



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:01 PM GMT

PDB ID : 4K4U  
Title : Poliovirus polymerase elongation complex (r5\_form)  
Authors : Gong, P.; Peersen, O.B.  
Deposited on : 2013-04-12  
Resolution : 2.85 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

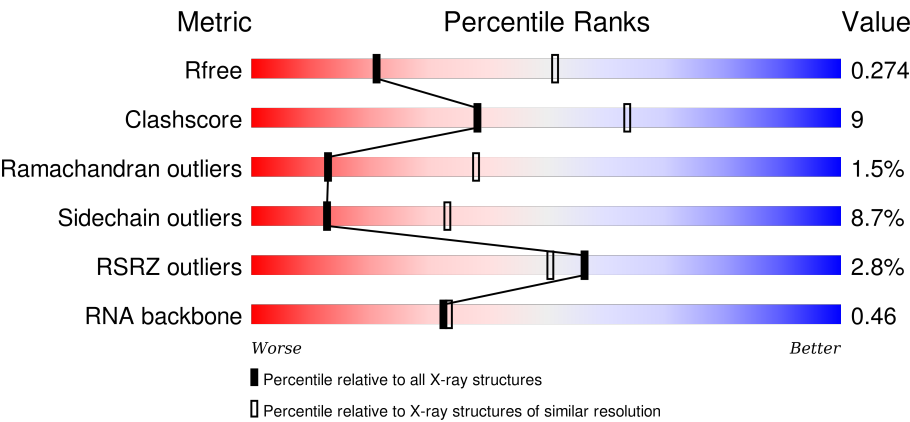
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)
RNA backbone	2183	1020 (3.22-2.50)

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><div></div><div>70%</div><div>25%</div><div>..</div></div></div>
1	E	471	<div><div>3%</div><div><div></div><div>73%</div><div>21%</div><div>..</div></div></div>
2	B	26	<div><div></div><div><div>42%</div><div>15%</div><div>15%</div><div>27%</div></div></div>
2	F	26	<div><div>4%</div><div><div></div><div>38%</div><div>19%</div><div>15%</div><div>27%</div></div></div>

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Mol	Chain	Length	Quality of chain
3	C	16	<div><div></div><div>38%50%6%6%</div></div>
3	G	16	<div><div></div><div>50%38%6%6%</div></div>
4	D	11	<div><div></div><div>9%18%82%</div></div>
4	H	11	<div><div></div><div>18%82%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9027 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
			3703	2374	611	696	22			
1	E	462	Total	C	N	O	S	0	0	0
			3703	2374	611	696	22			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	MET	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	MET	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(\*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	19	Total	C	N	O	P	0	0	0
			398	178	66	135	19			
2	F	19	Total	C	N	O	P	0	0	0
			398	178	66	135	19			

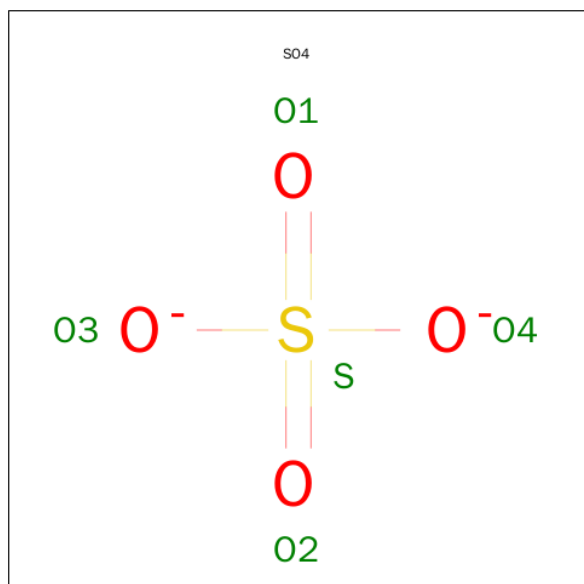
- Molecule 3 is a RNA chain called RNA (5'-R(\*UP\*GP\*UP\*UP\*CP\*GP\*AP\*CP\*GP\*AP\*GP\*AP\*GP\*AP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	15	Total	C	N	O	P	0	0	0
			328	146	65	102	15			
3	G	15	Total	C	N	O	P	0	0	0
			328	146	65	102	15			

- Molecule 4 is a RNA chain called RNA (5'-R(P\*GP\*GP\*GP\*GP\*GP\*AP\*GP\*AP\*UP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	2	Total	C	N	O	P	0	0	0
			46	20	10	14	2			
4	D	2	Total	C	N	O	P	0	0	0
			46	20	10	14	2			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0

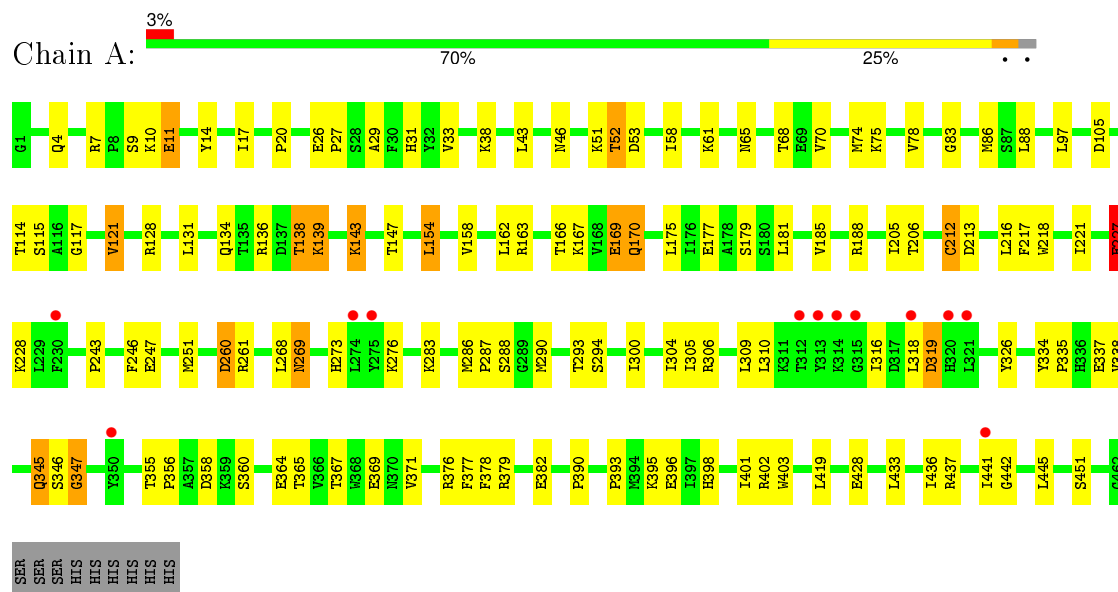
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	25	Total O 25 25	0	0
6	B	3	Total O 3 3	0	0
6	C	3	Total O 3 3	0	0
6	E	16	Total O 16 16	0	0
6	F	4	Total O 4 4	0	0
6	G	6	Total O 6 6	0	0

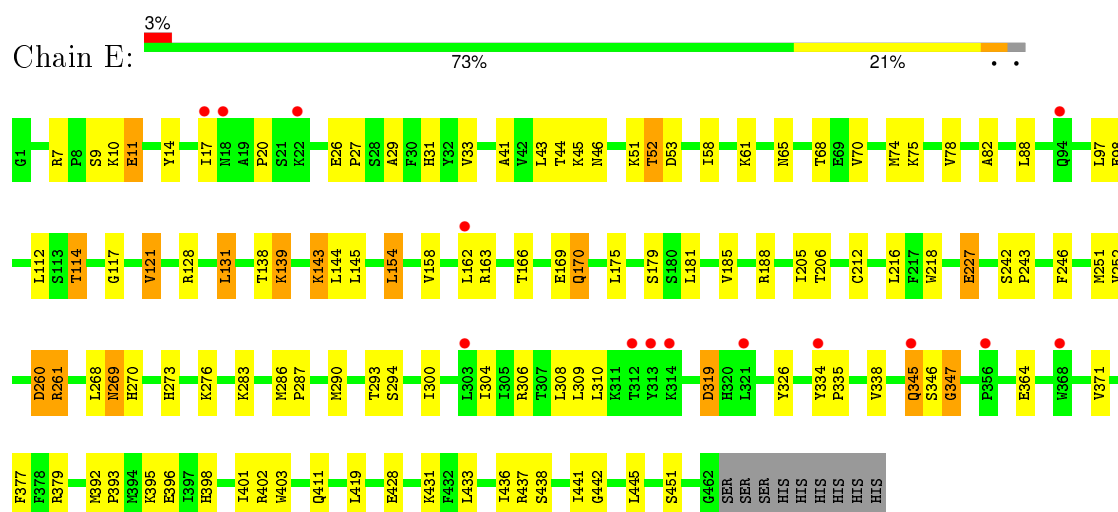
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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

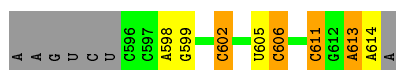


- Molecule 1: RNA-directed RNA polymerase 3D-POL



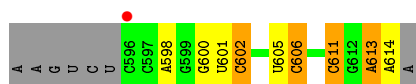
- Molecule 2: RNA (5'-R(\*AP\*AP\*GP\*UP\*CP\*UP\*CP\*CP\*AP\*GP\*GP\*UP\*CP\*UP\*CP\*UP\*CP\*UP\*CP\*GP\*UP\*CP\*GP\*AP\*AP\*A)-3')

Chain B: 



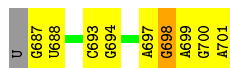
- Molecule 2: RNA (5'-R(\*AP\*AP\*GP\*UP\*CP\*UP\*CP\*CP\*AP\*GP\*GP\*UP\*CP\*UP\*CP\*UP\*CP\*UP\*CP\*GP\*UP\*CP\*GP\*AP\*AP\*A)-3')

Chain F: 



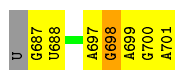
- Molecule 3: RNA (5'-R(\*UP\*GP\*UP\*UP\*CP\*GP\*AP\*CP\*GP\*AP\*GP\*AP\*GP\*AP\*GP\*A)-3')

Chain C: 



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

Chain G: 



- Molecule 4: RNA (5'-R(P\*GP\*GP\*GP\*GP\*GP\*AP\*GP\*AP\*UP\*GP\*A)-3')

Chain H: 



- Molecule 4: RNA (5'-R(P\*GP\*GP\*GP\*GP\*GP\*AP\*GP\*AP\*UP\*GP\*A)-3')

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.65Å 63.87Å 105.09Å 101.08° 106.22° 103.03°	Depositor
Resolution (Å)	43.26 – 2.85 43.26 – 2.82	Depositor EDS
% Data completeness (in resolution range)	98.0 (43.26-2.85) 88.5 (43.26-2.82)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.219 , 0.276 0.217 , 0.274	Depositor DCC
$R_{free}$ test set	1742 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	83.2	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 55.7	EDS
Estimated twinning fraction	0.439 for k,h,-h-k-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	0 of 35280 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9027	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.48	0/3793	0.63	0/5129
1	E	0.48	0/3793	0.63	0/5129
2	B	0.75	0/442	1.33	3/685 (0.4%)
2	F	0.68	0/442	1.21	3/685 (0.4%)
3	C	0.63	0/368	1.18	1/573 (0.2%)
3	G	0.69	0/368	1.18	1/573 (0.2%)
4	D	0.35	0/51	1.01	0/78
4	H	0.33	0/51	0.93	0/78
All	All	0.52	0/9308	0.79	8/12930 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	606	C	N3-C4-C5	-7.89	118.74	121.90
3	C	697	A	O5'-P-OP2	-6.72	99.65	105.70
2	F	606	C	N3-C4-C5	-6.48	119.31	121.90
2	F	606	C	N3-C4-N4	6.23	122.36	118.00
2	B	606	C	N3-C4-N4	5.40	121.78	118.00
3	G	697	A	O5'-P-OP1	-5.23	101.00	105.70
2	F	611	C	N1-C2-O2	5.15	121.99	118.90
2	B	611	C	N1-C2-O2	5.05	121.93	118.90

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	3703	0	3666	73	0
1	E	3703	0	3666	67	0
2	B	398	0	205	6	0
2	F	398	0	205	9	0
3	C	328	0	164	5	0
3	G	328	0	164	4	0
4	D	46	0	23	1	0
4	H	46	0	23	1	0
5	A	10	0	0	2	0
5	E	10	0	0	1	0
6	A	25	0	0	1	0
6	B	3	0	0	0	0
6	C	3	0	0	0	0
6	E	16	0	0	3	0
6	F	4	0	0	0	0
6	G	6	0	0	0	0
All	All	9027	0	8116	154	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 9.

All (154) 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:213:ASP:H	1:A:217:PHE:HD2	1.31	0.76
1:A:290:MET:HB2	1:A:293:THR:HG23	1.73	0.69
1:E:269:ASN:OD1	1:E:269:ASN:N	2.23	0.67
1:E:29:ALA:HB3	1:E:441:ILE:HD11	1.76	0.67
1:E:433:LEU:HD13	1:E:437:ARG:HH12	1.59	0.67
1:A:29:ALA:HB3	1:A:441:ILE:HD11	1.76	0.67
1:A:188:ARG:NH1	2:B:602:C:OP1	2.27	0.66
2:B:613:A:OP2	3:G:687:G:N2	2.27	0.66
1:A:65:ASN:OD1	1:A:243:PRO:HD3	1.96	0.66
3:C:687:G:N2	2:F:613:A:OP2	2.29	0.66
1:A:163:ARG:HH21	1:A:167:LYS:HD3	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:ASN:OD1	1:E:243:PRO:HD3	1.97	0.65
1:A:27:PRO:HB3	1:A:31:HIS:ND1	2.11	0.65
1:A:52:THR:OG1	1:A:53:ASP:N	2.30	0.65
2:F:605:U:H2'	2:F:606:C:C6	2.32	0.65
1:E:97:LEU:HD23	1:E:138:THR:HB	1.79	0.65
1:E:326:TYR:O	3:G:701:A:O2'	2.15	0.64
1:A:376:ARG:HD3	1:A:390:PRO:HB2	1.80	0.64
1:E:188:ARG:NH1	2:F:602:C:OP1	2.31	0.63
1:A:97:LEU:HD23	1:A:138:THR:HB	1.83	0.61
1:E:52:THR:OG1	1:E:53:ASP:N	2.33	0.61
1:E:166:THR:O	1:E:170:GLN:HB2	2.01	0.60
1:E:290:MET:HB2	1:E:293:THR:HG23	1.83	0.60
1:E:268:LEU:HD22	1:E:290:MET:HG3	1.82	0.60
1:E:163:ARG:NH2	5:E:502:SO4:O4	2.33	0.60
1:A:433:LEU:HD13	1:A:437:ARG:HH12	1.66	0.59
1:A:260:ASP:OD1	1:A:260:ASP:N	2.29	0.59
1:A:138:THR:OG1	1:A:139:LYS:N	2.35	0.59
1:A:326:TYR:O	3:C:701:A:O2'	2.18	0.58
1:E:7:ARG:NE	1:E:11:GLU:OE1	2.37	0.58
1:A:154:LEU:HD23	1:A:273:HIS:CE1	2.39	0.57
1:A:143:LYS:NZ	1:A:143:LYS:O	2.27	0.56
2:B:605:U:H2'	2:B:606:C:C6	2.39	0.56
1:E:436:ILE:O	1:E:442:GLY:HA3	2.05	0.56
1:E:29:ALA:CB	1:E:441:ILE:HD11	2.36	0.56
1:E:88:LEU:HD11	1:E:206:THR:HG22	1.88	0.55
1:E:27:PRO:HB3	1:E:31:HIS:ND1	2.21	0.55
1:A:436:ILE:O	1:A:442:GLY:HA3	2.06	0.55
1:E:74:MET:O	1:E:78:VAL:HG23	2.06	0.55
1:E:17:ILE:O	1:E:276:LYS:HA	2.07	0.55
1:A:88:LEU:HD11	1:A:206:THR:HG22	1.88	0.55
1:A:269:ASN:OD1	1:A:269:ASN:N	2.25	0.55
1:E:162:LEU:HD11	1:E:403:TRP:CD1	2.41	0.55
1:A:162:LEU:HD11	1:A:403:TRP:CD1	2.42	0.54
1:E:300:ILE:O	1:E:304:ILE:HG13	2.08	0.54
1:A:7:ARG:NE	1:A:11:GLU:OE1	2.40	0.54
1:A:287:PRO:O	1:A:293:THR:HG21	2.07	0.54
1:A:17:ILE:O	1:A:276:LYS:HA	2.08	0.53
1:E:138:THR:OG1	1:E:139:LYS:N	2.38	0.53
1:E:306:ARG:O	1:E:310:LEU:HG	2.09	0.53
1:E:269:ASN:O	1:E:283:LYS:HA	2.08	0.53
1:E:58:ILE:HD12	1:E:175:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:GLN:O	1:A:347:GLY:N	2.42	0.52
1:E:154:LEU:HD23	1:E:273:HIS:CE1	2.44	0.52
1:A:243:PRO:HA	1:A:246:PHE:HD2	1.75	0.52
1:E:260:ASP:HB2	1:E:261:ARG:HD3	1.92	0.52
1:A:300:ILE:O	1:A:304:ILE:HG13	2.10	0.52
1:E:243:PRO:HA	1:E:246:PHE:HD2	1.75	0.51
1:E:9:SER:HB3	1:E:14:TYR:O	2.09	0.51
1:A:83:GLY:O	1:A:86:MET:HB2	2.11	0.51
1:E:98:GLU:HG2	6:E:610:HOH:O	2.10	0.51
1:E:287:PRO:O	1:E:293:THR:HG21	2.10	0.51
2:F:600:G:H2'	2:F:601:U:H6	1.76	0.51
1:E:112:LEU:HD22	1:E:131:LEU:HD13	1.94	0.50
1:A:154:LEU:HD12	1:A:179:SER:HA	1.94	0.50
1:A:70:VAL:HG21	1:A:251:MET:HE3	1.93	0.50
1:A:166:THR:O	1:A:170:GLN:HB2	2.12	0.50
1:A:356:PRO:HB2	1:A:360:SER:HB2	1.94	0.49
1:E:419:LEU:HD11	2:F:606:C:H4'	1.94	0.49
1:E:58:ILE:HG13	1:E:175:LEU:HD11	1.94	0.49
2:F:600:G:H2'	2:F:601:U:C6	2.48	0.49
2:F:605:U:H2'	2:F:606:C:H6	1.77	0.49
1:E:269:ASN:ND2	6:E:612:HOH:O	2.43	0.49
1:E:154:LEU:HD12	1:E:179:SER:HA	1.94	0.48
1:E:117:GLY:C	1:E:121:VAL:HG12	2.34	0.48
1:A:143:LYS:NZ	1:A:147:THR:OG1	2.38	0.48
1:A:334:TYR:CD1	1:A:335:PRO:HD2	2.49	0.48
1:A:74:MET:O	1:A:78:VAL:HG23	2.14	0.47
1:A:38:LYS:NZ	5:A:501:SO4:O3	2.37	0.47
1:A:29:ALA:CB	1:A:441:ILE:HD11	2.44	0.47
4:H:804:G:H2'	4:H:805:G:C8	2.50	0.47
1:A:306:ARG:O	1:A:310:LEU:HG	2.15	0.47
1:A:163:ARG:NH2	5:A:502:SO4:O1	2.40	0.47
3:C:699:A:H2'	3:C:700:G:C8	2.50	0.47
3:C:698:G:H2'	3:C:699:A:C8	2.50	0.46
1:A:117:GLY:C	1:A:121:VAL:HG12	2.35	0.46
1:E:143:LYS:HD3	1:E:144:LEU:HD23	1.96	0.46
1:E:114:THR:HG22	2:F:600:G:P	2.56	0.46
1:E:377:PHE:HE1	1:E:393:PRO:HG3	1.80	0.46
1:A:269:ASN:O	1:A:283:LYS:HA	2.16	0.46
1:E:431:LYS:HB2	1:E:431:LYS:HE3	1.83	0.46
1:A:247:GLU:O	1:A:251:MET:HG3	2.15	0.46
1:A:212:CYS:HB2	1:A:217:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:334:TYR:CD1	1:E:335:PRO:HD2	2.51	0.46
1:E:319:ASP:OD1	1:E:319:ASP:N	2.48	0.45
1:A:268:LEU:HD22	1:A:290:MET:HG3	1.98	0.45
1:E:20:PRO:HG3	2:F:598:A:C4	2.52	0.45
1:A:337:GLU:OE2	1:A:365:THR:HG23	2.17	0.45
1:E:308:LEU:HD21	1:E:347:GLY:HA3	1.97	0.45
4:D:804:G:H2'	4:D:805:G:C8	2.53	0.44
1:A:177:GLU:H	1:A:288:SER:HB2	1.81	0.44
3:G:698:G:H2'	3:G:699:A:C8	2.53	0.44
3:G:699:A:H2'	3:G:700:G:C8	2.52	0.44
1:A:20:PRO:HG3	2:B:598:A:C4	2.53	0.44
1:A:9:SER:HB3	1:A:14:TYR:O	2.18	0.44
1:A:61:LYS:HE2	1:A:175:LEU:HD12	2.00	0.44
1:A:58:ILE:HD12	1:A:175:LEU:HD21	2.00	0.43
1:A:419:LEU:HD11	2:B:606:C:H4'	2.00	0.43
1:A:217:PHE:O	1:A:221:ILE:HG13	2.17	0.43
1:E:392:MET:HA	1:E:393:PRO:HD3	1.84	0.43
1:E:334:TYR:CG	1:E:335:PRO:HD2	2.53	0.43
1:E:345:GLN:O	1:E:347:GLY:N	2.52	0.43
1:A:134:GLN:O	1:A:136:ARG:HG3	2.19	0.43
1:A:310:LEU:HD21	1:A:318:LEU:HG	2.00	0.43
1:A:4:GLN:OE1	1:A:283:LYS:HB2	2.19	0.43
1:E:70:VAL:HG21	1:E:251:MET:HE3	2.01	0.43
1:A:355:THR:HB	1:A:356:PRO:CD	2.49	0.43
1:E:309:LEU:HA	1:E:309:LEU:HD23	1.74	0.43
1:E:395:LYS:O	1:E:398:HIS:HB2	2.19	0.42
1:A:398:HIS:O	1:A:401:ILE:HG22	2.19	0.42
1:E:411:GLN:HA	1:E:445:LEU:HD22	2.00	0.42
1:E:260:ASP:OD1	1:E:260:ASP:N	2.29	0.42
1:A:309:LEU:HD13	1:A:316:ILE:HD11	2.02	0.42
1:A:38:LYS:HE3	6:A:606:HOH:O	2.20	0.41
1:A:154:LEU:HD11	1:A:290:MET:HE1	2.02	0.41
1:E:441:ILE:O	1:E:445:LEU:HG	2.20	0.41
1:A:334:TYR:CG	1:A:335:PRO:HD2	2.55	0.41
1:A:395:LYS:O	1:A:398:HIS:HB2	2.20	0.41
1:A:227:GLU:HB3	1:A:228:LYS:H	1.71	0.41
1:E:41:ALA:HB2	1:E:163:ARG:HB2	2.01	0.41
1:E:145:LEU:HD23	1:E:145:LEU:HA	1.79	0.41
1:A:51:LYS:HB3	1:A:169:GLU:O	2.20	0.41
1:A:319:ASP:N	1:A:319:ASP:OD1	2.54	0.41
1:A:367:THR:C	1:A:369:GLU:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:HIS:ND1	1:E:283:LYS:HE3	2.35	0.41
1:E:75:LYS:HB2	1:E:75:LYS:HE3	1.91	0.41
1:E:379:ARG:HA	6:E:602:HOH:O	2.20	0.41
1:A:377:PHE:HE1	1:A:393:PRO:HG3	1.86	0.41
1:A:75:LYS:HB2	1:A:75:LYS:HE3	1.89	0.41
1:A:181:LEU:O	1:A:185:VAL:HG23	2.21	0.41
1:E:44:THR:OG1	1:E:45:LYS:N	2.54	0.41
1:E:398:HIS:O	1:E:401:ILE:HG22	2.21	0.41
1:A:309:LEU:HB3	1:A:316:ILE:HD13	2.03	0.41
1:E:181:LEU:O	1:E:185:VAL:HG23	2.21	0.41
1:E:51:LYS:HB3	1:E:169:GLU:O	2.20	0.41
1:A:378:PHE:O	1:A:379:ARG:HD3	2.20	0.41
1:A:286:MET:HB2	1:A:286:MET:HE2	2.01	0.40
1:A:441:ILE:O	1:A:445:LEU:HG	2.21	0.40
1:E:243:PRO:HA	1:E:246:PHE:CD2	2.55	0.40
1:E:82:ALA:HB2	1:E:252:VAL:HG13	2.02	0.40
1:A:115:SER:HB2	2:B:599:G:OP1	2.22	0.40
3:C:693:C:H2'	3:C:694:G:H8	1.85	0.40
1:E:286:MET:HA	1:E:287:PRO:HD3	1.99	0.40
1:E:61:LYS:HE2	1:E:175:LEU:HD12	2.04	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	460/471 (98%)	411 (89%)	41 (9%)	8 (2%)	11	35
1	E	460/471 (98%)	411 (89%)	43 (9%)	6 (1%)	15	42
All	All	920/942 (98%)	822 (89%)	84 (9%)	14 (2%)	13	38

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	LYS
1	A	227	GLU
1	E	139	LYS
1	E	227	GLU
1	A	33	VAL
1	A	346	SER
1	E	33	VAL
1	E	346	SER
1	A	105	ASP
1	A	138	THR
1	E	345	GLN
1	A	345	GLN
1	A	347	GLY
1	E	347	GLY

### 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	403/412 (98%)	367 (91%)	36 (9%)	12	32
1	E	403/412 (98%)	369 (92%)	34 (8%)	14	35
All	All	806/824 (98%)	736 (91%)	70 (9%)	13	33

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	11	GLU
1	A	26	GLU
1	A	43	LEU
1	A	46	ASN
1	A	52	THR
1	A	68	THR
1	A	114	THR
1	A	121	VAL
1	A	128	ARG

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Mol	Chain	Res	Type
1	A	131	LEU
1	A	143	LYS
1	A	154	LEU
1	A	158	VAL
1	A	169	GLU
1	A	170	GLN
1	A	205	ILE
1	A	212	CYS
1	A	216	LEU
1	A	218	TRP
1	A	227	GLU
1	A	260	ASP
1	A	261	ARG
1	A	269	ASN
1	A	294	SER
1	A	305	ILE
1	A	319	ASP
1	A	338	VAL
1	A	358	ASP
1	A	364	GLU
1	A	371	VAL
1	A	382	GLU
1	A	396	GLU
1	A	402	ARG
1	A	428	GLU
1	A	451	SER
1	E	10	LYS
1	E	11	GLU
1	E	26	GLU
1	E	43	LEU
1	E	46	ASN
1	E	52	THR
1	E	68	THR
1	E	114	THR
1	E	121	VAL
1	E	128	ARG
1	E	131	LEU
1	E	143	LYS
1	E	154	LEU
1	E	158	VAL
1	E	170	GLN
1	E	205	ILE

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Mol	Chain	Res	Type
1	E	212	CYS
1	E	216	LEU
1	E	218	TRP
1	E	227	GLU
1	E	242	SER
1	E	260	ASP
1	E	261	ARG
1	E	269	ASN
1	E	294	SER
1	E	319	ASP
1	E	338	VAL
1	E	364	GLU
1	E	371	VAL
1	E	396	GLU
1	E	402	ARG
1	E	428	GLU
1	E	438	SER
1	E	451	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	18/26 (69%)	4 (22%)	0
2	F	18/26 (69%)	4 (22%)	0
3	C	14/16 (87%)	2 (14%)	0
3	G	14/16 (87%)	2 (14%)	0
4	D	1/11 (9%)	0	0
4	H	1/11 (9%)	0	0
All	All	66/106 (62%)	12 (18%)	0

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	602	C
2	B	611	C
2	B	613	A
2	B	614	A
3	C	688	U

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Mol	Chain	Res	Type
3	C	698	G
2	F	602	C
2	F	611	C
2	F	613	A
2	F	614	A
3	G	688	U
3	G	698	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](#)

4 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	SO4	A	501	-	4,4,4	0.23	0	6,6,6	0.21	0
5	SO4	A	502	-	4,4,4	0.25	0	6,6,6	0.27	0
5	SO4	E	501	-	4,4,4	0.13	0	6,6,6	0.17	0
5	SO4	E	502	-	4,4,4	0.19	0	6,6,6	0.30	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
5	SO4	A	501	-	-	0/0/0/0	0/0/0/0
5	SO4	A	502	-	-	0/0/0/0	0/0/0/0
5	SO4	E	501	-	-	0/0/0/0	0/0/0/0
5	SO4	E	502	-	-	0/0/0/0	0/0/0/0

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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	SO4	1	0
5	A	502	SO4	1	0
5	E	502	SO4	1	0

## 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%)	0.08	12 (2%) 59 54	64, 92, 116, 132	0
1	E	462/471 (98%)	0.15	14 (3%) 54 47	66, 91, 116, 132	0
2	B	19/26 (73%)	-0.02	0 100 100	73, 105, 177, 198	0
2	F	19/26 (73%)	0.12	1 (5%) 30 24	75, 105, 177, 198	0
3	C	15/16 (93%)	-0.28	0 100 100	71, 97, 158, 161	0
3	G	15/16 (93%)	-0.27	0 100 100	71, 97, 158, 162	0
4	D	2/11 (18%)	1.55	1 (50%) 0 0	170, 170, 170, 185	0
4	H	2/11 (18%)	0.28	0 100 100	170, 170, 170, 184	0
All	All	996/1048 (95%)	0.10	28 (2%) 56 51	64, 92, 121, 198	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	321	LEU	4.7
1	A	312	THR	4.5
1	A	313	TYR	4.1
1	E	312	THR	4.1
1	A	321	LEU	4.0
2	F	596	C	3.6
1	A	314	LYS	3.5
1	A	275	TYR	3.3
1	E	368	TRP	2.9
1	A	318	LEU	2.8
1	E	334	TYR	2.8
1	E	17	ILE	2.8
1	E	18	ASN	2.7
1	E	303	LEU	2.6
1	A	274	LEU	2.6
1	E	22	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	350	TYR	2.5
1	A	315	GLY	2.4
1	A	320	HIS	2.3
1	E	313	TYR	2.3
1	E	94	GLN	2.3
4	D	805	G	2.2
1	A	441	ILE	2.2
1	E	356	PRO	2.2
1	A	230	PHE	2.2
1	E	314	LYS	2.1
1	E	345	GLN	2.1
1	E	162	LEU	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	SO4	A	501	5/5	0.86	0.14	-0.83	104,114,120,133	0
5	SO4	E	501	5/5	0.94	0.07	-2.91	103,114,123,131	0
5	SO4	A	502	5/5	0.90	0.09	-	121,123,126,140	0
5	SO4	E	502	5/5	0.82	0.12	-	118,123,128,138	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.