



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 06:11 pm BST

PDB ID : 6DWZ
Title : Hermes transposase deletion dimer complex with (C/G) DNA
Authors : Dyda, F.; Hickman, A.B.
Deposited on : 2018-06-28
Resolution : 3.20 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

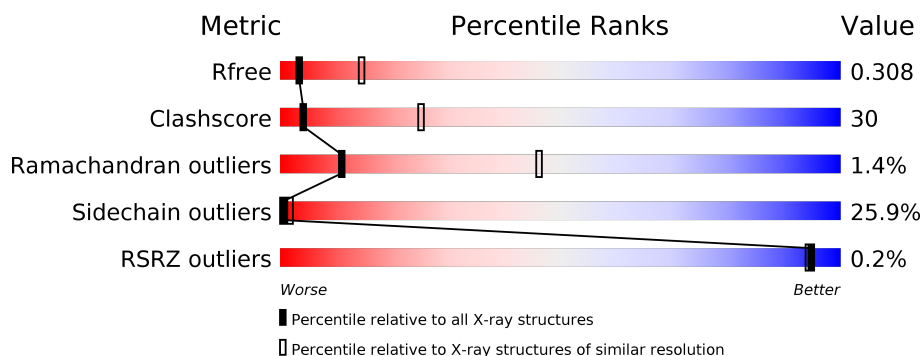
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	517	
1	E	517	
2	B	15	
2	F	15	
3	C	26	
3	G	26	

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Mol	Chain	Length	Quality of chain
4	D	7	<div><div></div><div>43%</div><div>57%</div></div>
4	H	7	<div><div></div><div>14%</div><div>43%</div><div>43%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9578 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 Hermes transposase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3832	2454	647	713	18			
1	E	476	Total	C	N	O	S	0	0	0
			3832	2454	647	713	18			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	GLY	-	expression tag	UNP Q25438
A	77	SER	-	expression tag	UNP Q25438
A	78	HIS	-	expression tag	UNP Q25438
A	79	MET	-	expression tag	UNP Q25438
A	128	GLY	LYS	conflict	UNP Q25438
A	?	-	ASP	deletion	UNP Q25438
A	?	-	ILE	deletion	UNP Q25438
A	?	-	SER	deletion	UNP Q25438
A	?	-	THR	deletion	UNP Q25438
A	?	-	THR	deletion	UNP Q25438
A	?	-	SER	deletion	UNP Q25438
A	?	-	PHE	deletion	UNP Q25438
A	?	-	PHE	deletion	UNP Q25438
A	?	-	PHE	deletion	UNP Q25438
A	?	-	PRO	deletion	UNP Q25438
A	?	-	GLN	deletion	UNP Q25438
A	?	-	LEU	deletion	UNP Q25438
A	?	-	THR	deletion	UNP Q25438
A	?	-	GLN	deletion	UNP Q25438
A	?	-	ASN	deletion	UNP Q25438
A	?	-	ASN	deletion	UNP Q25438
A	?	-	SER	deletion	UNP Q25438
A	?	-	ARG	deletion	UNP Q25438
A	?	-	GLU	deletion	UNP Q25438
A	?	-	PRO	deletion	UNP Q25438

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Chain	Residue	Modelled	Actual	Comment	Reference
A	519	SER	CYS	engineered mutation	UNP Q25438
E	76	GLY	-	expression tag	UNP Q25438
E	77	SER	-	expression tag	UNP Q25438
E	78	HIS	-	expression tag	UNP Q25438
E	79	MET	-	expression tag	UNP Q25438
E	128	GLY	LYS	conflict	UNP Q25438
E	?	-	ASP	deletion	UNP Q25438
E	?	-	ILE	deletion	UNP Q25438
E	?	-	SER	deletion	UNP Q25438
E	?	-	THR	deletion	UNP Q25438
E	?	-	THR	deletion	UNP Q25438
E	?	-	SER	deletion	UNP Q25438
E	?	-	PHE	deletion	UNP Q25438
E	?	-	PHE	deletion	UNP Q25438
E	?	-	PHE	deletion	UNP Q25438
E	?	-	PRO	deletion	UNP Q25438
E	?	-	GLN	deletion	UNP Q25438
E	?	-	LEU	deletion	UNP Q25438
E	?	-	THR	deletion	UNP Q25438
E	?	-	GLN	deletion	UNP Q25438
E	?	-	ASN	deletion	UNP Q25438
E	?	-	ASN	deletion	UNP Q25438
E	?	-	SER	deletion	UNP Q25438
E	?	-	ARG	deletion	UNP Q25438
E	?	-	GLU	deletion	UNP Q25438
E	?	-	PRO	deletion	UNP Q25438
E	519	SER	CYS	engineered mutation	UNP Q25438

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*AP*GP*AP*AP*CP*AP*AP*CP*AP*AP*CP*AP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	P	0	0	0
			309	147	69	79	14			
2	F	15	Total	C	N	O	P	0	0	0
			309	147	69	79	14			

- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	25	Total	C	N	O	P	0	0	0
			506	244	80	158	24			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	25	Total	C	N	O	P	0	0	0
			506	244	80	158	24			

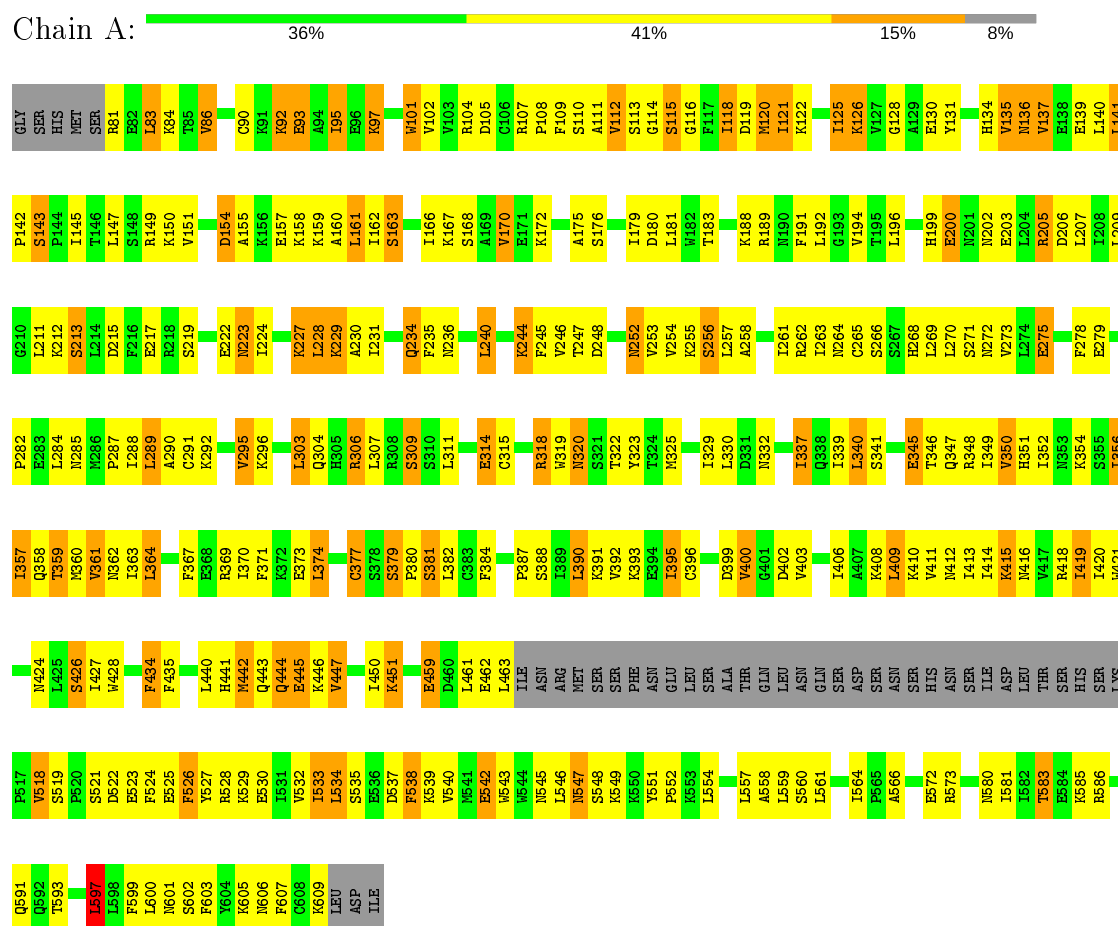
- Molecule 4 is a DNA chain called DNA (5'-D(*GP*CP*GP*TP*GP*AP*C)-3').

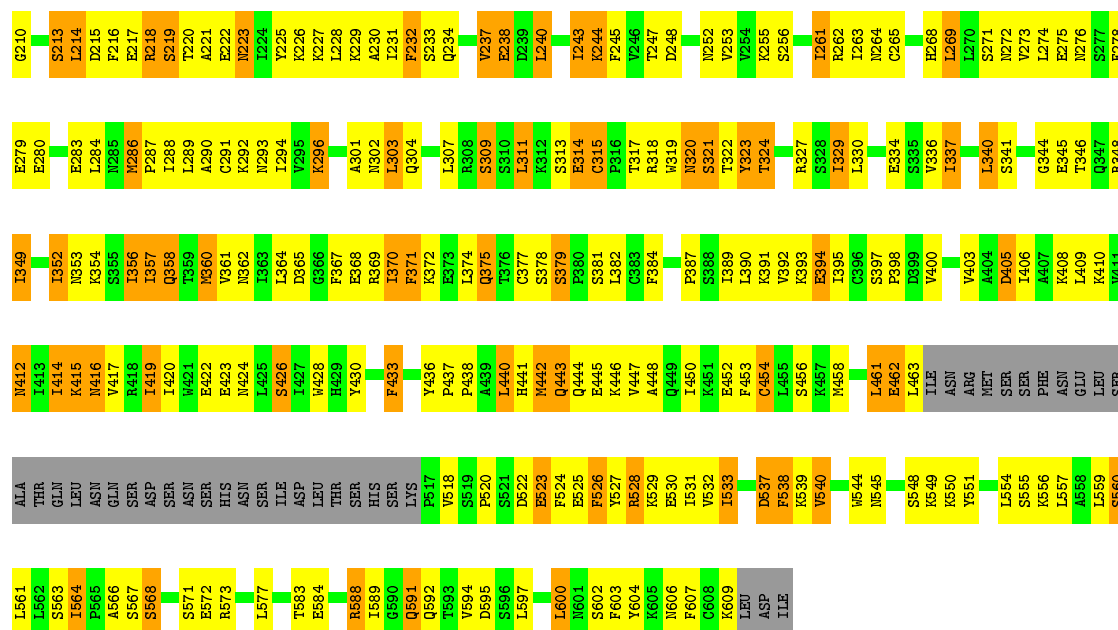
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	7	Total	C	N	O	P	0	0	0
			142	68	28	40	6			
4	H	7	Total	C	N	O	P	0	0	0
			142	68	28	40	6			

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Hermes transposase





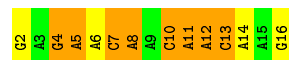
- Molecule 2: DNA (5'-D(*GP*AP*GP*AP*AP*CP*AP*AP*CP*AP*AP*CP*AP*AP*G)-3')

Chain B: 7% 20% 73%



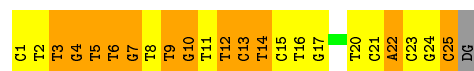
- Molecule 2: DNA (5'-D(*GP*AP*GP*AP*AP*CP*AP*AP*CP*AP*AP*CP*AP*AP*G)-3')

Chain F: 20% 27% 53%



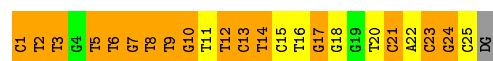
- Molecule 3: DNA (26-MER)

Chain C: 8% 42% 46%



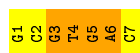
- Molecule 3: DNA (26-MER)

Chain G: 8% 27% 62%



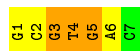
- Molecule 4: DNA (5'-D(*GP*CP*GP*TP*GP*AP*C)-3')

Chain D:  43% 57%



- Molecule 4: DNA (5'-D(*GP*CP*GP*TP*GP*AP*C)-3')

Chain H:  14% 43% 43%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.38Å 121.11Å 132.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.51 – 3.20 29.51 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.51-3.20) 99.1 (29.51-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.90Å)	Xtrriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, R_{free}	0.203 , 0.298 0.209 , 0.308	Depositor DCC
R_{free} test set	935 reflections (2.70%)	wwPDB-VP
Wilson B-factor (Å ²)	82.4	Xtrriage
Anisotropy	0.471	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 81.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9578	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1324e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.68	1/3905 (0.0%)	0.83	6/5268 (0.1%)
1	E	0.68	2/3905 (0.1%)	0.86	4/5268 (0.1%)
2	B	2.25	11/350 (3.1%)	1.83	18/538 (3.3%)
2	F	2.25	11/350 (3.1%)	1.80	18/538 (3.3%)
3	C	1.92	8/563 (1.4%)	1.97	27/868 (3.1%)
3	G	2.28	23/563 (4.1%)	1.86	22/868 (2.5%)
4	D	2.07	5/159 (3.1%)	1.46	3/244 (1.2%)
4	H	2.05	5/159 (3.1%)	1.47	2/244 (0.8%)
All	All	1.16	66/9954 (0.7%)	1.16	100/13836 (0.7%)

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	4
1	E	0	4
All	All	0	8

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	17	DG	N9-C4	10.86	1.46	1.38
3	G	24	DG	C6-N1	8.75	1.45	1.39
4	D	7	DC	C3'-O3'	8.41	1.54	1.44
3	G	23	DC	N3-C4	8.01	1.39	1.33
2	F	14	DA	C3'-O3'	-7.79	1.33	1.44

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	12	DT	O5'-P-OP1	-12.94	94.05	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	13	DC	O4'-C4'-C3'	-11.06	99.36	106.00
3	C	10	DG	O5'-P-OP1	-10.66	96.11	105.70
2	B	13	DC	O4'-C4'-C3'	-9.74	100.15	106.00
2	F	7	DC	O4'-C1'-N1	9.74	114.82	108.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	GLU	Peptide
1	A	318	ARG	Peptide
1	A	444	GLN	Peptide
1	A	445	GLU	Peptide
1	E	217	GLU	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	3832	0	3903	234	0
1	E	3832	0	3903	251	0
2	B	309	0	167	20	0
2	F	309	0	167	14	0
3	C	506	0	288	27	0
3	G	506	0	288	32	0
4	D	142	0	80	10	0
4	H	142	0	80	8	0
All	All	9578	0	8876	537	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 537 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)
2:B:16:DG:H1	3:C:1:DC:H42	1.17	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:5:DG:H2"	4:D:6:DA:H5"	1.54	0.89
1:E:412:ASN:O	1:E:416:ASN:ND2	2.04	0.88
1:E:341:SER:HA	1:E:346:THR:HB	1.54	0.87
3:C:22:DA:N6	4:D:4:DT:O4	2.07	0.86

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	472/517 (91%)	412 (87%)	52 (11%)	8 (2%)	9	42
1	E	472/517 (91%)	410 (87%)	57 (12%)	5 (1%)	14	51
All	All	944/1034 (91%)	822 (87%)	109 (12%)	13 (1%)	11	46

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	379	SER
1	A	252	ASN
1	A	320	ASN
1	A	157	GLU
1	A	200	GLU

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	436/475 (92%)	328 (75%)	108 (25%)	0	2
1	E	436/475 (92%)	318 (73%)	118 (27%)	0	1
All	All	872/950 (92%)	646 (74%)	226 (26%)	0	2

5 of 226 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	583	THR
1	E	181	LEU
1	E	538	PHE
1	A	597	LEU
1	E	119	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	332	ASN
1	E	416	ASN
1	E	358	GLN
1	A	234	GLN
1	E	362	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	476/517 (92%)	-0.49	0 100 100	41, 81, 131, 157	0
1	E	476/517 (92%)	-0.46	2 (0%) 92 89	37, 83, 132, 193	0
2	B	15/15 (100%)	-0.33	0 100 100	37, 57, 92, 111	0
2	F	15/15 (100%)	-0.49	0 100 100	39, 59, 84, 90	0
3	C	25/26 (96%)	-0.60	0 100 100	38, 69, 96, 127	0
3	G	25/26 (96%)	-0.56	0 100 100	40, 68, 92, 119	0
4	D	7/7 (100%)	-0.67	0 100 100	53, 55, 77, 81	0
4	H	7/7 (100%)	-0.63	0 100 100	49, 52, 98, 108	0
All	All	1046/1130 (92%)	-0.48	2 (0%) 95 94	37, 80, 131, 193	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	176	SER	2.5
1	E	178	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.