



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:46 PM GMT

PDB ID : 4W7S  
Title : Crystal structure of the yeast DEAD-box splicing factor Prp28 at 2.54 Angstroms resolution  
Authors : Jacewicz, A.; Smith, P.; Schwer, B.; Shuman, S.  
Deposited on : 2014-08-22  
Resolution : 2.54 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

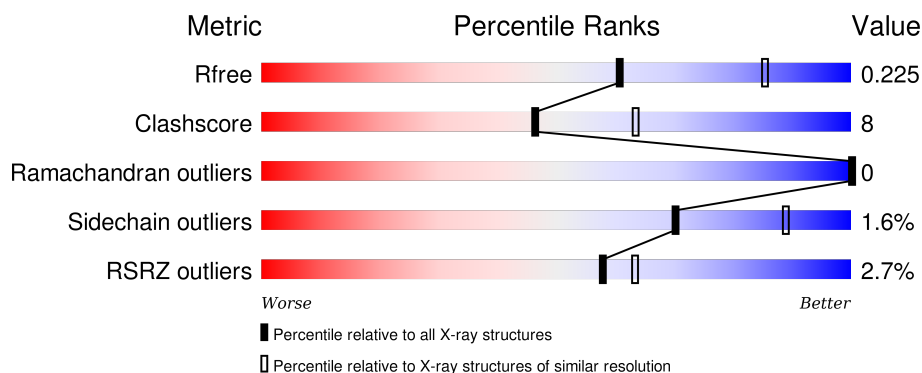
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.54 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	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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	463	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 83%, yellow 83%, yellow 98%, grey 98%, grey 100%);"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 83%, yellow 83%, yellow 98%, grey 98%, grey 100%);"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>83%</span> <span>15%</span> </div> </div>
1	B	463	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 4%, orange 4%, orange 83%, yellow 83%, yellow 98%, grey 98%, grey 100%);"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 4%, orange 4%, orange 83%, yellow 83%, yellow 98%, grey 98%, grey 100%);"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>83%</span> <span>13%</span> </div> </div>

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
2	P6G	A	601	-	-	-	X
2	P6G	A	602	-	-	-	X
2	P6G	A	603	-	-	-	X
2	P6G	A	604	-	-	-	X
2	P6G	A	605	-	-	-	X
2	P6G	B	602	-	-	X	X
2	P6G	B	603	-	-	X	-
2	P6G	B	604	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7553 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.

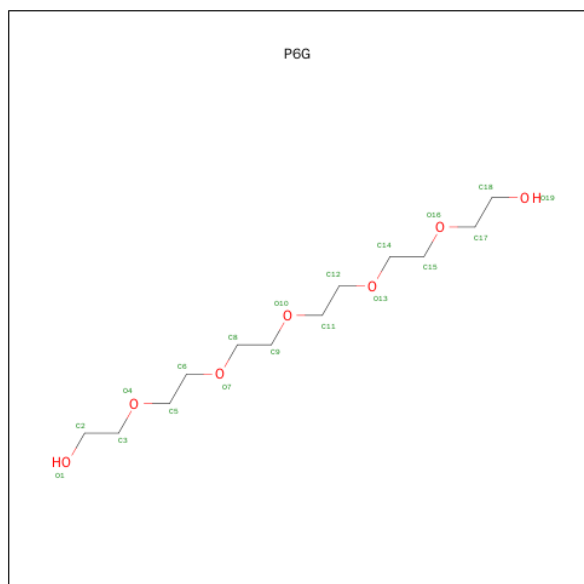
- Molecule 1 is a protein called Pre-mRNA-splicing ATP-dependent RNA helicase PRP28.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	Se	0	1	0
			3622	2306	623	679	3	11			
1	B	448	Total	C	N	O	S	Se	0	2	0
			3550	2259	607	670	3	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	SER	-	expression tag	UNP P23394
B	126	SER	-	expression tag	UNP P23394

- Molecule 2 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		

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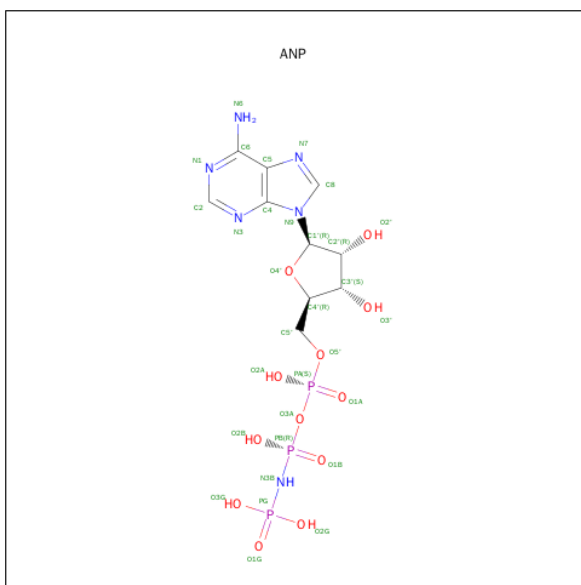
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			12	8	4		
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			19	12	7		
2	B	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			13	9	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Mg 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	141	Total O 141 141	0	0
6	B	108	Total O 110 110	0	2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.72Å 114.72Å 156.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	53.84 – 2.54 53.84 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.9 (53.84-2.54) 99.9 (53.84-2.54)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.53 (at 2.55Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.166 , 0.219 0.176 , 0.225	Depositor DCC
$R_{free}$ test set	1949 reflections (5.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.5	EDS
Estimated twinning fraction	0.031 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 39685 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7553	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: GOL, MG, ANP, P6G

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	0.47	1/3679 (0.0%)	0.60	0/4962
1	B	0.44	0/3606	0.60	0/4868
All	All	0.45	1/7285 (0.0%)	0.60	0/9830

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	CYS	CB-SG	-5.13	1.73	1.81

There are no bond angle outliers.

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	3622	0	3712	48	0
1	B	3550	0	3602	57	0
2	A	49	0	61	9	0
2	B	42	0	52	24	0
3	A	6	0	8	1	0
4	B	31	0	13	1	0
5	B	2	0	0	0	0
6	A	141	0	0	5	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	110	0	0	6	0
All	All	7553	0	7448	112	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 8.

All (112) 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)
2:A:604:P6G:H111	2:A:604:P6G:H152	1.19	1.09
2:A:604:P6G:C15	2:A:604:P6G:H111	2.07	0.84
1:A:242:SER:O	1:A:287:TYR:OH	2.02	0.78
1:B:149:ARG:HD2	2:B:603:P6G:H92	1.65	0.77
1:B:163:LYS:HE3	2:B:602:P6G:H141	1.70	0.71
1:A:353:ASP:HB3	2:A:605:P6G:H82	1.78	0.66
4:B:601:ANP:O2G	6:B:701:HOH:O	2.13	0.65
1:B:363:ASP:HA	1:B:372:ARG:NH2	2.12	0.65
1:B:172:ARG:HD3	1:B:176:GLU:OE2	1.97	0.65
1:B:152:ARG:HH12	2:B:603:P6G:H82	1.62	0.64
1:B:381:MSE:HE1	1:B:386:GLU:HG2	1.79	0.64
2:B:602:P6G:C15	2:B:602:P6G:H112	2.28	0.63
1:A:239:MSE:HE3	1:A:289:CYS:SG	2.38	0.63
1:A:172:ARG:NH1	1:A:176:GLU:OE2	2.30	0.62
1:B:458:LYS:HG3	1:B:459:GLU:HG3	1.80	0.62
1:A:564:ASN:OD1	6:A:815:HOH:O	2.16	0.61
1:B:152:ARG:NH1	2:B:603:P6G:O10	2.34	0.60
1:B:381:MSE:HE2	2:B:602:P6G:H81	1.83	0.59
1:B:161:VAL:HG12	2:B:602:P6G:H21	1.86	0.58
1:B:152:ARG:HD3	2:B:603:P6G:C12	2.33	0.57
1:B:218:LEU:HB2	1:B:393:MSE:HE1	1.85	0.56
1:B:363:ASP:HA	1:B:372:ARG:HH22	1.70	0.56
1:B:163:LYS:HZ1	2:B:602:P6G:H152	1.70	0.56
1:A:288:ASP:O	6:A:840:HOH:O	2.17	0.56
1:A:175:GLU:OE1	1:A:175:GLU:N	2.39	0.56
1:B:325:LEU:HD13	1:B:361:LYS:HD3	1.88	0.55
1:B:453:ALA:HB2	1:B:466:ILE:HD11	1.89	0.55
1:B:393:MSE:HE3	1:B:396:PRO:HG3	1.88	0.54
2:A:605:P6G:H32	6:B:770:HOH:O	2.06	0.54
1:A:174:TRP:HB3	1:A:185:LEU:HD11	1.87	0.54
1:B:163:LYS:NZ	2:B:602:P6G:H91	2.23	0.54
1:B:479:SER:HA	1:B:482:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ARG:HD3	2:B:603:P6G:H121	1.90	0.54
1:B:152:ARG:HH12	2:B:603:P6G:C8	2.21	0.53
1:A:410:LEU:HB3	1:A:563:LEU:HD21	1.90	0.53
1:B:163:LYS:HZ1	2:B:602:P6G:H91	1.72	0.53
1:A:480:LEU:O	1:A:484:ARG:HG3	2.09	0.52
1:B:541:VAL:HG13	1:B:545:GLU:HG3	1.92	0.52
1:B:163:LYS:NZ	2:B:602:P6G:H152	2.25	0.51
1:B:163:LYS:HD2	2:B:602:P6G:H171	1.91	0.51
1:A:223:THR:HG21	1:A:342:GLU:OE2	2.12	0.50
1:B:152:ARG:HD3	2:B:603:P6G:H122	1.94	0.50
2:B:602:P6G:H152	2:B:602:P6G:H112	1.94	0.50
1:B:398:TYR:HB3	2:B:602:P6G:H51	1.92	0.50
1:B:163:LYS:HZ3	2:B:602:P6G:H82	1.77	0.49
1:B:482:LEU:HD23	1:B:487:LYS:HD2	1.94	0.49
1:B:195:PRO:HD2	6:B:711:HOH:O	2.12	0.49
1:B:446:LYS:NZ	1:B:468:HIS:HB3	2.27	0.49
1:B:438:PRO:HB2	1:B:483:PHE:CZ	2.47	0.49
1:B:332:MSE:HE3	1:B:362:VAL:HG22	1.95	0.48
1:A:374:THR:HG22	1:A:393:MSE:HE3	1.94	0.48
1:B:467:LEU:HD21	1:B:476:ARG:HB2	1.96	0.47
1:B:210:ASN:HB3	1:B:212:LYS:HD2	1.97	0.47
1:A:398:TYR:HB3	2:A:601:P6G:H81	1.96	0.47
1:A:435:TYR:OH	2:A:603:P6G:H82	2.15	0.47
1:B:245:ARG:NH2	1:B:254:GLY:O	2.43	0.47
1:A:261:ALA:HB1	1:A:266:LEU:HD23	1.97	0.46
1:B:446:LYS:HZ2	1:B:468:HIS:HB3	1.81	0.46
1:B:183:ASP:HB2	6:B:778:HOH:O	2.15	0.46
1:A:211:MSE:HA	1:A:211:MSE:HE2	1.97	0.46
1:B:381:MSE:HE2	2:B:602:P6G:C8	2.46	0.46
1:A:227:LYS:O	1:A:230:ALA:HB3	2.17	0.45
1:A:321:LEU:HD23	1:A:358:ILE:HD13	1.98	0.45
1:A:353:ASP:HB3	2:A:605:P6G:C8	2.45	0.45
1:A:224:GLY:HA2	6:A:826:HOH:O	2.16	0.45
1:A:173:ASN:HD22	2:A:604:P6G:C17	2.29	0.45
1:A:172:ARG:HD3	1:A:176:GLU:OE1	2.17	0.44
1:A:443:ILE:HD11	1:A:449:ALA:HB2	1.99	0.44
1:A:374:THR:O	1:A:393:MSE:HE2	2.17	0.44
1:B:514:ILE:HD11	1:B:539:SER:HB3	2.00	0.44
1:A:548:SER:O	1:A:552:GLU:HG3	2.18	0.44
1:B:149:ARG:HE	2:B:603:P6G:H81	1.83	0.44
1:B:163:LYS:CE	2:B:602:P6G:H91	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:PRO:HB2	1:A:483:PHE:CZ	2.53	0.44
1:A:225:SER:HB2	6:A:753:HOH:O	2.17	0.44
1:A:381:MSE:HG3	2:A:601:P6G:H91	1.99	0.44
1:B:434:LYS:HB3	1:B:434:LYS:HE2	1.84	0.44
1:A:452:LEU:HA	1:A:452:LEU:HD23	1.85	0.43
1:A:233:ILE:HB	1:A:234:PRO:HD3	1.99	0.43
1:A:182:ARG:HD2	6:A:702:HOH:O	2.18	0.43
1:B:180:ILE:HA	1:B:181:PRO:HD2	1.86	0.43
1:B:163:LYS:HG2	2:B:602:P6G:H32	2.00	0.43
1:A:223:THR:HA	1:A:224:GLY:HA2	1.78	0.43
1:B:183:ASP:OD1	1:B:186:ARG:NH2	2.50	0.43
1:A:443:ILE:HD12	1:A:494:THR:HG22	2.00	0.43
1:B:275:GLN:HA	1:B:278[B]:THR:OG1	2.19	0.43
1:B:448:THR:HG21	1:B:513:GLN:NE2	2.34	0.43
1:A:138:TRP:HB2	1:A:146:MSE:SE	2.70	0.42
1:A:250:LYS:HE3	1:A:290:LYS:HE2	2.00	0.42
1:A:443:ILE:H	1:A:443:ILE:HG13	1.70	0.42
1:B:299:SER:OG	1:B:302:GLU:HG3	2.19	0.42
1:A:309:GLU:HG2	3:A:606:GOL:H11	2.01	0.42
1:B:210:ASN:CB	1:B:212:LYS:HD2	2.48	0.42
1:B:464:VAL:HG12	1:B:490:ILE:HB	2.02	0.42
1:B:267:VAL:HG13	1:B:315:VAL:HG12	2.02	0.42
1:A:183:ASP:O	1:A:187:VAL:HG23	2.20	0.42
1:B:186:ARG:NH1	1:B:284:GLU:OE2	2.47	0.41
1:A:293:SER:HA	1:A:315:VAL:O	2.20	0.41
1:B:227:LYS:NZ	1:B:341:ASP:OD1	2.43	0.41
1:B:245:ARG:HD3	6:B:773:HOH:O	2.20	0.41
1:A:451:TRP:CZ2	1:A:455:LYS:HD2	2.55	0.41
1:A:587:ILE:HA	1:A:587:ILE:HD13	1.86	0.41
1:A:295:VAL:O	1:A:320:ARG:HG2	2.21	0.41
1:A:143:LEU:HD13	1:A:172:ARG:HD2	2.03	0.41
1:A:396:PRO:HG2	1:A:398:TYR:CZ	2.55	0.41
1:A:558:ARG:HA	1:A:558:ARG:HD3	1.77	0.40
2:B:603:P6G:H61	6:B:703:HOH:O	2.22	0.40
1:A:387:LYS:HB3	1:A:387:LYS:HE2	1.76	0.40
1:B:376:MSE:HE2	1:B:376:MSE:HB2	2.01	0.40
1:B:467:LEU:HA	1:B:467:LEU:HD23	1.90	0.40
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.90	0.40
1:A:222:SER:O	1:A:225:SER:OG	2.23	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)
6:A:748:HOH:O	6:A:748:HOH:O[4_556]	2.03	0.17
6:A:750:HOH:O	6:A:750:HOH:O[4_556]	2.07	0.13

## 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	454/463 (98%)	445 (98%)	9 (2%)	0	100	100
1	B	446/463 (96%)	437 (98%)	9 (2%)	0	100	100
All	All	900/926 (97%)	882 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/402 (101%)	400 (98%)	6 (2%)	72	90
1	B	395/402 (98%)	388 (98%)	7 (2%)	66	87
All	All	801/804 (100%)	788 (98%)	13 (2%)	70	89

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	SER
1	A	326	GLU

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Mol	Chain	Res	Type
1	A	441	ILE
1	A	443	ILE
1	A	527	ARG
1	A	569	SER
1	B	152	ARG
1	B	211	MSE
1	B	367	ASP
1	B	376	MSE
1	B	447	GLN
1	B	488	VAL
1	B	575	LYS

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

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
2	P6G	A	601	-	12,12,18	0.93	0	11,11,17	0.38	0
2	P6G	A	602	-	6,6,18	0.75	0	5,5,17	0.33	0
2	P6G	A	603	-	6,6,18	0.75	0	5,5,17	0.32	0
2	P6G	A	604	-	11,11,18	0.90	0	10,10,17	0.43	0
2	P6G	A	605	-	9,9,18	0.83	0	8,8,17	0.28	0
3	GOL	A	606	-	5,5,5	0.33	0	5,5,5	0.27	0
4	ANP	B	601	5	27,33,33	1.40	4 (14%)	30,52,52	0.81	2 (6%)
2	P6G	B	602	-	18,18,18	0.81	0	17,17,17	0.41	0
2	P6G	B	603	-	9,9,18	0.95	0	8,8,17	0.61	0
2	P6G	B	604	-	12,12,18	0.95	0	11,11,17	0.61	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
2	P6G	A	601	-	-	0/10/10/16	0/0/0/0
2	P6G	A	602	-	-	0/4/4/16	0/0/0/0
2	P6G	A	603	-	-	0/4/4/16	0/0/0/0
2	P6G	A	604	-	-	0/9/9/16	0/0/0/0
2	P6G	A	605	-	-	0/7/7/16	0/0/0/0
3	GOL	A	606	-	-	0/4/4/4	0/0/0/0
4	ANP	B	601	5	-	0/12/38/38	0/3/3/3
2	P6G	B	602	-	-	0/16/16/16	0/0/0/0
2	P6G	B	603	-	-	0/7/7/16	0/0/0/0
2	P6G	B	604	-	-	0/10/10/16	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	ANP	PB-O3A	-2.48	1.56	1.59
4	B	601	ANP	PG-N3B	2.47	1.69	1.63
4	B	601	ANP	PB-O1B	3.72	1.50	1.46
4	B	601	ANP	PG-O1G	3.79	1.50	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	ANP	PA-O3A-PB	-2.42	124.56	132.67
4	B	601	ANP	O1G-PG-N3B	-2.16	108.59	111.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	P6G	2	0
2	A	603	P6G	1	0
2	A	604	P6G	3	0
2	A	605	P6G	3	0
3	A	606	GOL	1	0
4	B	601	ANP	1	0
2	B	602	P6G	15	0
2	B	603	P6G	9	0

## 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	443/463 (95%)	-0.19	4 (0%) 85 88	14, 30, 51, 73	0
1	B	436/463 (94%)	0.04	20 (4%) 36 42	14, 30, 71, 108	0
All	All	879/926 (94%)	-0.08	24 (2%) 58 63	14, 30, 63, 108	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	496	VAL	4.3
1	B	468	HIS	4.0
1	B	477	GLU	3.8
1	B	498	ALA	3.4
1	B	474	GLU	3.3
1	B	472	SER	3.2
1	B	500	GLY	3.0
1	B	481	GLN	2.7
1	B	471	LYS	2.7
1	B	446	LYS	2.7
1	A	213	GLN	2.5
1	A	135	GLY	2.5
1	B	450	ASP	2.5
1	B	497	ALA	2.4
1	A	531	ALA	2.3
1	B	144	HIS	2.2
1	B	407	SER	2.2
1	B	475	GLN	2.2
1	A	369	ALA	2.1
1	B	487	LYS	2.1
1	B	406	GLY	2.1
1	B	478	HIS	2.1
1	B	466	ILE	2.0
1	B	451	TRP	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(Å <sup>2</sup> )	Q<0.9
2	P6G	B	604	13/19	0.79	0.43	15.37	37,47,54,58	0
2	P6G	B	602	19/19	0.84	0.27	12.22	33,51,61,63	0
2	P6G	A	605	10/19	0.85	0.31	12.16	38,50,57,57	0
2	P6G	A	603	7/19	0.84	0.20	3.64	46,49,55,56	0
2	P6G	A	601	13/19	0.83	0.24	2.94	31,50,56,58	0
2	P6G	A	604	12/19	0.89	0.19	2.31	33,41,48,48	0
2	P6G	A	602	7/19	0.88	0.20	2.13	27,37,48,55	0
4	ANP	B	601	31/31	0.97	0.15	0.29	20,30,39,44	4
5	MG	B	606	1/1	0.96	0.05	-	38,38,38,38	0
3	GOL	A	606	6/6	0.85	0.24	-	55,59,62,63	0
5	MG	B	605	1/1	0.98	0.06	-	37,37,37,37	0
2	P6G	B	603	10/19	0.84	0.29	-	32,43,47,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.