



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:22 PM UTC

PDB ID : 3ZH2 / pdb_00003zh2
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

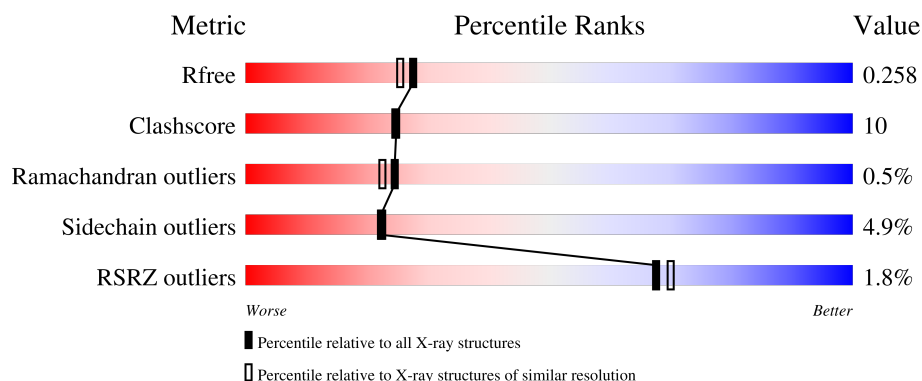
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	2% 73% 22% ..
1	B	316	2% 68% 24% ...
1	C	316	% 82% 16% .
1	D	316	2% 75% 20% ..
2	E	35	3% 23% 49% 6% 23%

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Mol	Chain	Length	Quality of chain
2	G	35	6% 34% 34% 9% 23%

2 Entry composition

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			

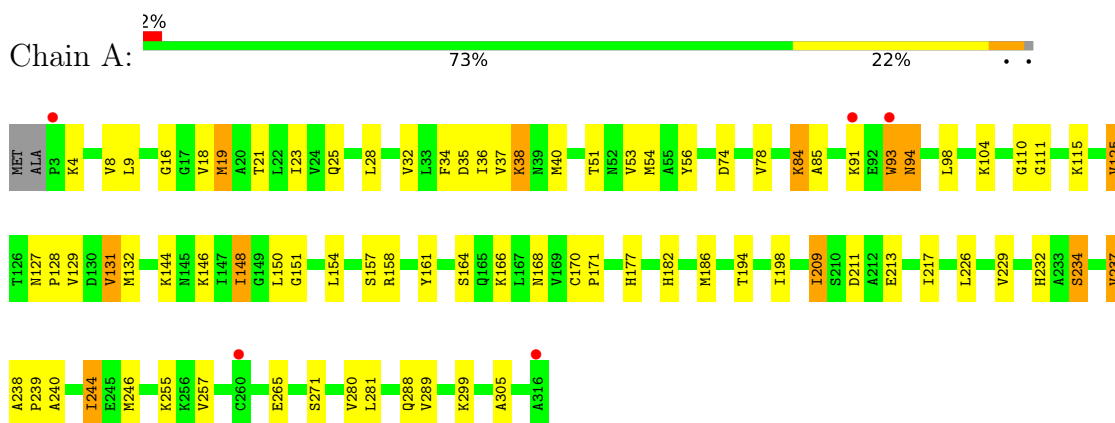
- Molecule 3 is water.

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		

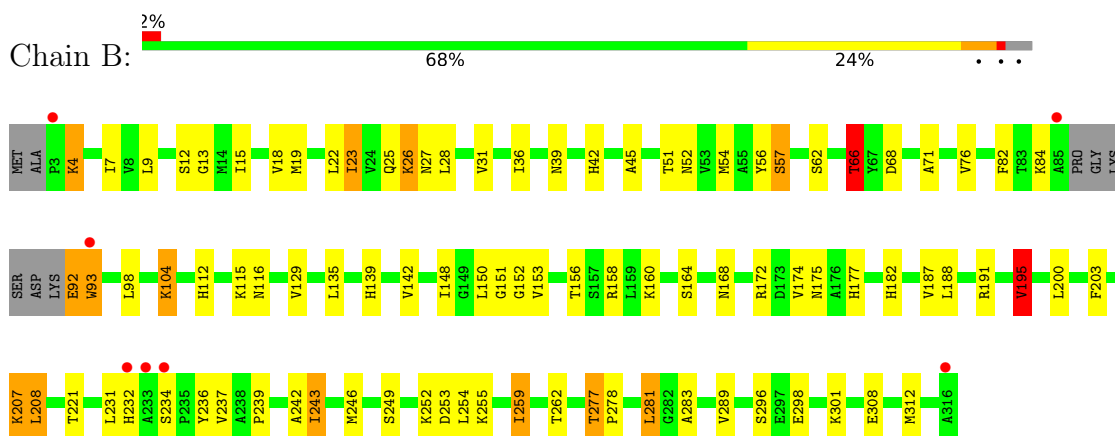
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

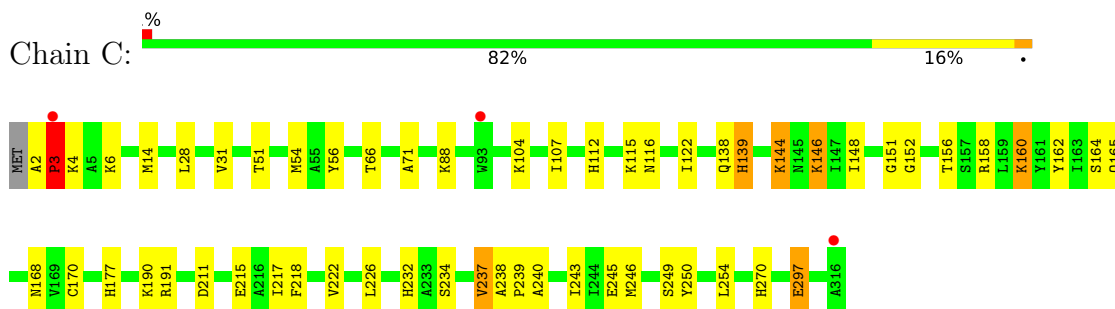
• Molecule 1: L-LACTATE DEHYDROGENASE



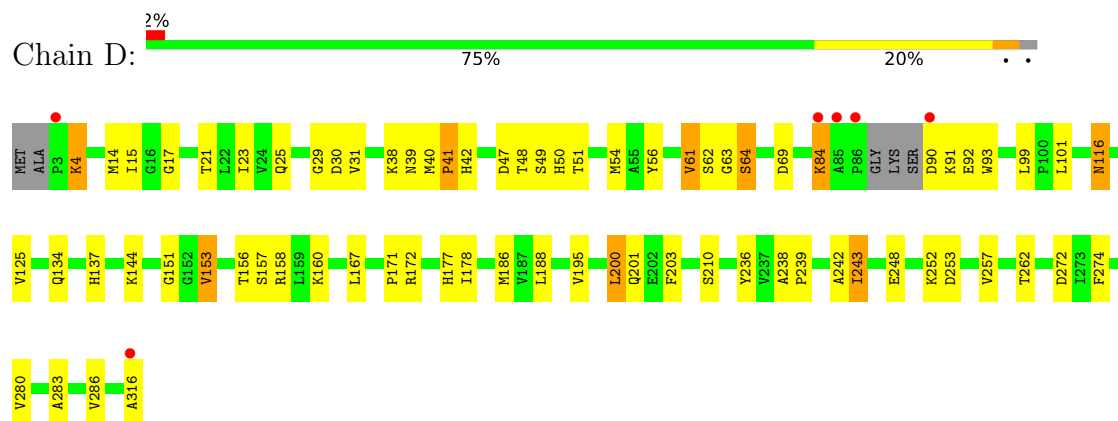
• Molecule 1: L-LACTATE DEHYDROGENASE



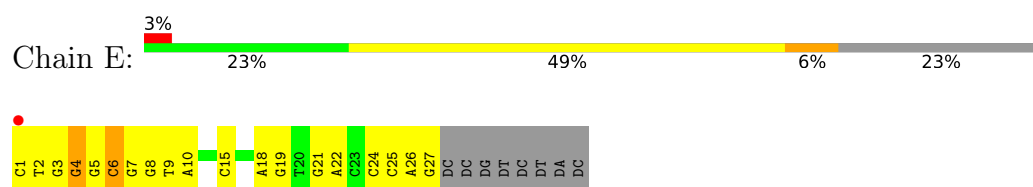
• Molecule 1: L-LACTATE DEHYDROGENASE



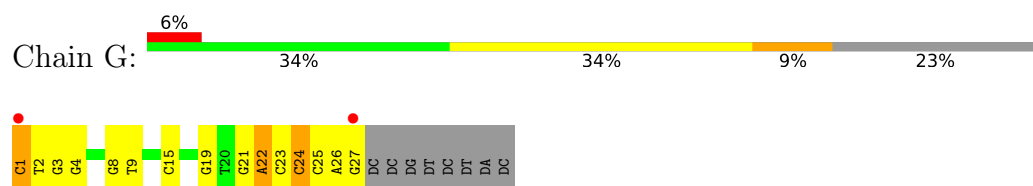
- Molecule 1: L-LACTATE DEHYDROGENASE



- Molecule 2: DNA APTAMER



- Molecule 2: DNA APTAMER



4 Data and refinement statistics

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 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-2.10) 97.4 (30.00-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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 ⓘ

5.1 Standard geometry ⓘ

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	1.49	17/2416 (0.7%)	1.48	23/3270 (0.7%)
1	B	1.42	11/2371 (0.5%)	1.42	20/3209 (0.6%)
1	C	1.33	7/2417 (0.3%)	1.34	11/3273 (0.3%)
1	D	1.31	7/2396 (0.3%)	1.33	12/3243 (0.4%)
2	E	0.41	0/628	1.15	5/966 (0.5%)
2	G	0.47	0/628	1.25	11/966 (1.1%)
All	All	1.31	42/10856 (0.4%)	1.37	82/14927 (0.5%)

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 (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	VAL	C-O	10.23	1.35	1.24
1	D	200	LEU	C-O	9.93	1.35	1.24
1	A	244	ILE	C-O	7.58	1.33	1.24
1	B	57	SER	CA-C	-7.35	1.43	1.53
1	D	158	ARG	C-O	7.09	1.32	1.24
1	C	139	HIS	CG-CD2	6.73	1.43	1.35
1	B	28	LEU	CA-C	6.54	1.61	1.52
1	B	45	ALA	C-O	6.12	1.31	1.24
1	A	8	VAL	C-O	6.00	1.30	1.24
1	B	25	GLN	C-O	-5.91	1.17	1.24
1	C	112	HIS	CG-CD2	5.84	1.42	1.35
1	A	177	HIS	ND1-CE1	5.80	1.38	1.32
1	D	41	PRO	C-O	5.80	1.31	1.24
1	A	182	HIS	CG-CD2	5.65	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	139	HIS	ND1-CE1	5.63	1.38	1.32
1	B	23	ILE	CA-CB	5.59	1.62	1.54
1	A	226	LEU	N-CA	5.53	1.53	1.46
1	D	286	VAL	C-O	5.51	1.29	1.23
1	B	18	VAL	N-CA	5.45	1.53	1.46
1	D	64	SER	N-CA	5.43	1.52	1.46
1	D	29	GLY	N-CA	5.40	1.51	1.45
1	C	165	GLN	CA-C	-5.40	1.46	1.52
1	A	131	VAL	C-O	5.32	1.29	1.24
1	B	112	HIS	CG-CD2	5.32	1.41	1.35
1	A	198	ILE	C-N	5.30	1.40	1.33
1	B	76	VAL	CA-C	-5.29	1.46	1.52
1	D	177	HIS	CA-C	-5.28	1.46	1.52
1	A	110	GLY	C-O	5.26	1.30	1.23
1	A	25	GLN	CA-C	5.21	1.59	1.52
1	A	240	ALA	N-CA	-5.21	1.40	1.46
1	B	164	SER	C-O	5.20	1.30	1.24
1	C	250	TYR	C-O	5.18	1.30	1.24
1	B	177	HIS	CG-CD2	5.18	1.41	1.35
1	C	240	ALA	CA-C	-5.18	1.46	1.52
1	A	32	VAL	CA-C	-5.17	1.46	1.52
1	A	177	HIS	CG-CD2	5.11	1.41	1.35
1	A	194	THR	CA-C	-5.10	1.46	1.52
1	A	161	TYR	N-CA	-5.08	1.40	1.46
1	A	78	VAL	N-CA	-5.08	1.40	1.46
1	A	177	HIS	CA-C	-5.06	1.46	1.52
1	B	182	HIS	CE1-NE2	5.01	1.37	1.32
1	C	177	HIS	CA-C	-5.00	1.46	1.52

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	8	DG	O3'-P-O5'	-11.15	87.27	104.00
1	B	66	THR	CB-CA-C	-9.29	91.63	109.37
2	E	22	DA	O3'-P-O5'	-9.07	90.39	104.00
1	A	127	ASN	N-CA-C	8.71	120.73	109.93
1	A	148	ILE	CA-C-N	-8.03	116.64	122.18
1	A	148	ILE	C-N-CA	-8.03	116.64	122.18
2	G	22	DA	O3'-P-O5'	-8.00	92.00	104.00
2	E	4	DG	P-O3'-C3'	7.74	131.82	120.20
1	C	115	LYS	N-CA-C	7.64	119.39	111.14
1	A	53	VAL	N-CA-C	-7.52	103.90	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	LEU	N-CA-C	-7.40	104.25	113.28
2	G	24	DC	P-O3'-C3'	7.36	131.25	120.20
2	E	15	DC	O3'-P-O5'	-7.11	93.33	104.00
1	A	21	THR	N-CA-C	7.09	119.62	111.11
1	D	242	ALA	N-CA-C	-6.84	103.61	112.23
2	G	1	DC	O3'-P-O5'	-6.80	93.81	104.00
1	B	142	VAL	CA-C-N	-6.78	113.70	120.21
1	B	142	VAL	C-N-CA	-6.78	113.70	120.21
1	B	289	VAL	N-CA-C	-6.76	97.87	107.75
1	D	63	GLY	N-CA-C	-6.64	99.90	112.51
1	A	229	VAL	N-CA-C	-6.61	103.80	111.00
1	C	164	SER	N-CA-C	-6.60	104.17	111.82
1	C	122	ILE	CB-CA-C	-6.52	100.97	110.63
1	B	152	GLY	N-CA-C	6.47	121.99	114.16
1	D	50	HIS	N-CA-C	6.45	119.12	111.71
2	G	4	DG	C2'-C3'-O3'	-6.45	101.83	111.50
1	B	243	ILE	CB-CA-C	-6.43	103.74	111.97
1	D	243	ILE	N-CA-C	-6.39	102.88	111.44
1	B	13	GLY	N-CA-C	-6.34	101.39	112.55
2	G	8	DG	P-O3'-C3'	6.29	129.63	120.20
1	C	165	GLN	N-CA-C	-6.20	104.45	111.14
1	A	125	VAL	N-CA-C	-6.17	107.85	113.71
1	C	170	CYS	CA-C-N	6.13	126.31	119.32
1	C	170	CYS	C-N-CA	6.13	126.31	119.32
1	B	259	ILE	N-CA-C	6.08	116.86	108.84
1	A	289	VAL	N-CA-C	-6.07	99.00	107.80
2	G	23	DC	P-O3'-C3'	6.07	129.30	120.20
1	A	8	VAL	N-CA-C	5.98	116.72	107.99
1	A	213	GLU	N-CA-C	-5.91	104.92	111.36
1	D	17	GLY	N-CA-C	5.91	119.79	112.64
1	D	30	ASP	N-CA-C	-5.90	102.74	110.53
1	B	7	ILE	CA-C-N	-5.88	115.44	123.14
1	B	7	ILE	C-N-CA	-5.88	115.44	123.14
2	G	9	DT	C2'-C3'-O3'	-5.84	102.73	111.50
2	E	21	DG	C2'-C3'-O3'	-5.83	102.76	111.50
1	B	195	VAL	CB-CA-C	-5.82	101.83	110.33
1	D	153	VAL	N-CA-C	-5.76	104.75	110.62
1	C	28	LEU	N-CA-C	5.75	118.49	111.82
1	A	168	ASN	CB-CA-C	-5.71	104.21	111.86
1	B	62	SER	CB-CA-C	-5.65	98.70	109.66
1	D	47	ASP	N-CA-C	-5.61	105.25	111.36
1	D	116	ASN	N-CA-C	5.61	120.24	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	281	LEU	N-CA-C	5.59	118.35	109.24
1	A	19	MET	N-CA-C	5.58	117.81	111.11
2	G	9	DT	O3'-P-O5'	5.58	112.38	104.00
1	A	164	SER	N-CA-C	-5.50	105.30	112.23
1	A	305	ALA	N-CA-C	-5.49	105.38	111.36
2	E	6	DC	P-O3'-C3'	-5.42	112.07	120.20
1	A	157	SER	N-CA-C	-5.38	105.98	112.54
1	B	277	THR	CA-C-N	-5.33	114.27	119.76
1	B	277	THR	C-N-CA	-5.33	114.27	119.76
1	A	18	VAL	N-CA-C	-5.32	104.84	112.35
1	C	237	VAL	N-CA-C	5.32	115.52	110.42
1	C	31	VAL	CB-CA-C	-5.31	102.77	110.63
1	C	160	LYS	N-CA-C	-5.30	105.58	111.36
1	A	111	GLY	N-CA-C	-5.28	106.01	112.77
1	B	54	MET	CA-C-N	-5.27	113.84	122.54
1	B	54	MET	C-N-CA	-5.27	113.84	122.54
1	A	170	CYS	CA-C-N	5.26	125.32	119.32
1	A	170	CYS	C-N-CA	5.26	125.32	119.32
1	A	186	MET	CA-C-N	-5.25	116.05	122.93
1	A	186	MET	C-N-CA	-5.25	116.05	122.93
2	G	9	DT	P-O3'-C3'	5.25	128.07	120.20
2	G	21	DG	P-O3'-C3'	5.18	127.98	120.20
1	C	270	HIS	N-CA-C	5.16	117.22	109.23
1	B	221	THR	N-CA-C	-5.12	105.77	111.36
1	D	262	THR	N-CA-C	5.10	117.17	109.41
1	A	37	VAL	N-CA-C	-5.10	102.93	109.30
1	D	167	LEU	N-CA-C	5.10	119.50	113.28
1	B	84	LYS	N-CA-C	5.06	117.98	110.14
1	D	137	HIS	N-CA-C	-5.05	105.86	111.36
1	A	211	ASP	N-CA-C	5.03	117.41	111.33

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

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	46	0
1	B	2336	0	2418	57	0
1	C	2380	0	2464	38	0
1	D	2360	0	2442	34	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	203	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 10.

All (203) 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
1:A:93:TRP:CD1	3:A:2059:HOH:O	2.30	0.83
1:A:54:MET:HE3	1:B:242:ALA:HB2	1.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:66:THR:HB	1:B:68:ASP:H	1.61	0.66
2:G:25:DC:C2'	2:G:26:DA:C8	2.79	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:C5'	2:G:15:DC:H6	2.13	0.60
1:A:93:TRP:CD1	3:A:2026:HOH:O	2.55	0.60
1:A:94:ASN:C	1:A:94:ASN:HD22	2.09	0.60
1:A:232:HIS:HE1	2:E:18:DA:N3	1.99	0.59
1:C:297:GLU:H	1:C:297:GLU:CD	2.10	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:C:232:HIS:ND1	3:C:2126:HOH:O	2.32	0.58
1:B:9:LEU:HD22	1:B:19:MET:HE3	1.86	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:C:168:ASN:CG	3:C:2092:HOH:O	2.45	0.57
1:A:84:LYS:HD2	1:A:85:ALA:O	2.05	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:MET:HE1	1:D:14:MET:HE1	1.86	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:B:148:ILE:HD12	1:B:246:MET:HE3	1.88	0.56
2:G:25:DC:H2'	2:G:26:DA:N7	2.22	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
1:A:51:THR:HG21	1:B:237:VAL:HG12	1.88	0.55
2:E:5:DG:H2'	2:E:5:DG:OP2	2.05	0.55
2:G:25:DC:H2''	2:G:26:DA:C8	2.40	0.55
1:C:218:PHE:O	1:C:222:VAL:HG23	2.07	0.54
2:G:1:DC:H2'	2:G:1:DC:P	2.47	0.54
1:A:16:GLY:HA2	1:A:19:MET:HE2	1.89	0.54
1:D:248:GLU:HG3	1:D:252:LYS:HD2	1.90	0.54
1:B:188:LEU:H	1:B:188:LEU:HD12	1.73	0.54
1:C:6:LYS:NZ	1:C:71:ALA:O	2.37	0.53
1:A:93:TRP:HZ2	1:A:98:LEU:CG	2.22	0.53
1:C:3:PRO:HA	1:C:4:LYS:C	2.33	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:HD2	1:B:158:ARG:N	2.24	0.52
1:A:38:LYS:HG2	3:A:2024:HOH:O	2.09	0.52
1:B:255:LYS:HA	1:B:281:LEU:O	2.10	0.52
1:C:238:ALA:N	1:C:239:PRO:CD	2.73	0.52
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:A:34:PHE:C	1:A:34:PHE:CD1	2.89	0.50
1:B:187:VAL:HG22	1:B:301:LYS:HB3	1.94	0.50
1:C:51:THR:HA	1:C:54:MET:HE2	1.94	0.50
1:D:200:LEU:O	1:D:201:GLN:C	2.54	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
2:E:2:DT:C2'	2:E:3:DG:C8	2.95	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:B:23:ILE:HG21	1:B:31:VAL:HG22	1.94	0.49
1:D:31:VAL:HB	1:D:61:VAL:HG13	1.94	0.49
1:A:56:TYR:CE2	1:B:172:ARG:HG2	2.48	0.49
1:A:93:TRP:CZ2	1:A:98:LEU:HG	2.48	0.49
1:B:191:ARG:HH21	1:B:298:GLU:CD	2.20	0.49
2:E:2:DT:H2''	2:E:3:DG:H5'	1.95	0.49
2:G:24:DC:H2''	2:G:25:DC:O5'	2.13	0.48
1:B:252:LYS:O	1:B:253:ASP:C	2.56	0.48
1:B:66:THR:HG22	3:B:2017:HOH:O	2.07	0.48
1:C:297:GLU:CD	1:C:297:GLU:N	2.71	0.48
1:A:40:MET:C	1:A:40:MET:SD	2.97	0.48
1:D:40:MET:N	1:D:41:PRO:HD2	2.28	0.48
1:B:158:ARG:HD2	1:B:158:ARG:H	1.79	0.48
1:D:101:LEU:HD23	1:D:101:LEU:HA	1.67	0.47
1:A:129:VAL:HG11	1:A:150:LEU:O	2.14	0.47
1:B:253:ASP:HB2	1:B:283:ALA:HB2	1.97	0.47
2:G:3:DG:OP2	2:G:3:DG:H2'	2.15	0.47
1:C:3:PRO:CD	3:C:2001:HOH:O	2.61	0.47
1:C:104:LYS:HB3	1:C:104:LYS:HE3	1.65	0.47
2:E:6:DC:C2'	2:E:7:DG:H5'	2.33	0.47
2:G:2:DT:OP2	2:G:2:DT:H6	1.97	0.47
1:A:132:MET:HE3	3:A:2065:HOH:O	2.14	0.46
1:D:186:MET:HG3	1:D:188:LEU:CD1	2.45	0.46
1:A:9:LEU:HD22	1:A:19:MET:HE3	1.96	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:93:TRP:HB2	3:A:2026:HOH:O	2.16	0.45
1:B:15:ILE:HG12	1:B:236:TYR:CB	2.46	0.45
1:A:104:LYS:HE3	3:A:2067:HOH:O	2.16	0.45
1:D:134:GLN:HB2	1:D:274:PHE:CD1	2.51	0.45
1:B:207:LYS:HE3	1:B:207:LYS:HB2	1.67	0.45
2:G:15:DC:H6	2:G:15:DC:H5''	1.81	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:B:22:LEU:HD23	1:B:22:LEU:HA	1.74	0.44
1:B:51:THR:O	1:B:52:ASN:C	2.58	0.44
1:B:203:PHE:HD2	1:B:208:LEU:HD12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:ILE:CG2	1:D:186:MET:HB2	2.47	0.44
1:A:93:TRP:HZ2	1:A:98:LEU:HG	1.82	0.44
1:A:125:VAL:HG12	1:A:125:VAL:O	2.18	0.44
1:A:36:ILE:HG12	2:E:9:DT:N3	2.33	0.44
1:A:244:ILE:HD13	1:A:244:ILE:HA	1.84	0.43
1:A:23:ILE:HG23	1:A:28:LEU:HB2	2.01	0.43
1:C:2:ALA:CA	1:C:3:PRO:C	2.91	0.43
1:C:144:LYS:H	1:C:144:LYS:HG3	1.37	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:A:148:ILE:HD12	1:A:246:MET:HE3	2.01	0.43
1:C:71:ALA:HA	1:C:116:ASN:HB3	2.01	0.43
1:C:156:THR:O	1:C:160:LYS:HG3	2.18	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:A:234:SER:HB2	2:E:19:DG:OP1	2.19	0.42
1:B:4:LYS:HE2	1:B:4:LYS:HB2	1.68	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:B:191:ARG:HD2	3:B:2095:HOH:O	2.18	0.42
1:C:158:ARG:O	1:C:162:TYR:CD2	2.72	0.42
1:C:249:SER:HA	1:C:254:LEU:HB2	2.00	0.42
1:D:257:VAL:HG22	1:D:280:VAL:HG22	2.01	0.42
2:G:26:DA:C2'	2:G:27:DG:H5''	2.34	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:B:308:GLU:HG3	1:B:312:MET:HE2	2.01	0.42
1:A:154:LEU:HD11	1:A:158:ARG:CZ	2.50	0.41
1:D:125:VAL:HG21	1:D:243:ILE:CD1	2.50	0.41
2:G:15:DC:H5''	2:G:15:DC:C6	2.56	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:82:PHE:HB3	1:B:98:LEU:HD22	2.03	0.41
1:B:160:LYS:HE3	1:B:175:ASN:HA	2.02	0.41
1:A:257:VAL:HG22	1:A:280:VAL:HG22	2.03	0.41
1:B:26:LYS:O	1:B:27:ASN:C	2.61	0.41
1:C:148:ILE:HD12	1:C:246:MET:HE3	2.01	0.41
1:D:156:THR:CB	1:D:160:LYS:HE3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:2:ALA:HA	1:C:3:PRO:C	2.46	0.41
1:B:27:ASN:ND2	1:C:254:LEU:HD21	2.36	0.40
1:B:239:PRO:C	1:B:243:ILE:HD12	2.44	0.40
1:C:191:ARG:HB2	3:C:2105:HOH:O	2.22	0.40
2:E:6:DC:C2'	2:E:7:DG: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:48:THR:O	1:D:49:SER:C	2.63	0.40
1:D:253:ASP:HB2	1:D:283:ALA:HB2	2.03	0.40
2:G:15:DC:C5'	2:G:15:DC:C6	2.98	0.40
1:B:15:ILE:O	1:B:19:MET:HG3	2.21	0.40
1:D:4:LYS:HE2	1:D:4:LYS:HB2	1.67	0.40
2:G:1:DC:P	2:G:1:DC:C3'	3.09	0.40
1:D:238:ALA:HB3	1:D:239:PRO:HD3	2.02	0.40
2:E:8:DG:H4'	2:E:10:DA:C4	2.56	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%)	36	36
1	B	304/316 (96%)	285 (94%)	17 (6%)	2 (1%)	18	15
1	C	313/316 (99%)	301 (96%)	10 (3%)	2 (1%)	21	18
1	D	307/316 (97%)	286 (93%)	20 (6%)	1 (0%)	36	36
All	All	1236/1264 (98%)	1169 (95%)	61 (5%)	6 (0%)	24	22

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 ⓘ

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%)	248 (95%)	14 (5%)	20	19
1	B	257/263 (98%)	239 (93%)	18 (7%)	14	11
1	C	261/263 (99%)	255 (98%)	6 (2%)	44	51
1	D	260/263 (99%)	247 (95%)	13 (5%)	22	22
All	All	1040/1052 (99%)	989 (95%)	51 (5%)	22	22

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	38	LYS
1	A	84	LYS
1	A	91	LYS
1	A	93	TRP
1	A	94	ASN
1	A	115	LYS
1	A	171	PRO
1	A	209	ILE
1	A	217	ILE
1	A	234	SER
1	A	271	SER
1	A	281	LEU
1	A	299	LYS

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Mol	Chain	Res	Type
1	B	4	LYS
1	B	12	SER
1	B	36	ILE
1	B	56	TYR
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	168	ASN
1	B	195	VAL
1	B	200	LEU
1	B	207	LYS
1	B	234	SER
1	B	262	THR
1	B	296	SER
1	C	66	THR
1	C	138	GLN
1	C	144	LYS
1	C	146	LYS
1	C	226	LEU
1	C	297	GLU
1	D	4	LYS
1	D	38	LYS
1	D	56	TYR
1	D	61	VAL
1	D	62	SER
1	D	84	LYS
1	D	90	ASP
1	D	91	LYS
1	D	92	GLU
1	D	93	TRP
1	D	144	LYS
1	D	171	PRO
1	D	210	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN

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Mol	Chain	Res	Type
1	A	116	ASN
1	A	184	ASN
1	A	201	GLN
1	A	205	ASN
1	A	223	ASN
1	A	232	HIS
1	A	284	ASN
1	B	42	HIS
1	B	116	ASN
1	B	206	ASN
1	B	223	ASN
1	B	293	GLN
1	C	103	ASN
1	C	112	HIS
1	C	165	GLN
1	C	175	ASN
1	C	223	ASN
1	C	293	GLN
1	D	116	ASN
1	D	137	HIS
1	D	201	GLN
1	D	205	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	314/316 (99%)	-0.03	5 (1%) 70 73	18, 29, 43, 77	0
1	B	308/316 (97%)	0.05	7 (2%) 61 64	17, 31, 46, 89	0
1	C	315/316 (99%)	-0.01	3 (0%) 79 81	21, 30, 47, 68	0
1	D	311/316 (98%)	0.12	6 (1%) 66 69	20, 34, 53, 98	0
2	E	27/35 (77%)	0.31	1 (3%) 45 47	33, 52, 91, 121	0
2	G	27/35 (77%)	0.29	2 (7%) 20 22	34, 49, 92, 126	0
All	All	1302/1334 (97%)	0.04	24 (1%) 67 70	17, 31, 53, 126	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	86	PRO	5.9
1	A	93	TRP	4.3
1	D	85	ALA	4.3
1	B	316	ALA	3.8
1	C	93	TRP	3.8
1	B	85	ALA	3.7
1	B	3	PRO	3.6
1	C	3	PRO	3.6
1	D	3	PRO	3.6
1	A	91	LYS	3.3
1	A	3	PRO	3.2
1	D	84	LYS	3.2
2	G	1	DC	3.0
2	E	1	DC	2.9
1	D	316	ALA	2.9
1	B	93	TRP	2.6
1	A	260	CYS	2.5
1	C	316	ALA	2.4
1	D	90	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	G	27	DG	2.3
1	A	316	ALA	2.3
1	B	233	ALA	2.2
1	B	232	HIS	2.1
1	B	234	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 oligosaccharides 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.