C5'	2.98	0.40
1:B:27:ASN:ND2	1:C:254:LEU:HD21	2.36	0.40
1:C:191:ARG:HB2	3:C:2105:HOH:O	2.22	0.40
2:G:15:DC:C6	2:G:15:DC:C5'	2.98	0.40
1:C:239:PRO:O	1:C:243:ILE:HG13	2.21	0.40
1:D:21:THR:O	1:D:25:GLN:HG2	2.21	0.40
1:D:253:ASP:HB2	1:D:283:ALA:HB2	2.03	0.40
2:G:1:DC:C3'	2:G:1:DC:P	3.09	0.40
1:B:15:ILE:O	1:B:19:MET:HG3	2.21	0.40
1:D:4:LYS:HB2	1:D:4:LYS:HE2	1.67	0.40
2:E:8:DG:H4'	2:E:10:DA:C4	2.56	0.40
1:D:238:ALA:HB3	1:D:239:PRO:HD3	2.02	0.40
2:E:27:DG:OP2	2:E:27:DG:H3'	2.22	0.40
1:A:93:TRP:HD1	3:A:2059:HOH:O	1.84	0.40
1:B:135:LEU:O	1:B:139:HIS:CD2	2.75	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	312/316 (99%)	297 (95%)	14 (4%)	1 (0%)	46	45
1	B	304/316 (96%)	285 (94%)	17 (6%)	2 (1%)	26	21
1	C	313/316 (99%)	301 (96%)	10 (3%)	2 (1%)	30	24
1	D	307/316 (97%)	286 (93%)	20 (6%)	1 (0%)	46	45
All	All	1236/1264 (98%)	1169 (95%)	61 (5%)	6 (0%)	34	30

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	151	GLY
1	A	151	GLY
1	B	26	LYS
1	D	151	GLY
1	B	151	GLY
1	C	3	PRO

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	262/263 (100%)	250 (95%)	12 (5%)	33	31
1	B	257/263 (98%)	239 (93%)	18 (7%)	19	15
1	C	261/263 (99%)	253 (97%)	8 (3%)	47	50
1	D	260/263 (99%)	249 (96%)	11 (4%)	36	35
All	All	1040/1052 (99%)	991 (95%)	49 (5%)	32	30

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	38	LYS
1	A	54	MET
1	A	56	TYR
1	A	84	LYS
1	A	93	TRP
1	A	94	ASN
1	A	115	LYS
1	A	171	PRO
1	A	234	SER
1	A	271	SER
1	A	299	LYS
1	B	4	LYS
1	B	12	SER
1	B	36	ILE
1	B	56	TYR

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Mol	Chain	Res	Type
1	B	57	SER
1	B	66	THR
1	B	92	GLU
1	B	93	TRP
1	B	104	LYS
1	B	115	LYS
1	B	129	VAL
1	B	165	GLN
1	B	168	ASN
1	B	184	ASN
1	B	200	LEU
1	B	207	LYS
1	B	234	SER
1	B	296	SER
1	C	56	TYR
1	C	66	THR
1	C	84	LYS
1	C	93	TRP
1	C	138	GLN
1	C	144	LYS
1	C	146	LYS
1	C	297	GLU
1	D	4	LYS
1	D	38	LYS
1	D	56	TYR
1	D	84	LYS
1	D	90	ASP
1	D	91	LYS
1	D	92	GLU
1	D	93	TRP
1	D	114	LYS
1	D	144	LYS
1	D	210	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	116	ASN
1	A	165	GLN
1	A	184	ASN
1	A	232	HIS

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Mol	Chain	Res	Type
1	A	284	ASN
1	B	42	HIS
1	B	116	ASN
1	B	206	ASN
1	C	116	ASN
1	D	112	HIS
1	D	165	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 carbohydrates in this entry.

5.6   Ligand geometry (i)

There are no ligands in this entry.

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(Å²)	Q<0.9
1	A	314/316 (99%)	-0.18	3 (0%) 84	87	18, 29, 43, 77	0
1	B	308/316 (97%)	-0.07	7 (2%) 64	70	17, 31, 46, 89	0
1	C	315/316 (99%)	-0.16	3 (0%) 84	87	21, 30, 47, 68	0
1	D	311/316 (98%)	0.05	11 (3%) 48	57	20, 34, 53, 98	0
2	E	27/35 (77%)	0.27	2 (7%) 17	24	33, 52, 91, 121	0
2	G	27/35 (77%)	0.27	2 (7%) 17	24	34, 49, 92, 126	0
All	All	1302/1334 (97%)	-0.08	28 (2%) 65	71	17, 31, 53, 126	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	86	PRO	4.5
1	D	92	GLU	4.0
1	D	91	LYS	3.9
1	B	316	ALA	3.8
1	D	90	ASP	3.8
1	B	93	TRP	3.7
1	A	93	TRP	3.6
1	D	85	ALA	3.6
1	B	92	GLU	3.6
1	D	93	TRP	3.1
2	G	1	DC	3.0
1	B	125	VAL	3.0
1	C	3	PRO	2.8
1	D	125	VAL	2.8
1	B	226	LEU	2.8
1	C	93	TRP	2.8
1	A	91	LYS	2.7
2	E	1	DC	2.6
1	A	316	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	3	PRO	2.4
1	B	124	VAL	2.4
2	E	27	DG	2.3
1	D	133	VAL	2.3
1	D	243	ILE	2.3
1	D	77	ILE	2.2
1	C	316	ALA	2.2
2	G	27	DG	2.2
1	D	84	LYS	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 carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.