wwPDB X-ray Structure Validation Summary Report (i)

Apr 29, 2024 – 04:59 am BST

PDB ID	:	4D1Q
Title	:	Hermes transposase bound to its terminal inverted repeat
Authors	:	Hickman, A.B.; Ewis, H.; Li, X.; Knapp, J.; Laver, T.; Doss, A.L.; Tolun, G.; Steven, A.; Grishaev, A.; Bax, A.; Atkinson, P.; Craig, N.L.; Dyda, F.
Deposited on	:	2014-05-04
Resolution	:	3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i)) were used in the production of this report:

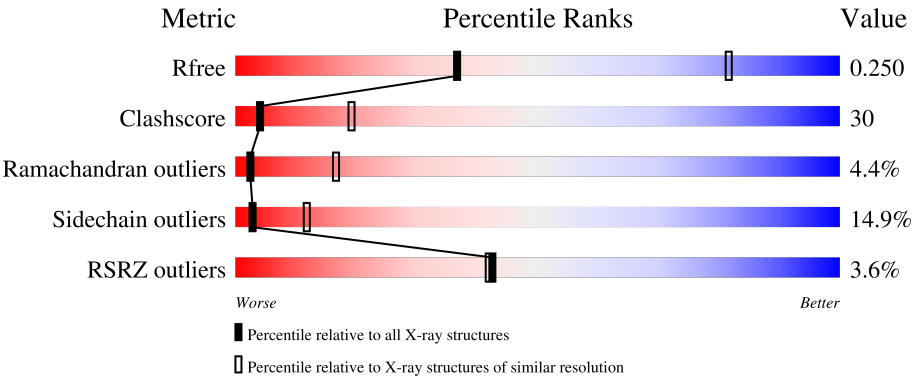
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.40 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	536	2% 38% 44% 11% • 6%
1	B	536	2% 45% 39% 10% • 6%
1	G	536	4% 42% 43% 7% • 7%
1	H	536	3% 45% 42% 8% • 5%
2	C	15	7% 20% 60% 13% 7%

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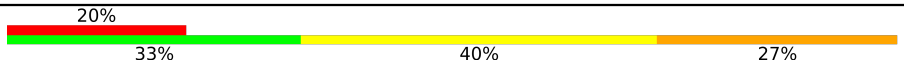
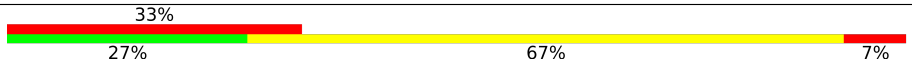
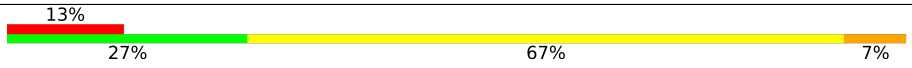
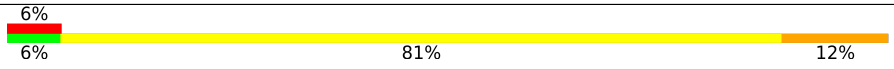
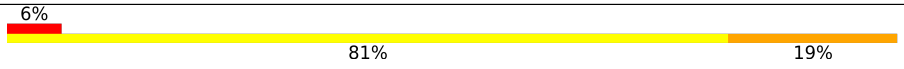
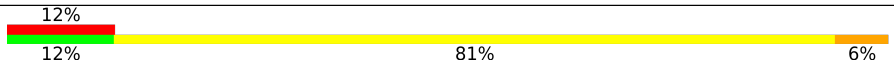
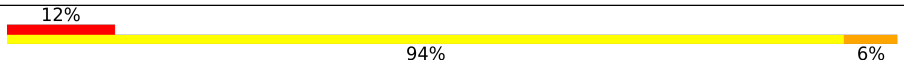
Mol	Chain	Length	Quality of chain
2	E	15	
2	I	15	
2	K	15	
3	D	16	
3	F	16	
3	J	16	
3	L	16	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18737 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 TRANSPOSASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	502	Total	C	N	O	S	0	0	0
			4041	2584	684	754	19			
1	B	505	Total	C	N	O	S	0	0	0
			4066	2599	689	758	20			
1	G	499	Total	C	N	O	S	0	0	0
			4013	2569	677	748	19			
1	H	509	Total	C	N	O	S	0	0	0
			4089	2613	691	765	20			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	HIS	-	expression tag	UNP Q25442
A	78	MET	-	expression tag	UNP Q25442
A	163	GLY	SER	conflict	UNP Q25442
A	233	SER	LEU	engineered mutation	UNP Q25442
A	286	MET	VAL	engineered mutation	UNP Q25442
B	77	HIS	-	expression tag	UNP Q25442
B	78	MET	-	expression tag	UNP Q25442
B	163	GLY	SER	conflict	UNP Q25442
B	233	SER	LEU	engineered mutation	UNP Q25442
B	286	MET	VAL	engineered mutation	UNP Q25442
B	519	CYS	CYS	conflict	UNP Q25442
G	77	HIS	-	expression tag	UNP Q25442
G	78	MET	-	expression tag	UNP Q25442
G	163	GLY	SER	conflict	UNP Q25442
G	233	SER	LEU	engineered mutation	UNP Q25442
G	286	MET	VAL	engineered mutation	UNP Q25442
H	77	HIS	-	expression tag	UNP Q25442
H	78	MET	-	expression tag	UNP Q25442
H	163	GLY	SER	conflict	UNP Q25442
H	233	SER	LEU	engineered mutation	UNP Q25442
H	286	MET	VAL	engineered mutation	UNP Q25442

- Molecule 2 is a DNA chain called TERMINAL INVERTED REPEAT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	P	0	0	0
			308	147	69	78	14			
2	E	15	Total	C	N	O	P	0	0	0
			308	147	69	78	14			
2	I	15	Total	C	N	O	P	0	0	0
			308	147	69	78	14			
2	K	15	Total	C	N	O	P	0	0	0
			308	147	69	78	14			

- Molecule 3 is a DNA chain called TERMINAL INVERTED REPEAT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	16	Total	C	N	O	P	0	0	0
			323	158	46	104	15			
3	F	16	Total	C	N	O	P	0	0	0
			323	158	46	104	15			
3	J	16	Total	C	N	O	P	0	0	0
			323	158	46	104	15			
3	L	16	Total	C	N	O	P	0	0	0
			323	158	46	104	15			

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

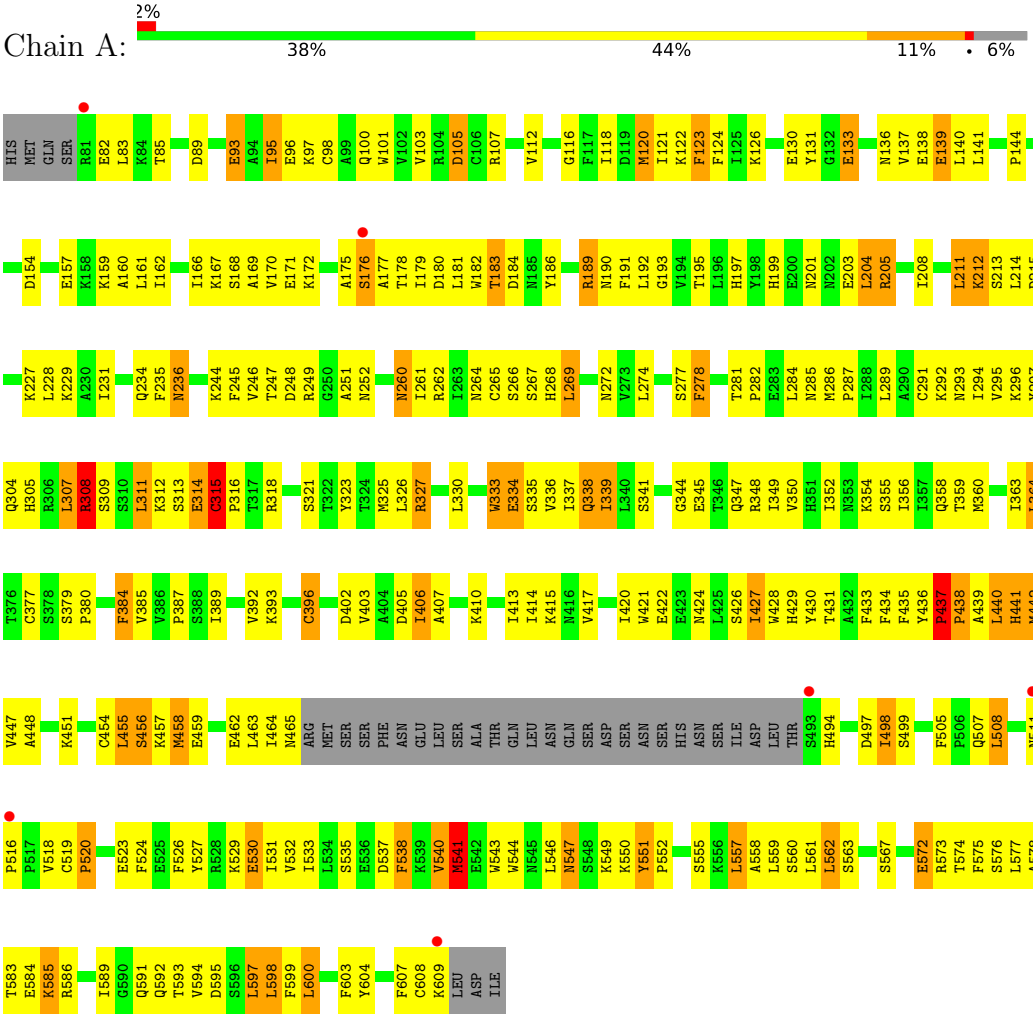
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		
4	G	1	Total	Na	0	0
			1	1		
4	H	1	Total	Na	0	0
			1	1		

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.

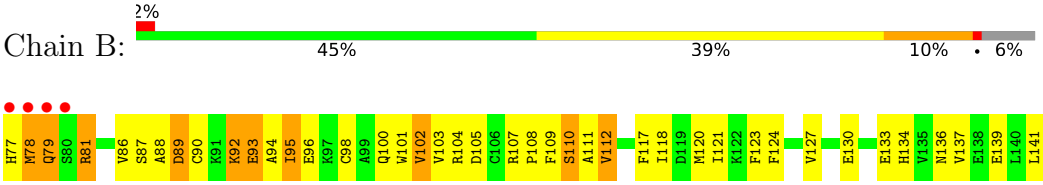
• Molecule 1: TRANSPOSASE

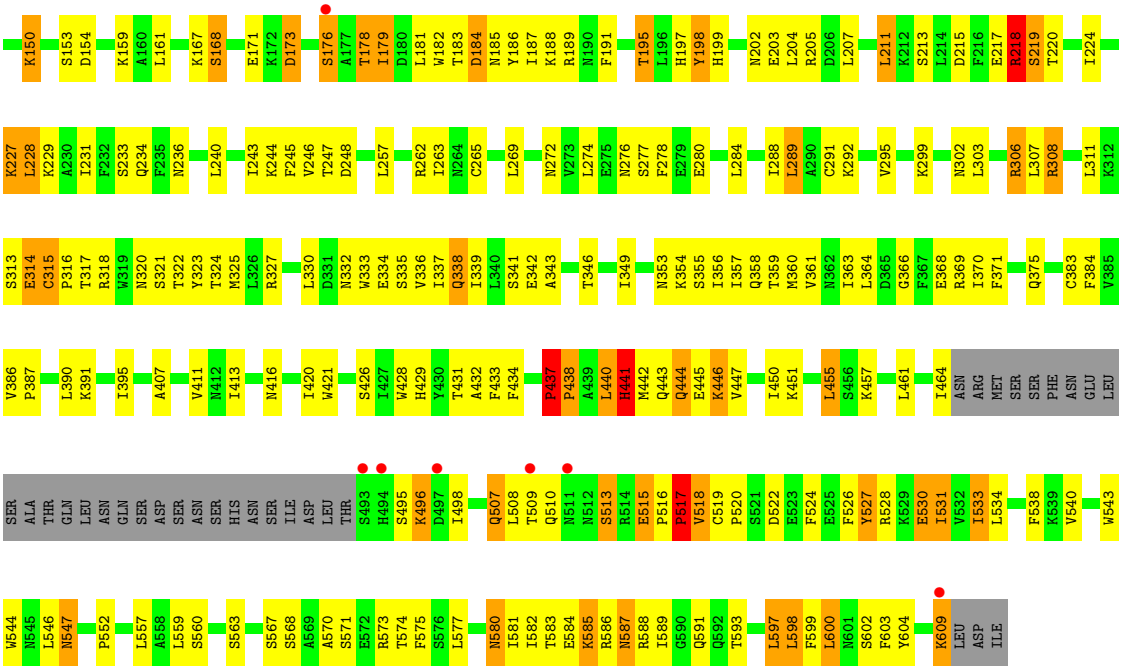
Chain A:



• Molecule 1: TRANSPOSASE

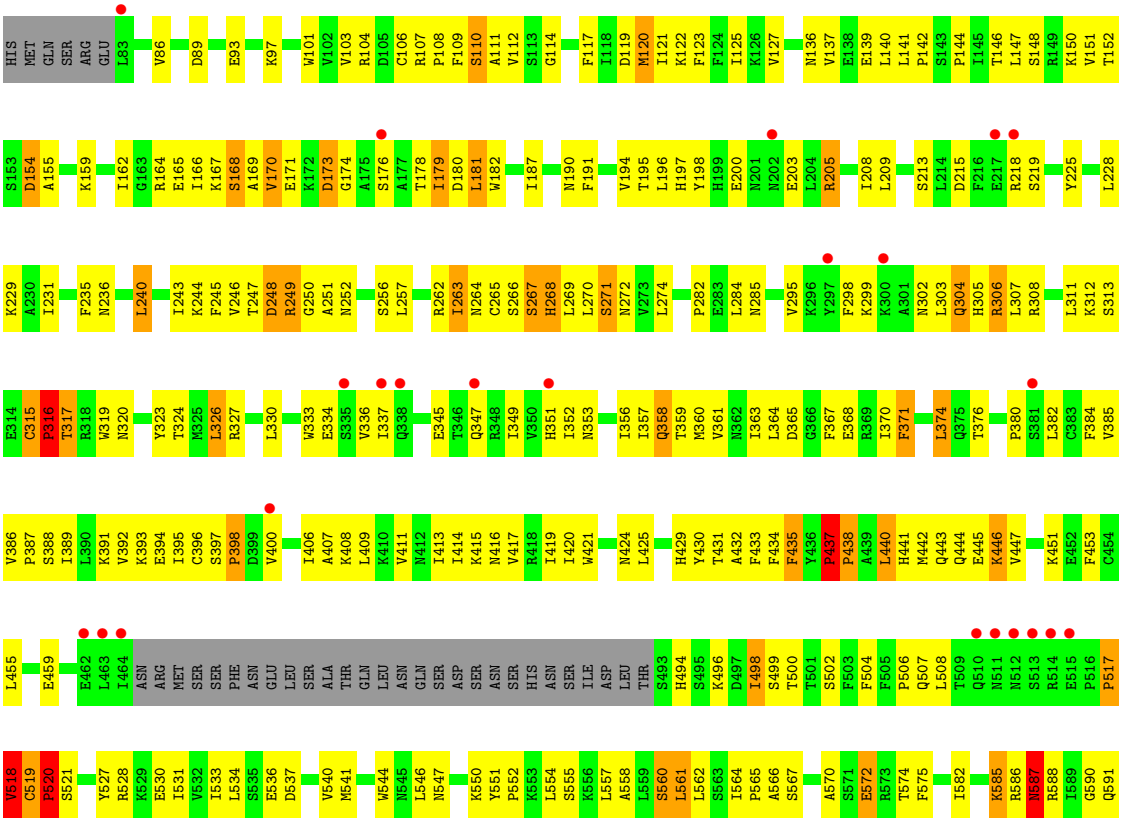
Chain B:

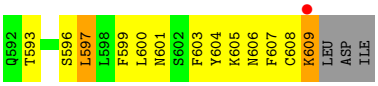




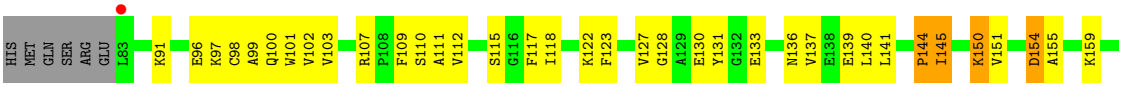
• Molecule 1: TRANSPOSASE

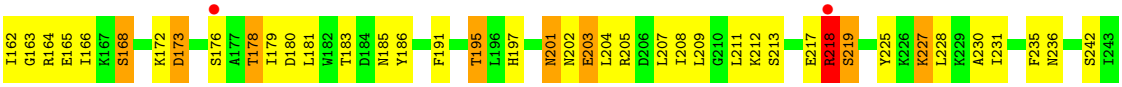
Chain G:

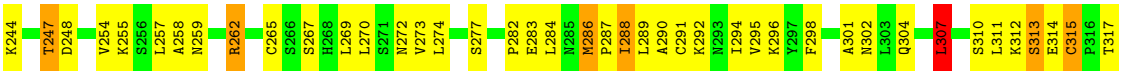


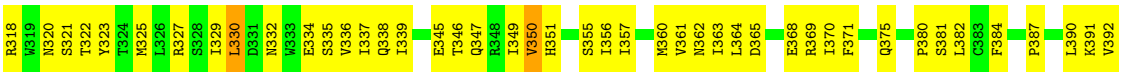


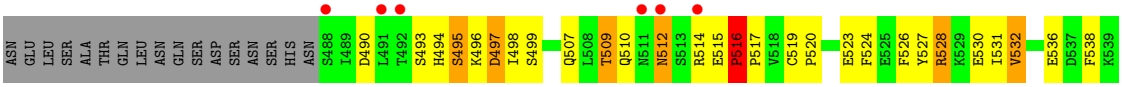
• Molecule 1: TRANSPOSASE

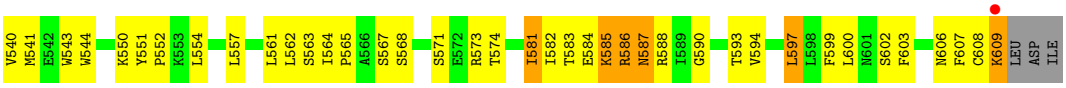




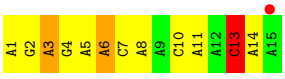




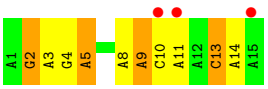




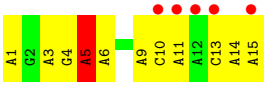
• Molecule 2: TERMINAL INVERTED REPEAT



• Molecule 2: TERMINAL INVERTED REPEAT



• Molecule 2: TERMINAL INVERTED REPEAT

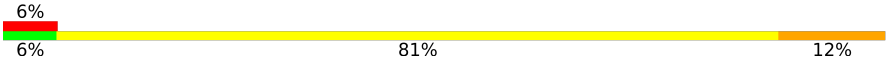


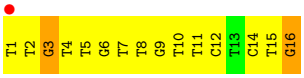
• Molecule 2: TERMINAL INVERTED REPEAT

Chain K:

• Molecule 3: TERMINAL INVERTED REPEAT

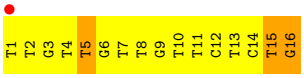
Chain D:





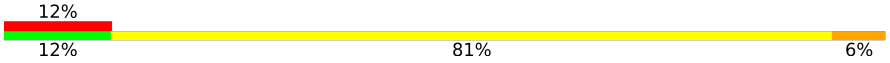
• Molecule 3: TERMINAL INVERTED REPEAT

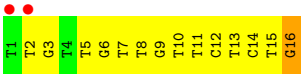
Chain F:



• Molecule 3: TERMINAL INVERTED REPEAT

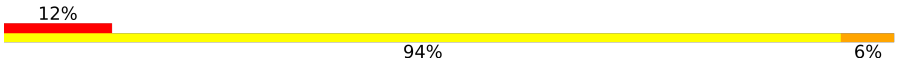
Chain J:

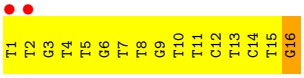




• Molecule 3: TERMINAL INVERTED REPEAT

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	265.15Å 265.15Å 157.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.40 29.86 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-3.40) 98.9 (29.86-3.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 3.31Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.212 , 0.254 0.212 , 0.250	Depositor DCC
R_{free} test set	947 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	88.4	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 93.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18737	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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

5.1 Standard geometry

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

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	1.02	11/4120 (0.3%)	1.08	10/5561 (0.2%)
1	B	0.83	2/4146 (0.0%)	0.95	4/5595 (0.1%)
1	G	0.70	1/4092 (0.0%)	0.87	3/5524 (0.1%)
1	H	0.76	2/4168 (0.0%)	0.91	6/5626 (0.1%)
2	C	1.30	3/349 (0.9%)	1.08	2/536 (0.4%)
2	E	1.07	0/349	1.06	3/536 (0.6%)
2	I	0.68	0/349	0.86	1/536 (0.2%)
2	K	0.74	0/349	0.91	1/536 (0.2%)
3	D	1.35	2/358 (0.6%)	1.05	1/552 (0.2%)
3	F	1.04	0/358	1.08	2/552 (0.4%)
3	J	0.77	0/358	0.84	0/552
3	L	0.82	0/358	0.91	0/552
All	All	0.86	21/19354 (0.1%)	0.96	33/26658 (0.1%)

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	2
1	B	0	2
1	G	0	2
1	H	0	3
2	C	0	3
2	E	0	2
2	I	0	1
2	K	0	1
3	D	0	1
3	F	0	1
3	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	1
All	All	0	20

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	438	PRO	CA-C	8.22	1.69	1.52
1	B	78	MET	CG-SD	8.14	2.02	1.81
1	A	439	ALA	CA-CB	7.91	1.69	1.52
1	H	438	PRO	CA-C	7.14	1.67	1.52
1	B	438	PRO	CA-C	7.04	1.67	1.52

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	5	DA	C1'-O4'-C4'	-7.75	102.35	110.10
3	D	16	DG	C1'-O4'-C4'	-7.12	102.98	110.10
1	B	441	HIS	N-CA-C	6.82	129.41	111.00
3	F	15	DT	C5'-C4'-O4'	-6.77	96.44	109.30
1	A	318	ARG	NE-CZ-NH1	-6.74	116.93	120.30

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	TYR	Sidechain
1	A	437	PRO	Mainchain
1	B	186	TYR	Sidechain
1	B	527	TYR	Sidechain
2	C	3	DA	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	4041	0	4097	277	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4066	0	4120	237	0
1	G	4013	0	4072	234	0
1	H	4089	0	4148	225	0
2	C	308	0	165	12	0
2	E	308	0	167	18	0
2	I	308	0	167	21	0
2	K	308	0	167	16	0
3	D	323	0	186	30	0
3	F	323	0	188	35	0
3	J	323	0	188	38	0
3	L	323	0	188	45	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
All	All	18737	0	17853	1096	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 30.

The worst 5 of 1096 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:78:MET:SD	1:B:78:MET:CG	2.02	1.45
1:A:541:MET:CE	1:A:541:MET:SD	2.07	1.42
1:A:438:PRO:CG	1:A:438:PRO:CB	1.75	1.41
3:D:2:DT:H2"	3:D:3:DG:H5"	1.29	1.14
3:J:2:DT:H2"	3:J:3:DG:H5"	1.15	1.13

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	498/536 (93%)	400 (80%)	80 (16%)	18 (4%)	3 21
1	B	501/536 (94%)	399 (80%)	83 (17%)	19 (4%)	3 19
1	G	495/536 (92%)	412 (83%)	61 (12%)	22 (4%)	2 16
1	H	505/536 (94%)	401 (79%)	75 (15%)	29 (6%)	1 12
All	All	1999/2144 (93%)	1612 (81%)	299 (15%)	88 (4%)	2 16

5 of 88 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	ARG
1	A	219	SER
1	A	444	GLN
1	A	445	GLU
1	A	494	HIS

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	461/494 (93%)	375 (81%)	86 (19%)	1 5
1	B	464/494 (94%)	395 (85%)	69 (15%)	3 12
1	G	458/494 (93%)	393 (86%)	65 (14%)	3 13
1	H	468/494 (95%)	412 (88%)	56 (12%)	5 19
All	All	1851/1976 (94%)	1575 (85%)	276 (15%)	3 12

5 of 276 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	203	GLU
1	H	288	ILE
1	H	490	ASP
1	B	154	ASP
1	B	146	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	272	ASN
1	G	429	HIS
1	G	304	GLN
1	G	362	ASN
1	G	547	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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

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, 95^{th} 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	502/536 (93%)	-0.35	10 (1%)	65	64	16, 68, 129, 200	0
1	B	505/536 (94%)	-0.33	11 (2%)	62	60	45, 83, 137, 200	0
1	G	499/536 (93%)	-0.04	24 (4%)	30	31	63, 116, 168, 200	0
1	H	509/536 (94%)	-0.23	16 (3%)	49	48	48, 102, 159, 200	0
2	C	15/15 (100%)	0.30	1 (6%)	17	19	61, 82, 164, 170	0
2	E	15/15 (100%)	0.81	3 (20%)	1	1	66, 91, 159, 177	0
2	I	15/15 (100%)	1.04	5 (33%)	0	0	103, 127, 188, 191	0
2	K	15/15 (100%)	0.81	2 (13%)	3	4	82, 118, 185, 195	0
3	D	16/16 (100%)	0.15	1 (6%)	20	21	62, 94, 149, 162	0
3	F	16/16 (100%)	0.10	1 (6%)	20	21	64, 104, 162, 164	0
3	J	16/16 (100%)	0.99	2 (12%)	3	4	109, 141, 184, 190	0
3	L	16/16 (100%)	0.54	2 (12%)	3	4	84, 140, 178, 183	0
All	All	2139/2268 (94%)	-0.19	78 (3%)	42	42	16, 95, 161, 200	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	77	HIS	7.4
1	A	513	SER	7.1
1	A	515	GLU	7.0
1	A	512	ASN	6.3
1	B	493	SER	6.0

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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	G	1610	1/1	0.80	0.19	77,77,77,77	0
4	NA	A	1610	1/1	0.87	0.14	44,44,44,44	0
4	NA	B	1610	1/1	0.88	0.24	57,57,57,57	0
4	NA	H	1610	1/1	0.98	0.16	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.