



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:47 PM UTC

PDB ID : 4YIG / pdb_00004yig
Title : vaccinia virus D4/A20(1-50) in complex with dsDNA containing an abasic site and free uracyl
Authors : tarbouriech, N.; burmeister, W.P.; iseni, F.
Deposited on : 2015-03-02
Resolution : 2.70 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:

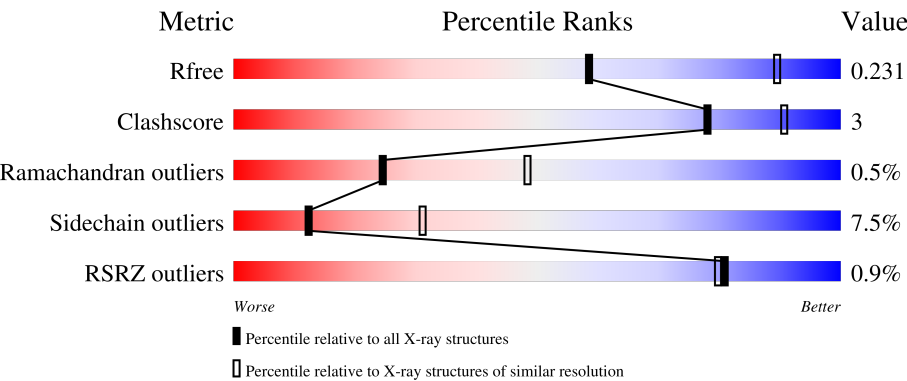
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



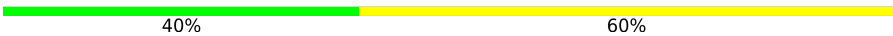
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	A	232	78%15%• 5%
1	E	232	% 84%11%5%
1	I	232	% 76%18%5%
2	B	52	2% 79%15%• •
2	F	52	2% 85%10%• •

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Mol	Chain	Length	Quality of chain
2	J	52	 81% 15%
3	C	10	 60% 30% 10%
3	G	10	 80% 20%
3	K	10	 70% 30%
4	D	10	 40% 60%
4	H	10	 80% 20%
4	L	10	 90% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	URA	A	301	-	X	-	-
5	URA	I	301	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7824 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 Uracil-DNA glycosylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1788	1158	295	329	6			
1	E	220	Total	C	N	O	S	0	0	0
			1788	1158	295	329	6			
1	I	220	Total	C	N	O	S	0	0	0
			1788	1158	295	329	6			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP P20536
A	-12	GLY	-	expression tag	UNP P20536
A	-11	SER	-	expression tag	UNP P20536
A	-10	SER	-	expression tag	UNP P20536
A	-9	HIS	-	expression tag	UNP P20536
A	-8	HIS	-	expression tag	UNP P20536
A	-7	HIS	-	expression tag	UNP P20536
A	-6	HIS	-	expression tag	UNP P20536
A	-5	HIS	-	expression tag	UNP P20536
A	-4	HIS	-	expression tag	UNP P20536
A	-3	SER	-	expression tag	UNP P20536
A	-2	GLN	-	expression tag	UNP P20536
A	-1	ASP	-	expression tag	UNP P20536
A	0	PRO	-	expression tag	UNP P20536
E	-13	MET	-	initiating methionine	UNP P20536
E	-12	GLY	-	expression tag	UNP P20536
E	-11	SER	-	expression tag	UNP P20536
E	-10	SER	-	expression tag	UNP P20536
E	-9	HIS	-	expression tag	UNP P20536
E	-8	HIS	-	expression tag	UNP P20536
E	-7	HIS	-	expression tag	UNP P20536
E	-6	HIS	-	expression tag	UNP P20536
E	-5	HIS	-	expression tag	UNP P20536

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP P20536
E	-3	SER	-	expression tag	UNP P20536
E	-2	GLN	-	expression tag	UNP P20536
E	-1	ASP	-	expression tag	UNP P20536
E	0	PRO	-	expression tag	UNP P20536
I	-13	MET	-	initiating methionine	UNP P20536
I	-12	GLY	-	expression tag	UNP P20536
I	-11	SER	-	expression tag	UNP P20536
I	-10	SER	-	expression tag	UNP P20536
I	-9	HIS	-	expression tag	UNP P20536
I	-8	HIS	-	expression tag	UNP P20536
I	-7	HIS	-	expression tag	UNP P20536
I	-6	HIS	-	expression tag	UNP P20536
I	-5	HIS	-	expression tag	UNP P20536
I	-4	HIS	-	expression tag	UNP P20536
I	-3	SER	-	expression tag	UNP P20536
I	-2	GLN	-	expression tag	UNP P20536
I	-1	ASP	-	expression tag	UNP P20536
I	0	PRO	-	expression tag	UNP P20536

- Molecule 2 is a protein called DNA polymerase processivity factor component A20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	50	Total	C	N	O	S	0	0	0
			398	256	63	78	1			
2	F	50	Total	C	N	O	S	0	0	0
			398	256	63	78	1			
2	J	50	Total	C	N	O	S	0	0	0
			398	256	63	78	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P20995
B	0	ALA	-	expression tag	UNP P20995
B	1	MET	-	expression tag	UNP P20995
B	2	ALA	-	expression tag	UNP P20995
F	-1	GLY	-	expression tag	UNP P20995
F	0	ALA	-	expression tag	UNP P20995
F	1	MET	-	expression tag	UNP P20995
F	2	ALA	-	expression tag	UNP P20995
J	-1	GLY	-	expression tag	UNP P20995

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Chain	Residue	Modelled	Actual	Comment	Reference
J	0	ALA	-	expression tag	UNP P20995
J	1	MET	-	expression tag	UNP P20995
J	2	ALA	-	expression tag	UNP P20995

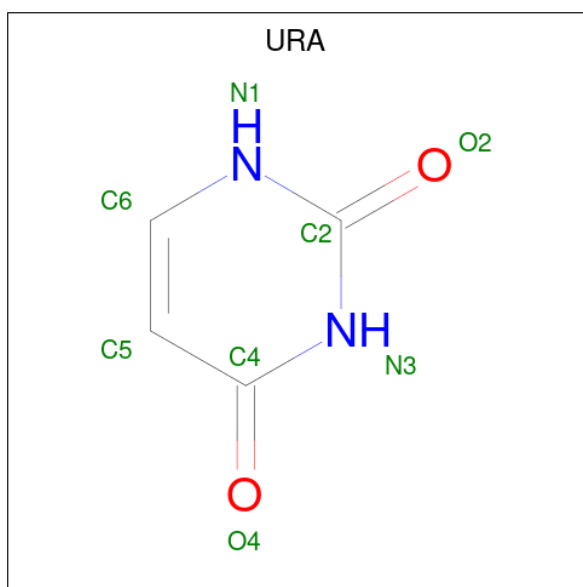
- Molecule 3 is a DNA chain called DNA (5'-D(*CP*TP*GP*TP*(ORP)P*AP*TP*CP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	P	0	0	0
			190	93	26	62	9			
3	G	10	Total	C	N	O	P	0	0	0
			190	93	26	62	9			
3	K	10	Total	C	N	O	P	0	0	0
			190	93	26	62	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	10	Total	C	N	O	P	0	0	0
			206	99	45	53	9			
4	H	10	Total	C	N	O	P	0	0	0
			206	99	45	53	9			
4	L	10	Total	C	N	O	P	0	0	0
			206	99	45	53	9			

- Molecule 5 is URACIL (CCD ID: URA) (formula: C₄H₄N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	2	2		
5	E	1	Total	C	N	O	0	0
			8	4	2	2		
5	I	1	Total	C	N	O	0	0
			8	4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total	O	0	0
			19	19		
6	B	2	Total	O	0	0
			2	2		
6	C	3	Total	O	0	0
			3	3		
6	E	10	Total	O	0	0
			10	10		
6	F	1	Total	O	0	0
			1	1		
6	G	1	Total	O	0	0
			1	1		
6	H	1	Total	O	0	0
			1	1		
6	I	13	Total	O	0	0
			13	13		
6	J	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	K	1	Total	O	0	0
			1	1		

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.

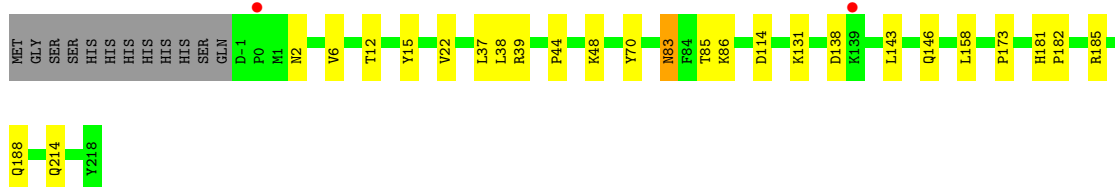
- Molecule 1: Uracil-DNA glycosylase

Chain A: 



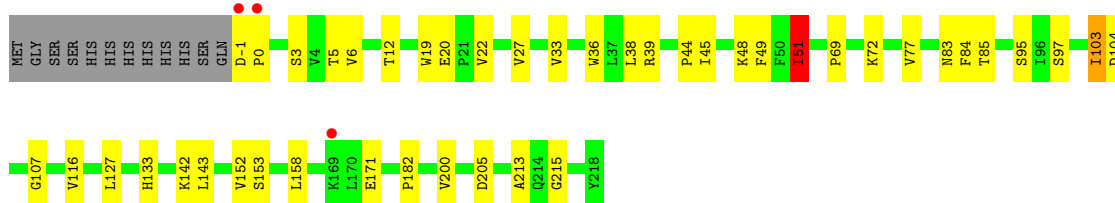
- Molecule 1: Uracil-DNA glycosylase

Chain E: 



- Molecule 1: Uracil-DNA glycosylase

Chain I: 

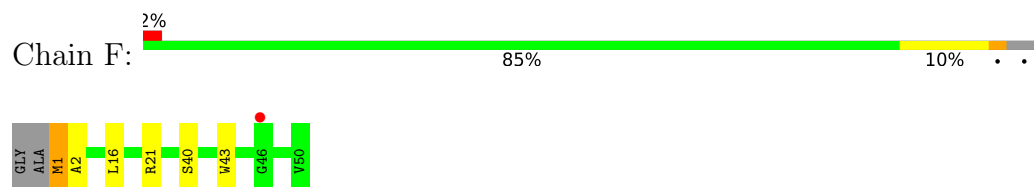


- Molecule 2: DNA polymerase processivity factor component A20

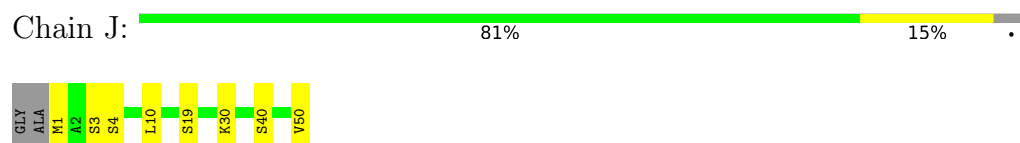
Chain B: 



- Molecule 2: DNA polymerase processivity factor component A20



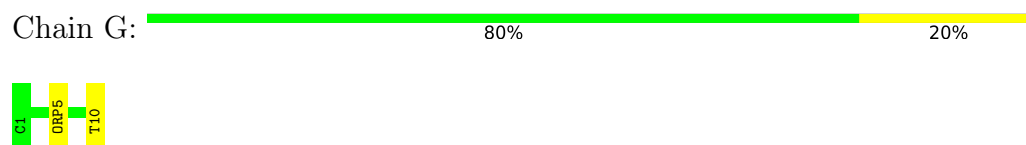
- Molecule 2: DNA polymerase processivity factor component A20



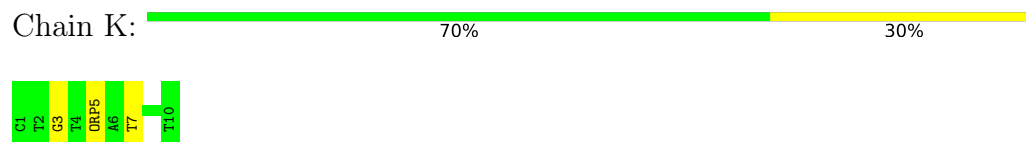
- Molecule 3: DNA (5'-D(*CP*TP*GP*TP*(ORP)P*AP*TP*CP*TP*T)-3')



- Molecule 3: DNA (5'-D(*CP*TP*GP*TP*(ORP)P*AP*TP*CP*TP*T)-3')



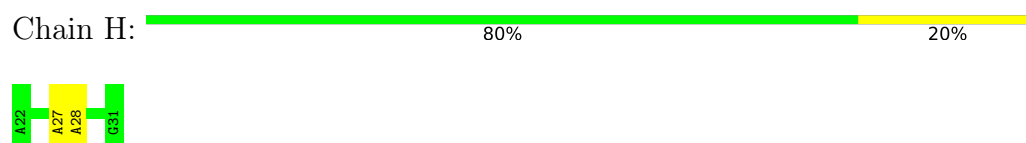
- Molecule 3: DNA (5'-D(*CP*TP*GP*TP*(ORP)P*AP*TP*CP*TP*T)-3')



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



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



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

Chain L:  90% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	136.09Å 136.09Å 161.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.86 – 2.70 48.86 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.86-2.70) 99.9 (48.86-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.180 , 0.228 0.187 , 0.231	Depositor DCC
R_{free} test set	2227 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	71.0	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.044 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7824	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.84% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.01	1/1838 (0.1%)	1.19	10/2500 (0.4%)
1	E	1.01	0/1838	1.15	5/2500 (0.2%)
1	I	0.94	1/1838 (0.1%)	1.10	7/2500 (0.3%)
2	B	1.11	0/405	1.16	1/545 (0.2%)
2	F	0.86	0/405	1.13	0/545
2	J	1.07	0/405	1.11	0/545
3	C	0.56	0/196	1.12	1/298 (0.3%)
3	G	0.57	0/196	1.05	0/298
3	K	0.42	0/196	1.02	1/298 (0.3%)
4	D	0.45	0/233	1.14	3/358 (0.8%)
4	H	0.44	0/233	1.02	0/358
4	L	0.44	0/233	1.04	1/358 (0.3%)
All	All	0.93	2/8016 (0.0%)	1.13	29/11103 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	33	VAL	N-CA	6.25	1.52	1.46
1	A	81	SER	C-O	-5.72	1.19	1.24

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	ASN	N-CA-C	12.51	127.65	112.38
1	A	83	ASN	CB-CA-C	-8.23	92.96	110.32
1	E	138	ASP	N-CA-C	7.47	120.07	111.11
1	I	33	VAL	N-CA-C	7.14	120.53	113.53
1	A	82	PRO	CA-C-N	6.70	131.32	120.60
1	A	82	PRO	C-N-CA	6.70	131.32	120.60
1	A	171	GLU	N-CA-C	-6.26	101.21	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	185	ARG	N-CA-C	6.25	119.93	112.93
1	E	83	ASN	N-CA-C	6.21	119.96	112.38
2	B	41	THR	N-CA-C	6.05	117.55	111.07
1	A	19	TRP	N-CA-C	6.04	120.50	113.20
1	E	39	ARG	CB-CA-C	-5.74	99.33	110.46
4	D	23	DA	C2'-C3'-O3'	5.71	120.07	111.50
1	I	33	VAL	CB-CA-C	-5.69	105.08	110.65
1	I	133	HIS	N-CA-C	5.67	119.82	113.02
1	A	154	VAL	N-CA-C	5.67	116.04	108.11
3	C	4	DT	C5'-C4'-O4'	-5.52	101.12	109.40
1	A	123	LEU	N-CA-C	5.40	119.85	113.16
1	E	83	ASN	CB-CA-C	-5.35	99.04	110.32
4	D	24	DG	C2'-C3'-O3'	5.34	119.52	111.50
1	A	172	SER	CA-C-N	-5.34	114.42	119.76
1	A	172	SER	C-N-CA	-5.34	114.42	119.76
1	I	45	ILE	CA-C-N	-5.32	114.19	119.56
1	I	45	ILE	C-N-CA	-5.32	114.19	119.56
4	D	30	DA	C2'-C3'-O3'	5.16	119.24	111.50
1	I	51	ILE	N-CA-CB	5.12	116.87	110.47
4	L	22	DA	C2'-C3'-O3'	5.05	119.08	111.50
1	I	116	VAL	N-CA-C	5.02	115.14	108.11
3	K	3	DG	C2'-C3'-O3'	5.02	119.03	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1788	0	1781	11	0
1	E	1788	0	1781	10	0
1	I	1788	0	1781	14	0
2	B	398	0	404	1	0
2	F	398	0	404	4	0
2	J	398	0	404	1	0
3	C	190	0	114	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	190	0	114	1	0
3	K	190	0	114	1	0
4	D	206	0	113	2	0
4	H	206	0	113	1	0
4	L	206	0	113	0	0
5	A	8	0	3	0	0
5	E	8	0	3	0	0
5	I	8	0	3	0	0
6	A	19	0	0	2	0
6	B	2	0	0	0	0
6	C	3	0	0	0	0
6	E	10	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
6	I	13	0	0	0	0
6	J	3	0	0	0	0
6	K	1	0	0	1	0
All	All	7824	0	7245	42	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 3.

All (42) 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:E:114:ASP:OD1	1:E:214:GLN:NE2	2.30	0.63
1:A:192:ASP:HB3	6:A:408:HOH:O	1.99	0.62
1:E:173:PRO:HB3	2:F:43:TRP:CE2	2.35	0.61
1:E:83:ASN:HB3	1:E:85:THR:HG23	1.86	0.57
1:A:109:ASN:ND2	6:A:401:HOH:O	2.38	0.55
1:I:36:TRP:O	1:I:39:ARG:HD3	2.06	0.54
1:A:7:SER:HB2	1:A:8:HIS:CD2	2.42	0.54
1:I:48:LYS:O	1:I:49:PHE:C	2.52	0.52
1:I:83:ASN:O	1:I:85:THR:HG23	2.09	0.52
1:A:187:ARG:NH1	4:D:29:DC:OP1	2.43	0.51
2:B:1:MET:HG3	2:B:2:ALA:N	2.25	0.51
3:C:3:DG:H1'	3:C:4:DT:H5''	1.94	0.50
1:A:184:ALA:HB1	1:A:188:GLN:NE2	2.27	0.49
4:H:27:DA:H2'	4:H:28:DA:C8	2.46	0.49
1:A:83:ASN:HB3	1:A:85:THR:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ALA:O	1:A:35:SER:C	2.56	0.48
1:I:19:TRP:O	1:I:20:GLU:C	2.57	0.47
1:E:173:PRO:HA	2:F:43:TRP:CZ3	2.49	0.47
1:I:6:VAL:HG12	1:I:27:VAL:HG13	1.96	0.47
4:D:27:DA:H2'	4:D:28:DA:C8	2.50	0.47
1:E:2:ASN:HB2	1:E:15:TYR:CZ	2.50	0.47
1:A:23:MET:O	1:A:27:VAL:HG23	2.15	0.46
1:I:153:SER:OG	1:I:205:ASP:OD2	2.28	0.46
1:I:158:LEU:HD23	1:I:182:PRO:HD3	1.98	0.45
1:I:103:ILE:H	1:I:103:ILE:HD13	1.82	0.44
1:I:44:PRO:HD3	1:I:69:PRO:HG2	1.98	0.44
1:E:22:VAL:HG12	1:E:143:LEU:HD11	2.00	0.44
1:E:173:PRO:HA	2:F:43:TRP:CH2	2.53	0.44
1:A:20:GLU:N	1:A:21:PRO:CD	2.81	0.43
3:K:7:DT:OP2	6:K:101:HOH:O	2.21	0.43
1:I:200:VAL:HG11	2:J:10:LEU:HB3	2.01	0.43
1:A:48:LYS:O	1:A:49:PHE:C	2.62	0.43
1:A:60:LYS:HD2	1:A:117:ILE:HB	2.01	0.42
1:I:84:PHE:CD1	1:I:107:GLY:HA2	2.54	0.42
1:I:213:ALA:C	1:I:215:GLY:H	2.28	0.42
1:I:22:VAL:HG12	1:I:143:LEU:HD11	2.00	0.41
1:E:181:HIS:CG	1:E:182:PRO:HD2	2.55	0.41
3:C:1:DC:O4'	3:G:10:DT:H2''	2.21	0.41
1:E:44:PRO:HB2	1:E:48:LYS:HB2	2.02	0.41
2:F:1:MET:HE3	2:F:2:ALA:H	1.85	0.41
1:I:51:ILE:HD12	1:I:77:VAL:HG23	2.01	0.41
1:E:70:TYR:CE1	1:E:86:LYS:HB3	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	Percentiles	
1	A	218/232 (94%)	205 (94%)	11 (5%)	2 (1%)	14	35
1	E	218/232 (94%)	203 (93%)	15 (7%)	0	100	100
1	I	218/232 (94%)	199 (91%)	17 (8%)	2 (1%)	14	35
2	B	48/52 (92%)	47 (98%)	1 (2%)	0	100	100
2	F	48/52 (92%)	46 (96%)	2 (4%)	0	100	100
2	J	48/52 (92%)	47 (98%)	1 (2%)	0	100	100
All	All	798/852 (94%)	747 (94%)	47 (6%)	4 (0%)	24	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	171	GLU
1	A	138	ASP
1	A	172	SER
1	I	0	PRO

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	
1	A	202/213 (95%)	187 (93%)	15 (7%)	13	32
1	E	202/213 (95%)	194 (96%)	8 (4%)	28	56
1	I	202/213 (95%)	188 (93%)	14 (7%)	14	34
2	B	44/44 (100%)	37 (84%)	7 (16%)	2	7
2	F	44/44 (100%)	40 (91%)	4 (9%)	9	22
2	J	44/44 (100%)	37 (84%)	7 (16%)	2	7
All	All	738/771 (96%)	683 (92%)	55 (8%)	12	31

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL

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Mol	Chain	Res	Type
1	A	5	THR
1	A	7	SER
1	A	12	THR
1	A	37	LEU
1	A	38	LEU
1	A	131	LYS
1	A	135	ILE
1	A	150	LYS
1	A	169	LYS
1	A	177	ILE
1	A	186	ASP
1	A	188	GLN
1	A	192	ASP
1	A	196	GLU
2	B	1	MET
2	B	20	LEU
2	B	25	SER
2	B	33	SER
2	B	40	SER
2	B	48	GLN
2	B	50	VAL
1	E	6	VAL
1	E	12	THR
1	E	37	LEU
1	E	38	LEU
1	E	131	LYS
1	E	146	GLN
1	E	158	LEU
1	E	188	GLN
2	F	1	MET
2	F	16	LEU
2	F	21	ARG
2	F	40	SER
1	I	-1	ASP
1	I	3	SER
1	I	5	THR
1	I	12	THR
1	I	38	LEU
1	I	51	ILE
1	I	72	LYS
1	I	95	SER
1	I	97	SER

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Mol	Chain	Res	Type
1	I	103	ILE
1	I	104	ASP
1	I	127	LEU
1	I	142	LYS
1	I	152	VAL
2	J	1	MET
2	J	3	SER
2	J	4	SER
2	J	19	SER
2	J	30	LYS
2	J	40	SER
2	J	50	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	16	HIS
1	A	109	ASN
1	A	165	ASN
1	A	188	GLN
1	A	206	ASN
1	E	8	HIS
1	E	16	HIS
1	E	109	ASN
1	E	146	GLN
1	I	2	ASN
1	I	8	HIS
1	I	146	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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
3	ORP	K	5	3	9,12,13	0.99	1 (11%)	7,16,19	0.72	0
3	ORP	C	5	3	9,12,13	1.23	1 (11%)	7,16,19	1.19	1 (14%)
3	ORP	G	5	3	9,12,13	1.24	1 (11%)	7,16,19	0.59	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
3	ORP	K	5	3	-	0/3/17/18	0/1/1/1
3	ORP	C	5	3	-	1/3/17/18	0/1/1/1
3	ORP	G	5	3	-	2/3/17/18	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5	ORP	O1-C1	2.56	1.47	1.39
3	G	5	ORP	O4-C4	-2.27	1.40	1.45
3	K	5	ORP	O1-C1	2.24	1.46	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	ORP	C1-C2-C3	2.32	107.09	103.93

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	5	ORP	C3-C4-C5-O5
3	G	5	ORP	O4-C4-C5-O5
3	C	5	ORP	C3-C4-C5-O5

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

3 ligands 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	$\# Z > 2$
5	URA	A	301	-	8,8,8	1.83	2 (25%)	10,10,10	3.30	6 (60%)
5	URA	I	301	-	8,8,8	1.80	3 (37%)	10,10,10	2.84	6 (60%)
5	URA	E	301	-	8,8,8	1.32	1 (12%)	10,10,10	3.67	6 (60%)

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
5	URA	A	301	-	-	-	0/1/1/1
5	URA	I	301	-	-	-	0/1/1/1
5	URA	E	301	-	-	-	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	301	URA	C5-C4	-3.00	1.37	1.43
5	I	301	URA	C6-C5	2.53	1.40	1.35
5	I	301	URA	C4-N3	-2.52	1.34	1.38
5	A	301	URA	C6-C5	2.44	1.40	1.35
5	I	301	URA	C5-C4	-2.43	1.38	1.43
5	E	301	URA	C5-C4	-2.40	1.38	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	301	URA	C4-N3-C2	-5.82	119.91	125.55
5	E	301	URA	O4-C4-C5	-5.18	116.23	125.16
5	I	301	URA	N1-C2-N3	4.92	120.36	115.17
5	E	301	URA	N1-C2-N3	4.91	120.34	115.17
5	A	301	URA	N1-C2-N3	4.65	120.08	115.17
5	A	301	URA	C6-N1-C2	-4.65	119.55	122.40
5	A	301	URA	O4-C4-C5	-4.57	117.27	125.16
5	E	301	URA	O2-C2-N1	-4.54	118.11	122.79
5	A	301	URA	O4-C4-N3	4.06	125.16	119.27
5	I	301	URA	C4-N3-C2	-3.81	121.86	125.55
5	E	301	URA	C5-C4-N3	3.80	120.12	114.80
5	A	301	URA	O2-C2-N1	-3.68	118.99	122.79
5	I	301	URA	C6-N1-C2	-3.43	120.29	122.40
5	A	301	URA	C4-N3-C2	-3.24	122.40	125.55
5	I	301	URA	O4-C4-C5	-3.09	119.83	125.16
5	E	301	URA	O4-C4-N3	3.02	123.65	119.27
5	I	301	URA	C5-C4-N3	2.79	118.71	114.80
5	I	301	URA	O2-C2-N1	-2.69	120.01	122.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	220/232 (94%)	-0.38	1 (0%) 87 86	47, 62, 90, 130	0
1	E	220/232 (94%)	-0.14	2 (0%) 81 80	50, 74, 100, 148	0
1	I	220/232 (94%)	-0.02	3 (1%) 73 72	49, 80, 111, 139	0
2	B	50/52 (96%)	-0.34	1 (2%) 65 62	45, 60, 79, 97	0
2	F	50/52 (96%)	0.15	1 (2%) 65 62	63, 86, 107, 108	0
2	J	50/52 (96%)	-0.47	0 100 100	52, 61, 81, 99	0
3	C	9/10 (90%)	-0.86	0 100 100	54, 57, 75, 87	0
3	G	9/10 (90%)	-0.73	0 100 100	58, 63, 82, 89	0
3	K	9/10 (90%)	-0.36	0 100 100	67, 77, 102, 115	0
4	D	10/10 (100%)	-0.67	0 100 100	65, 72, 82, 86	0
4	H	10/10 (100%)	-0.61	0 100 100	75, 81, 96, 107	0
4	L	10/10 (100%)	0.05	0 100 100	88, 98, 105, 119	0
All	All	867/912 (95%)	-0.21	8 (0%) 81 80	45, 72, 104, 148	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	0	PRO	3.3
2	B	1	MET	2.9
2	F	46	GLY	2.5
1	A	0	PRO	2.5
1	I	169	LYS	2.4
1	E	0	PRO	2.3
1	E	139	LYS	2.2
1	I	-1	ASP	2.1

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($\text{\AA}^2$)	Q<0.9
3	ORP	K	5	12/13	0.97	0.07	56,64,78,79	0
3	ORP	G	5	12/13	0.99	0.06	50,56,65,74	0
3	ORP	C	5	12/13	0.99	0.05	45,53,60,71	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	URA	A	301	8/8	0.96	0.08	62,69,72,77	0
5	URA	I	301	8/8	0.96	0.07	76,80,82,86	0
5	URA	E	301	8/8	0.97	0.08	61,71,82,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.