



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:02 PM GMT

PDB ID : 3SIU  
Title : Structure of a hPrp31-15.5K-U4atac 5' stem loop complex, monomeric form  
Authors : Liu, S.; Ghalei, H.; Luhrmann, R.; Wahl, M.C.  
Deposited on : 2011-06-20  
Resolution : 2.63 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

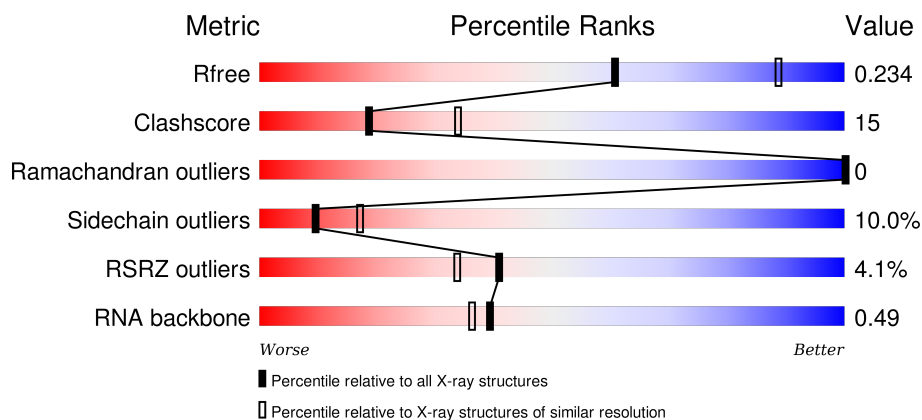
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.63 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	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)
RNA backbone	2183	1036 (3.04-2.20)

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	130	<div> <div>4%</div> <div>70% 24% . .</div> </div>
1	D	130	<div> <div>4%</div> <div>64% 28% . .</div> </div>
2	B	254	<div> <div>4%</div> <div>59% 27% 6% 7%</div> </div>
2	E	254	<div> <div>3%</div> <div>67% 22% . 7%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	28	<div><div></div><div>11%</div><div>50%</div><div>29%</div><div>21%</div></div>
3	F	28	<div><div></div><div>7%</div><div>39%</div><div>46%</div><div>14%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6896 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 NHP2-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			967	611	172	179	5			
1	D	125	Total	C	N	O	S	0	0	0
			968	611	172	180	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P55769
A	0	SER	-	EXPRESSION TAG	UNP P55769
D	-1	GLY	-	EXPRESSION TAG	UNP P55769
D	0	SER	-	EXPRESSION TAG	UNP P55769

- Molecule 2 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	0
			1844	1158	319	357	10			
2	E	236	Total	C	N	O	S	0	0	0
			1848	1161	319	358	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	80	GLY	-	EXPRESSION TAG	UNP Q8WWY3
B	81	PRO	-	EXPRESSION TAG	UNP Q8WWY3
B	82	LEU	-	EXPRESSION TAG	UNP Q8WWY3
B	83	GLY	-	EXPRESSION TAG	UNP Q8WWY3
B	84	SER	-	EXPRESSION TAG	UNP Q8WWY3
E	80	GLY	-	EXPRESSION TAG	UNP Q8WWY3
E	81	PRO	-	EXPRESSION TAG	UNP Q8WWY3
E	82	LEU	-	EXPRESSION TAG	UNP Q8WWY3

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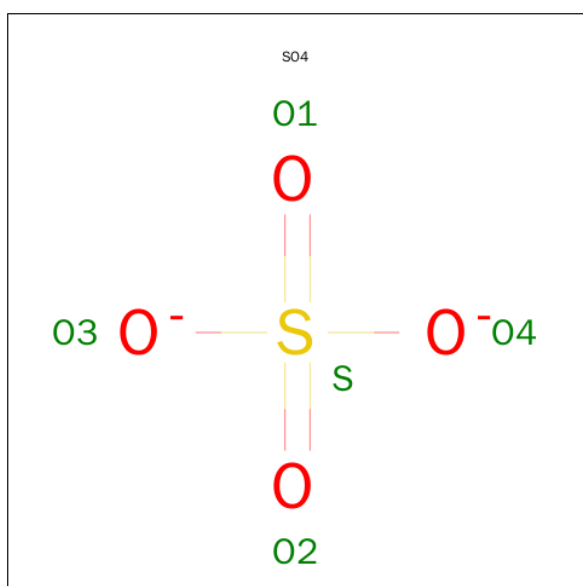
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Chain	Residue	Modelled	Actual	Comment	Reference
E	83	GLY	-	EXPRESSION TAG	UNP Q8WWY3
E	84	SER	-	EXPRESSION TAG	UNP Q8WWY3

- Molecule 3 is a RNA chain called U4atac snRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	28	Total	C	N	O	P	0	0	0
			601	269	113	192	27			
3	F	28	Total	C	N	O	P	0	0	0
			601	269	113	192	27			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		
5	B	11	Total	O	0	0
			11	11		

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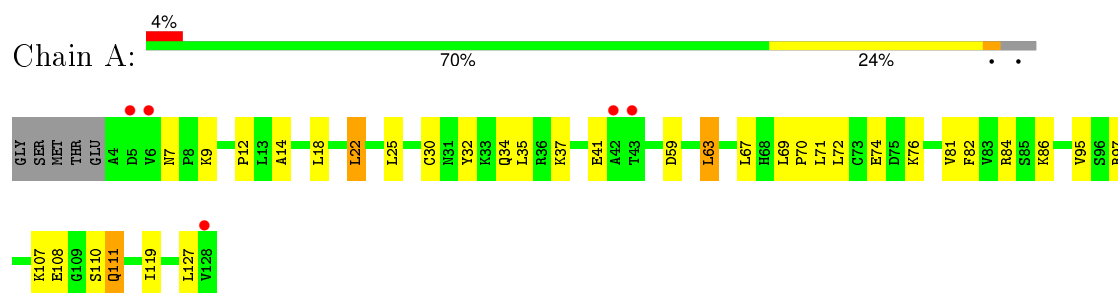
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	9	Total 9	O 9	0	0
5	D	9	Total 9	O 9	0	0
5	E	10	Total 10	O 10	0	0
5	F	14	Total 14	O 14	0	0

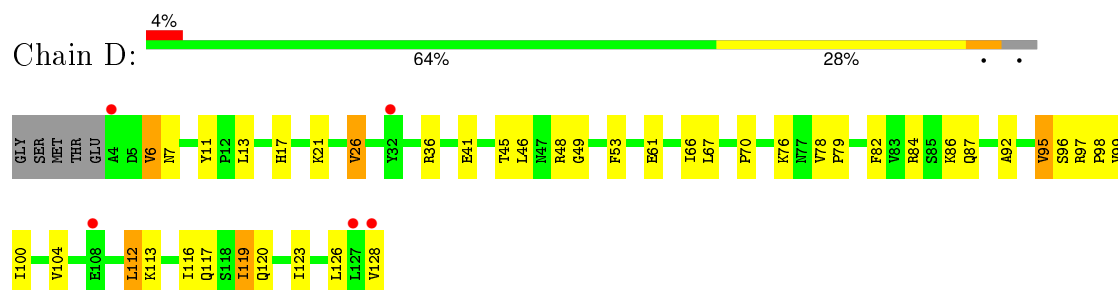
### 3 Residue-property plots [i](#)

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.

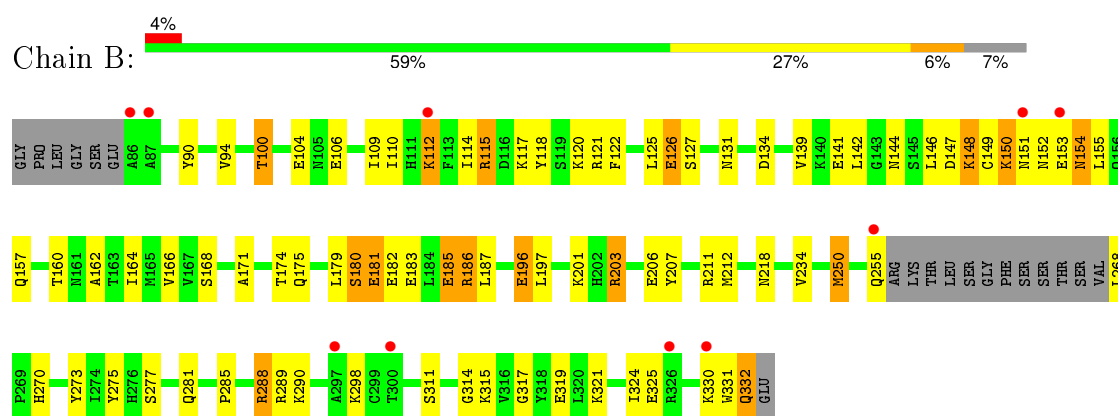
- Molecule 1: NHP2-like protein 1



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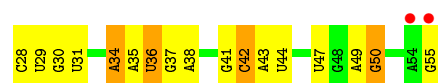


- Molecule 2: U4/U6 small nuclear ribonucleoprotein Prp31



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.50 Å 111.26 Å 110.86 Å 90.00° 101.81° 90.00°	Depositor
Resolution (Å)	29.45 – 2.63 30.32 – 2.63	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.45-2.63) 98.9 (30.32-2.63)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.64 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.198 , 0.241 0.185 , 0.234	Depositor DCC
$R_{free}$ test set	1748 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.0	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 50.4	EDS
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 34743 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% 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](#)

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	0.45	0/979	0.62	0/1323
1	D	0.40	0/980	0.58	0/1323
2	B	0.42	0/1870	0.56	0/2526
2	E	0.45	0/1874	0.56	0/2532
3	C	0.47	0/673	0.97	3/1049 (0.3%)
3	F	0.58	0/673	1.19	5/1049 (0.5%)
All	All	0.45	0/7049	0.71	8/9802 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	C	48	G	N9-C4-C5	-6.70	102.72	105.40
3	F	42	C	C2-N1-C1'	6.34	125.78	118.80
3	F	34	A	N1-C6-N6	6.33	122.40	118.60
3	F	34	A	C5-C6-N6	-5.57	119.25	123.70
3	C	48	G	N1-C6-O6	5.51	123.20	119.90
3	F	36	U	C5-C4-O4	5.44	129.16	125.90
3	F	34	A	N9-C4-C5	-5.33	103.67	105.80
3	C	48	G	C8-N9-C4	5.19	108.47	106.40

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	967	0	1017	30	0
1	D	968	0	1017	35	0
2	B	1844	0	1864	69	0
2	E	1848	0	1870	51	0
3	C	601	0	305	22	0
3	F	601	0	305	15	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
5	A	4	0	0	0	0
5	B	11	0	0	1	0
5	C	9	0	0	2	0
5	D	9	0	0	0	0
5	E	10	0	0	0	0
5	F	14	0	0	1	0
All	All	6896	0	6378	204	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 15.

All (204) 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)
3:C:45:A:H4'	3:C:46:G:H5''	1.31	1.11
2:B:285:PRO:HA	2:B:288:ARG:HD2	1.40	1.03
1:A:32:TYR:CE1	1:A:111:GLN:HG3	1.95	1.00
1:A:32:TYR:HE1	1:A:111:GLN:HG3	1.18	1.00
2:B:218:ASN:HD22	2:B:317:GLY:H	1.07	1.00
3:C:40:C:C2'	3:C:41:G:H5'	1.99	0.92
2:B:112:LYS:HD3	2:B:115:ARG:NH2	1.88	0.88
2:B:218:ASN:ND2	2:B:317:GLY:H	1.71	0.88
2:B:186:ARG:HG3	2:E:211:ARG:NH1	1.89	0.86
2:B:147:ASP:O	2:B:148:LYS:HG3	1.77	0.85
3:C:40:C:H2'	3:C:41:G:H5'	1.59	0.82
3:C:45:A:H1'	3:C:46:G:OP2	1.81	0.81
2:B:186:ARG:HG3	2:E:211:ARG:HH12	1.44	0.80
2:B:311:SER:OG	2:B:315:LYS:HG2	1.81	0.80
1:A:95:VAL:HG12	1:A:97:ARG:H	1.47	0.79
1:D:119:ILE:O	1:D:123:ILE:HG13	1.85	0.77
2:B:218:ASN:HD22	2:B:317:GLY:N	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:PRO:HA	2:B:288:ARG:CD	2.18	0.73
1:D:86:LYS:HG3	1:D:98:PRO:HB3	1.69	0.72
2:B:117:LYS:HG2	2:B:187:LEU:HD13	1.71	0.71
2:E:121:ARG:HD2	2:E:121:ARG:O	1.92	0.70
2:B:147:ASP:O	2:B:148:LYS:HE3	1.93	0.68
3:C:45:A:H3'	3:C:45:A:OP1	1.92	0.68
3:C:45:A:C1'	3:C:46:G:OP2	2.43	0.66
2:B:315:LYS:O	2:B:319:GLU:HG3	1.95	0.66
2:B:121:ARG:NH1	2:B:144:ASN:O	2.26	0.65
2:B:270:HIS:CE1	3:C:42:C:H5"	2.31	0.65
1:A:71:LEU:HD12	1:A:71:LEU:N	2.12	0.65
2:E:108:ASN:HD22	2:E:109:ILE:N	1.94	0.65
2:B:117:LYS:NZ	2:B:183:GLU:O	2.30	0.65
2:B:185:GLU:HB3	2:B:186:ARG:NH1	2.12	0.64
2:B:112:LYS:HD3	2:B:115:ARG:HH22	1.59	0.64
2:B:106:GLU:O	2:B:110:ILE:HG13	1.97	0.64
2:B:250:MET:HE1	3:C:41:G:H1	1.63	0.63
2:E:108:ASN:HD22	2:E:108:ASN:C	2.01	0.63
1:D:49:GLY:HA2	1:D:76:LYS:NZ	2.13	0.63
3:C:29:U:H2'	3:C:30:G:C8	2.34	0.63
1:D:113:LYS:O	1:D:117:GLN:HG2	1.99	0.63
1:A:35:LEU:HD23	1:A:37:LYS:HE2	1.81	0.62
2:E:152:ASN:OD1	2:E:155:LEU:HB2	2.00	0.62
2:B:196:GLU:HA	2:B:196:GLU:OE1	1.98	0.62
2:B:331:TRP:O	2:B:332:GLN:HG2	1.98	0.62
1:D:95:VAL:HG13	1:D:97:ARG:H	1.64	0.62
3:C:29:U:H2'	3:C:30:G:H8	1.64	0.61
2:B:196:GLU:CA	2:B:196:GLU:OE1	2.48	0.61
2:E:147:ASP:HA	2:E:150:LYS:NZ	2.15	0.61
2:E:133:LEU:O	2:E:133:LEU:HD13	2.01	0.61
1:A:59:ASP:HB3	1:A:86:LYS:HD3	1.83	0.60
1:D:116:ILE:O	1:D:120:GLN:HG3	2.03	0.59
1:A:41:GLU:HG3	3:C:37:G:O6	2.03	0.59
2:E:109:ILE:HG22	2:E:110:ILE:N	2.18	0.59
2:E:106:GLU:OE1	2:E:106:GLU:HA	2.02	0.59
2:B:146:LEU:HD12	2:B:174:THR:HG21	1.85	0.58
2:E:115:ARG:HG3	2:E:116:ASP:N	2.18	0.58
2:B:211:ARG:NH2	2:E:186:ARG:HB2	2.17	0.58
1:D:49:GLY:HA2	1:D:76:LYS:HZ2	1.69	0.58
2:E:331:TRP:O	2:E:332:GLN:HG2	2.04	0.58
2:E:117:LYS:HB2	2:E:187:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:LYS:HG2	2:B:151:ASN:N	2.19	0.57
3:F:28:C:H5'	5:F:23:HOH:O	2.05	0.57
3:C:47:U:C2'	3:C:48:G:H5'	2.35	0.56
2:B:90:TYR:O	2:B:94:VAL:HG23	2.05	0.56
2:E:153:GLU:O	2:E:157:GLN:HG2	2.05	0.56
2:E:165:MET:HG3	2:E:166:VAL:N	2.21	0.56
1:A:67:LEU:O	1:A:71:LEU:HD13	2.07	0.55
3:C:32:C:H5'	5:C:58:HOH:O	2.06	0.55
2:B:285:PRO:CA	2:B:288:ARG:HD2	2.27	0.55
2:B:131:ASN:HD22	2:B:134:ASP:CG	2.10	0.54
1:A:34:GLN:NE2	1:A:110:SER:OG	2.37	0.54
2:B:179:LEU:HB3	2:B:183:GLU:HG3	1.89	0.54
2:E:200:SER:O	2:E:204:ILE:HG13	2.06	0.54
2:B:149:CYS:SG	2:B:168:SER:HA	2.47	0.54
2:B:154:ASN:HA	2:B:157:GLN:NE2	2.22	0.54
2:B:270:HIS:HB2	2:B:289:ARG:HH21	1.72	0.53
2:E:119:SER:O	2:E:123:PRO:HG3	2.08	0.53
1:A:81:VAL:HG22	1:A:82:PHE:N	2.24	0.53
2:E:289:ARG:NH2	3:F:41:G:OP2	2.41	0.53
1:D:17:HIS:CD2	1:D:21:LYS:HE2	2.43	0.53
2:B:185:GLU:OE1	2:B:186:ARG:NH1	2.42	0.53
2:B:117:LYS:NZ	2:B:183:GLU:HB2	2.24	0.53
1:D:46:LEU:HA	1:D:76:LYS:NZ	2.24	0.53
2:B:207:TYR:O	2:B:211:ARG:HG2	2.08	0.53
2:E:121:ARG:CZ	2:E:146:LEU:HD13	2.39	0.52
2:E:155:LEU:C	2:E:164:ILE:HD11	2.30	0.52
2:B:290:LYS:HG3	2:B:331:TRP:CH2	2.44	0.52
1:D:97:ARG:HD3	3:F:34:A:C6	2.44	0.52
2:B:218:ASN:ND2	2:B:314:GLY:HA2	2.23	0.52
2:E:148:LYS:O	2:E:152:ASN:ND2	2.39	0.52
1:A:74:GLU:OE1	1:A:74:GLU:HA	2.09	0.52
3:C:40:C:O2'	3:C:41:G:H5'	2.10	0.52
2:B:154:ASN:HA	2:B:157:GLN:HE21	1.75	0.52
1:A:25:LEU:HD23	1:A:119:ILE:HG13	1.92	0.51
2:B:186:ARG:N	2:B:186:ARG:HD2	2.26	0.51
2:E:322:ASP:O	2:E:326:ARG:HG3	2.11	0.51
1:D:67:LEU:O	1:D:70:PRO:HD2	2.10	0.50
2:E:193:MET:HA	2:E:193:MET:CE	2.42	0.50
2:B:180:SER:OG	2:B:183:GLU:HG2	2.12	0.50
1:A:71:LEU:CD1	1:A:71:LEU:N	2.74	0.49
2:E:133:LEU:HD12	2:E:137:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:GLU:OE1	2:B:182:GLU:HA	2.12	0.49
2:B:117:LYS:CE	2:B:183:GLU:HB2	2.42	0.49
1:D:95:VAL:CG1	1:D:97:ARG:H	2.25	0.49
1:D:13:LEU:HD12	1:D:82:PHE:O	2.11	0.49
1:D:112:LEU:HB3	1:D:116:ILE:HG13	1.94	0.49
1:D:26:VAL:HG22	1:D:92:ALA:HB1	1.95	0.49
2:B:152:ASN:OD1	2:B:155:LEU:N	2.21	0.48
3:F:42:C:H4'	3:F:43:A:O5'	2.14	0.48
2:B:275:TYR:CE2	2:B:288:ARG:HB3	2.49	0.48
2:E:331:TRP:O	2:E:332:GLN:CB	2.61	0.48
3:C:43:A:O2'	3:C:44:U:H5'	2.13	0.48
2:E:160:THR:O	2:E:164:ILE:HG13	2.13	0.48
2:B:212:MET:HA	2:B:212:MET:CE	2.44	0.48
2:E:212:MET:CE	2:E:212:MET:HA	2.43	0.48
3:F:49:A:O3'	3:F:50:G:H4'	2.14	0.47
2:E:161:ASN:O	2:E:165:MET:HB3	2.14	0.47
2:B:115:ARG:HD2	2:B:126:GLU:HG3	1.95	0.47
1:D:97:ARG:HD3	3:F:34:A:C5	2.49	0.47
2:B:186:ARG:CG	2:E:211:ARG:HH12	2.23	0.47
1:A:34:GLN:HG2	1:A:107:LYS:HD3	1.97	0.47
2:E:193:MET:HA	2:E:193:MET:HE3	1.97	0.46
3:C:43:A:H3'	3:C:44:U:H6	1.79	0.46
2:B:162:ALA:O	2:B:166:VAL:HG23	2.15	0.46
1:A:67:LEU:O	1:A:70:PRO:HD2	2.16	0.46
1:A:18:LEU:HG	1:A:22:LEU:HD22	1.97	0.46
3:F:38:A:C8	3:F:49:A:C6	3.04	0.46
2:E:147:ASP:HA	2:E:150:LYS:HZ2	1.79	0.46
2:E:155:LEU:O	2:E:164:ILE:HD11	2.16	0.46
1:A:72:LEU:O	1:A:76:LYS:HG2	2.15	0.46
2:B:321:LYS:HE2	2:B:325:GLU:OE2	2.16	0.46
2:B:147:ASP:O	2:B:148:LYS:CE	2.63	0.46
1:D:123:ILE:HA	1:D:126:LEU:HD12	1.98	0.46
1:A:41:GLU:OE1	3:C:37:G:N1	2.45	0.46
2:E:320:LEU:O	2:E:324:ILE:HG13	2.16	0.46
1:D:48:ARG:NH2	3:F:47:U:OP1	2.49	0.46
2:B:277:SER:O	2:B:281:GLN:HG2	2.16	0.46
2:E:150:LYS:HD2	2:E:150:LYS:N	2.31	0.45
2:E:270:HIS:CD2	3:F:44:U:C2	3.05	0.45
2:B:197:LEU:HA	2:B:197:LEU:HD23	1.52	0.45
1:A:22:LEU:CD1	1:A:119:ILE:HD12	2.46	0.45
2:B:234:VAL:HG21	2:B:273:TYR:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:121:ARG:HD3	2:E:177:GLN:O	2.16	0.45
1:D:36:ARG:HD3	1:D:36:ARG:HA	1.76	0.45
1:D:76:LYS:HG2	1:D:76:LYS:O	2.16	0.45
2:B:298:LYS:HB2	2:B:324:ILE:HD11	1.98	0.45
2:B:115:ARG:CD	2:B:126:GLU:HG3	2.47	0.45
2:B:100:THR:O	2:B:104:GLU:HG3	2.16	0.45
1:A:7:ASN:OD1	1:A:9:LYS:HB2	2.16	0.45
1:D:95:VAL:HG12	1:D:97:ARG:O	2.16	0.45
2:B:109:ILE:HG22	2:E:92:VAL:HG22	1.98	0.45
2:B:154:ASN:O	2:B:157:GLN:HB2	2.17	0.45
1:A:14:ALA:HB1	1:A:18:LEU:HB3	1.99	0.44
1:A:74:GLU:CA	1:A:74:GLU:OE1	2.66	0.44
1:A:63:LEU:HD13	1:A:67:LEU:HD21	1.99	0.44
3:C:31:U:H2'	3:C:32:C:C6	2.52	0.44
3:C:32:C:C5'	5:C:58:HOH:O	2.65	0.44
2:E:135:TYR:O	2:E:139:VAL:HG13	2.17	0.44
1:A:12:PRO:HG3	1:A:127:LEU:CD2	2.48	0.44
1:D:100:ILE:HG12	3:F:36:U:P	2.58	0.44
2:E:221:ILE:O	2:E:321:LYS:HD2	2.17	0.44
1:D:6:VAL:HG13	1:D:7:ASN:N	2.33	0.43
2:B:131:ASN:HB3	5:B:8:HOH:O	2.18	0.43
3:F:30:G:C6	3:F:31:U:C4	3.06	0.43
2:E:117:LYS:HD3	2:E:117:LYS:HA	1.85	0.43
2:B:171:ALA:O	2:B:174:THR:HG22	2.17	0.43
2:E:89:GLU:OE2	2:E:211:ARG:NE	2.49	0.43
1:A:67:LEU:HA	1:A:67:LEU:HD23	1.79	0.43
1:A:30:CYS:HB2	1:A:35:LEU:HD22	2.00	0.43
2:B:118:TYR:CD1	2:B:139:VAL:HG22	2.54	0.43
2:E:110:ILE:HG21	2:E:194:ALA:HB2	2.00	0.43
2:B:152:ASN:ND2	2:B:154:ASN:HD22	2.16	0.43
2:B:212:MET:HE2	2:B:212:MET:HA	2.01	0.43
3:C:40:C:C3'	3:C:41:G:H5'	2.49	0.43
2:E:283:LEU:HD23	2:E:291:ALA:HB2	1.99	0.43
1:D:87:GLN:HA	1:D:87:GLN:NE2	2.33	0.43
1:D:41:GLU:O	1:D:45:THR:HG23	2.18	0.42
1:D:76:LYS:HE3	1:D:76:LYS:HB3	1.71	0.42
2:B:152:ASN:HD21	2:B:154:ASN:HD22	1.67	0.42
2:B:120:LYS:HG2	2:B:179:LEU:HD21	2.00	0.42
2:B:203:ARG:NH2	2:B:206:GLU:OE2	2.44	0.42
1:D:46:LEU:HA	1:D:76:LYS:HZ1	1.83	0.42
2:E:147:ASP:HA	2:E:150:LYS:HZ3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:PHE:CZ	1:D:104:VAL:HG21	2.55	0.42
1:D:99:VAL:HG22	3:F:35:A:O2'	2.20	0.42
3:C:45:A:C4'	3:C:46:G:H5''	2.23	0.42
2:E:331:TRP:O	2:E:332:GLN:HB2	2.20	0.41
3:F:29:U:H2'	3:F:30:G:C8	2.55	0.41
2:E:250:MET:HE3	2:E:293:ARG:N	2.35	0.41
2:B:181:GLU:HG3	2:B:181:GLU:H	1.67	0.41
1:D:126:LEU:C	1:D:128:VAL:H	2.23	0.41
1:D:48:ARG:HH22	3:F:47:U:P	2.44	0.41
2:B:330:LYS:HA	2:B:330:LYS:HD3	1.77	0.41
1:A:25:LEU:O	1:A:25:LEU:HD12	2.21	0.41
2:E:228:ALA:O	2:E:232:MET:HB2	2.20	0.41
1:A:111:GLN:HG2	1:A:111:GLN:H	1.39	0.41
3:C:45:A:H3'	3:C:45:A:P	2.61	0.41
1:A:107:LYS:HG3	1:A:108:GLU:N	2.35	0.41
2:E:89:GLU:O	2:E:93:ILE:HG12	2.21	0.41
1:D:67:LEU:HD23	1:D:67:LEU:HA	1.72	0.41
2:E:146:LEU:HD23	2:E:171:ALA:HB1	2.02	0.40
1:D:41:GLU:HG3	3:F:37:G:O6	2.21	0.40
1:D:78:VAL:HA	1:D:79:PRO:HD3	1.86	0.40
1:A:69:LEU:HB2	1:A:70:PRO:HD3	2.02	0.40
1:D:17:HIS:NE2	1:D:21:LYS:HE2	2.37	0.40
2:E:332:GLN:OE1	2:E:332:GLN:HA	2.21	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	123/130 (95%)	118 (96%)	5 (4%)	0	100	100
1	D	123/130 (95%)	121 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	231/254 (91%)	223 (96%)	8 (4%)	0	100	100
2	E	232/254 (91%)	228 (98%)	4 (2%)	0	100	100
All	All	709/768 (92%)	690 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	108/112 (96%)	104 (96%)	4 (4%)	41	68
1	D	108/112 (96%)	98 (91%)	10 (9%)	11	20
2	B	203/219 (93%)	174 (86%)	29 (14%)	4	6
2	E	204/219 (93%)	185 (91%)	19 (9%)	11	20
All	All	623/662 (94%)	561 (90%)	62 (10%)	9	17

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	63	LEU
1	A	84	ARG
1	A	111	GLN
2	B	100	THR
2	B	112	LYS
2	B	114	ILE
2	B	115	ARG
2	B	122	PHE
2	B	125	LEU
2	B	126	GLU
2	B	127	SER
2	B	141	GLU
2	B	142	LEU

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Mol	Chain	Res	Type
2	B	148	LYS
2	B	150	LYS
2	B	153	GLU
2	B	154	ASN
2	B	160	THR
2	B	164	ILE
2	B	175	GLN
2	B	180	SER
2	B	181	GLU
2	B	185	GLU
2	B	186	ARG
2	B	196	GLU
2	B	201	LYS
2	B	203	ARG
2	B	250	MET
2	B	255	GLN
2	B	268	LEU
2	B	288	ARG
2	B	332	GLN
1	D	6	VAL
1	D	11	TYR
1	D	26	VAL
1	D	61	GLU
1	D	66	ILE
1	D	84	ARG
1	D	95	VAL
1	D	96	SER
1	D	112	LEU
1	D	119	ILE
2	E	91	ARG
2	E	108	ASN
2	E	109	ILE
2	E	115	ARG
2	E	133	LEU
2	E	145	SER
2	E	149	CYS
2	E	155	LEU
2	E	159	LEU
2	E	165	MET
2	E	170	THR
2	E	173	THR
2	E	177	GLN

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Mol	Chain	Res	Type
2	E	186	ARG
2	E	192	ASP
2	E	193	MET
2	E	267	VAL
2	E	274	ILE
2	E	283	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	34	GLN
2	B	131	ASN
2	B	154	ASN
2	B	157	GLN
2	B	218	ASN
2	B	332	GLN
1	D	87	GLN
2	E	108	ASN
2	E	177	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	27/28 (96%)	5 (18%)	1 (3%)
3	F	27/28 (96%)	2 (7%)	0
All	All	54/56 (96%)	7 (12%)	1 (1%)

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	41	G
3	C	42	C
3	C	43	A
3	C	45	A
3	C	46	G
3	F	50	G
3	F	55	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	C	45	A

## 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](#)

2 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	$\# Z  > 2$
4	SO4	B	1	-	4,4,4	0.23	0	6,6,6	0.10	0
4	SO4	D	129	-	4,4,4	0.19	0	6,6,6	0.41	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
4	SO4	B	1	-	-	0/0/0/0	0/0/0/0
4	SO4	D	129	-	-	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.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	125/130 (96%)	0.11	5 (4%)	42 35	52, 67, 110, 168	0
1	D	125/130 (96%)	0.21	5 (4%)	42 35	52, 75, 125, 177	0
2	B	235/254 (92%)	0.05	10 (4%)	39 32	49, 76, 122, 166	0
2	E	236/254 (92%)	-0.02	7 (2%)	54 47	54, 73, 126, 177	0
3	C	28/28 (100%)	0.45	3 (10%)	8 5	59, 94, 149, 185	0
3	F	28/28 (100%)	-0.14	2 (7%)	19 13	57, 75, 116, 139	0
All	All	777/824 (94%)	0.07	32 (4%)	41 34	49, 73, 125, 185	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	43	A	6.1
1	D	4	ALA	5.5
1	A	5	ASP	4.5
2	E	87	ALA	4.2
2	E	153	GLU	4.2
2	E	86	ALA	3.9
2	B	151	ASN	3.9
1	D	128	VAL	3.6
2	B	86	ALA	3.3
3	C	42	C	3.2
1	A	6	VAL	3.2
1	D	127	LEU	3.2
2	E	150	LYS	3.1
2	B	255	GLN	2.8
2	B	300	THR	2.8
2	E	148	LYS	2.7
2	B	112	LYS	2.6
3	F	55	G	2.6
1	D	32	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	108	GLU	2.4
2	B	153	GLU	2.4
2	B	87	ALA	2.3
2	E	326	ARG	2.3
1	A	128	VAL	2.3
3	F	54	A	2.2
2	E	151	ASN	2.2
3	C	28	C	2.2
2	B	297	ALA	2.2
2	B	330	LYS	2.1
2	B	326	ARG	2.1
1	A	43	THR	2.0
1	A	42	ALA	2.0

## 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( $\text{\AA}^2$ )	Q<0.9
4	SO4	D	129	5/5	0.95	0.20	0.03	100,101,108,117	0
4	SO4	B	1	5/5	0.91	0.16	-0.64	127,128,141,147	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.