



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:59 PM GMT

PDB ID : 4K4W  
Title : Poliovirus polymerase elongation complex (r5+2\_form)  
Authors : Gong, P.; Peersen, O.B.  
Deposited on : 2013-04-12  
Resolution : 2.69 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

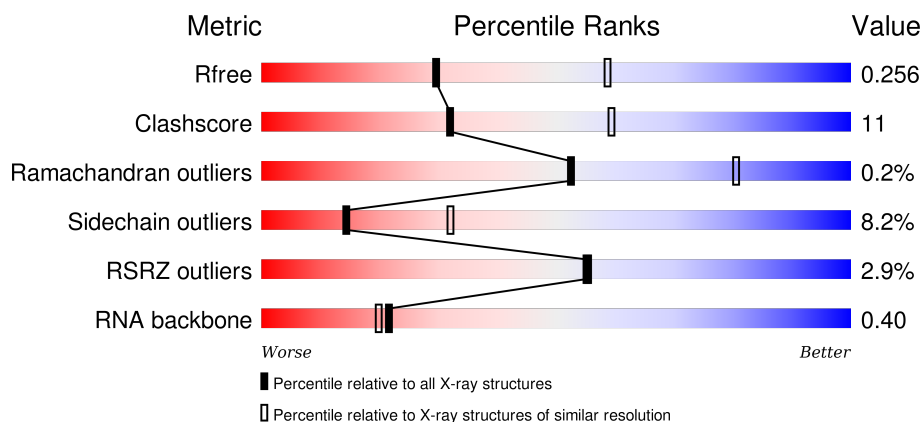
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.69 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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)
RNA backbone	2183	1069 (3.10-2.30)

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. 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	471	<div> <div>3%</div> <div>70%</div> <div>25%</div> <div>..</div> </div>
1	E	471	<div> <div>2%</div> <div>73%</div> <div>23%</div> <div>..</div> </div>
2	B	35	<div> <div>9%</div> <div>14%</div> <div>31%</div> <div>14%</div> <div>40%</div> </div>
2	F	35	<div> <div>9%</div> <div>11%</div> <div>37%</div> <div>11%</div> <div>40%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	18	<div><div></div><div></div><div></div><div></div><div></div></div> <div>33%22%17%6%22%</div>
3	G	18	<div><div></div><div></div><div></div><div></div><div></div></div> <div>33%22%28%17%</div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9029 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 RNA-directed RNA polymerase 3D-POL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3700	2372	611	696	21			
1	E	462	Total	C	N	O	S	0	0	0
			3700	2372	611	696	21			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	ALA	CYS	ENGINEERED MUTATION	UNP P03300
A	446	ASP	LEU	ENGINEERED MUTATION	UNP P03300
A	462	GLY	-	EXPRESSION TAG	UNP P03300
A	463	SER	-	EXPRESSION TAG	UNP P03300
A	464	SER	-	EXPRESSION TAG	UNP P03300
A	465	SER	-	EXPRESSION TAG	UNP P03300
A	466	HIS	-	EXPRESSION TAG	UNP P03300
A	467	HIS	-	EXPRESSION TAG	UNP P03300
A	468	HIS	-	EXPRESSION TAG	UNP P03300
A	469	HIS	-	EXPRESSION TAG	UNP P03300
A	470	HIS	-	EXPRESSION TAG	UNP P03300
A	471	HIS	-	EXPRESSION TAG	UNP P03300
E	290	ALA	CYS	ENGINEERED MUTATION	UNP P03300
E	446	ASP	LEU	ENGINEERED MUTATION	UNP P03300
E	462	GLY	-	EXPRESSION TAG	UNP P03300
E	463	SER	-	EXPRESSION TAG	UNP P03300
E	464	SER	-	EXPRESSION TAG	UNP P03300
E	465	SER	-	EXPRESSION TAG	UNP P03300
E	466	HIS	-	EXPRESSION TAG	UNP P03300
E	467	HIS	-	EXPRESSION TAG	UNP P03300
E	468	HIS	-	EXPRESSION TAG	UNP P03300
E	469	HIS	-	EXPRESSION TAG	UNP P03300
E	470	HIS	-	EXPRESSION TAG	UNP P03300
E	471	HIS	-	EXPRESSION TAG	UNP P03300

- Molecule 2 is a RNA chain called RNA (5'-R(P\*GP\*GP\*GP\*AP\*GP\*AP\*UP\*GP\*AP\*AP\*AP\*GP\*UP\*CP\*UP\*CP\*CP\*AP\*GP\*GP\*UP\*CP\*UP\*CP\*UP\*CP\*UP\*CP\*GP\*UP\*CP\*GP\*AP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	21	Total	C	N	O	P	0	0	0
			445	198	76	150	21			
2	F	21	Total	C	N	O	P	0	0	0
			445	198	76	150	21			

- Molecule 3 is a RNA chain called RNA (5'-R(\*UP\*GP\*UP\*UP\*CP\*GP\*AP\*CP\*GP\*AP\*GP\*AP\*GP\*AP\*GP\*AP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	14	Total	C	N	O	P	0	0	0
			305	136	62	93	14			
3	G	15	Total	C	N	O	P	0	0	0
			325	145	64	101	15			

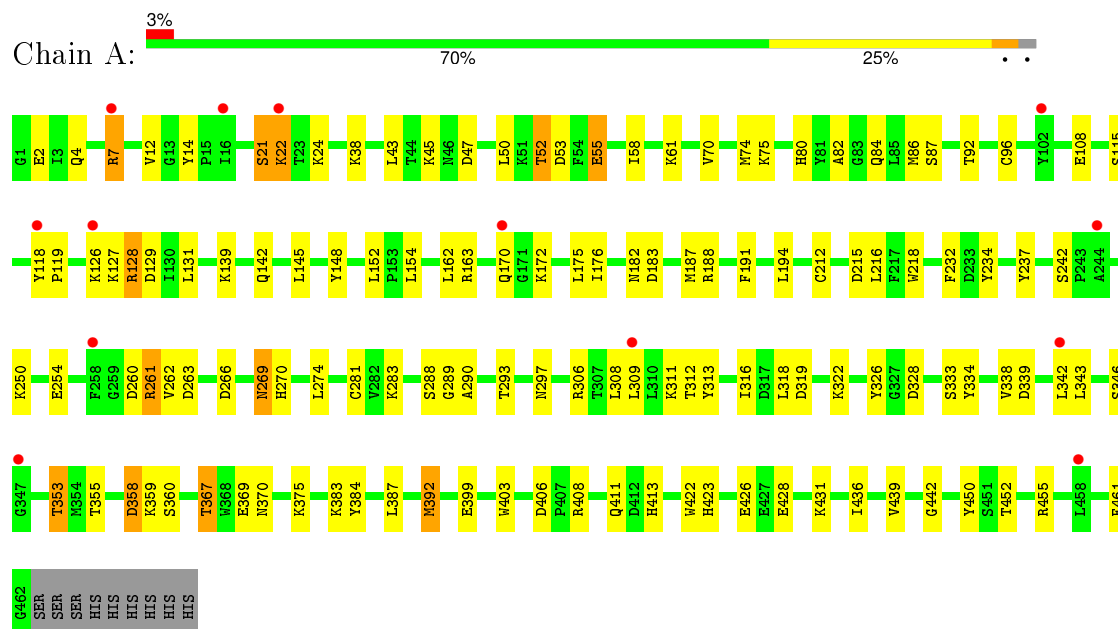
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	7	Total	O	0	0
			7	7		
4	C	4	Total	O	0	0
			4	4		
4	E	39	Total	O	0	0
			39	39		
4	G	3	Total	O	0	0
			3	3		
4	F	4	Total	O	0	0
			4	4		

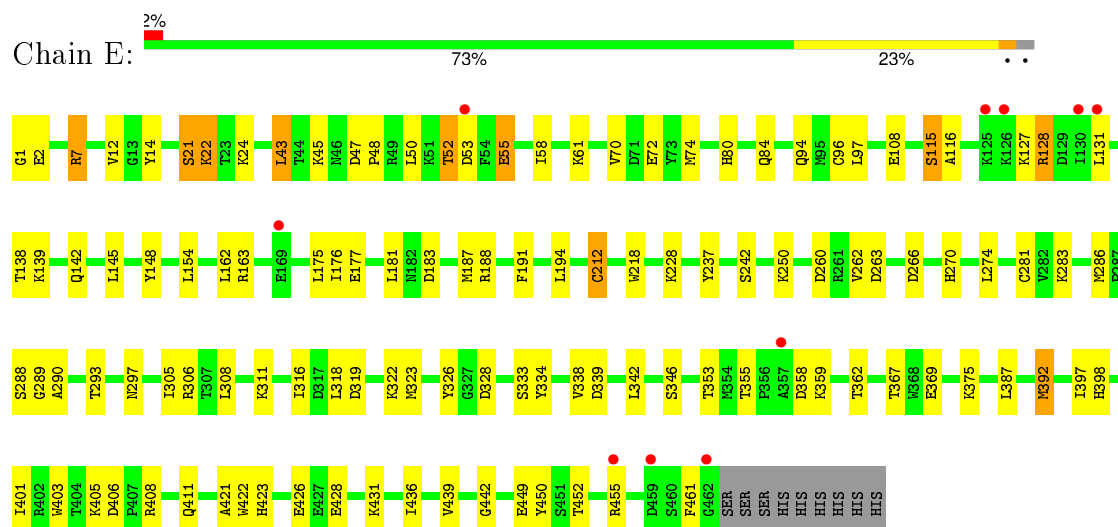
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

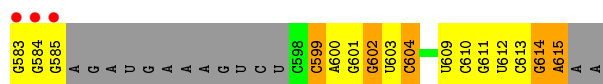
#### • Molecule 1: RNA-directed RNA polymerase 3D-POL



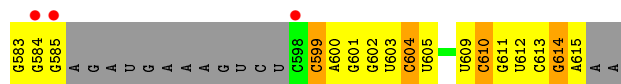
#### • Molecule 1: RNA-directed RNA polymerase 3D-POL



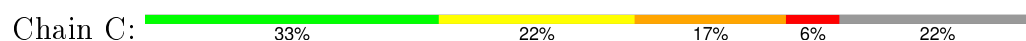
- Molecule 2: RNA (5'-R(P\*GP\*GP\*GP\*AP\*GP\*AP\*UP\*GP\*AP\*AP\*AP\*GP\*UP\*CP\*UP\*CP\*CP\*AP\*GP\*GP\*UP\*CP\*UP\*CP\*UP\*CP\*UP\*CP\*UP\*CP\*GP\*UP\*CP\*GP\*AP\*AP\*A)-3')



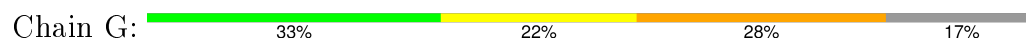
- Molecule 2: RNA (5'-R(P\*GP\*GP\*GP\*AP\*GP\*AP\*UP\*GP\*AP\*AP\*AP\*GP\*UP\*CP\*UP\*CP\*CP\*AP\*GP\*GP\*UP\*CP\*UP\*CP\*UP\*CP\*UP\*CP\*UP\*CP\*GP\*UP\*CP\*GP\*AP\*AP\*A)-3')



- Molecule 3: RNA (5'-R(\*UP\*GP\*UP\*UP\*CP\*GP\*AP\*CP\*GP\*AP\*GP\*AP\*GP\*AP\*GP\*AP\*GP\*AP\*CP\*C)-3')



- Molecule 3: RNA (5'-R(\*UP\*GP\*UP\*UP\*CP\*GP\*AP\*CP\*GP\*AP\*GP\*AP\*GP\*AP\*GP\*AP\*GP\*AP\*CP\*C)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.49 Å 64.37 Å 102.28 Å 73.65° 73.56° 72.20°	Depositor
Resolution (Å)	42.38 – 2.69 42.38 – 2.69	Depositor EDS
% Data completeness (in resolution range)	97.8 (42.38-2.69) 90.1 (42.38-2.69)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.69 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.213 , 0.256 0.211 , 0.256	Depositor DCC
$R_{free}$ test set	2021 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.1	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 54.1	EDS
Estimated twinning fraction	0.419 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	0 of 39825 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9029	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.50	0/3790	0.62	1/5126 (0.0%)
1	E	0.49	0/3790	0.62	1/5126 (0.0%)
2	B	0.59	0/494	1.13	1/765 (0.1%)
2	F	0.62	0/494	1.20	3/765 (0.4%)
3	C	0.56	0/342	1.18	1/532 (0.2%)
3	G	0.58	0/364	1.18	0/566
All	All	0.51	0/9274	0.77	7/12880 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	CYS	CA-CB-SG	6.02	124.83	114.00
3	C	697	A	N1-C6-N6	-5.63	115.22	118.60
2	F	605	U	N3-C2-O2	-5.31	118.48	122.20
2	B	604	C	N1-C2-O2	-5.12	115.83	118.90
2	F	604	C	N1-C2-O2	-5.10	115.84	118.90
1	E	212	CYS	CA-CB-SG	5.07	123.12	114.00
2	F	610	C	C6-N1-C2	-5.03	118.29	120.30

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	A	3700	0	3662	80	2
1	E	3700	0	3662	65	2
2	B	445	0	228	13	0
2	F	445	0	228	15	0
3	C	305	0	155	9	0
3	G	325	0	165	9	0
4	A	52	0	0	5	0
4	B	7	0	0	0	0
4	C	4	0	0	0	0
4	E	39	0	0	0	0
4	F	4	0	0	0	0
4	G	3	0	0	0	0
All	All	9029	0	8100	177	2

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 11.

All (177) 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:A:84:GLN:OE1	1:A:306:ARG:NH2	2.15	0.79
1:A:215:ASP:OD2	4:A:544:HOH:O	2.00	0.78
3:C:693:A:H2'	3:C:694:G:H8	1.50	0.75
1:E:84:GLN:OE1	1:E:306:ARG:NH2	2.23	0.71
1:A:399:GLU:OE1	4:A:504:HOH:O	2.09	0.70
3:G:692:G:N2	2:F:610:C:O2	2.25	0.69
2:B:600:A:H2'	2:B:601:G:C8	2.29	0.67
1:E:52:THR:OG1	1:E:53:ASP:N	2.26	0.67
1:E:250:LYS:HG2	1:E:262:VAL:HB	1.78	0.66
3:C:692:G:H2'	3:C:693:A:C8	2.30	0.66
1:A:52:THR:OG1	1:A:53:ASP:N	2.30	0.65
2:B:600:A:H2'	2:B:601:G:H8	1.63	0.64
1:A:128:ARG:NH1	3:C:695:A:OP1	2.32	0.63
1:A:353:THR:HG23	4:A:510:HOH:O	1.99	0.62
1:E:108:GLU:O	1:E:188:ARG:NH2	2.23	0.62
1:E:21:SER:H	1:E:22:LYS:HE2	1.66	0.61
3:C:693:A:H2'	3:C:694:G:C8	2.35	0.60
1:E:61:LYS:HE2	1:E:175:LEU:HD12	1.84	0.60
1:A:290:ALA:O	1:A:293:THR:HG23	2.00	0.59
1:E:311:LYS:HE2	1:E:346:SER:HB3	1.85	0.59
1:A:53:ASP:OD2	4:A:514:HOH:O	2.17	0.59
3:C:690:A:H2'	3:C:691:C:H5'	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:ALA:O	1:E:293:THR:HG23	2.03	0.58
1:E:7:ARG:HE	1:E:12:VAL:HG23	1.68	0.58
1:E:80:HIS:CE1	1:E:318:LEU:HB3	2.39	0.58
1:A:436:ILE:O	1:A:442:GLY:HA3	2.05	0.57
1:E:375:LYS:HB3	1:E:392:MET:CE	2.35	0.56
1:E:115:SER:OG	2:F:599:C:OP1	2.18	0.56
1:A:306:ARG:HG2	1:A:318:LEU:HD13	1.88	0.56
1:E:270:HIS:CE1	1:E:283:LYS:HE2	2.40	0.56
2:F:600:A:H2'	2:F:601:G:H8	1.71	0.56
1:E:128:ARG:NH1	3:G:695:A:OP1	2.40	0.55
2:B:602:G:H2'	2:B:603:U:C6	2.42	0.55
3:C:694:G:H2'	3:C:695:A:O4'	2.06	0.54
1:A:183:ASP:O	1:A:187:MET:HG2	2.07	0.54
2:F:609:U:H2'	2:F:610:C:H6	1.73	0.54
1:E:449:GLU:OE1	1:E:449:GLU:N	2.37	0.54
2:B:609:U:H2'	2:B:610:C:H6	1.70	0.54
1:A:92:THR:O	1:A:261:ARG:NH2	2.40	0.54
2:F:614:G:H2'	2:F:615:A:C8	2.43	0.54
2:F:600:A:H2'	2:F:601:G:C8	2.43	0.54
1:E:24:LYS:HD2	2:F:599:C:H42	1.72	0.54
1:A:316:ILE:HG13	1:A:334:TYR:OH	2.08	0.54
1:E:306:ARG:HG2	1:E:318:LEU:HD13	1.89	0.53
1:A:80:HIS:CE1	1:A:318:LEU:HB3	2.43	0.53
1:E:436:ILE:O	1:E:442:GLY:HA3	2.07	0.53
1:A:375:LYS:HB3	1:A:392:MET:CE	2.39	0.53
3:G:690:A:H2'	3:G:691:C:H5'	1.90	0.53
1:E:308:LEU:HD22	1:E:346:SER:HB2	1.91	0.53
1:E:127:LYS:O	1:E:131:LEU:HD12	2.08	0.53
1:A:322:LYS:HB2	1:A:333:SER:OG	2.09	0.53
1:A:21:SER:H	1:A:22:LYS:HE2	1.74	0.53
1:A:127:LYS:O	1:A:131:LEU:HD12	2.09	0.53
1:E:260:ASP:OD1	1:E:260:ASP:N	2.38	0.53
1:A:308:LEU:HD22	1:A:346:SER:HB2	1.91	0.53
1:A:311:LYS:O	1:A:311:LYS:HE3	2.08	0.52
2:F:612:U:H2'	2:F:613:C:O4'	2.08	0.52
1:A:250:LYS:HG2	1:A:262:VAL:HB	1.90	0.52
2:F:602:G:H2'	2:F:603:U:C6	2.44	0.52
1:A:387:LEU:HD22	1:A:461:PHE:CZ	2.45	0.52
1:E:316:ILE:HG13	1:E:334:TYR:OH	2.10	0.52
1:E:14:TYR:CD2	1:E:274:LEU:HD21	2.45	0.51
1:A:422:TRP:CZ2	1:A:423:HIS:CE1	2.98	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ILE:HG13	1:A:334:TYR:CZ	2.46	0.51
1:E:286:MET:HG2	1:E:297:ASN:HD21	1.76	0.51
2:B:612:U:H2'	2:B:613:C:O4'	2.12	0.50
1:A:55:GLU:HA	1:A:58:ILE:HG12	1.93	0.50
3:G:694:G:H2'	3:G:695:A:O4'	2.11	0.50
1:A:176:ILE:HA	1:A:288:SER:OG	2.12	0.50
1:E:387:LEU:HD22	1:E:461:PHE:CZ	2.47	0.50
1:A:61:LYS:HE2	1:A:175:LEU:HD12	1.92	0.50
1:A:254:GLU:HG3	1:A:262:VAL:HG11	1.93	0.50
1:A:339:ASP:HB3	1:A:342:LEU:HB2	1.93	0.50
3:G:692:G:H2'	3:G:693:A:C8	2.47	0.50
1:A:142:GLN:HA	1:A:145:LEU:HD12	1.93	0.49
1:E:142:GLN:HA	1:E:145:LEU:HD12	1.93	0.49
1:A:309:LEU:HD23	1:A:343:LEU:HD21	1.94	0.49
1:A:270:HIS:CE1	1:A:283:LYS:HE2	2.48	0.49
1:A:406:ASP:OD1	1:A:408:ARG:HG3	2.13	0.49
1:E:22:LYS:H	1:E:22:LYS:HE2	1.78	0.49
3:G:697:A:O2'	3:G:698:G:H5'	2.12	0.49
1:A:126:LYS:O	1:A:129:ASP:HB2	2.13	0.49
2:B:614:G:H2'	2:B:615:A:C8	2.48	0.49
1:A:4:GLN:HG3	1:A:283:LYS:HG3	1.95	0.48
1:A:22:LYS:H	1:A:22:LYS:HE2	1.78	0.48
1:E:162:LEU:HD11	1:E:403:TRP:CD1	2.49	0.48
1:E:288:SER:OG	1:E:289:GLY:N	2.45	0.48
1:E:398:HIS:O	1:E:401:ILE:HG22	2.13	0.48
1:E:183:ASP:O	1:E:187:MET:HG2	2.13	0.48
2:B:603:U:H2'	2:B:604:C:C6	2.49	0.48
1:A:311:LYS:HE2	1:A:346:SER:HB3	1.96	0.48
1:A:70:VAL:HG23	1:A:74:MET:HE2	1.96	0.48
1:A:452:THR:HA	1:A:455:ARG:HE	1.79	0.48
1:E:339:ASP:HB3	1:E:342:LEU:HB2	1.97	0.47
1:E:24:LYS:HG2	2:F:583:G:O6	2.14	0.47
1:A:387:LEU:HD22	1:A:461:PHE:CE2	2.49	0.47
1:A:452:THR:HA	1:A:455:ARG:HH21	1.80	0.47
1:A:162:LEU:HD11	1:A:403:TRP:CD1	2.49	0.47
1:E:191:PHE:O	1:E:194:LEU:HB3	2.15	0.47
1:A:375:LYS:HB3	1:A:392:MET:HE3	1.97	0.46
3:G:688:C:H42	2:F:614:G:H1	1.64	0.46
1:E:263:ASP:O	1:E:266:ASP:HB2	2.15	0.46
1:E:97:LEU:HD23	1:E:138:THR:HB	1.97	0.46
1:E:422:TRP:CZ2	1:E:423:HIS:CE1	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LYS:NZ	2:B:601:G:OP1	2.49	0.46
1:A:269:ASN:HD22	1:A:269:ASN:C	2.19	0.46
2:F:603:U:H2'	2:F:604:C:C6	2.50	0.45
3:C:697:A:O2'	3:C:698:G:H5'	2.15	0.45
1:E:237:TYR:CG	1:E:328:ASP:HB3	2.51	0.45
1:A:22:LYS:HD3	2:B:585:G:O4'	2.17	0.45
3:G:691:C:H1'	3:G:692:G:H5'	1.98	0.45
1:E:375:LYS:HB3	1:E:392:MET:HE3	1.97	0.45
2:B:602:G:H2'	2:B:603:U:H6	1.81	0.45
1:E:22:LYS:HD3	2:F:585:G:O4'	2.16	0.45
1:A:152:LEU:HD12	1:A:182:ASN:HB2	1.99	0.45
1:E:286:MET:HG2	1:E:297:ASN:ND2	2.31	0.45
1:E:177:GLU:N	1:E:288:SER:OG	2.41	0.45
1:A:38:LYS:NZ	4:A:527:HOH:O	2.49	0.45
1:E:55:GLU:HA	1:E:58:ILE:HG12	1.99	0.44
1:A:216:LEU:HA	1:A:216:LEU:HD23	1.68	0.44
1:E:43:LEU:HA	1:E:43:LEU:HD12	1.84	0.44
1:E:311:LYS:HE2	1:E:346:SER:CB	2.47	0.44
1:A:237:TYR:CG	1:A:328:ASP:HB3	2.53	0.44
3:C:692:G:H2'	3:C:693:A:H8	1.82	0.44
1:E:47:ASP:O	1:E:50:LEU:HD12	2.18	0.44
1:E:80:HIS:ND1	1:E:318:LEU:HB3	2.32	0.44
1:A:24:LYS:HG2	2:B:583:G:O6	2.17	0.44
1:A:108:GLU:O	1:A:188:ARG:NH2	2.36	0.44
1:A:84:GLN:O	1:A:87:SER:OG	2.27	0.44
1:A:293:THR:O	1:A:297:ASN:ND2	2.51	0.44
1:A:312:THR:HG22	1:A:313:TYR:CD1	2.53	0.44
1:E:70:VAL:HG13	1:E:74:MET:HE2	2.00	0.43
1:A:7:ARG:HE	1:A:12:VAL:HG23	1.82	0.43
1:E:452:THR:HA	1:E:455:ARG:HE	1.84	0.43
1:E:116:ALA:O	1:E:181:LEU:N	2.45	0.43
1:A:80:HIS:ND1	1:A:318:LEU:HB3	2.33	0.42
1:E:1:GLY:HA2	1:E:283:LYS:O	2.19	0.42
1:A:384:TYR:HB2	1:A:387:LEU:HD12	2.02	0.42
1:A:263:ASP:O	1:A:266:ASP:HB2	2.20	0.42
1:A:70:VAL:HG13	1:A:75:LYS:HE3	2.02	0.42
1:A:118:TYR:CG	1:A:119:PRO:HA	2.55	0.42
1:A:358:ASP:O	1:A:360:SER:N	2.52	0.42
1:E:406:ASP:OD1	1:E:408:ARG:HG3	2.18	0.42
1:A:24:LYS:HD2	2:B:599:C:H42	1.84	0.42
1:A:426:GLU:HG3	1:A:450:TYR:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:LYS:HE3	1:E:139:LYS:HB2	1.84	0.42
1:E:322:LYS:HB2	1:E:333:SER:OG	2.20	0.42
1:E:449:GLU:H	1:E:449:GLU:CD	2.23	0.42
1:A:4:GLN:CG	1:A:283:LYS:HG3	2.50	0.42
1:E:426:GLU:HG3	1:E:450:TYR:CD1	2.55	0.42
1:E:342:LEU:HD23	1:E:342:LEU:HA	1.88	0.41
3:G:693:A:H2'	3:G:694:G:H8	1.85	0.41
1:A:290:ALA:H	1:A:293:THR:HG21	1.85	0.41
1:A:413:HIS:ND1	3:C:698:G:H5''	2.36	0.41
1:A:170:GLN:HB3	1:A:172:LYS:HG3	2.01	0.41
1:A:47:ASP:O	1:A:50:LEU:HD12	2.20	0.41
1:A:288:SER:OG	1:A:289:GLY:N	2.52	0.41
1:E:47:ASP:HA	1:E:48:PRO:HD3	1.79	0.41
1:A:261:ARG:C	1:A:263:ASP:H	2.24	0.41
1:A:82:ALA:O	1:A:86:MET:HG2	2.21	0.41
1:A:139:LYS:HE3	1:A:139:LYS:HB2	1.83	0.41
1:E:80:HIS:HE1	1:E:318:LEU:O	2.03	0.41
2:F:600:A:C2	2:F:601:G:C5	3.09	0.41
1:A:383:LYS:HB3	1:A:384:TYR:CD1	2.55	0.41
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.82	0.41
1:A:367:THR:HG23	1:A:370:ASN:OD1	2.20	0.41
1:A:191:PHE:O	1:A:194:LEU:HB3	2.21	0.41
1:E:449:GLU:OE2	1:E:452:THR:OG1	2.38	0.40
1:E:405:LYS:O	1:E:406:ASP:HB2	2.21	0.40
1:E:397:ILE:HD13	1:E:421:ALA:HB2	2.03	0.40
1:E:127:LYS:NZ	2:F:601:G:OP1	2.54	0.40
1:E:176:ILE:HA	1:E:288:SER:OG	2.20	0.40
1:A:14:TYR:CD2	1:A:274:LEU:HD21	2.56	0.40
1:E:305:ILE:HD12	1:E:323:MET:CE	2.51	0.40
1:A:128:ARG:HE	1:A:128:ARG:HB3	1.76	0.40
2:B:600:A:C2	2:B:601:G:C5	3.10	0.40
1:A:232:PHE:HE1	1:A:234:TYR:CZ	2.40	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:VAL:O	1:E:148:TYR:OH[1_664]	2.06	0.14
1:A:148:TYR:OH	1:E:12:VAL:O[1_664]	2.10	0.10

## 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	
1	A	460/471 (98%)	429 (93%)	30 (6%)	1 (0%)	52	80
1	E	460/471 (98%)	429 (93%)	30 (6%)	1 (0%)	52	80
All	All	920/942 (98%)	858 (93%)	60 (6%)	2 (0%)	52	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	359	LYS
1	E	359	LYS

### 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	402/411 (98%)	370 (92%)	32 (8%)	15	33
1	E	402/411 (98%)	368 (92%)	34 (8%)	13	30
All	All	804/822 (98%)	738 (92%)	66 (8%)	14	32

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	7	ARG
1	A	21	SER
1	A	22	LYS

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Mol	Chain	Res	Type
1	A	43	LEU
1	A	45	LYS
1	A	52	THR
1	A	55	GLU
1	A	96	CYS
1	A	115	SER
1	A	128	ARG
1	A	154	LEU
1	A	163	ARG
1	A	218	TRP
1	A	242	SER
1	A	260	ASP
1	A	261	ARG
1	A	269	ASN
1	A	281	CYS
1	A	319	ASP
1	A	326	TYR
1	A	338	VAL
1	A	353	THR
1	A	355	THR
1	A	358	ASP
1	A	367	THR
1	A	369	GLU
1	A	392	MET
1	A	411	GLN
1	A	428	GLU
1	A	431	LYS
1	A	439	VAL
1	E	2	GLU
1	E	7	ARG
1	E	21	SER
1	E	22	LYS
1	E	43	LEU
1	E	45	LYS
1	E	52	THR
1	E	55	GLU
1	E	72	GLU
1	E	94	GLN
1	E	96	CYS
1	E	115	SER
1	E	128	ARG
1	E	154	LEU

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Mol	Chain	Res	Type
1	E	163	ARG
1	E	212	CYS
1	E	218	TRP
1	E	228	LYS
1	E	242	SER
1	E	281	CYS
1	E	319	ASP
1	E	326	TYR
1	E	338	VAL
1	E	353	THR
1	E	355	THR
1	E	358	ASP
1	E	362	THR
1	E	367	THR
1	E	369	GLU
1	E	392	MET
1	E	411	GLN
1	E	428	GLU
1	E	431	LYS
1	E	439	VAL

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

Mol	Chain	Res	Type
1	E	272	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	19/35 (54%)	6 (31%)	0
2	F	19/35 (54%)	4 (21%)	0
3	C	13/18 (72%)	4 (30%)	0
3	G	14/18 (77%)	5 (35%)	0
All	All	65/106 (61%)	19 (29%)	0

All (19) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	584	G
2	B	599	C

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Mol	Chain	Res	Type
2	B	602	G
2	B	611	G
2	B	614	G
2	B	615	A
3	C	690	A
3	C	692	G
3	C	695	A
3	C	697	A
3	G	688	C
3	G	690	A
3	G	692	G
3	G	695	A
3	G	697	A
2	F	584	G
2	F	599	C
2	F	611	G
2	F	614	G

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	462/471 (98%)	0.20	13 (2%) 56 57	51, 74, 101, 115	0
1	E	462/471 (98%)	0.14	10 (2%) 65 66	50, 75, 100, 115	0
2	B	21/35 (60%)	0.25	3 (14%) 4 3	62, 96, 153, 156	0
2	F	21/35 (60%)	0.46	3 (14%) 4 3	63, 97, 154, 157	0
3	C	14/18 (77%)	-0.13	0 100 100	64, 107, 161, 173	0
3	G	15/18 (83%)	-0.19	0 100 100	64, 107, 174, 181	0
All	All	995/1048 (94%)	0.17	29 (2%) 55 55	50, 75, 107, 181	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	585	G	5.7
1	A	309	LEU	4.7
2	B	584	G	4.6
1	A	22	LYS	4.4
1	E	126	LYS	3.9
2	F	584	G	3.6
1	A	7	ARG	3.6
1	E	53	ASP	3.4
1	E	130	ILE	3.3
2	B	583	G	3.0
1	A	16	ILE	3.0
1	A	118	TYR	2.9
2	F	598	C	2.8
1	A	170	GLN	2.7
1	E	459	ASP	2.6
1	E	169	GLU	2.5
1	A	347	GLY	2.5
1	A	126	LYS	2.4
1	E	125	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	462	GLY	2.2
2	B	585	G	2.2
1	A	258	PHE	2.2
1	A	102	TYR	2.2
1	A	458	LEU	2.2
1	E	455	ARG	2.2
1	E	131	LEU	2.1
1	E	357	ALA	2.1
1	A	342	LEU	2.1
1	A	244	ALA	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.