wwPDB X-ray Structure Validation Summary Report (i)

Sep 14, 2026 – 05:15 PM EDT

PDB ID	:	6U6X / pdb_00006u6x
Title	:	Human SAMHD1 bound to deoxyribo(C*G*C*C*T)-oligonucleotide
Authors	:	Taylor, A.B.; Bhattacharya, A.; Wang, Z.; Ivanov, D.N.
Deposited on	:	2019-08-30
Resolution	:	2.58 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 (1)) were used in the production of this report:

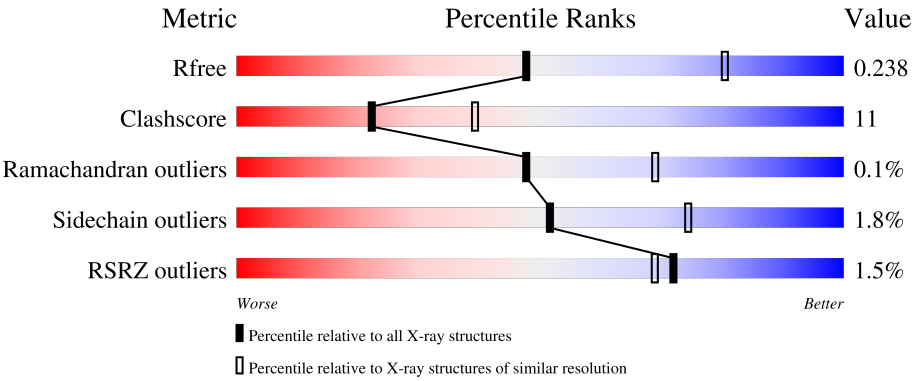
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.58 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	533	65% 14% 20%
1	B	533	2% 48% 22% 28%
1	C	533	50% 19% 29%
1	D	533	68% 13% 19%
2	E	5	40% 40% 20%

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Mol	Chain	Length	Quality of chain
2	F	5	20% 60% 20%
2	G	5	20% 60% 20%
2	H	5	60% 20% 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13531 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 Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	1	0
			3497	2243	605	630	19			
1	B	383	Total	C	N	O	S	0	0	0
			3139	2019	547	556	17			
1	C	376	Total	C	N	O	S	0	0	0
			3075	1973	532	554	16			
1	D	430	Total	C	N	O	S	0	1	0
			3531	2265	613	634	19			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	MET	-	initiating methionine	UNP Q9Y3Z3
A	95	TRP	-	expression tag	UNP Q9Y3Z3
A	96	SER	-	expression tag	UNP Q9Y3Z3
A	97	HIS	-	expression tag	UNP Q9Y3Z3
A	98	PRO	-	expression tag	UNP Q9Y3Z3
A	99	GLN	-	expression tag	UNP Q9Y3Z3
A	100	PHE	-	expression tag	UNP Q9Y3Z3
A	101	GLU	-	expression tag	UNP Q9Y3Z3
A	102	LYS	-	expression tag	UNP Q9Y3Z3
A	103	GLY	-	expression tag	UNP Q9Y3Z3
A	104	SER	-	expression tag	UNP Q9Y3Z3
A	105	GLY	-	expression tag	UNP Q9Y3Z3
A	106	SER	-	expression tag	UNP Q9Y3Z3
A	107	GLU	-	expression tag	UNP Q9Y3Z3
A	108	ASN	-	expression tag	UNP Q9Y3Z3
A	109	LEU	-	expression tag	UNP Q9Y3Z3
A	110	TYR	-	expression tag	UNP Q9Y3Z3
A	111	PHE	-	expression tag	UNP Q9Y3Z3
A	112	GLN	-	expression tag	UNP Q9Y3Z3
A	113	GLY	-	expression tag	UNP Q9Y3Z3
A	311	ALA	ASP	engineered mutation	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	94	MET	-	initiating methionine	UNP Q9Y3Z3
B	95	TRP	-	expression tag	UNP Q9Y3Z3
B	96	SER	-	expression tag	UNP Q9Y3Z3
B	97	HIS	-	expression tag	UNP Q9Y3Z3
B	98	PRO	-	expression tag	UNP Q9Y3Z3
B	99	GLN	-	expression tag	UNP Q9Y3Z3
B	100	PHE	-	expression tag	UNP Q9Y3Z3
B	101	GLU	-	expression tag	UNP Q9Y3Z3
B	102	LYS	-	expression tag	UNP Q9Y3Z3
B	103	GLY	-	expression tag	UNP Q9Y3Z3
B	104	SER	-	expression tag	UNP Q9Y3Z3
B	105	GLY	-	expression tag	UNP Q9Y3Z3
B	106	SER	-	expression tag	UNP Q9Y3Z3
B	107	GLU	-	expression tag	UNP Q9Y3Z3
B	108	ASN	-	expression tag	UNP Q9Y3Z3
B	109	LEU	-	expression tag	UNP Q9Y3Z3
B	110	TYR	-	expression tag	UNP Q9Y3Z3
B	111	PHE	-	expression tag	UNP Q9Y3Z3
B	112	GLN	-	expression tag	UNP Q9Y3Z3
B	113	GLY	-	expression tag	UNP Q9Y3Z3
B	311	ALA	ASP	engineered mutation	UNP Q9Y3Z3
C	94	MET	-	initiating methionine	UNP Q9Y3Z3
C	95	TRP	-	expression tag	UNP Q9Y3Z3
C	96	SER	-	expression tag	UNP Q9Y3Z3
C	97	HIS	-	expression tag	UNP Q9Y3Z3
C	98	PRO	-	expression tag	UNP Q9Y3Z3
C	99	GLN	-	expression tag	UNP Q9Y3Z3
C	100	PHE	-	expression tag	UNP Q9Y3Z3
C	101	GLU	-	expression tag	UNP Q9Y3Z3
C	102	LYS	-	expression tag	UNP Q9Y3Z3
C	103	GLY	-	expression tag	UNP Q9Y3Z3
C	104	SER	-	expression tag	UNP Q9Y3Z3
C	105	GLY	-	expression tag	UNP Q9Y3Z3
C	106	SER	-	expression tag	UNP Q9Y3Z3
C	107	GLU	-	expression tag	UNP Q9Y3Z3
C	108	ASN	-	expression tag	UNP Q9Y3Z3
C	109	LEU	-	expression tag	UNP Q9Y3Z3
C	110	TYR	-	expression tag	UNP Q9Y3Z3
C	111	PHE	-	expression tag	UNP Q9Y3Z3
C	112	GLN	-	expression tag	UNP Q9Y3Z3
C	113	GLY	-	expression tag	UNP Q9Y3Z3
C	311	ALA	ASP	engineered mutation	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	94	MET	-	initiating methionine	UNP Q9Y3Z3
D	95	TRP	-	expression tag	UNP Q9Y3Z3
D	96	SER	-	expression tag	UNP Q9Y3Z3
D	97	HIS	-	expression tag	UNP Q9Y3Z3
D	98	PRO	-	expression tag	UNP Q9Y3Z3
D	99	GLN	-	expression tag	UNP Q9Y3Z3
D	100	PHE	-	expression tag	UNP Q9Y3Z3
D	101	GLU	-	expression tag	UNP Q9Y3Z3
D	102	LYS	-	expression tag	UNP Q9Y3Z3
D	103	GLY	-	expression tag	UNP Q9Y3Z3
D	104	SER	-	expression tag	UNP Q9Y3Z3
D	105	GLY	-	expression tag	UNP Q9Y3Z3
D	106	SER	-	expression tag	UNP Q9Y3Z3
D	107	GLU	-	expression tag	UNP Q9Y3Z3
D	108	ASN	-	expression tag	UNP Q9Y3Z3
D	109	LEU	-	expression tag	UNP Q9Y3Z3
D	110	TYR	-	expression tag	UNP Q9Y3Z3
D	111	PHE	-	expression tag	UNP Q9Y3Z3
D	112	GLN	-	expression tag	UNP Q9Y3Z3
D	113	GLY	-	expression tag	UNP Q9Y3Z3
D	311	ALA	ASP	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is a DNA chain called DNA SC-GS-SC-SC-DT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	P	S	0	0	0
			76	37	14	19	3	3			
2	G	4	Total	C	N	O	P	S	0	0	0
			53	24	8	15	3	3			
2	F	4	Total	C	N	O	P	S	0	0	0
			68	33	11	18	3	3			
2	H	4	Total	C	N	O	P	S	0	0	0
			76	37	14	19	3	3			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Zn 1 1	0	0

- Molecule 4 is water.

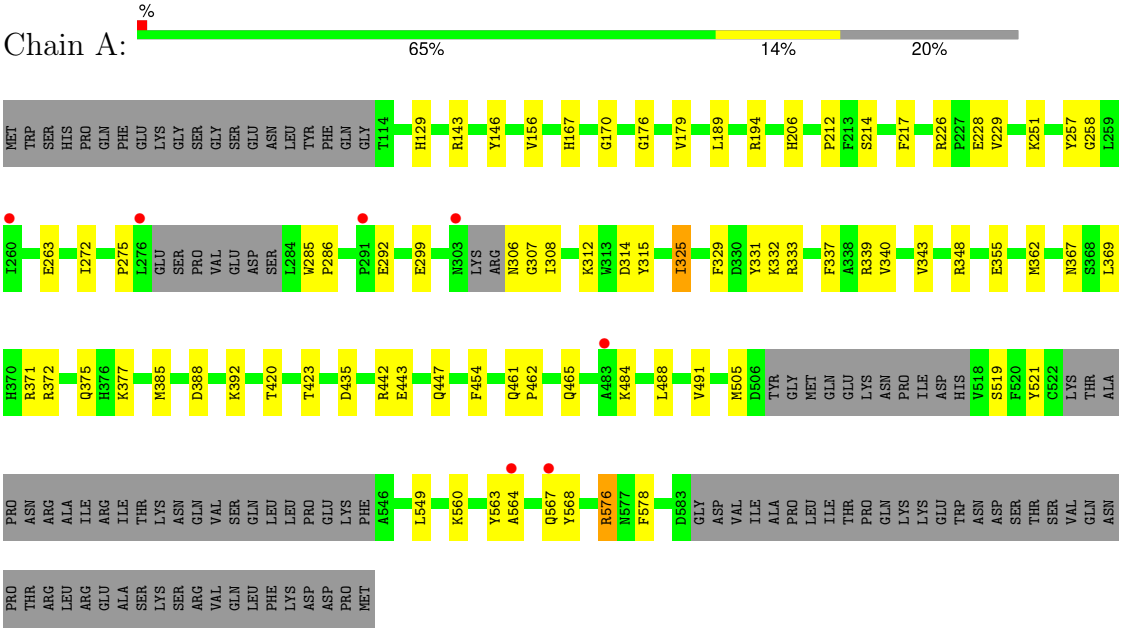
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total O 4 4	0	0
4	D	8	Total O 8 8	0	0

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.

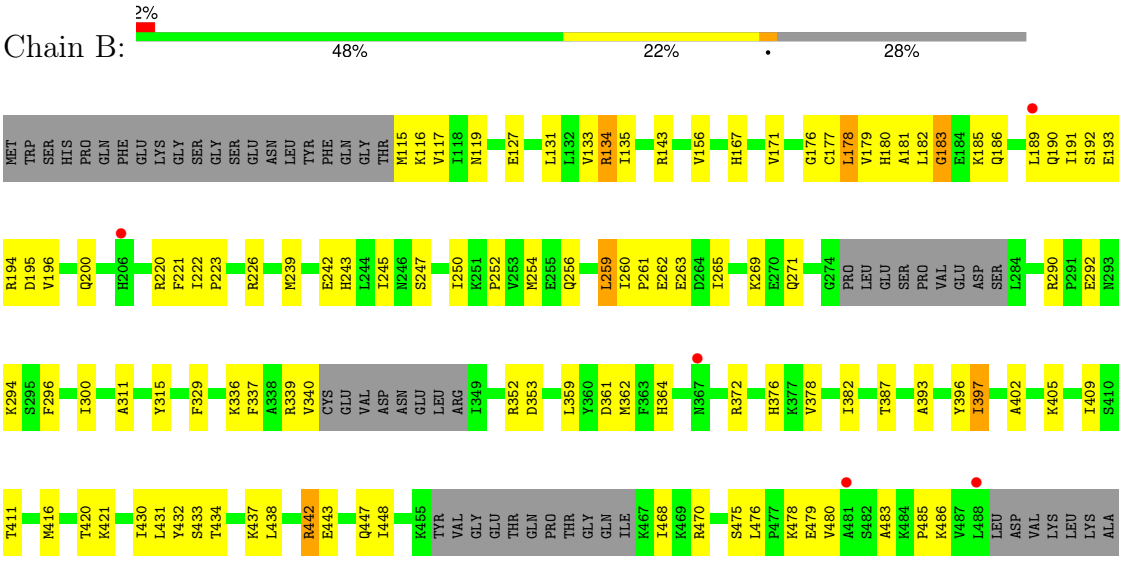
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

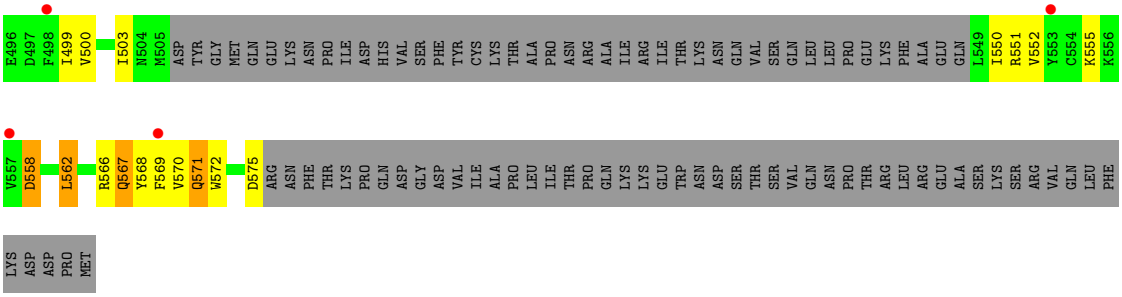
Chain A:



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain B:

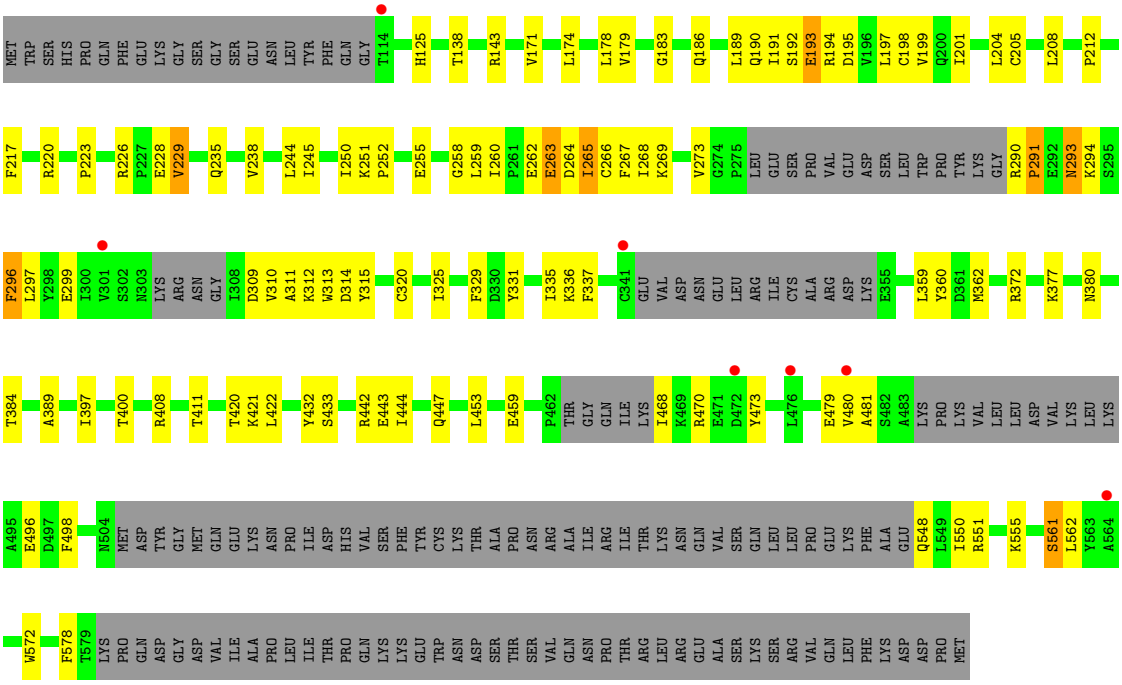




• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain C:

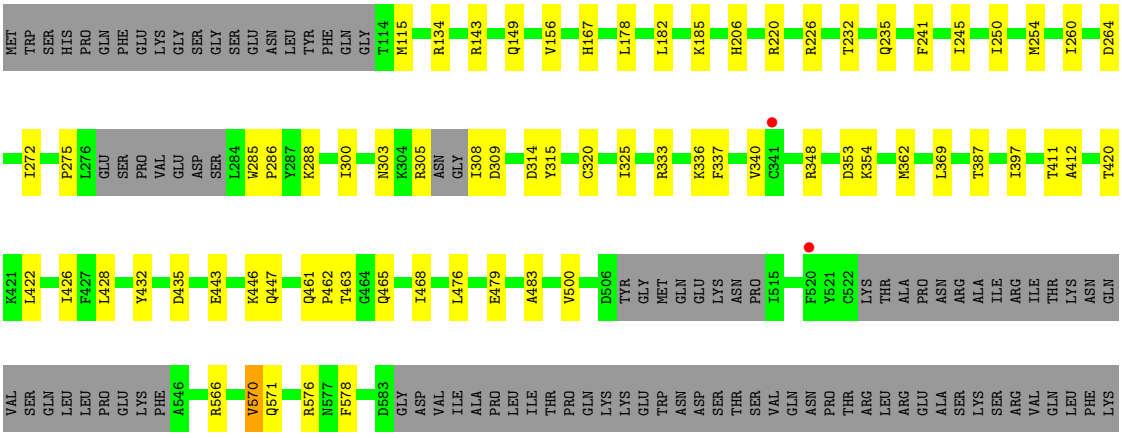




• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain D:

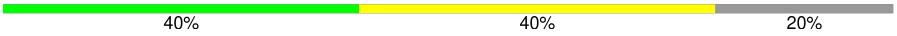






• Molecule 2: DNA SC-GS-SC-SC-DT

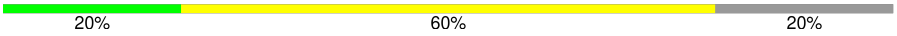
Chain E:





• Molecule 2: DNA SC-GS-SC-SC-DT

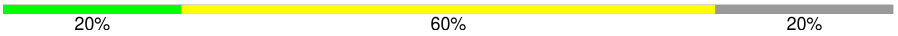
Chain G:





• Molecule 2: DNA SC-GS-SC-SC-DT

Chain F:





• Molecule 2: DNA SC-GS-SC-SC-DT

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.36Å 81.87Å 106.00Å 69.72° 76.30° 82.77°	Depositor
Resolution (Å)	61.66 – 2.58 61.66 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.8 (61.66-2.58) 97.8 (61.66-2.58)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.196 , 0.236 0.197 , 0.238	Depositor DCC
R_{free} test set	2276 reflections (3.41%)	wwPDB-VP
Wilson B-factor (Å^2)	67.2	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 75.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13531	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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: GS, SC, ZN

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	0.45	0/3578	0.65	5/4825 (0.1%)
1	B	0.46	0/3211	0.77	7/4322 (0.2%)
1	C	0.42	0/3145	0.73	6/4239 (0.1%)
1	D	0.39	0/3613	0.62	2/4871 (0.0%)
All	All	0.43	0/13547	0.69	20/18257 (0.1%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	397	ILE	N-CA-C	8.46	118.87	106.85
1	C	263	GLU	CA-C-N	-6.83	109.63	121.52
1	C	263	GLU	C-N-CA	-6.83	109.63	121.52
1	A	325	ILE	CA-C-N	-6.79	113.35	122.72
1	A	325	ILE	C-N-CA	-6.79	113.35	122.72

There are no chirality outliers.

There are no planarity outliers.

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	3497	0	3461	51	0
1	B	3139	0	3126	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3075	0	3027	88	0
1	D	3531	0	3500	45	0
2	E	76	0	46	4	0
2	F	68	0	41	4	0
2	G	53	0	29	3	0
2	H	76	0	46	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	4	0	0	0	0
4	D	8	0	0	1	0
All	All	13531	0	13276	285	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 11.

The worst 5 of 285 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:552:VAL:HG21	1:B:569:PHE:CE1	2.00	0.96
1:B:552:VAL:HG21	1:B:569:PHE:CD1	2.00	0.96
1:B:393:ALA:HB1	1:B:397:ILE:CD1	1.95	0.95
1:C:191:ILE:HG23	1:C:191:ILE:O	1.67	0.92
1:B:372:ARG:NH2	2:G:804:SC:S2P	2.45	0.90

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	418/533 (78%)	405 (97%)	13 (3%)	0	100	100
1	B	371/533 (70%)	353 (95%)	17 (5%)	1 (0%)	36	56
1	C	362/533 (68%)	349 (96%)	12 (3%)	1 (0%)	36	56
1	D	421/533 (79%)	413 (98%)	8 (2%)	0	100	100
All	All	1572/2132 (74%)	1520 (97%)	50 (3%)	2 (0%)	48	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	558	ASP
1	C	291	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	378/474 (80%)	377 (100%)	1 (0%)	86	94
1	B	337/474 (71%)	325 (96%)	12 (4%)	31	56
1	C	331/474 (70%)	323 (98%)	8 (2%)	43	68
1	D	382/474 (81%)	377 (99%)	5 (1%)	61	81
All	All	1428/1896 (75%)	1402 (98%)	26 (2%)	51	74

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	262	GLU
1	C	293	ASN
1	D	468	ILE
1	C	266	CYS
1	C	359	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	375	GLN
1	D	243	HIS
1	D	577	ASN
1	D	200	GLN
1	B	186	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)

16 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SC	H	801	2	17,17,21	0.42	0	24,24,31	0.44	0
2	SC	E	803	2	17,20,21	0.59	0	23,28,31	0.42	0
2	SC	F	801	2	8,8,21	0.41	0	9,10,31	0.65	0
2	SC	G	804	2	0,3,21	-	-	0,3,31	-	-
2	SC	E	804	2	17,20,21	0.35	0	23,28,31	0.40	0
2	GS	F	802	2	21,24,25	0.47	0	30,35,38	0.45	0
2	SC	G	803	2	17,20,21	0.39	0	23,28,31	0.39	0
2	SC	F	804	2	17,20,21	0.41	0	23,28,31	0.38	0
2	SC	H	803	2	17,20,21	0.53	0	23,28,31	0.43	0
2	GS	E	802	2	21,24,25	0.43	0	30,35,38	0.43	0
2	GS	G	802	2	21,24,25	0.40	0	30,35,38	0.32	0
2	SC	H	804	2	17,20,21	0.36	0	23,28,31	0.37	0
2	SC	E	801	2	17,17,21	0.48	0	24,24,31	0.47	0
2	GS	H	802	2	21,24,25	0.45	0	30,35,38	0.49	0
2	SC	F	803	2	17,20,21	0.46	0	23,28,31	0.39	0
2	SC	G	801	2	8,8,21	0.44	0	9,10,31	0.92	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SC	H	801	2	-	0/6/18/22	0/2/2/2
2	SC	E	803	2	-	4/7/21/22	0/2/2/2
2	SC	F	801	2	-	0/2/12/22	0/1/1/2
2	SC	E	804	2	-	0/7/21/22	0/2/2/2
2	GS	F	802	2	-	0/7/21/22	0/3/3/3
2	SC	G	803	2	-	3/7/21/22	0/2/2/2
2	SC	F	804	2	-	2/7/21/22	0/2/2/2
2	SC	H	803	2	-	4/7/21/22	0/2/2/2
2	GS	E	802	2	-	0/7/21/22	0/3/3/3
2	GS	G	802	2	-	1/7/21/22	0/3/3/3
2	SC	H	804	2	-	5/7/21/22	0/2/2/2
2	SC	E	801	2	-	2/6/18/22	0/2/2/2
2	GS	H	802	2	-	1/7/21/22	0/3/3/3
2	SC	F	803	2	-	0/7/21/22	0/2/2/2
2	SC	G	801	2	-	2/2/12/22	0/1/1/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	801	SC	C1'-C2'-C3'	-2.46	100.63	103.26

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	801	SC	C3'-C4'-C5'-O5'
2	G	801	SC	O4'-C4'-C5'-O5'
2	H	803	SC	C2'-C1'-N1-C6
2	E	801	SC	C3'-C4'-C5'-O5'
2	E	801	SC	O4'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	804	SC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	804	SC	3	0
2	F	802	GS	1	0
2	F	804	SC	2	0
2	E	802	GS	1	0
2	G	802	GS	1	0
2	H	802	GS	1	0
2	F	803	SC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides 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, 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	427/533 (80%)	-0.10	7 (1%)	70	67	31, 74, 133, 181	1 (0%)
1	B	383/533 (71%)	0.14	9 (2%)	61	56	70, 112, 166, 192	0
1	C	376/533 (70%)	0.25	7 (1%)	66	62	65, 116, 166, 201	0
1	D	430/533 (80%)	-0.11	2 (0%)	87	86	32, 79, 138, 175	1 (0%)
2	E	0/5	-	-			-	-
2	F	0/5	-	-			-	-
2	G	0/5	-	-			-	-
2	H	0/5	-	-			-	-
All	All	1616/2152 (75%)	0.04	25 (1%)	72	69	31, 93, 159, 201	2 (0%)

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	341	CYS	4.0
1	A	564	ALA	4.0
1	C	564	ALA	3.1
1	C	480	VAL	3.0
1	C	301	VAL	2.8

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

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	SC	G	801	8/20	0.63	0.11	133,141,145,146	0
2	SC	F	801	8/20	0.72	0.13	106,122,127,131	0
2	SC	E	801	16/20	0.81	0.11	80,122,143,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SC	F	804	19/20	0.81	0.10	149,166,176,185	0
2	SC	H	801	16/20	0.82	0.10	85,118,149,149	0
2	SC	E	804	19/20	0.83	0.11	105,135,150,155	0
2	SC	H	804	19/20	0.84	0.12	127,146,157,158	0
2	SC	G	803	19/20	0.88	0.09	115,152,173,175	0
2	SC	G	804	4/20	0.88	0.12	157,157,158,160	0
2	SC	F	803	19/20	0.92	0.09	105,122,134,154	0
2	GS	G	802	22/23	0.93	0.07	105,113,125,146	0
2	SC	H	803	19/20	0.93	0.09	72,113,130,133	0
2	SC	E	803	19/20	0.94	0.07	74,112,125,128	1
2	GS	F	802	22/23	0.94	0.08	81,94,101,123	0
2	GS	H	802	22/23	0.95	0.08	54,62,72,82	0
2	GS	E	802	22/23	0.96	0.06	58,70,75,94	0

6.3 Carbohydrates (i)

There are no oligosaccharides 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
3	ZN	B	701	1/1	0.92	0.08	99,99,99,99	1
3	ZN	A	701	1/1	0.96	0.08	89,89,89,89	1
3	ZN	C	701	1/1	0.96	0.07	146,146,146,146	0
3	ZN	D	701	1/1	0.97	0.06	106,106,106,106	1

6.5 Other polymers (i)

There are no such residues in this entry.