



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 10:23 PM GMT

PDB ID : 3C5F  
Title : Structure of a binary complex of the R517A Pol lambda mutant  
Authors : Garcia-Diaz, M.; Bebenek, K.; Foley, M.C.; Pedersen, L.C.; Schlick, T.; Kunkel, T.A.  
Deposited on : 2008-01-31  
Resolution : 2.25 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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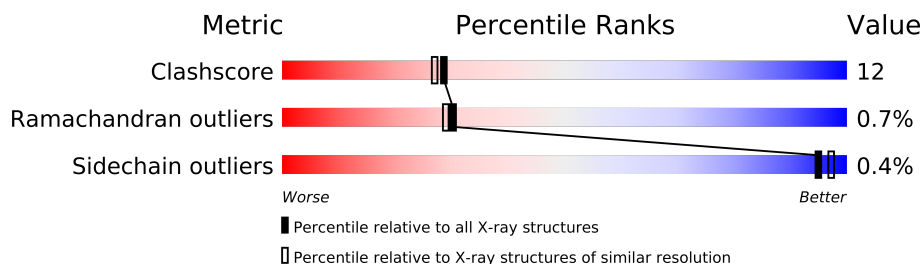
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : **FAILED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.25 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))
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1-T	11	
1	1-U	11	
1	2-T	11	
1	2-U	11	
2	1-P	6	
2	1-Q	6	
2	2-P	6	
2	2-Q	6	
3	1-D	4	
3	1-E	4	
3	2-D	4	
3	2-E	4	
4	1-A	335	
4	1-B	335	
4	2-A	335	
4	2-B	335	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13157 atoms, of which 0 are hydrogen and 0 are deuterium.

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 (5'-D(\*DCP\*DGP\*DGP\*DCP\*DCP\*DGP\*DTP\*DAP\*DCP\*DTP\*DG)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-T	11	Total	C	N	O	P	0	11	0
			222	106	41	65	10			
1	1-U	11	Total	C	N	O	P	0	11	0
			222	106	41	65	10			
1	2-T	11	Total	C	N	O	P	0	11	0
			222	106	41	65	10			
1	2-U	11	Total	C	N	O	P	0	11	0
			222	106	41	65	10			

- Molecule 2 is a DNA chain called DNA (5'-D(\*DCP\*DAP\*DGP\*DTP\*DAP\*DC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1-P	6	Total	C	N	O	P	0	6	0
			119	58	23	33	5			
2	1-Q	6	Total	C	N	O	P	0	6	0
			119	58	23	33	5			
2	2-P	6	Total	C	N	O	P	0	6	0
			119	58	23	33	5			
2	2-Q	6	Total	C	N	O	P	0	6	0
			119	58	23	33	5			

- Molecule 3 is a DNA chain called DNA (5'-D(P\*DGP\*DCP\*DCP\*DG)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1-D	4	Total	C	N	O	P	0	4	0
			83	38	16	25	4			
3	1-E	4	Total	C	N	O	P	0	4	0
			83	38	16	25	4			
3	2-D	4	Total	C	N	O	P	0	4	0
			83	38	16	25	4			
3	2-E	4	Total	C	N	O	P	0	4	0
			83	38	16	25	4			

- Molecule 4 is a protein called DNA polymerase lambda.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	1-A	326	Total	C	N	O	S	0	326	0
			2541	1598	462	469	12			
4	1-B	326	Total	C	N	O	S	0	326	0
			2551	1604	467	468	12			
4	2-A	326	Total	C	N	O	S	0	326	0
			2541	1598	462	469	12			
4	2-B	325	Total	C	N	O	S	0	325	0
			2538	1597	465	464	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	MET	-	expression tag	UNP Q9UGP5
A	517	ALA	ARG	engineered	UNP Q9UGP5
B	241	MET	-	expression tag	UNP Q9UGP5
B	517	ALA	ARG	engineered	UNP Q9UGP5

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	2-A	3	Total	Na	0	3
			3	3		
5	1-B	3	Total	Na	0	3
			3	3		
5	1-A	3	Total	Na	0	3
			3	3		
5	2-B	3	Total	Na	0	3
			3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1-A	321	Total	O	0	321
			321	321		
6	1-B	259	Total	O	0	259
			259	259		
6	1-D	3	Total	O	0	3
			3	3		
6	1-E	3	Total	O	0	3
			3	3		
6	1-P	18	Total	O	0	18
			18	18		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1-Q	11	Total 11	O 11	0	11
6	1-T	16	Total 16	O 16	0	16
6	1-U	8	Total 8	O 8	0	8
6	2-A	324	Total 324	O 324	0	324
6	2-B	257	Total 257	O 257	0	257
6	2-D	3	Total 3	O 3	0	3
6	2-E	2	Total 2	O 2	0	2
6	2-P	18	Total 18	O 18	0	18
6	2-Q	11	Total 11	O 11	0	11
6	2-T	11	Total 11	O 11	0	11
6	2-U	13	Total 13	O 13	0	13

### 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 errors 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.

Note EDS failed to run properly.

- Molecule 1: DNA (5'-D(\*DCP\*DGP\*DGP\*DCP\*DCP\*DGP\*DTP\*DAP\*DCP\*DTP\*DG)-3')

Chain 1-T: 



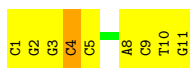
- Molecule 1: DNA (5'-D(\*DCP\*DGP\*DGP\*DCP\*DCP\*DGP\*DTP\*DAP\*DCP\*DTP\*DG)-3')

Chain 1-U: 



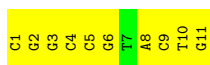
- Molecule 1: DNA (5'-D(\*DCP\*DGP\*DGP\*DCP\*DCP\*DGP\*DTP\*DAP\*DCP\*DTP\*DG)-3')

Chain 2-T: 



- Molecule 1: DNA (5'-D(\*DCP\*DGP\*DGP\*DCP\*DCP\*DGP\*DTP\*DAP\*DCP\*DTP\*DG)-3')

Chain 2-U: 



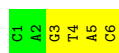
- Molecule 2: DNA (5'-D(\*DCP\*DAP\*DGP\*DTP\*DAP\*DC)-3')

Chain 1-P: 

There are no outlier residues recorded for this chain.

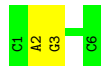
- Molecule 2: DNA (5'-D(\*DCP\*DAP\*DGP\*DTP\*DAP\*DC)-3')

Chain 1-Q: 



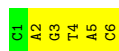
- Molecule 2: DNA (5'-D(\*DCP\*DAP\*DGP\*DTP\*DAP\*DC)-3')

Chain 2-P:



- Molecule 2: DNA (5'-D(\*DCP\*DAP\*DGP\*DTP\*DAP\*DC)-3')

Chain 2-Q:



- Molecule 3: DNA (5'-D(P\*DGP\*DCP\*DCP\*DG)-3')

Chain 1-D:



- Molecule 3: DNA (5'-D(P\*DGP\*DCP\*DCP\*DG)-3')

Chain 1-E:



- Molecule 3: DNA (5'-D(P\*DGP\*DCP\*DCP\*DG)-3')

Chain 2-D:



- Molecule 3: DNA (5'-D(P\*DGP\*DCP\*DCP\*DG)-3')

Chain 2-E:



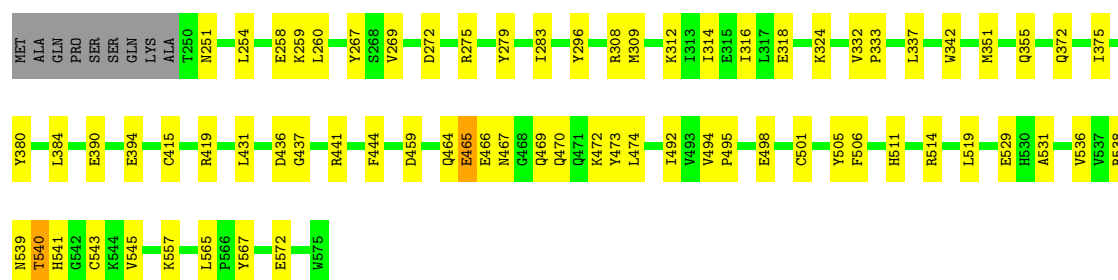
- Molecule 4: DNA polymerase lambda

Chain 1-A:



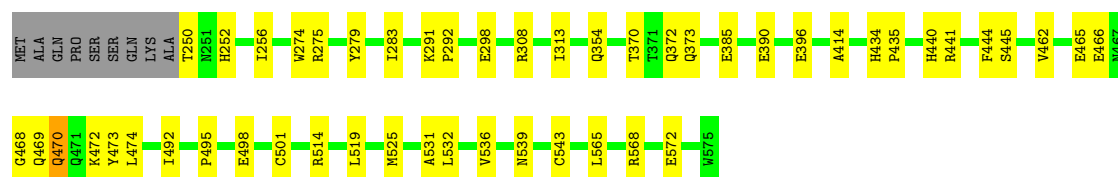
- Molecule 4: DNA polymerase lambda

Chain 1-B:



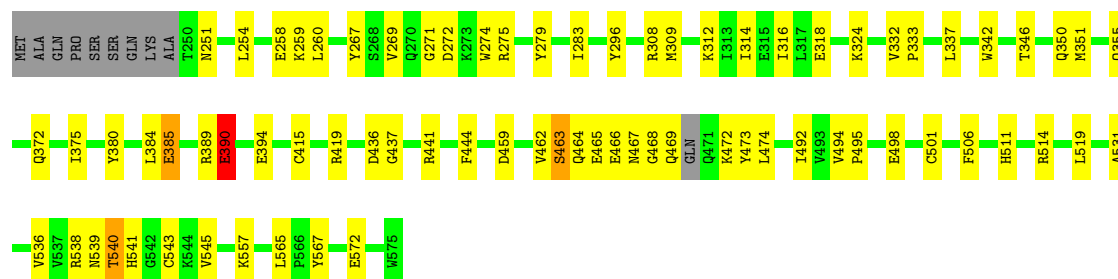
• Molecule 4: DNA polymerase lambda

Chain 2-A:



• Molecule 4: DNA polymerase lambda

Chain 2-B:



## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.24Å 151.88Å 85.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25	Depositor
% Data completeness (in resolution range)	85.2 (50.00-2.25)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.24Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.224 , 0.263	Depositor
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtriage
Anisotropy	0.223	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	5 of 56789 reflections (0.009%)	Xtriage
Total number of atoms	13157	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.39 % 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 3.1954e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	1-T	0.46	0/248	0.72	0/381
1	1-U	0.38	0/248	0.76	0/381
2	1-P	0.45	0/133	0.74	0/203
2	1-Q	0.49	0/133	0.71	0/203
3	1-D	1.03	1/92 (1.1%)	0.80	0/138
3	1-E	1.07	1/92 (1.1%)	0.76	0/138
4	1-A	0.37	0/2594	0.60	2/3502 (0.1%)
4	1-B	0.37	0/2604	0.59	0/3515
All	All	0.42	2/6144 (0.0%)	0.62	2/8461 (0.0%)

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	2-T	0	1
2	1-Q	0	1
2	2-Q	0	1
3	1-E	0	1
3	2-E	0	1
4	2-B	0	3
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-E	1[A]	DG	OP3-P	-7.66	1.51	1.61
3	1-D	1[A]	DG	OP3-P	-7.00	1.52	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1-A	368[A]	SER	CB-CA-C	5.82	121.16	110.10
4	1-A	471[A]	GLN	N-CA-C	5.73	126.47	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	1-E	1[A]	DG	Sidechain
2	1-Q	6[A]	DC	Sidechain
4	2-B	385[B]	GLU	Mainchain
4	2-B	389[B]	ARG	Mainchain
4	2-B	390[B]	GLU	Mainchain
3	2-E	1[B]	DG	Sidechain
2	2-Q	6[B]	DC	Sidechain
1	2-T	4[B]	DC	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-T	222	0	125	5	0
1	1-U	222	0	125	22	0
1	2-T	222	0	126	43	0
1	2-U	222	0	125	26	0
2	1-P	119	0	69	0	0
2	1-Q	119	0	69	2	0
2	2-P	119	0	69	6	0
2	2-Q	119	0	69	8	0
3	1-D	83	0	45	3	0
3	1-E	83	0	45	3	0
3	2-D	83	0	45	3	0
3	2-E	83	0	45	3	0
4	1-A	2541	0	2520	31	0
4	1-B	2551	0	2539	76	0
4	2-A	2541	0	2518	47	0
4	2-B	2538	0	2528	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	1-A	3	0	0	0	0
5	1-B	3	0	0	0	0
5	2-A	3	0	0	0	0
5	2-B	3	0	0	0	0
6	1-A	321	0	0	6	0
6	1-B	259	0	0	6	0
6	1-D	3	0	0	0	0
6	1-E	3	0	0	0	0
6	1-P	18	0	0	0	0
6	1-Q	11	0	0	0	0
6	1-T	16	0	0	1	0
6	1-U	8	0	0	0	0
6	2-A	324	0	0	6	0
6	2-B	257	0	0	8	0
6	2-D	3	0	0	0	0
6	2-E	2	0	0	0	0
6	2-P	18	0	0	0	0
6	2-Q	11	0	0	0	0
6	2-T	11	0	0	1	0
6	2-U	13	0	0	0	0
All	All	13157	0	11062	286	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (286) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:T:10[B]:DT:H3'	1:T:11[B]:DG:P	1.66	1.36
1:T:10[B]:DT:C3'	1:T:11[B]:DG:P	2.19	1.28
1:T:10[B]:DT:O3'	1:T:11[B]:DG:H5'	1.08	1.24
1:U:9[B]:DC:OP2	4:B:464[B]:GLN:OE1	1.56	1.23
1:T:10[B]:DT:O3'	1:T:11[B]:DG:C5'	1.86	1.22
1:T:3[B]:DG:O3'	1:T:4[B]:DC:P	1.99	1.20
1:U:9[A]:DC:C4'	4:B:465[A]:GLU:HG2	1.78	1.09
1:T:10[B]:DT:O3'	1:T:11[B]:DG:P	2.11	1.08
4:A:469[B]:GLN:N	4:B:469[B]:GLN:HA	1.67	1.01
1:T:3[B]:DG:C3'	1:T:4[B]:DC:OP2	2.08	1.01
4:A:469[B]:GLN:NE2	4:B:468[B]:GLY:O	1.93	1.00
1:T:4[B]:DC:H3'	1:T:5[B]:DC:H5''	1.43	0.99
4:B:519[B]:LEU:HD23	4:B:565[B]:LEU:HD11	1.44	0.99
4:B:519[A]:LEU:HD23	4:B:565[A]:LEU:HD11	1.44	0.99
1:U:8[B]:DA:H2''	1:U:9[B]:DC:OP1	1.70	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:T:5[B]:DC:OP2	4:A:514[B]:ARG:NH2	2.07	0.87
4:A:354[B]:GLN:HG2	6:A:1114[B]:HOH:O	1.75	0.85
4:B:472[B]:LYS:HD3	4:B:474[B]:LEU:HD21	1.56	0.85
4:B:472[A]:LYS:HD3	4:B:474[A]:LEU:HD21	1.56	0.85
4:A:354[A]:GLN:HG2	6:A:1114[A]:HOH:O	1.75	0.85
1:U:9[A]:DC:H4'	4:B:465[A]:GLU:HG2	1.58	0.82
4:A:469[B]:GLN:HA	4:B:469[B]:GLN:N	1.93	0.82
4:B:470[A]:GLN:HG2	4:B:494[A]:VAL:HG12	1.63	0.81
1:T:3[B]:DG:O3'	1:T:4[B]:DC:OP1	1.96	0.81
1:T:4[B]:DC:C3'	1:T:5[B]:DC:H5''	2.09	0.81
1:T:3[B]:DG:H3'	1:T:4[B]:DC:OP2	1.79	0.81
1:T:9[B]:DC:N4	2:P:2[B]:DA:H61	1.79	0.80
1:U:9[A]:DC:OP2	4:B:466[A]:GLU:C	2.16	0.80
4:B:572[B]:GLU:HG3	6:B:864[B]:HOH:O	1.82	0.79
4:B:572[A]:GLU:HG3	6:B:864[A]:HOH:O	1.82	0.79
1:T:3[B]:DG:O3'	1:T:4[B]:DC:OP2	1.94	0.79
1:U:9[A]:DC:O4'	4:B:465[A]:GLU:HG2	1.81	0.79
1:T:10[B]:DT:HO3'	1:T:11[B]:DG:H5'	0.99	0.78
1:U:8[A]:DA:H3'	4:B:467[A]:ASN:CA	1.82	0.78
4:B:260[B]:LEU:HD13	4:B:309[B]:MET:HE1	1.64	0.76
4:B:260[A]:LEU:HD13	4:B:309[A]:MET:HE1	1.64	0.76
1:U:9[A]:DC:OP2	4:B:467[A]:ASN:N	2.18	0.76
1:U:4[B]:DC:H2'	4:B:274[B]:TRP:CZ3	2.21	0.76
1:T:10[B]:DT:C4	1:T:11[B]:DG:C6	2.75	0.74
1:U:8[A]:DA:H1'	4:B:465[A]:GLU:CD	2.08	0.74
4:A:525[B]:MET:HE1	4:A:532[B]:LEU:HD21	1.70	0.73
4:A:525[A]:MET:HE1	4:A:532[A]:LEU:HD21	1.70	0.73
1:U:9[B]:DC:N4	2:Q:2[B]:DA:H61	1.86	0.72
4:A:465[B]:GLU:HA	6:A:1090[B]:HOH:O	1.89	0.72
4:A:465[A]:GLU:HA	6:A:1090[A]:HOH:O	1.89	0.72
1:U:9[B]:DC:H6	1:U:9[B]:DC:H5''	1.54	0.71
4:B:539[B]:ASN:ND2	4:B:543[B]:CYS:HB2	2.06	0.71
4:B:539[A]:ASN:ND2	4:B:543[A]:CYS:HB2	2.06	0.71
1:U:8[B]:DA:N6	2:Q:3[B]:DG:O6	2.23	0.71
4:B:540[B]:THR:OG1	4:B:541[B]:HIS:CD2	2.44	0.71
4:B:540[A]:THR:OG1	4:B:541[A]:HIS:CD2	2.44	0.71
4:B:538[B]:ARG:HA	4:B:543[B]:CYS:O	1.91	0.70
4:B:538[A]:ARG:HA	4:B:543[A]:CYS:O	1.91	0.70
4:B:540[B]:THR:OG1	4:B:541[B]:HIS:HD2	1.74	0.70
4:B:540[A]:THR:OG1	4:B:541[A]:HIS:HD2	1.74	0.70
4:A:468[B]:GLY:C	4:B:469[B]:GLN:HA	2.12	0.69
1:U:5[B]:DC:C2'	1:U:6[B]:DG:H5'	2.21	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:T:6[A]:DG:OP1	4:A:521[A]:LYS:HD2	1.92	0.69
1:T:10[B]:DT:N3	1:T:11[B]:DG:C6	2.62	0.68
1:T:9[B]:DC:H42	2:P:2[B]:DA:N6	1.92	0.68
1:U:10[B]:DT:H2''	1:U:11[B]:DG:H5'	1.76	0.68
4:A:469[B]:GLN:HA	4:B:469[B]:GLN:H	1.59	0.67
4:B:279[B]:TYR:OH	4:B:312[B]:LYS:HE2	1.93	0.67
4:B:279[A]:TYR:OH	4:B:312[A]:LYS:HE2	1.93	0.67
1:T:9[B]:DC:N4	2:P:2[B]:DA:N6	2.42	0.67
1:U:9[B]:DC:N3	2:Q:3[B]:DG:N1	2.41	0.66
4:B:467[B]:ASN:ND2	4:B:469[B]:GLN:H	1.94	0.66
1:U:1[B]:DC:H2''	1:U:2[B]:DG:H5'	1.77	0.65
4:A:372[B]:GLN:HG3	6:A:982[B]:HOH:O	1.94	0.65
4:A:372[A]:GLN:HG3	6:A:982[A]:HOH:O	1.94	0.65
1:U:1[A]:DC:H2''	1:U:2[A]:DG:O5'	1.96	0.65
1:T:4[B]:DC:H2''	4:A:274[B]:TRP:CZ3	2.32	0.64
4:B:351[B]:MET:HG2	4:B:355[B]:GLN:HE21	1.61	0.64
4:B:351[A]:MET:HG2	4:B:355[A]:GLN:HE21	1.61	0.64
4:B:260[B]:LEU:HD13	4:B:309[B]:MET:CE	2.27	0.64
4:B:260[A]:LEU:HD13	4:B:309[A]:MET:CE	2.27	0.64
4:B:519[B]:LEU:HD21	4:B:565[B]:LEU:HD21	1.81	0.63
4:B:519[A]:LEU:HD21	4:B:565[A]:LEU:HD21	1.81	0.63
4:A:444[B]:PHE:CZ	4:A:473[B]:TYR:HB2	2.34	0.62
4:A:444[A]:PHE:CZ	4:A:473[A]:TYR:HB2	2.34	0.62
1:T:10[B]:DT:H3'	1:T:11[B]:DG:OP2	2.00	0.61
4:A:308[B]:ARG:HG3	4:A:308[B]:ARG:HH11	1.66	0.60
4:A:308[A]:ARG:HG3	4:A:308[A]:ARG:HH11	1.66	0.60
4:A:536[B]:VAL:HG22	6:A:950[B]:HOH:O	2.00	0.60
4:A:536[A]:VAL:HG22	6:A:950[A]:HOH:O	2.00	0.60
4:B:254[B]:LEU:O	4:B:258[B]:GLU:HG2	2.01	0.60
4:A:396[B]:GLU:HG3	4:A:414[B]:ALA:HB2	1.83	0.60
4:B:254[A]:LEU:O	4:B:258[A]:GLU:HG2	2.01	0.60
4:A:396[A]:GLU:HG3	4:A:414[A]:ALA:HB2	1.83	0.60
1:T:10[B]:DT:O4	1:T:11[B]:DG:O6	2.20	0.60
4:B:470[A]:GLN:HG2	4:B:494[A]:VAL:CG1	2.31	0.60
1:U:9[B]:DC:N4	2:Q:2[B]:DA:N6	2.49	0.59
4:A:519[B]:LEU:HD21	4:A:565[B]:LEU:HD21	1.84	0.58
1:U:9[A]:DC:H4'	4:B:465[A]:GLU:CG	2.32	0.58
1:U:8[A]:DA:H3'	4:B:467[A]:ASN:N	2.18	0.58
1:T:4[B]:DC:C3'	1:T:5[B]:DC:C5'	2.81	0.57
1:U:5[B]:DC:H2'	1:U:6[B]:DG:H5'	1.84	0.57
1:T:10[B]:DT:C4	1:T:11[B]:DG:O6	2.58	0.57
4:B:465[A]:GLU:O	4:B:466[A]:GLU:C	2.38	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:385[B]:GLU:HG2	6:B:979[B]:HOH:O	2.04	0.57
4:A:252[B]:HIS:HB3	4:A:292[B]:PRO:HG3	1.86	0.57
4:A:252[A]:HIS:HB3	4:A:292[A]:PRO:HG3	1.86	0.57
1:T:8[B]:DA:C6	2:P:3[B]:DG:O6	2.58	0.56
1:T:8[B]:DA:N1	2:P:3[B]:DG:O6	2.39	0.56
4:B:279[B]:TYR:O	4:B:283[B]:ILE:HG13	2.06	0.56
4:B:279[A]:TYR:O	4:B:283[A]:ILE:HG13	2.06	0.56
4:A:441[B]:ARG:CZ	4:B:465[B]:GLU:O	2.54	0.56
1:U:9[A]:DC:C4'	4:B:465[A]:GLU:CG	2.67	0.56
4:B:346[B]:THR:O	4:B:350[B]:GLN:HG3	2.06	0.56
4:B:372[B]:GLN:HG3	6:B:903[B]:HOH:O	2.06	0.55
4:B:372[A]:GLN:HG3	6:B:903[A]:HOH:O	2.06	0.55
4:A:492[B]:ILE:HD12	4:A:492[B]:ILE:N	2.21	0.55
4:A:492[A]:ILE:HD12	4:A:492[A]:ILE:N	2.21	0.55
4:B:539[B]:ASN:C	4:B:539[B]:ASN:OD1	2.45	0.55
4:B:539[A]:ASN:C	4:B:539[A]:ASN:OD1	2.45	0.55
1:T:10[B]:DT:C3'	1:T:11[B]:DG:OP2	2.54	0.55
4:A:466[B]:GLU:HG2	4:B:437[B]:GLY:O	2.06	0.55
4:A:466[A]:GLU:HG2	4:B:437[A]:GLY:O	2.06	0.55
1:U:8[B]:DA:H2'	1:U:9[B]:DC:C6	2.42	0.55
1:U:8[B]:DA:H2'	1:U:9[B]:DC:H5''	1.89	0.55
4:B:296[B]:TYR:N	4:B:314[B]:ILE:HD11	2.22	0.54
4:B:464[A]:GLN:O	4:B:465[A]:GLU:HB2	2.06	0.54
4:B:296[A]:TYR:N	4:B:314[A]:ILE:HD11	2.22	0.54
1:T:5[B]:DC:P	4:A:514[B]:ARG:HH21	2.29	0.54
4:A:501[B]:CYS:SG	4:A:531[B]:ALA:HA	2.48	0.54
4:A:501[A]:CYS:SG	4:A:531[A]:ALA:HA	2.48	0.54
1:T:10[B]:DT:C4	1:T:11[B]:DG:C5	2.96	0.53
4:B:519[B]:LEU:CD2	4:B:565[B]:LEU:HD11	2.29	0.53
4:B:519[A]:LEU:CD2	4:B:565[A]:LEU:HD11	2.29	0.53
4:B:390[B]:GLU:O	4:B:394[B]:GLU:HG3	2.08	0.53
3:D:3[B]:DC:H2''	3:D:4[B]:DG:C8	2.44	0.53
1:T:1[B]:DC:H2'	1:T:2[B]:DG:C8	2.44	0.53
3:D:3[A]:DC:H2''	3:D:4[A]:DG:C8	2.44	0.53
1:T:1[A]:DC:H2'	1:T:2[A]:DG:C8	2.44	0.53
1:T:5[B]:DC:H2'	6:T:591[B]:HOH:O	2.08	0.52
1:T:4[B]:DC:H3'	1:T:5[B]:DC:C5'	2.28	0.52
1:T:10[B]:DT:O3'	1:T:11[B]:DG:O5'	2.23	0.52
4:B:511[B]:HIS:O	4:B:514[B]:ARG:HG3	2.09	0.52
4:B:464[A]:GLN:O	4:B:465[A]:GLU:CB	2.58	0.52
4:B:511[A]:HIS:O	4:B:514[A]:ARG:HG3	2.09	0.52
1:T:10[B]:DT:C5	1:T:11[B]:DG:N7	2.78	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:501[B]:CYS:SG	4:B:531[B]:ALA:HA	2.50	0.52
4:B:501[A]:CYS:SG	4:B:531[A]:ALA:HA	2.50	0.52
1:T:10[B]:DT:N3	1:T:11[B]:DG:C5	2.79	0.51
4:A:519[B]:LEU:HD22	4:A:565[B]:LEU:HD11	1.91	0.51
1:T:6[A]:DG:H1'	6:T:229[A]:HOH:O	2.10	0.51
4:B:390[A]:GLU:O	4:B:394[A]:GLU:HG3	2.11	0.51
4:A:539[B]:ASN:N	4:A:543[B]:CYS:O	2.41	0.51
4:A:539[A]:ASN:N	4:A:543[A]:CYS:O	2.41	0.51
1:U:1[A]:DC:H2'	1:U:2[A]:DG:C8	2.46	0.51
1:T:9[B]:DC:H4'	4:A:462[B]:VAL:HG13	1.93	0.50
1:U:7[A]:DT:H2''	4:B:467[A]:ASN:ND2	2.27	0.50
1:T:3[B]:DG:C2'	1:T:4[B]:DC:OP2	2.60	0.50
1:U:7[A]:DT:H4'	4:B:529[A]:GLU:OE1	2.13	0.49
4:B:314[B]:ILE:O	4:B:318[B]:GLU:HG3	2.11	0.49
3:E:1[B]:DG:H2'	3:E:2[B]:DC:C6	2.48	0.49
4:B:384[B]:LEU:HD23	6:B:946[B]:HOH:O	2.11	0.49
4:B:314[A]:ILE:O	4:B:318[A]:GLU:HG3	2.11	0.49
3:E:1[A]:DG:H2'	3:E:2[A]:DC:C6	2.48	0.49
4:B:384[A]:LEU:HD23	6:B:946[A]:HOH:O	2.11	0.49
4:B:269[B]:VAL:HG21	4:B:332[B]:VAL:HG13	1.94	0.49
4:B:337[B]:LEU:HD12	4:B:380[B]:TYR:OH	2.12	0.49
4:B:269[A]:VAL:HG21	4:B:332[A]:VAL:HG13	1.94	0.49
4:B:337[A]:LEU:HD12	4:B:380[A]:TYR:OH	2.12	0.49
4:B:259[B]:LYS:HD2	4:B:316[B]:ILE:HD13	1.94	0.49
4:B:259[A]:LYS:HD2	4:B:316[A]:ILE:HD13	1.94	0.49
4:B:519[B]:LEU:CD2	4:B:565[B]:LEU:HD21	2.42	0.49
4:B:519[A]:LEU:CD2	4:B:565[A]:LEU:HD21	2.42	0.49
4:A:568[B]:ARG:HG3	4:A:572[B]:GLU:HB2	1.95	0.49
4:A:568[A]:ARG:HG3	4:A:572[A]:GLU:HB2	1.95	0.49
1:T:10[B]:DT:C6	1:T:11[B]:DG:N7	2.81	0.48
4:B:467[B]:ASN:HD22	4:B:468[B]:GLY:N	2.11	0.48
1:U:1[B]:DC:H2'	1:U:2[B]:DG:C8	2.49	0.48
4:A:441[B]:ARG:NH1	4:B:465[B]:GLU:HB3	2.28	0.48
1:T:10[B]:DT:C2	1:T:11[B]:DG:C5	3.01	0.48
1:U:8[B]:DA:C6	2:Q:3[B]:DG:O6	2.67	0.48
1:U:8[B]:DA:C2'	1:U:9[B]:DC:H5''	2.44	0.48
1:U:8[A]:DA:H1'	4:B:465[A]:GLU:OE2	2.13	0.48
4:B:492[B]:ILE:HD13	4:B:506[B]:PHE:CZ	2.48	0.48
4:B:462[B]:VAL:O	4:B:463[B]:SER:HB2	2.12	0.48
4:B:492[A]:ILE:HD13	4:B:506[A]:PHE:CZ	2.48	0.48
3:E:3[B]:DC:H2''	3:E:4[B]:DG:C8	2.48	0.47
3:E:3[A]:DC:H2''	3:E:4[A]:DG:C8	2.48	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:8[A]:DA:H1'	4:B:465[A]:GLU:OE1	2.13	0.47
1:U:9[B]:DC:H42	2:Q:2[B]:DA:N6	2.13	0.47
4:A:291[B]:LYS:HE3	4:A:298[B]:GLU:OE2	2.14	0.47
4:A:291[A]:LYS:HE3	4:A:298[A]:GLU:OE2	2.14	0.47
1:U:5[B]:DC:N4	1:U:6[B]:DG:C6	2.82	0.47
1:T:9[B]:DC:O2	2:P:3[B]:DG:N2	2.41	0.47
4:B:271[B]:GLY:HA2	4:B:346[B]:THR:HG21	1.96	0.46
4:A:440[B]:HIS:CE1	4:B:466[B]:GLU:O	2.68	0.46
1:U:9[B]:DC:H4'	1:U:9[B]:DC:OP1	2.15	0.46
4:B:351[B]:MET:HG2	4:B:355[B]:GLN:NE2	2.29	0.46
1:U:9[A]:DC:P	4:B:467[A]:ASN:N	2.88	0.46
4:B:470[A]:GLN:CG	4:B:494[A]:VAL:HG12	2.40	0.46
4:B:351[A]:MET:HG2	4:B:355[A]:GLN:NE2	2.29	0.46
4:A:467[A]:ASN:OD1	4:B:469[A]:GLN:HA	2.15	0.46
4:B:536[B]:VAL:HG22	6:B:958[B]:HOH:O	2.15	0.46
4:B:495[B]:PRO:HG2	4:B:498[B]:GLU:HG3	1.98	0.46
4:B:495[A]:PRO:HG2	4:B:498[A]:GLU:HG3	1.98	0.46
4:B:536[A]:VAL:HG22	6:B:958[A]:HOH:O	2.15	0.46
4:A:308[B]:ARG:HG3	4:A:308[B]:ARG:NH1	2.26	0.46
4:B:390[B]:GLU:HG2	6:B:947[B]:HOH:O	2.16	0.46
4:A:308[A]:ARG:HG3	4:A:308[A]:ARG:NH1	2.26	0.46
4:A:256[B]:ILE:HD13	4:A:313[B]:ILE:HG23	1.98	0.46
4:A:256[A]:ILE:HD13	4:A:313[A]:ILE:HG23	1.98	0.46
1:U:9[B]:DC:OP1	1:U:9[B]:DC:C4'	2.64	0.46
4:A:385[B]:GLU:HB3	6:A:842[B]:HOH:O	2.14	0.46
4:A:385[A]:GLU:HB3	6:A:842[A]:HOH:O	2.14	0.46
1:U:5[B]:DC:C3'	1:U:6[B]:DG:H5'	2.46	0.45
4:A:441[B]:ARG:HH12	4:B:465[B]:GLU:HB3	1.81	0.45
4:B:415[B]:CYS:HA	4:B:419[B]:ARG:HB2	1.97	0.45
4:B:415[A]:CYS:HA	4:B:419[A]:ARG:HB2	1.97	0.45
1:U:6[A]:DG:C2	4:B:505[A]:TYR:OH	2.61	0.45
2:Q:3[B]:DG:H2''	2:Q:4[B]:DT:O5'	2.16	0.45
2:Q:3[A]:DG:H2''	2:Q:4[A]:DT:O5'	2.16	0.45
3:D:1[B]:DG:H2''	3:D:2[B]:DC:H5'	1.98	0.45
3:D:1[A]:DG:H2''	3:D:2[A]:DC:H5'	1.98	0.45
4:A:279[B]:TYR:O	4:A:283[B]:ILE:HG13	2.17	0.44
4:A:495[B]:PRO:HG2	4:A:498[B]:GLU:HG3	1.99	0.44
4:A:279[A]:TYR:O	4:A:283[A]:ILE:HG13	2.17	0.44
4:A:495[A]:PRO:HG2	4:A:498[A]:GLU:HG3	1.99	0.44
3:E:2[B]:DC:P	4:B:308[B]:ARG:HB2	2.57	0.44
4:B:545[B]:VAL:O	4:B:545[B]:VAL:HG22	2.17	0.44
3:E:2[A]:DC:P	4:B:308[A]:ARG:HB2	2.57	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:545[A]:VAL:O	4:B:545[A]:VAL:HG22	2.17	0.44
1:U:3[A]:DG:H2''	1:U:4[A]:DC:O5'	2.18	0.44
4:B:464[A]:GLN:O	4:B:472[A]:LYS:O	2.35	0.44
1:U:9[B]:DC:C6	1:U:9[B]:DC:H5''	2.43	0.44
1:U:1[B]:DC:C2'	1:U:2[B]:DG:H5'	2.47	0.43
4:B:375[B]:ILE:HD13	4:B:459[B]:ASP:HB3	2.01	0.43
4:B:375[A]:ILE:HD13	4:B:459[A]:ASP:HB3	2.01	0.43
4:A:472[B]:LYS:HE2	4:A:474[B]:LEU:HD21	2.00	0.43
4:A:472[A]:LYS:HE2	4:A:474[A]:LEU:HD21	2.00	0.43
4:A:469[B]:GLN:O	4:A:470[B]:GLN:C	2.57	0.43
4:A:469[A]:GLN:O	4:A:470[A]:GLN:C	2.57	0.43
4:B:539[B]:ASN:CG	4:B:543[B]:CYS:HB2	2.39	0.43
1:U:8[A]:DA:H3'	4:B:467[A]:ASN:HA	1.86	0.43
4:B:539[A]:ASN:CG	4:B:543[A]:CYS:HB2	2.39	0.43
2:Q:5[B]:DA:H4'	4:B:342[B]:TRP:CZ2	2.54	0.43
2:Q:5[A]:DA:H4'	4:B:342[A]:TRP:CZ2	2.54	0.43
4:A:370[B]:THR:HG23	4:A:373[B]:GLN:OE1	2.18	0.43
4:B:272[B]:ASP:OD1	4:B:275[B]:ARG:HB2	2.19	0.43
4:B:272[A]:ASP:OD1	4:B:275[A]:ARG:HB2	2.19	0.43
4:A:370[A]:THR:HG23	4:A:373[A]:GLN:OE1	2.18	0.43
1:T:9[A]:DC:H2''	1:T:10[A]:DT:H6	1.85	0.42
4:B:436[B]:ASP:C	4:B:436[B]:ASP:OD1	2.58	0.42
4:B:436[A]:ASP:OD1	4:B:436[A]:ASP:C	2.58	0.42
1:U:3[B]:DG:H2''	1:U:4[B]:DC:C6	2.55	0.42
3:D:1[B]:DG:OP2	4:A:275[B]:ARG:NH1	2.52	0.42
4:A:434[B]:HIS:HA	4:A:435[B]:PRO:HD3	1.85	0.42
3:D:1[A]:DG:OP2	4:A:275[A]:ARG:NH1	2.52	0.42
4:A:434[A]:HIS:HA	4:A:435[A]:PRO:HD3	1.85	0.42
4:A:445[B]:SER:HB3	4:B:441[B]:ARG:NH1	2.34	0.42
4:A:445[A]:SER:HB3	4:B:441[A]:ARG:NH1	2.34	0.42
4:A:250[B]:THR:HG22	6:A:1118[B]:HOH:O	2.19	0.42
4:A:250[A]:THR:HG22	6:A:1118[A]:HOH:O	2.19	0.42
4:B:572[B]:GLU:CG	6:B:864[B]:HOH:O	2.55	0.42
4:B:332[B]:VAL:HB	4:B:333[B]:PRO:HD3	2.02	0.42
4:B:572[A]:GLU:CG	6:B:864[A]:HOH:O	2.55	0.42
4:B:332[A]:VAL:HB	4:B:333[A]:PRO:HD3	2.02	0.42
4:A:468[B]:GLY:O	4:B:468[B]:GLY:C	2.57	0.42
1:U:8[A]:DA:OP1	4:B:467[A]:ASN:C	2.58	0.42
4:B:541[B]:HIS:N	4:B:541[B]:HIS:CD2	2.87	0.41
4:B:541[A]:HIS:CD2	4:B:541[A]:HIS:N	2.87	0.41
4:A:519[B]:LEU:CD2	4:A:565[B]:LEU:HD21	2.50	0.41
1:T:1[B]:DC:H2''	1:T:2[B]:DG:H5'	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:267[B]:TYR:CE1	4:B:275[B]:ARG:HD2	2.55	0.41
1:U:9[A]:DC:H4'	4:B:464[A]:GLN:C	2.40	0.41
1:T:1[A]:DC:H2''	1:T:2[A]:DG:H5'	2.01	0.41
4:B:267[A]:TYR:CE1	4:B:275[A]:ARG:HD2	2.55	0.41
1:T:5[B]:DC:OP2	4:A:514[B]:ARG:CZ	2.66	0.41
4:A:250[B]:THR:O	4:A:250[B]:THR:HG22	2.20	0.41
4:A:250[A]:THR:O	4:A:250[A]:THR:HG22	2.20	0.41
4:B:494[B]:VAL:HB	4:B:495[B]:PRO:HD2	2.03	0.41
4:B:494[A]:VAL:HB	4:B:495[A]:PRO:HD2	2.03	0.41
4:B:324[B]:LYS:HD2	6:B:1025[B]:HOH:O	2.22	0.40
4:B:444[B]:PHE:CZ	4:B:473[B]:TYR:HB2	2.56	0.40
4:A:390[B]:GLU:H	4:A:390[B]:GLU:CD	2.25	0.40
4:B:324[A]:LYS:HD2	6:B:1025[A]:HOH:O	2.22	0.40
4:B:444[A]:PHE:CZ	4:B:473[A]:TYR:HB2	2.56	0.40
4:A:390[A]:GLU:H	4:A:390[A]:GLU:CD	2.25	0.40
1:T:3[B]:DG:O3'	1:T:4[B]:DC:O5'	2.39	0.40
1:U:4[B]:DC:H5'	1:U:5[B]:DC:H5'	2.04	0.40
4:B:557[B]:LYS:HE3	4:B:567[B]:TYR:CZ	2.56	0.40
4:B:557[A]:LYS:HE3	4:B:567[A]:TYR:CZ	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	
4	1-A	324/335 (97%)	315 (97%)	8 (2%)	1 (0%)	50	54
4	1-B	324/335 (97%)	311 (96%)	10 (3%)	3 (1%)	25	20
4	2-A	324/335 (97%)	315 (97%)	8 (2%)	1 (0%)	50	54
4	2-B	321/335 (96%)	309 (96%)	8 (2%)	4 (1%)	19	13
All	All	1293/1340 (96%)	1250 (97%)	34 (3%)	9 (1%)	30	29

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	2-B	463[B]	SER
4	1-A	470[A]	GLN
4	1-B	465[A]	GLU
4	2-A	470[B]	GLN
4	1-B	251[A]	ASN
4	2-B	251[B]	ASN
4	2-B	390[B]	GLU
4	1-B	540[A]	THR
4	2-B	540[B]	THR

### 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	
4	1-A	267/280 (95%)	266 (100%)	1 (0%)	95	97
4	1-B	269/280 (96%)	268 (100%)	1 (0%)	95	97
All	All	536/560 (96%)	534 (100%)	2 (0%)	95	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	1-A	300[A]	CYS
4	1-B	431[A]	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
4	1-A	327[A]	HIS
4	1-A	379[A]	HIS
4	1-A	486[A]	HIS
4	1-B	355[A]	GLN
4	1-B	379[A]	HIS
4	1-B	486[A]	HIS
4	1-B	541[A]	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 12 ligands modelled in this entry, 12 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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.