



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2026 – 11:39 pm BST

PDB ID : 5NNU / pdb_00005nnu
Title : KSHV uracil-DNA glycosylase, product complex with dsDNA exhibiting duplex nucleotide flipping
Authors : Earl, C.; Bagneris, C.; Barrett, T.; Savva, R.
Deposited on : 2017-04-10
Resolution : 2.97 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
Mogul : 1.8.4, CSD as541be (2020)
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

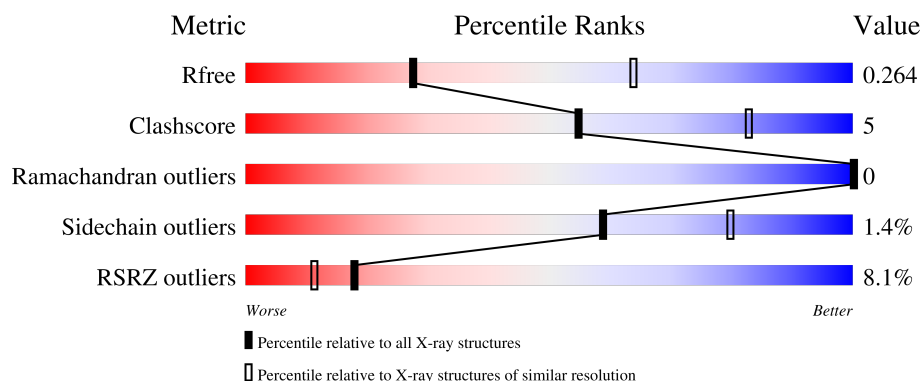
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	S	11	9% 73% 27%
1	U	11	9% 82% 18%
1	W	11	18% 73% 27%
1	Y	11	82% 18%
2	A	240	6% 87% 8% ••

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Mol	Chain	Length	Quality of chain
2	B	240	5% 84% 12% .
2	D	240	10% 79% 16% . .
2	E	240	9% 80% 12% 8%
3	T	11	82% 18%
3	V	11	9% 100%
3	X	11	18% 73% 27%
3	Z	11	18% 91% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8844 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 DNA chain called DNA containing an abasic site.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	11	Total	C	N	O	P	0	0	0
			213	104	33	66	10			
1	U	11	Total	C	N	O	P	0	0	0
			213	104	33	66	10			
1	W	11	Total	C	N	O	P	0	0	0
			213	104	33	66	10			
1	Y	11	Total	C	N	O	P	0	0	0
			213	104	33	66	10			

- Molecule 2 is a protein called Uracil-DNA glycosylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	231	Total	C	N	O	S	0	1	0
			1759	1134	315	303	7			
2	B	230	Total	C	N	O	S	0	0	0
			1783	1155	316	305	7			
2	D	230	Total	C	N	O	S	0	1	0
			1757	1138	312	300	7			
2	E	222	Total	C	N	O	S	0	0	0
			1674	1090	293	284	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	SER	-	expression tag	UNP Q76RG8
A	20	ALA	-	expression tag	UNP Q76RG8
A	21	SER	-	expression tag	UNP Q76RG8
B	19	SER	-	expression tag	UNP Q76RG8
B	20	ALA	-	expression tag	UNP Q76RG8
B	21	SER	-	expression tag	UNP Q76RG8
D	19	SER	-	expression tag	UNP Q76RG8
D	20	ALA	-	expression tag	UNP Q76RG8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	21	SER	-	expression tag	UNP Q76RG8
E	19	SER	-	expression tag	UNP Q76RG8
E	20	ALA	-	expression tag	UNP Q76RG8
E	21	SER	-	expression tag	UNP Q76RG8

- Molecule 3 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	11	Total	C	N	O	P	0	0	0
			227	109	44	63	11			
3	V	11	Total	C	N	O	P	0	0	0
			227	109	44	63	11			
3	X	11	Total	C	N	O	P	0	0	0
			227	109	44	63	11			
3	Z	11	Total	C	N	O	P	0	0	0
			227	109	44	63	11			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	S	2	Total	O	0	0
			2	2		
4	A	18	Total	O	0	0
			18	18		
4	B	17	Total	O	0	0
			17	17		
4	D	17	Total	O	0	0
			17	17		
4	E	11	Total	O	0	0
			11	11		
4	T	4	Total	O	0	0
			4	4		
4	U	5	Total	O	0	0
			5	5		
4	V	7	Total	O	0	0
			7	7		
4	W	8	Total	O	0	0
			8	8		
4	X	12	Total	O	0	0
			12	12		
4	Y	3	Total	O	0	0
			3	3		

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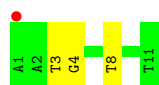
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Z	7	Total	O	0	0
			7	7		

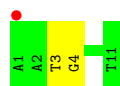
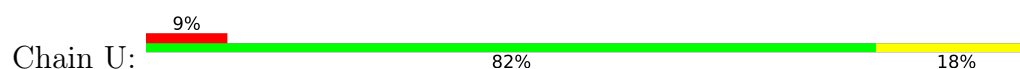
3 Residue-property plots [i](#)

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.

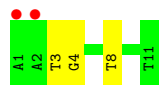
- Molecule 1: DNA containing an abasic site



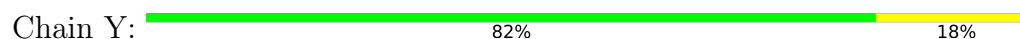
- Molecule 1: DNA containing an abasic site



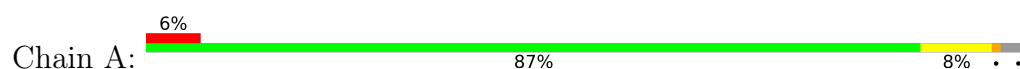
- Molecule 1: DNA containing an abasic site



- Molecule 1: DNA containing an abasic site

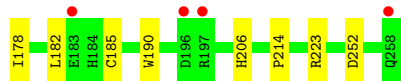
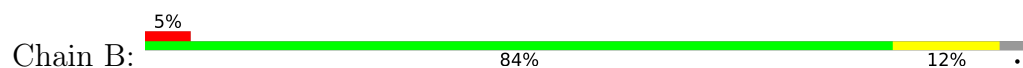


- Molecule 2: Uracil-DNA glycosylase

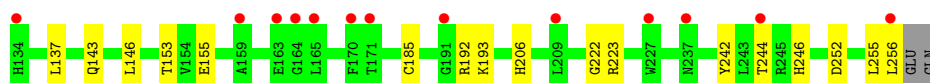
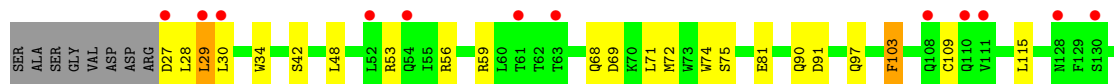
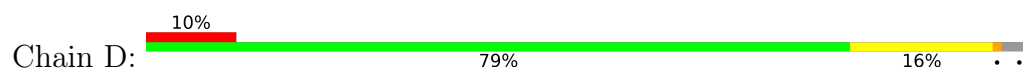




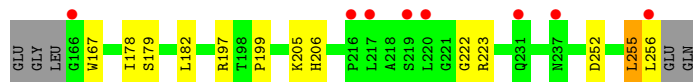
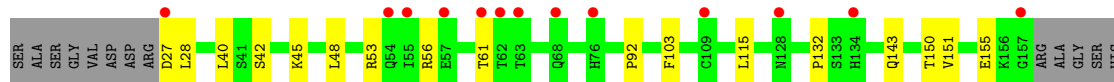
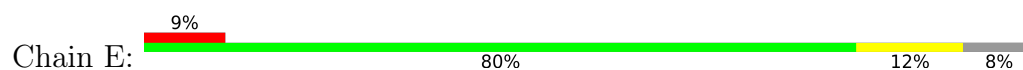
- Molecule 2: Uracil-DNA glycosylase



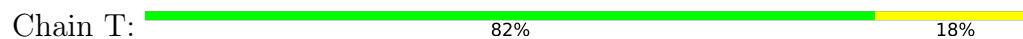
- Molecule 2: Uracil-DNA glycosylase



- Molecule 2: Uracil-DNA glycosylase



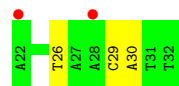
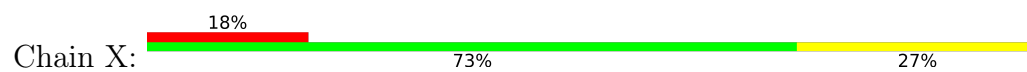
- Molecule 3: DNA



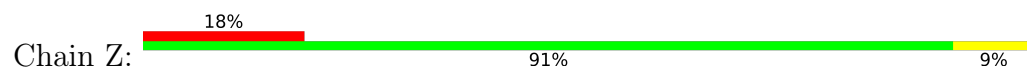
- Molecule 3: DNA



● Molecule 3: DNA



● Molecule 3: DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.10Å 70.80Å 140.25Å 90.00° 94.36° 90.00°	Depositor
Resolution (Å)	49.20 – 2.97 49.20 – 2.97	Depositor EDS
% Data completeness (in resolution range)	97.0 (49.20-2.97) 97.0 (49.20-2.97)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0158, PHENIX 1.10-2155	Depositor
R, R_{free}	0.244 , 0.269 0.239 , 0.264	Depositor DCC
R_{free} test set	1717 reflections (5.28%)	wwPDB-VP
Wilson B-factor (Å ²)	68.6	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8844	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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 ⓘ

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

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	S	0.51	0/223	0.71	0/340
1	U	0.45	0/223	0.71	0/340
1	W	0.46	0/223	0.67	0/340
1	Y	0.47	0/223	0.67	0/340
2	A	0.85	0/1811	1.31	4/2477 (0.2%)
2	B	0.89	0/1835	1.29	3/2504 (0.1%)
2	D	0.88	0/1814	1.36	11/2481 (0.4%)
2	E	0.88	0/1724	1.34	8/2361 (0.3%)
3	T	0.51	0/255	0.72	0/391
3	V	0.47	0/255	0.69	0/391
3	X	0.48	0/255	0.70	0/391
3	Z	0.43	0/255	0.67	0/391
All	All	0.81	0/9096	1.21	26/12747 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	223	ARG	N-CA-C	-7.97	103.69	113.50
2	E	255	LEU	CA-C-N	7.53	135.25	121.70
2	E	255	LEU	C-N-CA	7.53	135.25	121.70
2	E	223	ARG	N-CA-C	-6.37	105.51	113.28
2	B	69	ASP	CA-CB-CG	6.30	118.90	112.60
2	D	223	ARG	N-CA-C	-6.28	105.62	113.28
2	B	91	ASP	CA-CB-CG	6.23	118.83	112.60
2	D	103	PHE	CB-CA-C	-6.23	101.08	111.23
2	A	69	ASP	CA-CB-CG	6.07	118.67	112.60
2	B	223	ARG	N-CA-C	-6.00	105.78	113.23
2	D	69	ASP	CA-CB-CG	5.82	118.42	112.60
2	D	81	GLU	CB-CG-CD	5.74	122.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	91	ASP	CA-CB-CG	5.38	117.98	112.60
2	D	27	ASP	CA-C-N	5.29	131.43	122.65
2	D	27	ASP	C-N-CA	5.29	131.43	122.65
2	A	91	ASP	CA-CB-CG	5.25	117.85	112.60
2	E	27	ASP	CA-C-N	5.18	131.25	122.65
2	E	27	ASP	C-N-CA	5.18	131.25	122.65
2	E	61	THR	N-CA-C	5.16	119.45	111.56
2	D	244	THR	CA-C-N	5.12	127.14	120.28
2	D	244	THR	C-N-CA	5.12	127.14	120.28
2	A	151	VAL	CB-CA-C	5.04	118.09	110.63
2	E	42	SER	CA-C-N	5.02	127.32	120.54
2	E	42	SER	C-N-CA	5.02	127.32	120.54
2	D	42	SER	CA-C-N	5.00	127.30	120.54
2	D	42	SER	C-N-CA	5.00	127.30	120.54

There are no chirality outliers.

There are no planarity outliers.

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	S	213	0	125	4	0
1	U	213	0	125	1	0
1	W	213	0	125	4	0
1	Y	213	0	125	2	0
2	A	1759	0	1628	12	0
2	B	1783	0	1713	15	0
2	D	1757	0	1675	20	0
2	E	1674	0	1579	17	0
3	T	227	0	125	5	0
3	V	227	0	125	0	0
3	X	227	0	125	6	0
3	Z	227	0	125	1	0
4	A	18	0	0	2	0
4	B	17	0	0	2	0
4	D	17	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	11	0	0	0	0
4	S	2	0	0	0	0
4	T	4	0	0	0	0
4	U	5	0	0	0	0
4	V	7	0	0	0	0
4	W	8	0	0	0	0
4	X	12	0	0	1	0
4	Y	3	0	0	0	0
4	Z	7	0	0	0	0
All	All	8844	0	7595	78	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 5.

All (78) 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:S:4:DG:H1	3:T:29:DC:H5	1.05	0.95
1:W:4:DG:H1	3:X:29:DC:H5	1.24	0.86
2:D:29:LEU:HD23	2:D:72:MET:HG2	1.59	0.83
1:S:4:DG:N1	3:T:29:DC:H5	1.81	0.78
3:T:29:DC:H2''	3:T:30:DA:C2	2.29	0.68
3:X:26:DT:H71	4:X:106:HOH:O	1.95	0.66
3:X:29:DC:H2''	3:X:30:DA:C2	2.30	0.66
2:B:125:SER:CB	4:B:301:HOH:O	2.44	0.65
2:D:185:CYS:H	2:D:206:HIS:HD2	1.43	0.64
2:D:103:PHE:O	2:D:115:LEU:HD13	1.97	0.64
2:D:185:CYS:H	2:D:206:HIS:CD2	2.15	0.64
3:T:29:DC:H2'	3:T:29:DC:O2	1.97	0.63
3:X:29:DC:H2'	3:X:29:DC:O2	1.99	0.62
2:A:178:ILE:HG23	2:A:182:LEU:HD12	1.83	0.60
2:E:179:SER:O	2:E:205:LYS:HE3	2.03	0.59
2:D:143:GLN:HE22	2:D:252:ASP:H	1.51	0.57
2:E:205:LYS:HG3	2:E:206:HIS:CD2	2.40	0.57
2:D:29:LEU:CD2	2:D:71:LEU:HB2	2.35	0.57
2:E:143:GLN:HE22	2:E:252:ASP:H	1.52	0.56
2:B:70:LYS:HD3	4:B:316:HOH:O	2.05	0.56
2:E:132:PRO:HG3	2:E:256:LEU:HD22	1.88	0.55
2:D:53:ARG:HA	2:D:56:ARG:HD3	1.89	0.55
1:W:4:DG:N1	3:X:29:DC:H5	2.00	0.54
2:E:150:THR:HB	2:E:197:ARG:NH2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:GLN:HB2	2:B:109:CYS:SG	2.49	0.53
2:A:98:ALA:HB3	4:A:310:HOH:O	2.08	0.53
2:D:34:TRP:CD1	2:D:75:SER:HB2	2.43	0.53
2:D:143:GLN:NE2	2:D:252:ASP:H	2.07	0.52
2:A:143:GLN:HE22	2:A:252:ASP:H	1.56	0.52
2:A:151:VAL:HG22	2:A:167:TRP:HB2	1.91	0.52
2:A:143:GLN:NE2	2:A:252:ASP:H	2.08	0.52
2:B:143:GLN:NE2	2:B:252:ASP:H	2.08	0.52
2:E:143:GLN:NE2	2:E:252:ASP:H	2.08	0.52
2:B:143:GLN:HE22	2:B:252:ASP:H	1.56	0.51
2:D:97:GLN:HB2	2:D:109:CYS:SG	2.51	0.50
2:D:28:LEU:HD22	2:D:48:LEU:HD23	1.93	0.50
2:E:53:ARG:HA	2:E:56:ARG:HD2	1.93	0.50
2:E:255:LEU:HA	2:E:256:LEU:C	2.37	0.50
2:B:53:ARG:HA	2:B:56:ARG:HD3	1.93	0.49
2:E:103:PHE:O	2:E:115:LEU:HD13	2.12	0.48
2:E:28:LEU:HD22	2:E:48:LEU:HD23	1.95	0.48
2:D:256:LEU:C	4:D:301:HOH:O	2.57	0.48
2:D:185:CYS:O	2:D:206:HIS:HB3	2.13	0.47
2:D:59:ARG:HE	2:D:68:GLN:HG2	1.80	0.47
2:B:103:PHE:O	2:B:115:LEU:HD13	2.16	0.46
2:D:90:GLN:HG3	2:D:193:LYS:HG3	1.98	0.45
2:B:47:LYS:HE3	2:B:169:TRP:CE2	2.50	0.45
2:E:151:VAL:HG13	2:E:167:TRP:HD1	1.82	0.45
2:A:103:PHE:O	2:A:115:LEU:HD13	2.17	0.45
2:B:104:SER:HB2	2:B:137:LEU:HB2	2.00	0.44
2:D:115:LEU:HD11	2:D:137:LEU:HD21	1.98	0.44
2:A:65:TYR:HB3	4:A:310:HOH:O	2.17	0.44
3:X:29:DC:O2	3:X:29:DC:C2'	2.65	0.44
2:A:192:ARG:HE	2:E:199:PRO:HB2	1.83	0.44
2:D:71:LEU:HD21	2:D:153:THR:HG22	1.99	0.43
2:E:92:PRO:HD3	2:E:151:VAL:O	2.18	0.43
2:E:28:LEU:HD11	2:E:45:LYS:HG2	2.01	0.43
2:E:178:ILE:HG23	2:E:182:LEU:HD13	1.99	0.43
2:B:178:ILE:HG23	2:B:182:LEU:HD13	1.99	0.43
2:B:185:CYS:HB2	2:B:206:HIS:ND1	2.33	0.43
2:A:28:LEU:HD22	2:A:48:LEU:HD23	2.00	0.43
2:A:220:LEU:O	2:A:223:ARG:HD3	2.19	0.43
2:B:190:TRP:HB3	2:B:214:PRO:HD3	2.01	0.43
2:D:222:GLY:HA3	1:W:8:DT:H4'	2.01	0.43
3:T:29:DC:O2	3:T:29:DC:C2'	2.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:8:DT:H4'	2:A:222:GLY:HA3	2.01	0.43
2:B:70:LYS:O	2:B:100:GLY:HA3	2.19	0.43
2:B:28:LEU:HD22	2:B:48:LEU:HD23	2.01	0.42
2:A:66:PRO:HG2	2:A:71:LEU:HD23	2.01	0.42
2:D:242:TYR:CE1	2:D:246:HIS:CE1	3.07	0.42
1:W:3:DT:H2''	1:W:4:DG:C8	2.55	0.41
1:Y:4:DG:N2	3:Z:30:DA:C2	2.90	0.40
2:B:77:CYS:HB3	2:B:141:ALA:CB	2.51	0.40
2:D:74:TRP:CE3	2:D:146:LEU:HD11	2.56	0.40
2:E:40:LEU:HB2	2:E:45:LYS:HE3	2.04	0.40
1:U:3:DT:H2''	1:U:4:DG:C8	2.56	0.40
1:S:3:DT:H2''	1:S:4:DG:C8	2.56	0.40
2:E:222:GLY:HA3	1:Y:8:DT:H4'	2.03	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	
2	A	226/240 (94%)	215 (95%)	11 (5%)	0	100	100
2	B	224/240 (93%)	215 (96%)	9 (4%)	0	100	100
2	D	229/240 (95%)	221 (96%)	8 (4%)	0	100	100
2	E	218/240 (91%)	210 (96%)	8 (4%)	0	100	100
All	All	897/960 (93%)	861 (96%)	36 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	A	172/213 (81%)	168 (98%)	4 (2%)	44	72
2	B	182/213 (85%)	182 (100%)	0	100	100
2	D	177/213 (83%)	172 (97%)	5 (3%)	38	69
2	E	164/213 (77%)	163 (99%)	1 (1%)	78	88
All	All	695/852 (82%)	685 (99%)	10 (1%)	59	80

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	151	VAL
2	A	192	ARG
2	A	255	LEU
2	A	257	GLU
2	D	29	LEU
2	D	30	LEU
2	D	155	GLU
2	D	192	ARG
2	D	255	LEU
2	E	155	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	76	HIS
2	A	90	GLN
2	A	143	GLN
2	A	149	ASN
2	B	68	GLN
2	B	90	GLN
2	B	143	GLN
2	B	149	ASN
2	B	212	GLN

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Mol	Chain	Res	Type
2	D	90	GLN
2	D	143	GLN
2	D	149	ASN
2	D	184	HIS
2	D	206	HIS
2	D	212	GLN
2	D	231	GLN
2	D	246	HIS
2	E	90	GLN
2	E	143	GLN
2	E	212	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 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	$\# Z > 2$
1	AAB	Y	6	1	9,12,13	0.62	0	8,16,19	0.72	0
1	AAB	U	6	1	9,12,13	0.68	0	8,16,19	0.63	0
1	AAB	W	6	1	9,12,13	0.77	0	8,16,19	0.82	0
1	AAB	S	6	1	9,12,13	0.64	0	8,16,19	0.58	0

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
1	AAB	Y	6	1	-	0/3/17/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	AAB	U	6	1	-	0/3/17/18	0/1/1/1
1	AAB	W	6	1	-	0/3/17/18	0/1/1/1
1	AAB	S	6	1	-	0/3/17/18	0/1/1/1

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.

5.5 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	S	10/11 (90%)	0.71	1 (10%) 12 8	54, 70, 132, 140	0
1	U	10/11 (90%)	0.50	1 (10%) 12 8	51, 68, 107, 110	0
1	W	10/11 (90%)	1.06	2 (20%) 3 2	72, 85, 115, 117	0
1	Y	10/11 (90%)	0.87	0 100 100	63, 91, 108, 111	0
2	A	231/240 (96%)	0.81	14 (6%) 27 16	34, 67, 97, 114	1 (0%)
2	B	230/240 (95%)	0.67	12 (5%) 33 20	38, 61, 87, 102	0
2	D	230/240 (95%)	0.91	25 (10%) 10 7	36, 71, 103, 118	1 (0%)
2	E	222/240 (92%)	1.00	21 (9%) 14 9	42, 72, 104, 136	0
3	T	11/11 (100%)	0.59	0 100 100	66, 80, 91, 116	0
3	V	11/11 (100%)	0.47	1 (9%) 15 9	64, 72, 89, 103	0
3	X	11/11 (100%)	1.27	2 (18%) 3 2	103, 105, 117, 121	0
3	Z	11/11 (100%)	1.26	2 (18%) 3 2	97, 105, 116, 134	0
All	All	997/1048 (95%)	0.85	81 (8%) 18 11	34, 69, 105, 140	2 (0%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	27	ASP	5.8
2	D	27	ASP	5.6
2	A	161	SER	4.1
2	E	237	ASN	3.8
2	E	157	GLY	3.6
2	B	159	ALA	3.4
2	B	258	GLN	3.3
2	B	163	GLU	3.3
1	S	1	DA	3.2
2	D	237	ASN	3.1
2	D	164	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
2	A	197	ARG	3.1
2	D	209	LEU	3.1
2	B	197	ARG	3.0
2	D	163	GLU	3.0
2	E	256	LEU	3.0
2	D	159	ALA	3.0
2	A	157	GLY	3.0
2	E	134	HIS	3.0
2	E	220	LEU	2.9
2	E	219	SER	2.9
2	E	61	THR	2.9
2	E	55	ILE	2.9
2	D	256	LEU	2.8
2	E	128	ASN	2.8
2	B	150	THR	2.7
2	E	62	THR	2.7
2	B	161	SER	2.7
2	D	110	GLN	2.7
2	D	29	LEU	2.6
2	A	128	ASN	2.6
2	A	24	ASP	2.6
3	X	22	DA	2.5
2	B	89	GLY	2.5
2	D	191	GLY	2.5
2	E	166	GLY	2.5
2	B	27	ASP	2.5
2	A	61	THR	2.5
2	A	167	TRP	2.5
2	D	54	GLN	2.5
1	W	1	DA	2.5
2	E	54	GLN	2.4
2	E	68	GLN	2.4
2	E	231	GLN	2.4
2	A	122	LEU	2.4
2	D	30	LEU	2.4
2	D	111	VAL	2.3
2	D	170	PHE	2.3
2	A	163	GLU	2.3
2	A	162	HIS	2.3
2	E	217	LEU	2.3
2	D	61	THR	2.3
3	Z	27	DA	2.2

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Mol	Chain	Res	Type	RSRZ
2	A	133	SER	2.2
2	B	183	GLU	2.2
2	D	134	HIS	2.2
2	D	227	TRP	2.2
2	E	57	GLU	2.2
2	D	171	THR	2.2
2	D	52	LEU	2.2
2	D	165	LEU	2.2
2	E	76	HIS	2.1
1	U	1	DA	2.1
2	D	130	SER	2.1
2	D	108	GLN	2.1
2	B	126	VAL	2.1
2	D	128	ASN	2.1
2	E	109	CYS	2.1
2	E	216	PRO	2.1
2	B	158	ARG	2.1
2	B	196	ASP	2.1
2	D	63	THR	2.1
2	A	134	HIS	2.0
2	A	258	GLN	2.0
1	W	2	DA	2.0
2	E	63	THR	2.0
3	V	22	DA	2.0
3	X	28	DA	2.0
3	Z	22	DA	2.0
2	A	150	THR	2.0
2	D	244	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	AAB	W	6	12/13	0.91	0.12	85,88,92,94	0
1	AAB	Y	6	12/13	0.94	0.10	77,84,91,91	0
1	AAB	S	6	12/13	0.95	0.10	58,62,66,67	0
1	AAB	U	6	12/13	0.96	0.10	62,65,72,73	0

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.