



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 04:04 PM BST

PDB ID : 6R02  
Title : Psychrobacter arcticus ATP phosphoribosyltransferase bound to histidine and PRPP  
Authors : Alphey, M.S.; da Silva, R.G.; Thomson, C.M.  
Deposited on : 2019-03-12  
Resolution : 2.65 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

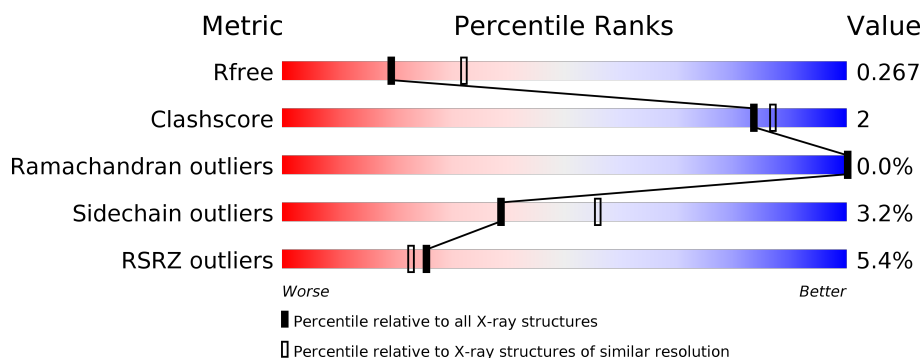
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	388	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>• •</div> </div> </div>
1	B	388	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>• •</div> </div> </div>
1	C	388	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>•</div> </div> </div>
1	D	388	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>•</div> </div> </div>
2	E	232	<div> <div>12%</div> <div> <div></div> <div>81%</div> <div>6%</div> <div>13%</div> </div> </div>
2	F	232	<div> <div>10%</div> <div> <div></div> <div>78%</div> <div>7%</div> <div>• 14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	232	
2	H	232	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18055 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 ATP phosphoribosyltransferase regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	1	0
			2935	1855	511	555	14			
1	B	378	Total	C	N	O	S	0	0	0
			2943	1859	516	554	14			
1	C	379	Total	C	N	O	S	0	0	0
			2947	1863	515	555	14			
1	D	378	Total	C	N	O	S	0	0	0
			2918	1845	508	551	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q4FTX3
B	0	GLY	-	expression tag	UNP Q4FTX3
C	0	GLY	-	expression tag	UNP Q4FTX3
D	0	GLY	-	expression tag	UNP Q4FTX3

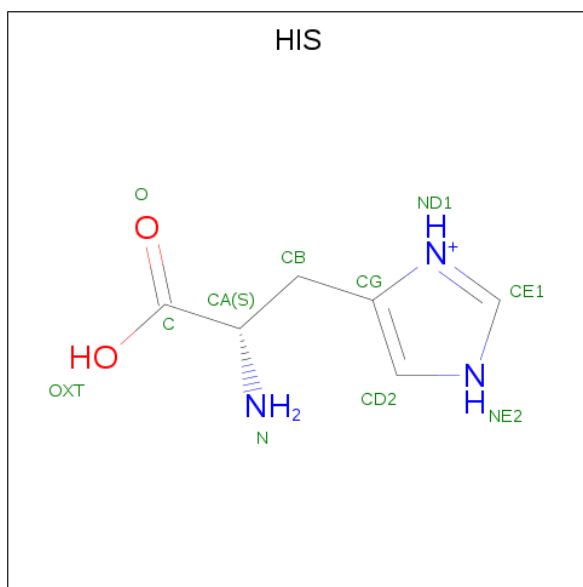
- Molecule 2 is a protein called ATP phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	202	Total	C	N	O	S	0	0	0
			1532	975	266	286	5			
2	F	200	Total	C	N	O	S	0	0	0
			1481	942	257	277	5			
2	G	208	Total	C	N	O	S	0	0	0
			1585	1010	277	293	5			
2	H	203	Total	C	N	O	S	0	0	0
			1528	976	261	286	5			

There are 4 discrepancies between the modelled and reference sequences:

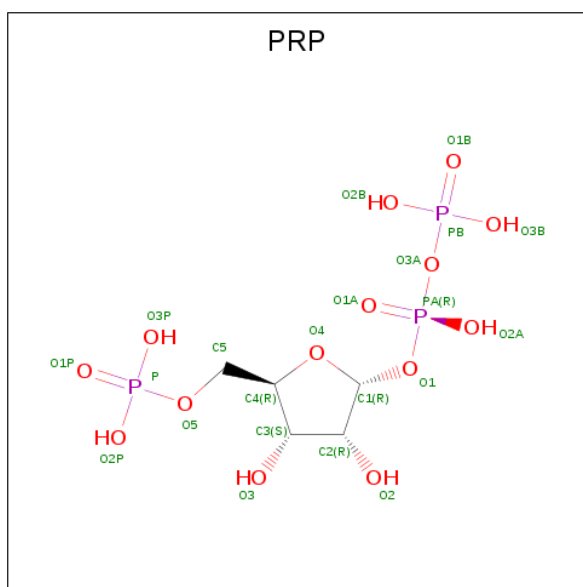
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	GLY	-	expression tag	UNP Q4FQF7
F	0	GLY	-	expression tag	UNP Q4FQF7
G	0	GLY	-	expression tag	UNP Q4FQF7
H	0	GLY	-	expression tag	UNP Q4FQF7

- Molecule 3 is HISTIDINE (three-letter code: HIS) (formula:  $C_6H_{10}N_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	6	3	2		
3	B	1	Total	C	N	O	0	0
			11	6	3	2		
3	C	1	Total	C	N	O	0	0
			11	6	3	2		
3	D	1	Total	C	N	O	0	0
			11	6	3	2		

- Molecule 4 is 1-O-pyrophosphono-5-O-phosphono-alpha-D-ribofuranose (three-letter code: PRP) (formula:  $C_5H_{13}O_{14}P_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	O	P	0	0
			22	5	14	3		
4	F	1	Total	C	O	P	0	0
			22	5	14	3		
4	G	1	Total	C	O	P	0	0
			22	5	14	3		
4	H	1	Total	C	O	P	0	0
			22	5	14	3		

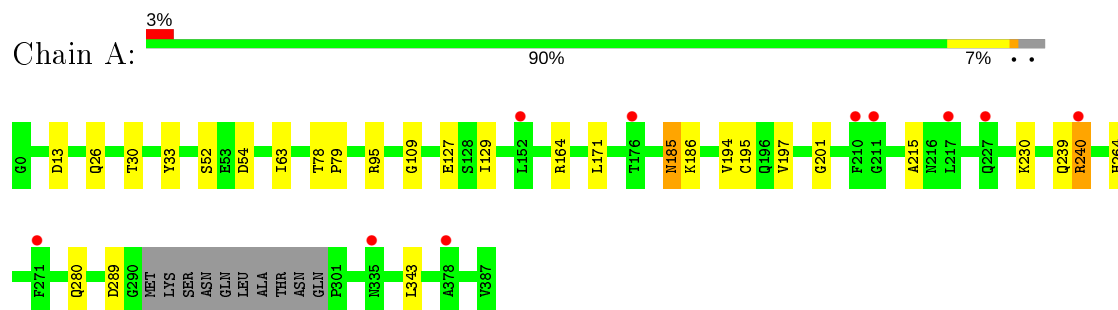
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	O	0	0
			10	10		
5	B	15	Total	O	0	0
			15	15		
5	C	12	Total	O	0	0
			12	12		
5	D	10	Total	O	0	0
			10	10		
5	E	3	Total	O	0	0
			3	3		
5	F	1	Total	O	0	0
			1	1		
5	H	3	Total	O	0	0
			3	3		

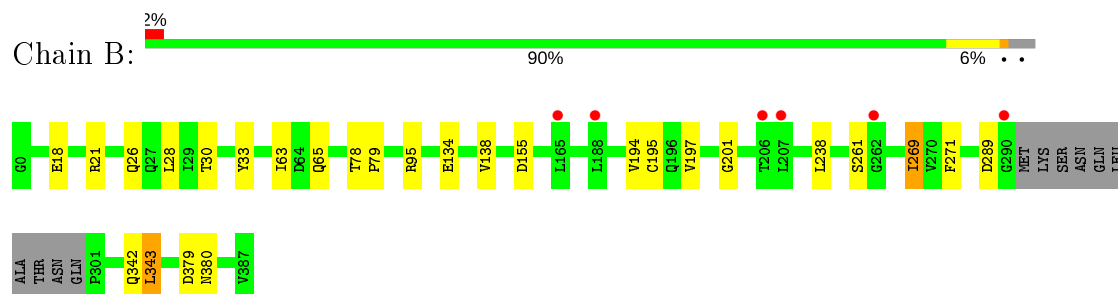
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

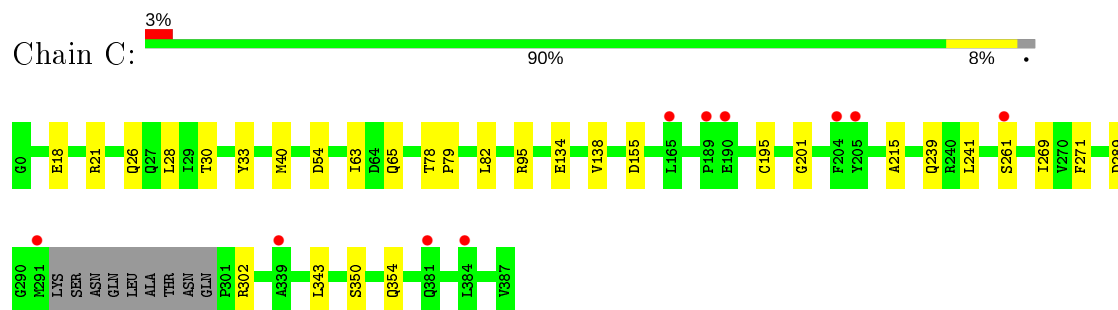
- Molecule 1: ATP phosphoribosyltransferase regulatory subunit



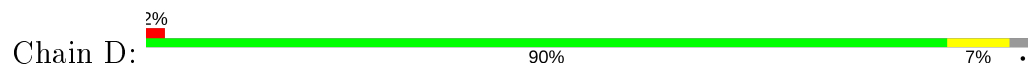
- Molecule 1: ATP phosphoribosyltransferase regulatory subunit

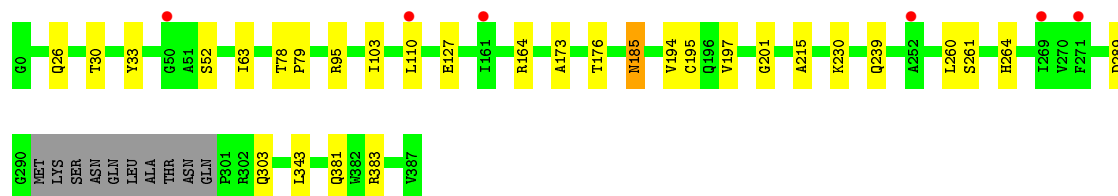


- Molecule 1: ATP phosphoribosyltransferase regulatory subunit

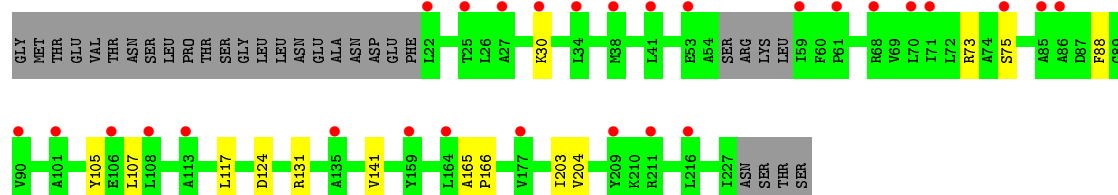
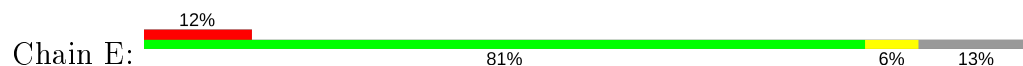


- Molecule 1: ATP phosphoribosyltransferase regulatory subunit

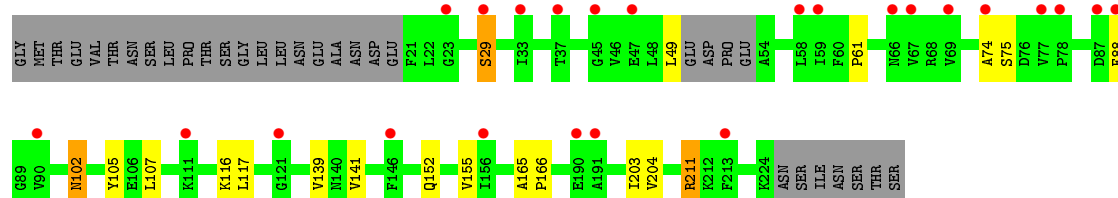
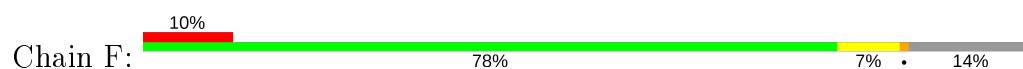




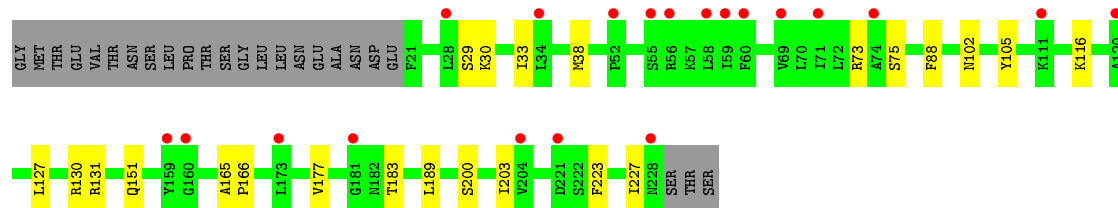
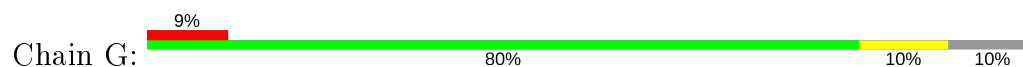
- Molecule 2: ATP phosphoribosyltransferase



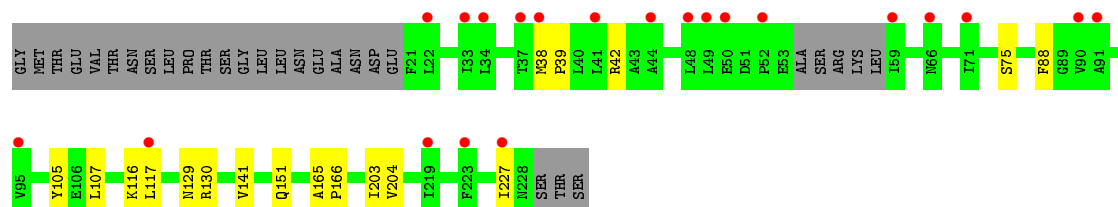
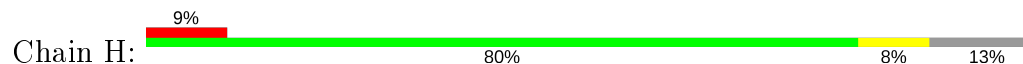
- Molecule 2: ATP phosphoribosyltransferase



- Molecule 2: ATP phosphoribosyltransferase



- Molecule 2: ATP phosphoribosyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.25Å 147.31Å 99.33Å 90.00° 103.11° 90.00°	Depositor
Resolution (Å)	77.31 – 2.65 77.31 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (77.31-2.65) 99.9 (77.31-2.65)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 2.65Å)	Xtriage
Refinement program	REFMAC refmac_5.8.0238	Depositor
R, $R_{free}$	0.236 , 0.270 0.234 , 0.267	Depositor DCC
$R_{free}$ test set	3726 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.9	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 28.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18055	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9041e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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

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	0.65	0/2992	0.73	0/4062
1	B	0.65	0/2997	0.74	0/4066
1	C	0.65	0/3001	0.74	0/4071
1	D	0.65	0/2972	0.73	0/4037
2	E	0.67	0/1554	0.76	0/2110
2	F	0.69	0/1502	0.76	0/2045
2	G	0.67	0/1609	0.77	0/2183
2	H	0.67	0/1551	0.75	0/2110
All	All	0.66	0/18178	0.75	0/24684

There are no bond length outliers.

There are no bond angle outliers.

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	2935	0	2904	18	0
1	B	2943	0	2925	12	0
1	C	2947	0	2929	19	0
1	D	2918	0	2876	15	0
2	E	1532	0	1569	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1481	0	1482	10	0
2	G	1585	0	1632	9	0
2	H	1528	0	1549	6	0
3	A	11	0	6	1	0
3	B	11	0	6	0	0
3	C	11	0	6	1	0
3	D	11	0	6	0	0
4	E	22	0	8	0	0
4	F	22	0	8	0	0
4	G	22	0	8	1	0
4	H	22	0	8	0	0
5	A	10	0	0	0	0
5	B	15	0	0	0	0
5	C	12	0	0	0	0
5	D	10	0	0	0	0
5	E	3	0	0	0	0
5	F	1	0	0	0	0
5	H	3	0	0	0	0
All	All	18055	0	17922	85	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 2.

All (85) 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:C:241:LEU:HD12	1:C:269:ILE:CD1	2.01	0.90
1:C:241:LEU:HD12	1:C:269:ILE:HD11	1.60	0.83
1:A:52:SER:OG	1:A:264:HIS:HB2	1.90	0.71
1:C:241:LEU:HD12	1:C:269:ILE:HD13	1.71	0.70
1:D:127:GLU:HG3	1:D:303:GLN:HG3	1.74	0.69
2:G:33:ILE:CD1	2:G:200:SER:OG	2.44	0.66
2:F:49:LEU:HD13	2:F:61:PRO:HG2	1.77	0.64
1:C:241:LEU:CD1	1:C:269:ILE:CD1	2.75	0.64
1:C:241:LEU:CD1	1:C:269:ILE:HD13	2.29	0.62
2:G:223:PHE:O	2:G:227:ILE:HG12	2.02	0.59
2:E:107:LEU:HD12	2:E:204:VAL:HG21	1.85	0.59
1:C:215:ALA:HA	1:C:239:GLN:HE21	1.69	0.57
2:G:33:ILE:HD13	2:G:200:SER:OG	2.05	0.56
1:B:65:GLN:O	1:D:63:ILE:HG21	2.06	0.55
1:A:52:SER:HB2	1:A:54:ASP:OD1	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LYS:HB2	2:G:105:TYR:CD1	2.43	0.54
1:A:215:ALA:HA	1:A:239:GLN:HE21	1.73	0.54
2:F:107:LEU:HD12	2:F:204:VAL:HG21	1.91	0.53
1:B:63:ILE:HD11	1:C:63:ILE:HD11	1.91	0.53
1:C:18:GLU:OE1	1:C:21:ARG:NH1	2.40	0.52
1:D:215:ALA:HA	1:D:239:GLN:HE21	1.74	0.52
2:F:165:ALA:HB3	2:F:166:PRO:HD3	1.92	0.52
2:H:165:ALA:HB3	2:H:166:PRO:HD3	1.92	0.51
1:B:18:GLU:OE1	1:B:21:ARG:NH1	2.42	0.51
2:E:165:ALA:HB3	2:E:166:PRO:HD3	1.92	0.50
2:G:165:ALA:HB3	2:G:166:PRO:HD3	1.93	0.50
2:G:183:THR:OG1	4:G:301:PRP:O3P	2.20	0.49
1:B:28:LEU:HD23	1:B:138:VAL:CG1	2.42	0.49
1:B:195:CYS:O	1:B:201:GLY:HA3	2.12	0.49
1:C:195:CYS:O	1:C:201:GLY:HA3	2.13	0.49
1:D:195:CYS:O	1:D:201:GLY:HA3	2.12	0.49
1:C:78:THR:HG1	3:C:401:HIS:N	2.11	0.49
1:A:129:ILE:HG21	1:A:240:ARG:NH2	2.29	0.48
1:A:195:CYS:O	1:A:201:GLY:HA3	2.13	0.48
1:A:78:THR:HB	1:A:79:PRO:HD3	1.96	0.47
1:C:78:THR:HB	1:C:79:PRO:HD3	1.96	0.47
2:F:29:SER:HB2	2:F:74:ALA:HA	1.96	0.47
1:A:78:THR:HG1	3:A:401:HIS:N	2.11	0.47
1:A:33:TYR:CD2	1:A:95:ARG:HB3	2.50	0.47
1:C:241:LEU:CD1	1:C:269:ILE:HD11	2.39	0.46
1:D:78:THR:HB	1:D:79:PRO:HD3	1.97	0.46
1:D:52:SER:HB3	1:D:264:HIS:HB2	1.97	0.46
1:D:33:TYR:CD2	1:D:95:ARG:HB3	2.51	0.46
1:C:33:TYR:CD2	1:C:95:ARG:HB3	2.51	0.46
1:B:33:TYR:CD2	1:B:95:ARG:HB3	2.51	0.45
2:F:107:LEU:HD12	2:F:204:VAL:CG2	2.47	0.45
1:A:63:ILE:HG21	1:C:65:GLN:O	2.17	0.45
1:B:238:LEU:HD23	1:B:269:ILE:HD11	1.98	0.44
1:B:343:LEU:HD22	1:B:343:LEU:HA	1.86	0.44
1:D:381:GLN:NE2	1:D:383:ARG:HD2	2.32	0.44
2:F:117:LEU:HD13	2:F:141:VAL:HG11	1.99	0.44
1:B:78:THR:HB	1:B:79:PRO:HD3	2.00	0.44
2:H:107:LEU:HD12	2:H:204:VAL:HG21	2.00	0.44
1:B:134:GLU:O	1:B:138:VAL:HG23	2.18	0.43
2:F:102:ASN:ND2	2:F:102:ASN:H	2.17	0.43
1:C:28:LEU:HD23	1:C:138:VAL:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:HD3	1:A:230:LYS:HD2	2.00	0.43
1:B:26:GLN:O	1:B:30:THR:HG23	2.18	0.43
1:C:26:GLN:O	1:C:30:THR:HG23	2.18	0.43
1:D:164:ARG:HD3	1:D:230:LYS:HD2	2.00	0.43
2:F:211:ARG:HD3	2:F:211:ARG:HA	1.89	0.43
1:A:109:GLY:HA3	1:A:280[B]:GLN:CD	2.39	0.43
1:A:185:ASN:O	2:G:105:TYR:HA	2.19	0.43
2:H:38:MET:HB2	2:H:39:PRO:HD3	2.00	0.43
1:A:26:GLN:O	1:A:30:THR:HG23	2.19	0.42
1:A:13:ASP:OD2	2:H:129:ASN:OD1	2.36	0.42
1:D:173:ALA:O	1:D:176:THR:OG1	2.36	0.42
1:D:26:GLN:O	1:D:30:THR:HG23	2.20	0.42
2:E:105:TYR:O	2:E:203:ILE:HA	2.20	0.42
2:F:139:VAL:HG13	2:F:155:VAL:HG11	2.02	0.42
2:H:117:LEU:HD13	2:H:141:VAL:HG11	2.01	0.42
2:F:105:TYR:O	2:F:203:ILE:HA	2.20	0.42
1:C:134:GLU:O	1:C:138:VAL:HG23	2.20	0.41
2:H:105:TYR:O	2:H:203:ILE:HA	2.21	0.41
1:C:350:SER:O	1:C:354:GLN:HG3	2.21	0.41
2:G:105:TYR:O	2:G:203:ILE:HA	2.21	0.41
1:D:194:VAL:O	1:D:197:VAL:HG22	2.21	0.40
1:D:215:ALA:HA	1:D:239:GLN:NE2	2.36	0.40
1:A:215:ALA:HA	1:A:239:GLN:NE2	2.35	0.40
1:A:186:LYS:CB	2:G:105:TYR:CD1	3.04	0.40
1:B:194:VAL:O	1:B:197:VAL:HG22	2.21	0.40
1:A:194:VAL:O	1:A:197:VAL:HG22	2.22	0.40
1:D:185:ASN:O	2:E:105:TYR:HA	2.22	0.40
2:E:117:LEU:HD13	2:E:141:VAL:HG11	2.02	0.40
1:C:40:MET:HB2	1:D:103:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

## 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	375/388 (97%)	364 (97%)	11 (3%)	0	100	100
1	B	374/388 (96%)	366 (98%)	8 (2%)	0	100	100
1	C	375/388 (97%)	364 (97%)	11 (3%)	0	100	100
1	D	374/388 (96%)	366 (98%)	7 (2%)	1 (0%)	41	56
2	E	198/232 (85%)	193 (98%)	5 (2%)	0	100	100
2	F	196/232 (84%)	190 (97%)	6 (3%)	0	100	100
2	G	206/232 (89%)	200 (97%)	6 (3%)	0	100	100
2	H	199/232 (86%)	193 (97%)	6 (3%)	0	100	100
All	All	2297/2480 (93%)	2236 (97%)	60 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	110	LEU

### 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	316/329 (96%)	310 (98%)	6 (2%)	57	74
1	B	318/329 (97%)	309 (97%)	9 (3%)	43	61
1	C	318/329 (97%)	310 (98%)	8 (2%)	47	66
1	D	312/329 (95%)	307 (98%)	5 (2%)	62	78
2	E	164/195 (84%)	158 (96%)	6 (4%)	34	50
2	F	153/195 (78%)	146 (95%)	7 (5%)	27	41
2	G	170/195 (87%)	156 (92%)	14 (8%)	11	17
2	H	163/195 (84%)	156 (96%)	7 (4%)	29	44
All	All	1914/2096 (91%)	1852 (97%)	62 (3%)	39	56

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

Mol	Chain	Res	Type
1	A	127	GLU
1	A	171	LEU
1	A	185	ASN
1	A	240	ARG
1	A	289	ASP
1	A	343	LEU
1	B	155	ASP
1	B	261	SER
1	B	269	ILE
1	B	271	PHE
1	B	289	ASP
1	B	342	GLN
1	B	343	LEU
1	B	379	ASP
1	B	380	ASN
1	C	54	ASP
1	C	82	LEU
1	C	155	ASP
1	C	261	SER
1	C	271	PHE
1	C	289	ASP
1	C	302	ARG
1	C	343	LEU
1	D	185	ASN
1	D	260	LEU
1	D	261	SER
1	D	289	ASP
1	D	343	LEU
2	E	30	LYS
2	E	73	ARG
2	E	75	SER
2	E	88	PHE
2	E	124	ASP
2	E	131	ARG
2	F	29	SER
2	F	75	SER
2	F	88	PHE
2	F	102	ASN
2	F	116	LYS
2	F	152	GLN
2	F	211	ARG
2	G	29	SER
2	G	30	LYS

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Mol	Chain	Res	Type
2	G	38	MET
2	G	73	ARG
2	G	75	SER
2	G	88	PHE
2	G	102	ASN
2	G	116	LYS
2	G	127	LEU
2	G	130	ARG
2	G	131	ARG
2	G	151	GLN
2	G	177	VAL
2	G	189	LEU
2	H	42	ARG
2	H	75	SER
2	H	88	PHE
2	H	116	LYS
2	H	130	ARG
2	H	151	GLN
2	H	227	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	144	ASN
1	A	239	GLN
1	A	353	GLN
1	B	144	ASN
1	B	226	GLN
1	B	266	HIS
1	B	272	ASN
1	B	280	GLN
1	B	380	ASN
1	C	196	GLN
1	C	224	ASN
1	C	239	GLN
1	C	266	HIS
1	C	272	ASN
1	D	144	ASN
1	D	239	GLN
1	D	353	GLN
1	D	381	GLN

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Mol	Chain	Res	Type
2	E	66	ASN
2	E	83	HIS
2	E	206	GLN
2	F	66	ASN
2	F	102	ASN
2	F	206	GLN
2	G	206	GLN
2	H	151	GLN
2	H	194	HIS
2	H	206	GLN
2	H	225	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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	PRP	G	301	-	19,22,22	0.63	0	33,35,35	1.17	2 (6%)
4	PRP	H	301	-	19,22,22	0.59	0	33,35,35	1.12	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PRP	E	301	-	19,22,22	0.61	0	33,35,35	1.06	2 (6%)
4	PRP	F	301	-	19,22,22	0.62	0	33,35,35	1.12	2 (6%)

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	PRP	G	301	-	-	7/16/33/33	0/1/1/1
4	PRP	H	301	-	-	3/16/33/33	0/1/1/1
4	PRP	E	301	-	-	3/16/33/33	0/1/1/1
4	PRP	F	301	-	-	6/16/33/33	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	301	PRP	C1-C2-C3	2.84	105.90	102.30
4	H	301	PRP	C1-C2-C3	2.81	105.85	102.30
4	F	301	PRP	PA-O3A-PB	-2.76	123.36	132.83
4	G	301	PRP	O1-C1-C2	2.73	111.35	106.72
4	E	301	PRP	PA-O3A-PB	-2.41	124.57	132.83
4	H	301	PRP	O1-C1-C2	2.11	110.28	106.72
4	F	301	PRP	O1-C1-C2	2.10	110.28	106.72
4	H	301	PRP	PA-O3A-PB	-2.06	125.77	132.83
4	E	301	PRP	P-O5-C5	2.02	123.85	118.30

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	301	PRP	C1-O1-PA-O3A
4	G	301	PRP	C5-O5-P-O2P
4	G	301	PRP	C5-O5-P-O3P
4	H	301	PRP	C1-O1-PA-O2A
4	E	301	PRP	C5-O5-P-O2P
4	E	301	PRP	C5-O5-P-O3P
4	F	301	PRP	C5-O5-P-O1P
4	F	301	PRP	C5-O5-P-O2P

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Mol	Chain	Res	Type	Atoms
4	F	301	PRP	C3-C4-C5-O5
4	F	301	PRP	C1-O1-PA-O3A
4	F	301	PRP	O4-C4-C5-O5
4	H	301	PRP	C1-O1-PA-O3A
4	G	301	PRP	C5-O5-P-O1P
4	G	301	PRP	PA-O3A-PB-O1B
4	H	301	PRP	O4-C4-C5-O5
4	F	301	PRP	C5-O5-P-O3P
4	G	301	PRP	PA-O3A-PB-O2B
4	G	301	PRP	PA-O3A-PB-O3B
4	E	301	PRP	O4-C4-C5-O5

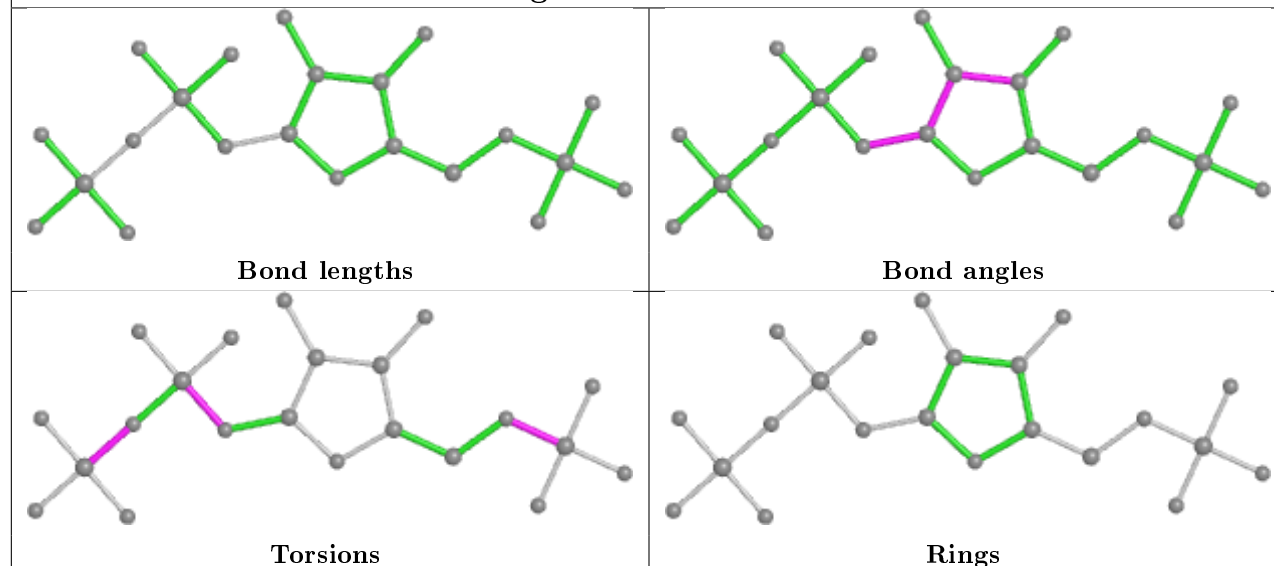
There are no ring outliers.

1 monomer is involved in 1 short contact:

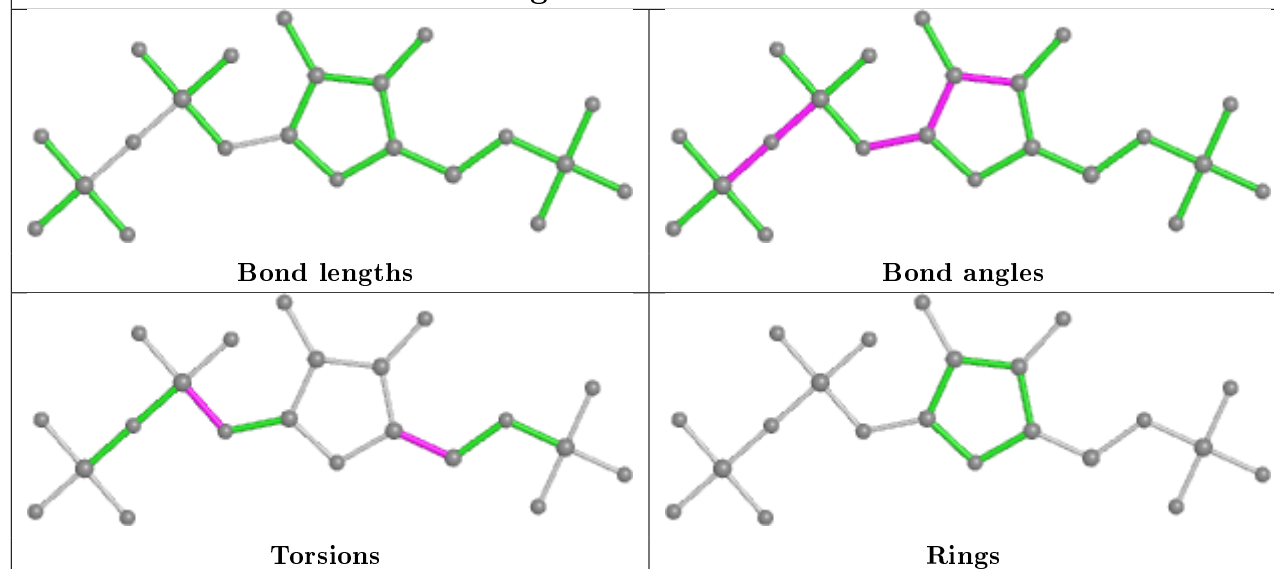
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	301	PRP	1	0

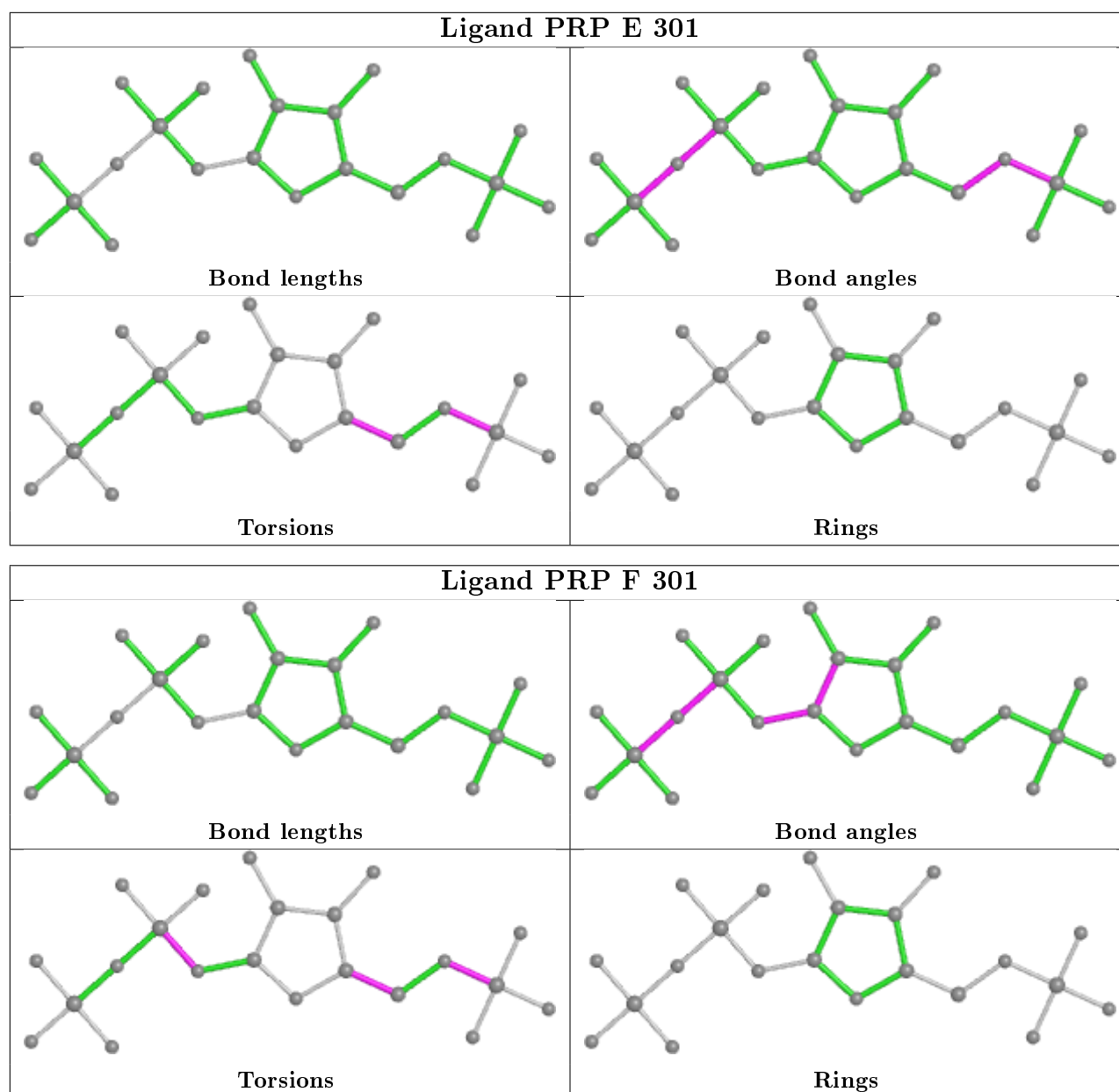
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand PRP G 301



## Ligand PRP H 301





## 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	378/388 (97%)	0.13	10 (2%) 56 52	53, 77, 115, 124	0
1	B	378/388 (97%)	0.15	6 (1%) 72 69	45, 70, 101, 124	0
1	C	379/388 (97%)	0.21	10 (2%) 56 52	45, 71, 111, 133	0
1	D	378/388 (97%)	0.14	6 (1%) 72 69	53, 80, 132, 158	0
2	E	202/232 (87%)	0.64	28 (13%) 2 2	73, 98, 127, 146	0
2	F	200/232 (86%)	0.69	24 (12%) 4 3	67, 96, 132, 141	0
2	G	208/232 (89%)	0.45	20 (9%) 8 6	66, 85, 111, 126	0
2	H	203/232 (87%)	0.60	21 (10%) 6 4	59, 87, 118, 141	0
All	All	2326/2480 (93%)	0.31	125 (5%) 25 23	45, 81, 120, 158	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	74	ALA	6.0
2	F	37	THR	4.8
1	D	252	ALA	4.6
2	F	69	VAL	4.6
2	F	33	ILE	4.5
2	G	58	LEU	4.3
2	E	59	ILE	4.2
1	A	271	PHE	4.1
2	F	90	VAL	4.0
2	F	66	ASN	3.9
2	E	41	LEU	3.8
2	F	29	SER	3.8
2	H	49	LEU	3.7
2	F	67	VAL	3.6
2	H	22	LEU	3.6
2	H	227	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	165	LEU	3.6
2	H	38	MET	3.6
2	G	60	PHE	3.6
2	H	219	ILE	3.5
2	H	59	ILE	3.5
2	E	113	ALA	3.4
2	E	85	ALA	3.4
2	F	121	GLY	3.4
2	H	34	LEU	3.4
1	A	378	ALA	3.3
1	C	189	PRO	3.3
2	H	52	PRO	3.3
2	G	228	ASN	3.3
2	E	159	TYR	3.3
2	G	55	SER	3.3
2	H	223	PHE	3.3
1	A	217	LEU	3.2
1	D	271	PHE	3.2
2	G	69	VAL	3.2
2	H	71	ILE	3.2
2	F	78	PRO	3.2
2	H	44	ALA	3.1
2	E	61	PRO	3.1
2	H	50	GLU	3.1
1	B	207	LEU	3.1
1	D	269	ILE	3.1
2	E	75	SER	3.0
2	H	41	LEU	3.0
2	E	70	LEU	3.0
2	G	52	PRO	3.0
2	E	27	ALA	2.9
1	A	211	GLY	2.9
2	F	88	PHE	2.9
2	H	66	ASN	2.9
2	F	45	GLY	2.8
2	E	30	LYS	2.8
2	G	56	ARG	2.8
1	B	188	LEU	2.8
2	H	37	THR	2.8
2	E	135	ALA	2.8
2	E	177	VAL	2.8
1	A	240	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	95	VAL	2.7
2	E	25	THR	2.7
2	E	209	TYR	2.7
2	F	59	ILE	2.7
2	G	111	LYS	2.7
2	E	90	VAL	2.7
1	D	161	ILE	2.7
1	A	152	LEU	2.6
2	G	59	ILE	2.6
2	F	190	GLU	2.6
2	F	87	ASP	2.6
2	F	191	ALA	2.5
2	G	159	TYR	2.5
2	E	68	ARG	2.5
1	C	190	GLU	2.5
2	E	71	ILE	2.5
2	H	33	ILE	2.5
2	E	108	LEU	2.5
1	B	165	LEU	2.5
1	A	176	THR	2.5
2	F	47	GLU	2.5
2	G	173	LEU	2.5
2	H	48	LEU	2.5
2	E	106	GLU	2.4
2	G	34	LEU	2.4
1	A	335	ASN	2.4
1	C	384	LEU	2.4
2	F	58	LEU	2.4
2	F	77	VAL	2.4
2	E	101	ALA	2.4
2	E	216	LEU	2.4
2	G	28	LEU	2.4
2	G	160	GLY	2.4
1	A	210	PHE	2.3
1	C	339	ALA	2.3
2	H	91	ALA	2.3
2	F	146	PHE	2.3
2	G	120	ALA	2.3
1	B	206	THR	2.3
2	G	74	ALA	2.3
2	G	221	ASP	2.3
2	F	23	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	G	204	VAL	2.3
2	H	117	LEU	2.2
2	H	90	VAL	2.2
1	C	381	GLN	2.2
1	D	110	LEU	2.2
2	E	22	LEU	2.2
2	G	181	GLY	2.2
2	F	111	LYS	2.2
2	E	86	ALA	2.2
1	C	261	SER	2.1
1	B	290	GLY	2.1
2	E	53	GLU	2.1
2	F	156	ILE	2.1
1	A	227	GLN	2.1
1	C	204	PHE	2.1
2	F	213	PHE	2.1
1	B	262	GLY	2.1
2	E	38	MET	2.1
2	E	34	LEU	2.1
2	G	71	ILE	2.1
1	C	291	MET	2.0
2	E	164	LEU	2.0
1	C	205	TYR	2.0
2	E	211	ARG	2.0
1	D	50	GLY	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 ⓘ

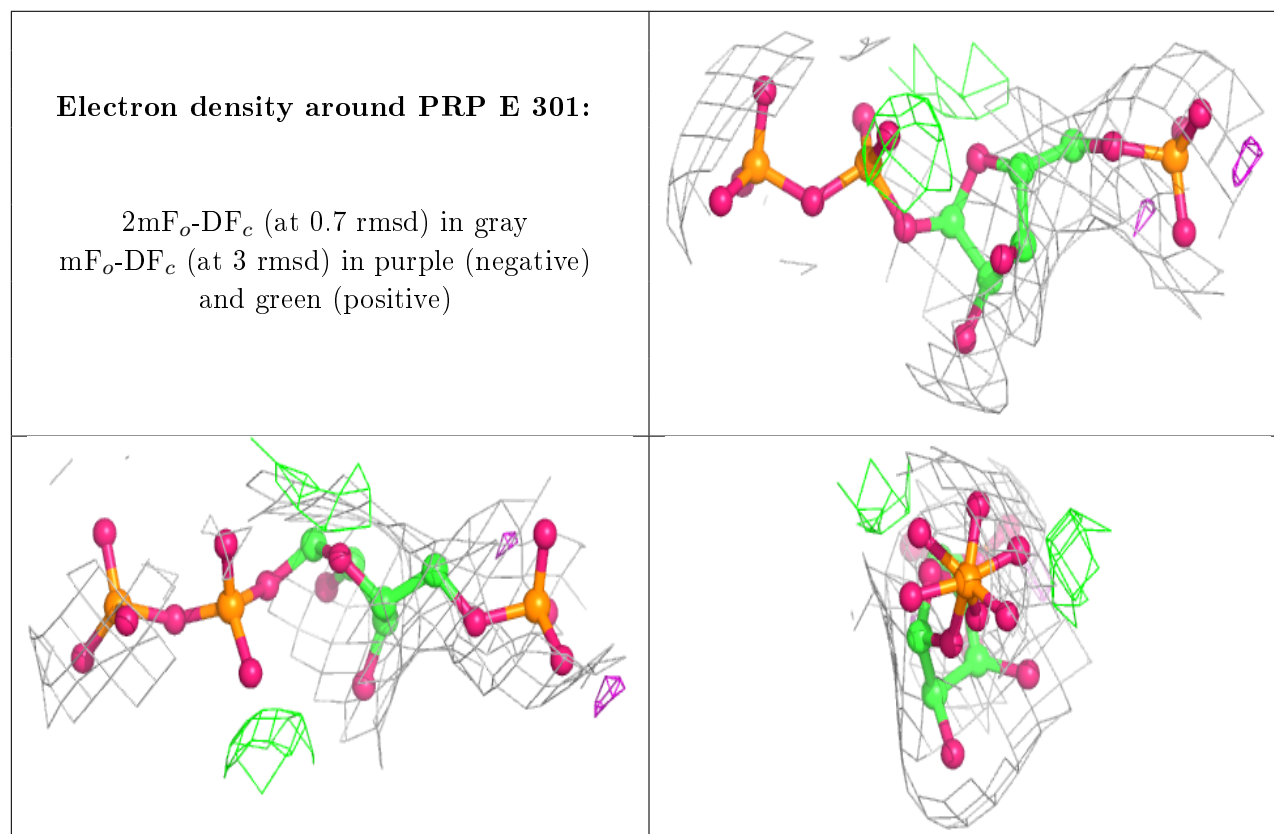
There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

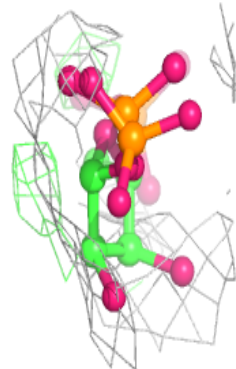
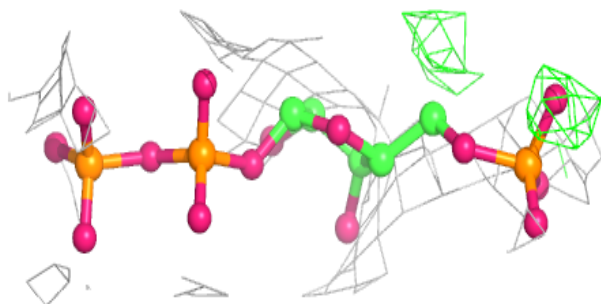
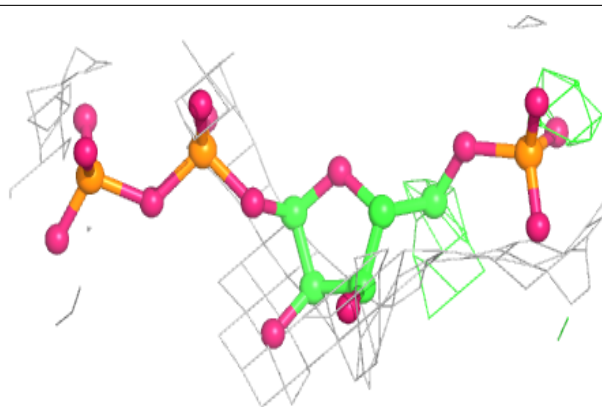
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PRP	E	301	22/22	0.69	0.14	118,131,161,163	0
4	PRP	F	301	22/22	0.77	0.13	122,151,171,175	0
4	PRP	G	301	22/22	0.80	0.15	100,120,142,143	0
4	PRP	H	301	22/22	0.83	0.11	117,123,148,149	0
3	HIS	D	401	11/11	0.85	0.16	70,72,73,73	0
3	HIS	C	401	11/11	0.85	0.22	65,70,74,75	0
3	HIS	B	401	11/11	0.89	0.19	73,76,85,85	0
3	HIS	A	401	11/11	0.92	0.15	70,73,77,79	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

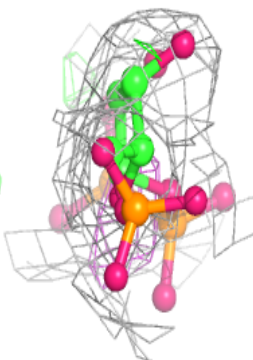
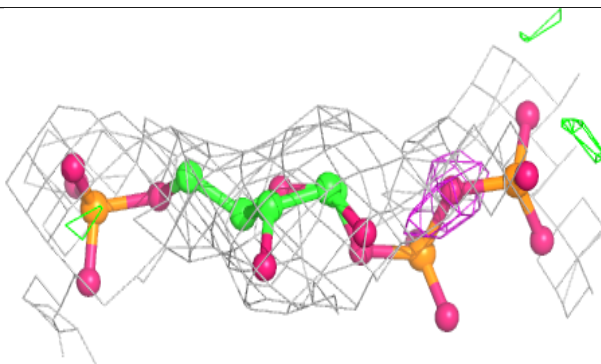
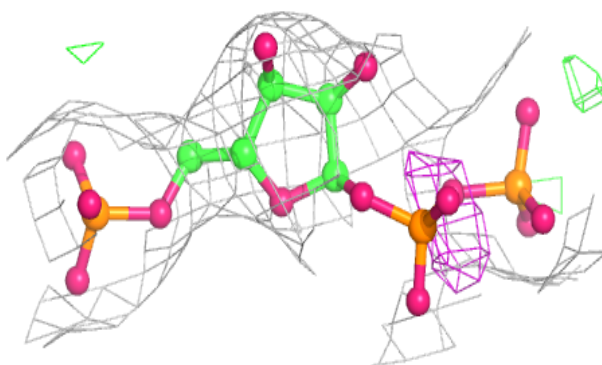


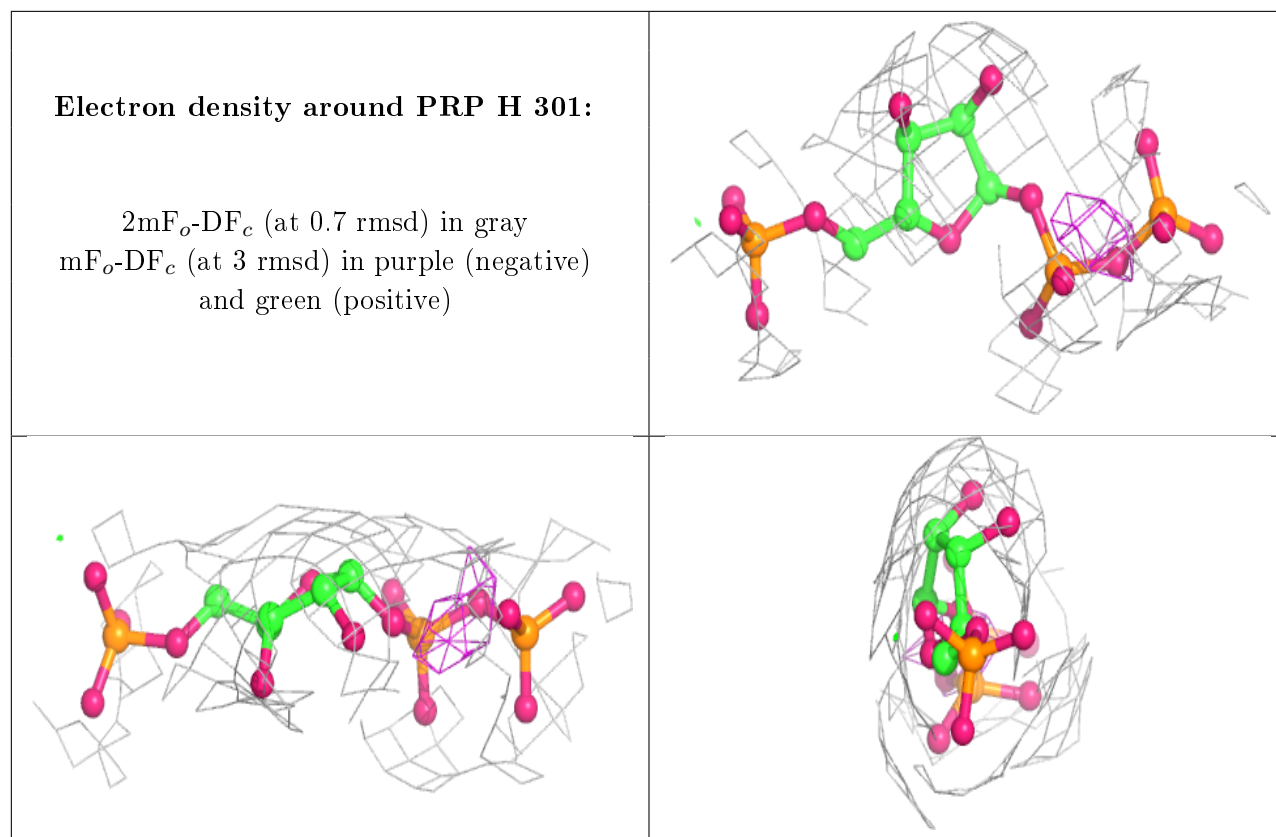
**Electron density around PRP F 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around PRP G 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.