

Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 07:41 AM EDT

PDB ID	:	5W6Q
Title	:	Structural basis for recognition of artificial DNA by an evolved KlenTaq variant
Authors	:	Singh, I.; Georgiadis, M.M.
Deposited on	:	2017-06-16
Resolution	:	2.66 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 (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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
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)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.66 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	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m A}))$
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349(2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	А	540	% •		9%	5%				
-	G	510	% •		570	570				
	С	540			12%	•				
1	G	540	86%		12%	•				
2	В	12	58%	33%	89	%				
2	Е	12	50%	50%						



Mol	Chain	Length	Quality of chain							
2	Н	12	50%	50%						
3	D	13	69%	31%						
3	F	13	62%	38%						
3	Ι	13	<u>8%</u> 69%	31%						



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2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14188 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	515	Total	С	Ν	0	\mathbf{S}	0	1	0
	I A	515	4069	2587	730	742	10	0	1	
1	C	521	Total	С	Ν	0	S	0	1	0
			4117	2617	743	747	10	0		U
1	C	597	Total	С	Ν	0	S	0	0	0
I G	027	4165	2652	746	756	11	0		0	

• Molecule 1 is a protein called DNA polymerase I, thermostable.

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There are 12	discrepancies	between	the modelled	and	reference	sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	444	VAL	MET	engineered mutation	UNP P19821
А	527	ALA	PRO	engineered mutation	UNP P19821
А	551	GLU	ASP	engineered mutation	UNP P19821
А	832	VAL	GLU	engineered mutation	UNP P19821
С	444	VAL	MET	engineered mutation	UNP P19821
С	527	ALA	PRO	engineered mutation	UNP P19821
С	551	GLU	ASP	engineered mutation	UNP P19821
С	832	VAL	GLU	engineered mutation	UNP P19821
G	444	VAL	MET	engineered mutation	UNP P19821
G	527	ALA	PRO	engineered mutation	UNP P19821
G	551	GLU	ASP	engineered mutation	UNP P19821
G	832	VAL	GLU	engineered mutation	UNP P19821

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
0	Р	19	Total	С	Ν	Ο	Р	0	0	0
	Z D	12	244	115	48	70	11	0		
0	F	12	Total	С	Ν	Ο	Р	0	0	0
			244	115	48	70	11	0	0	U



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Н	12	Total 244	C 115	N 48	O 70	Р 11	0	0	0

• Molecule 3 is a DNA chain called DNA (5'-D(P*GP*(1WA)P*GP*CP*GP*CP*GP*T P*GP*GP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Л	12	Total	С	Ν	Ο	Р	0	0	0
5 D	10	270	126	51	80	13	0	0	0	
2	Б	13	Total	С	Ν	Ο	Р	0	0	0
J	Г		270	126	51	80	13			
2	т	13	Total	С	Ν	Ο	Р	0	0	0
3 1			270	126	51	80	13		0	U

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	83	Total O 83 83	0	0
4	В	5	Total O 5 5	0	0
4	D	15	Total O 15 15	0	0
4	С	64	Total O 64 64	0	0
4	Е	8	Total O 8 8	0	0
4	F	14	Total O 14 14	0	0
4	G	85	Total O 85 85	0	0
4	Н	11	Total O 11 11	0	0
4	Ι	10	Total O 10 10	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: DNA polymerase I, thermostable

1693 E694 6694 R704 R771 R771 E774 E776 E776 E777 E776 E777 E776 E777 E776 E776

• Molecule 2: DNA (5'-D(*GP*AP*CP*CP*AP*CP*GP*GP*CP*GP*CP*(1W5))-3')

Chain B:	58%	33%	8%
G101 C104 A105 G107 G107 G108 105112			
• Molecule 2:	DNA (5'-D(*GP*AP*CP*Cl	P*AP*CP*GP*GP*CP*	GP*CP*(1W5))-3')
Chain E:	50%	50%	
6101 A102 C103 C104 A105 106 108 105 115 112			
• Molecule 2:	DNA $(5'-D(*GP*AP*CP*C)$	P*AP*CP*GP*GP*CP*	GP*CP*(1W5))-3')
Chain H:	50%	50%	
6101 C104 A105 C106 C106 G107 G108 108 111 105112			
• Molecule 3:)	DNA $(5'-D(P*GP*(1WA)))$	P*GP*CP*GP*CP*CP	P*GP*TP*GP*GP*TP*C)-3'
Chain D:	69%	31%	
5204 1WA205 208 208 7209 7210 6211 6211			
• Molecule 3:)	DNA $(5'-D(P*GP*(1WA)))$	P*GP*CP*GP*CP*CP	P*GP*TP*GP*GP*TP*C)-3'
Chain F:	62%	38%	
2216 14A205 2210 2211 7212 7215 7216			
• Molecule 3:)	DNA (5'-D(P*GP*(1WA))	P*GP*CP*GP*CP*CP	P*GP*TP*GP*GP*TP*C)-3'
Chain I:	69%	31%	







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	199.28Å 114.61Å 90.52Å	Deperitor
a, b, c, α , β , γ	90.00° 91.88° 90.00°	Depositor
Bosolution (Å)	49.13 - 2.66	Depositor
Resolution (A)	99.34 - 2.66	EDS
% Data completeness	98.5(49.13-2.66)	Depositor
(in resolution range)	98.5 (99.34 - 2.66)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	0.08	Depositor
$< I/\sigma(I) > 1$	$2.19 (at 2.65 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
D D	0.211 , 0.247	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.215 , 0.247	DCC
R_{free} test set	2819 reflections (4.89%)	wwPDB-VP
Wilson B-factor $(Å^2)$	39.8	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32, 31.8	EDS
L-test for $twinning^2$	$< L > = 0.49, < L^2 > = 0.32$	Xtriage
	0.017 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l	
	0.016 for -1/2 *h+3/2 *k, 1/2 *h+1/2 *k, -1	
Estimated twinning fraction	0.056 for $1/2$ *h- $3/2$ *k,- $1/2$ *h- $1/2$ *k,-l	Xtriage
	0.085 for 1/2 *h + 3/2 *k, 1/2 *h - 1/2 *k, -1	
	0.024 for -h,-k,l	
F_o, F_c correlation	0.91	EDS
Total number of atoms	14188	wwPDB-VP
Average B, all atoms $(Å^2)$	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 1W5, $1\mathrm{WA}$

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).

Mal	Chain	Bond	lengths	Bond	angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.24	0/4153	0.38	0/5625
1	С	0.21	0/4203	0.36	0/5693
1	G	0.21	0/4256	0.38	0/5767
2	В	0.50	0/249	0.72	0/382
2	Ε	0.54	0/249	0.75	0/382
2	Н	0.52	0/249	0.73	0/382
3	D	0.50	0/276	0.84	0/422
3	F	0.52	0/276	0.85	0/422
3	Ι	0.50	0/276	0.84	0/422
All	All	0.27	0/14187	0.45	0/19497

There are no bond length outliers.

There are no bond angle outliers.

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	А	4069	0	4117	31	0
1	С	4117	0	4167	39	0
1	G	4165	0	4205	37	0
2	В	244	0	133	4	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Е	244	0	133	3	0
2	Н	244	0	133	4	0
3	D	270	0	147	2	0
3	F	270	0	147	3	0
3	Ι	270	0	147	2	0
4	А	83	0	0	0	0
4	В	5	0	0	0	0
4	С	64	0	0	0	0
4	D	15	0	0	0	0
4	Е	8	0	0	0	0
4	F	14	0	0	0	0
4	G	85	0	0	0	0
4	Н	11	0	0	0	0
4	Ι	10	0	0	0	0
All	All	14188	0	13329	113	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 4.

All (113) c	close co	ontacts	within	the same	$\operatorname{asymmetric}$	unit	are	listed	below,	sorted	by	their	clash
magnitude.													

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:639:HIS:HA	1:A:642:THR:HG22	1.60	0.83	
1:G:684:ILE:HG13	1:G:685:PRO:HD2	1.61	0.81	
1:C:794:GLU:HG3	1:C:795:ARG:HG2	1.66	0.78	
1:A:302:PRO:HG2	1:A:328:ARG:HD3	1.68	0.76	
1:A:584:ILE:O	1:A:595:ARG:NH1	2.23	0.70	
1:A:642:THR:HG23	1:A:662:ALA:HB1	1.76	0.68	
1:C:584:ILE:O	1:C:595:ARG:NH1	2.30	0.64	
1:C:328:ARG:O	1:C:331:ARG:NH1	2.31	0.63	
1:C:527:ALA:O	1:C:531:LYS:HG2	1.98	0.63	
1:G:487[A]:ARG:NH1	2:H:108:DG:OP1	2.32	0.62	
1:A:453:VAL:HG13	1:A:550:PRO:HB3	1.81	0.62	
1:A:487[A]:ARG:NH1	2:B:108:DG:OP1	2.33	0.62	
1:C:713:GLU:OE2	1:C:717:ARG:NH1	2.32	0.61	
1:C:487[B]:ARG:NE	1:C:488:ASP:OD1	2.34	0.60	
1:G:670:LEU:HD22	1:G:753:VAL:HG11	1.84	0.60	
1:G:584:ILE:O	1:G:595:ARG:NH1	2.32	0.59	
1:G:453:VAL:HG13	1:G:550:PRO:HB3	1.86	0.58	
1:A:607:VAL:HB	1:A:789:LEU:HB2	1.85	0.58	
1:C:639:HIS:HB2	1:C:659:ARG:HH21	1.69	0.57	



	• p ~ g ~	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:G:466:GLU:OE2	1:G:469:ARG:NH2	2.38	0.57	
1:A:466:GLU:OE1	1:A:469:ARG:NH2	2.38	0.56	
1:C:339:TYR:O	1:C:343:ARG:NH1	2.39	0.56	
1:G:694[A]:GLU:OE2	1:G:704:ARG:NH1	2.34	0.56	
1:A:587:ARG:NH2	2:B:112:1W5:OP2	2.39	0.56	
1:C:800:ALA:HB1	1:C:821:VAL:HG11	1.87	0.55	
1:C:600:ALA:HB2	1:C:606:LEU:HG	1.88	0.55	
1:C:453:VAL:HG13	1:C:550:PRO:HB3	1.88	0.55	
1:A:514:THR:O	1:A:536:ARG:NH1	2.29	0.54	
1:C:304:GLY:O	1:C:349:ARG:NH1	2.41	0.53	
1:C:503:ILE:HG22	1:C:518:VAL:HG13	1.90	0.53	
1:C:607:VAL:HB	1:C:789:LEU:HB2	1.91	0.53	
2:B:104:DC:H2"	2:B:105:DA:C8	2.44	0.53	
1:C:670:LEU:HD22	1:C:753:VAL:HG11	1.90	0.52	
1:G:339:TYR:O	1:G:343:ARG:NH1	2.43	0.51	
1:G:541:LEU:HD12	1:G:590:LEU:HD23	1.94	0.50	
1:A:595:ARG:HG2	1:A:827:TRP:HB3	1.93	0.50	
1:G:487[A]:ARG:HD3	2:H:107:DG:H4'	1.93	0.49	
1:G:463:VAL:HG13	1:G:538:LEU:HD22	1.95	0.49	
1:C:611:TYR:HB3	1:C:614:ILE:HB	1.95	0.48	
1:A:670:LEU:HD22	1:A:753:VAL:HG11	1.96	0.48	
1:C:639:HIS:HB2	1:C:659:ARG:NH2	2.28	0.48	
1:A:487[B]:ARG:NH2	1:A:511:LYS:HD3	2.29	0.48	
1:C:694:GLU:O	1:C:698:GLN:HG2	2.13	0.48	
1:G:659:ARG:HG3	1:G:660:ARG:N	2.28	0.48	
1:G:586:VAL:HG12	2:H:111:DC:H5"	1.95	0.48	
1:C:542:LYS:NZ	1:C:547:ASP:OD2	2.42	0.47	
1:C:486:SER:HA	3:F:212:DT:H4'	1.96	0.47	
1:G:487[B]:ARG:NH2	1:G:511:LYS:HD3	2.29	0.47	
1:A:311:LEU:HB3	1:A:319:ALA:HB1	1.96	0.47	
1:A:633:GLN:NE2	1:C:801:ARG:HH11	2.13	0.47	
1:G:783:VAL:HB	1:G:786:GLU:HB2	1.94	0.47	
1:G:637:ASP:HB3	1:G:640:THR:HB	1.95	0.47	
1:C:320:ASP:OD1	1:C:339:TYR:OH	2.23	0.47	
1:G:503:ILE:HD13	1:G:518:VAL:HG13	1.97	0.47	
1:C:595:ARG:HG2	1:C:827:TRP:HB3	1.97	0.47	
1:A:638:ILE:HB	1:A:639:HIS:HD2	1.79	0.47	
1:A:376:LEU:HD22	1:A:420:LEU:HD12	1.98	0.46	
1:C:541:LEU:HB3	1:C:594:ILE:HD11	1.97	0.46	
1:A:662:ALA:O	1:A:666:ASN:HB2	2.16	0.45	
1:G:303:GLU:OE2	1:G:346:LYS:HB2	2.17	0.45	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:G:299:TRP:CG	1:G:300:PRO:HA	2.51	0.45	
1:G:311:LEU:HB3	1:G:319:ALA:HB1	1.99	0.45	
1:G:484:LEU:HD11	1:G:532:ILE:HG12	1.98	0.45	
1:G:490:LEU:HD11	1:G:532:ILE:HD13	1.98	0.45	
1:C:348:ALA:HB3	1:C:369:PRO:HA	1.99	0.45	
1:G:611:TYR:HB3	1:G:614:ILE:HB	1.99	0.44	
1:C:684:ILE:HG13	1:C:685:PRO:HD2	1.99	0.44	
1:C:775:MET:O	1:C:795:ARG:NH1	2.49	0.44	
2:E:102:DA:H2'	2:E:103:DC:C6	2.53	0.44	
1:G:631:VAL:HG13	1:G:641:GLU:HB3	1.98	0.44	
1:G:771:ARG:O	1:G:774:GLU:HG2	2.18	0.44	
1:A:549:LEU:HD22	1:A:560:LEU:HD21	2.00	0.43	
1:A:783:VAL:HB	1:A:786:GLU:HB2	2.01	0.43	
3:F:210:DC:H2'	3:F:211:DG:C8	2.53	0.43	
3:D:210:DC:H2'	3:D:211:DG:C8	2.54	0.43	
1:G:487[B]:ARG:NH2	1:G:491:GLU:OE1	2.38	0.43	
1:G:676:HIS:O	1:G:679:SER:N	2.49	0.43	
1:C:487[A]:ARG:NH1	2:E:108:DG:OP1	2.52	0.43	
1:G:425:ARG:NH2	1:G:723:LEU:O	2.52	0.43	
1:G:351:LEU:HD11	1:G:412:LEU:HD12	2.01	0.42	
3:I:210:DC:H2'	3:I:211:DG:C8	2.54	0.42	
1:A:746:ARG:HA	1:A:749:PHE:CE2	2.54	0.42	
1:A:299:TRP:CG	1:A:300:PRO:HA	2.53	0.42	
1:C:299:TRP:CG	1:C:300:PRO:HA	2.55	0.42	
1:G:793:LYS:HE2	1:G:793:LYS:HB2	1.83	0.42	
1:G:576:SER:O	3:I:208:DG:H4'	2.19	0.42	
1:C:475:PHE:CD1	1:C:481:PRO:HA	2.54	0.42	
1:C:487[B]:ARG:HH12	1:C:491:GLU:HB2	1.85	0.42	
1:C:587:ARG:HG3	1:C:588:THR:HG23	2.02	0.42	
1:A:542:LYS:HA	1:A:546:ILE:HB	2.01	0.41	
1:A:401:GLU:OE1	1:A:404:GLU:N	2.41	0.41	
1:A:696:TYR:O	1:A:699:SER:OG	2.35	0.41	
1:C:453:VAL:O	1:C:457:ARG:HG2	2.20	0.41	
1:G:600:ALA:HB2	1:G:606:LEU:HG	2.03	0.41	
2:H:104:DC:H2"	2:H:105:DA:C8	2.55	0.41	
1:A:781:LEU:HB2	1:A:788:VAL:HB	2.03	0.41	
1:A:576:SER:O	3:D:208:DG:H4'	2.20	0.41	
1:A:717:ARG:HE	1:A:717:ARG:HB2	1.54	0.41	
1:C:673:MET:HA	3:F:204:DG:H5'	2.02	0.41	
1:G:549:LEU:HD22	1:G:560:LEU:HD21	2.02	0.41	
1:G:689:ALA:O	1:G:693:ILE:HG12	2.21	0.41	



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
2:E:104:DC:H2'	2:E:105:DA:C8	2.56	0.41
1:A:609:LEU:HG	1:A:821:VAL:HG23	2.03	0.40
1:C:584:ILE:HA	1:C:585:PRO:HD3	1.97	0.40
1:C:492:ARG:O	1:C:496:ASP:HB2	2.21	0.40
1:A:805:GLU:OE1	1:A:805:GLU:HA	2.21	0.40
1:C:574:LEU:HD12	1:C:782:GLN:OE1	2.21	0.40
1:G:337:GLU:HA	1:G:338:PRO:HD3	1.87	0.40
1:A:487[A]:ARG:HD3	2:B:107:DG:H4'	2.04	0.40
1:C:337:GLU:HA	1:C:338:PRO:HD3	1.90	0.40
1:C:372:ASP:HB3	1:C:375:LEU:HG	2.04	0.40
1:G:523:ARG:HH11	1:G:523:ARG:HG3	1.86	0.40
1:G:554:HIS:CG	1:G:555:PRO:HD2	2.57	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	Perce	ntiles
1	А	510/540~(94%)	487 (96%)	22 (4%)	1 (0%)	47	64
1	С	518/540~(96%)	499 (96%)	18 (4%)	1 (0%)	47	64
1	G	525/540~(97%)	503 (96%)	21 (4%)	1 (0%)	47	64
All	All	1553/1620~(96%)	1489 (96%)	61 (4%)	3 (0%)	47	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	586	VAL
1	G	586	VAL
1	А	586	VAL



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	417/440~(95%)	412 (99%)	5 (1%)	71 84
1	С	420/440~(96%)	417 (99%)	3 (1%)	84 91
1	G	424/440 (96%)	421 (99%)	3 (1%)	84 91
All	All	1261/1320~(96%)	1250 (99%)	11 (1%)	86 87

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	346	LYS
1	А	487[A]	ARG
1	А	487[B]	ARG
1	А	633	GLN
1	А	641	GLU
1	С	303	GLU
1	С	487[A]	ARG
1	С	487[B]	ARG
1	G	487[A]	ARG
1	G	487[B]	ARG
1	G	698	GLN

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such side chains are listed below:

Mol	Chain	Res	Type
1	А	633	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)

6 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).

Mal Type Che		Chain	Thein Dec	Tinle	Bond lengths			Bond angles		
IVIOI	туре	Type Chain I	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	1W5	Н	112	2	18,23,24	1.45	3 (16%)	20,33,36	2.10	3 (15%)
3	1WA	F	205	3	$17,\!24,\!25$	0.79	0	19,35,38	1.32	3 (15%)
2	1W5	В	112	2	18,23,24	1.45	3 (16%)	20,33,36	2.13	3 (15%)
2	1W5	Е	112	2	18,23,24	1.46	3 (16%)	20,33,36	2.12	4 (20%)
3	1WA	Ι	205	3	17,24,25	0.79	0	19,35,38	1.34	3 (15%)
3	1WA	D	205	3	17,24,25	0.80	0	19,35,38	1.35	3 (15%)

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	1W5	Н	112	2	-	0/8/25/26	0/2/2/2
3	1WA	F	205	3	-	2/3/21/22	0/3/3/3
2	1W5	В	112	2	-	0/8/25/26	0/2/2/2
2	1W5	Ε	112	2	-	0/8/25/26	0/2/2/2
3	1WA	Ι	205	3	-	3/3/21/22	0/3/3/3
3	1WA	D	205	3	-	1/3/21/22	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Е	112	1W5	C6-C1	-3.25	1.34	1.39
2	В	112	1W5	C6-C1	-3.24	1.34	1.39
2	Н	112	1W5	C6-C1	-3.19	1.34	1.39
2	Н	112	1W5	C6-C5	2.37	1.43	1.39
2	В	112	1W5	C6-C5	2.30	1.43	1.39
2	Ε	112	1W5	C6-C5	2.26	1.43	1.39
2	В	112	1W5	O2-C2	-2.04	1.19	1.29
2	Н	112	1W5	O2-C2	-2.03	1.19	1.29
2	Е	112	1W5	O2-C2	-2.03	1.19	1.29



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	112	1W5	C4-N3-C2	8.31	126.89	116.76
2	Е	112	1W5	C4-N3-C2	8.28	126.85	116.76
2	Н	112	1W5	C4-N3-C2	8.19	126.74	116.76
3	D	205	1WA	C8-N9-C1'	4.31	129.66	125.40
3	F	205	1WA	C8-N9-C1'	4.18	129.53	125.40
3	Ι	205	1WA	C8-N9-C1'	3.64	129.00	125.40
3	D	205	1WA	C2-N3-C4	-2.76	112.07	115.78
3	F	205	1WA	C2-N3-C4	-2.72	112.13	115.78
3	Ι	205	1WA	C2-N3-C4	-2.55	112.35	115.78
2	В	112	1W5	O4'-C1'-C2'	2.22	107.14	103.57
2	Н	112	1W5	C6-C1-C1'	2.18	127.82	120.89
2	В	112	1W5	C6-C1-C1'	2.15	127.73	120.89
3	D	205	1WA	N2-C2-N3	-2.13	114.32	117.79
3	Ι	205	1WA	N2-C2-N3	-2.10	114.37	117.79
2	Н	112	1W5	O4'-C1'-C2'	2.09	106.93	103.57
3	F	205	1WA	N2-C2-N3	-2.08	114.40	117.79
2	Е	112	1W5	C6-C1-C1'	2.06	127.44	120.89
2	Е	112	1W5	C5-C6-C1	2.01	122.58	119.53
2	Е	112	1W5	C5-C4-N4	2.01	127.28	125.22

All (19) bond angle outliers are listed below:

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Ι	205	1WA	C3'-C4'-C5'-O5'
3	Ι	205	1WA	O4'-C4'-C5'-O5'
3	F	205	1WA	O4'-C4'-C5'-O5'
3	D	205	1WA	O4'-C4'-C5'-O5'
3	Ι	205	1WA	C4'-C5'-O5'-P
3	F	205	1WA	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	112	1W5	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	Ι	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ι	205:1WA	O3'	206:DG	Р	1.36



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	515/540~(95%)	-0.04	6 (1%) 79 77	22, 38, 67, 82	0
1	С	521/540~(96%)	-0.01	3 (0%) 89 89	27, 39, 63, 71	0
1	G	527/540~(97%)	-0.08	7 (1%) 77 75	23, 35, 62, 82	0
2	В	11/12~(91%)	-0.23	0 100 100	32, 36, 42, 43	0
2	Е	11/12~(91%)	-0.36	0 100 100	31, 33, 43, 44	0
2	Н	11/12~(91%)	-0.30	0 100 100	33, 38, 58, 58	0
3	D	12/13~(92%)	-0.31	0 100 100	29, 33, 43, 58	0
3	F	12/13~(92%)	-0.40	0 100 100	31, 33, 43, 52	0
3	Ι	12/13~(92%)	-0.00	1 (8%) 11 9	31, 36, 48, 68	0
All	All	$163\overline{2/1695}\ (96\%)$	-0.05	17 (1%) 82 81	22, 37, 64, 82	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	640	THR	4.4
1	А	661	ALA	3.6
1	С	665	ILE	3.1
1	А	686	TYR	3.0
3	Ι	204	DG	3.0
1	С	634	GLU	2.8
1	С	484	LEU	2.6
1	G	645	TRP	2.3
1	А	526	HIS	2.3
1	А	642	THR	2.3
1	G	643	ALA	2.2
1	G	658	MET	2.2
1	А	638	ILE	2.2
1	G	675	ALA	2.1
1	G	820	GLU	2.1



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Mol	Chain	Res	Type	RSRZ
1	G	667	PHE	2.1
1	G	641	GLU	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
2	1W5	Н	112	22/23	0.93	0.18	28,34,41,45	0
3	1WA	Ι	205	22/23	0.93	0.17	33,39,46,56	0
3	1WA	D	205	22/23	0.96	0.15	29,35,41,43	0
2	1W5	В	112	22/23	0.96	0.17	26,31,40,45	0
3	1WA	F	205	22/23	0.97	0.14	31,36,41,43	0
2	1W5	Е	112	22/23	0.97	0.16	28,32,35,39	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.

