



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:13 AM UTC

PDB ID : 6R02 / pdb_00006r02
Title : Psychrobacter arcticus ATP phosphoribosyltransferase bound to histidine and PRPP
Authors : Alpey, 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

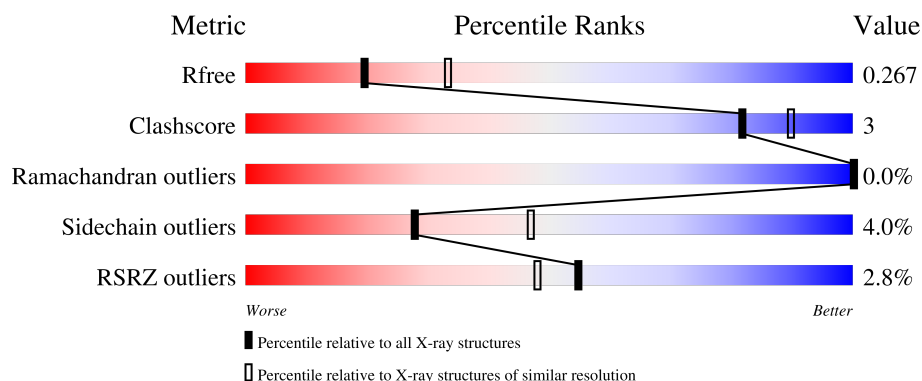
1 Overall quality at a glance

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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	2% 89% 7% ..
1	B	388	2% 89% 7% ..
1	C	388	2% 90% 8% .
1	D	388	3% 88% 10% .
2	E	232	4% 80% 7% 13%

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Mol	Chain	Length	Quality of chain
2	F	232	6% 76% 9% 14%
2	G	232	3% 79% 10% 10%
2	H	232	% 79% 9% 12%

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

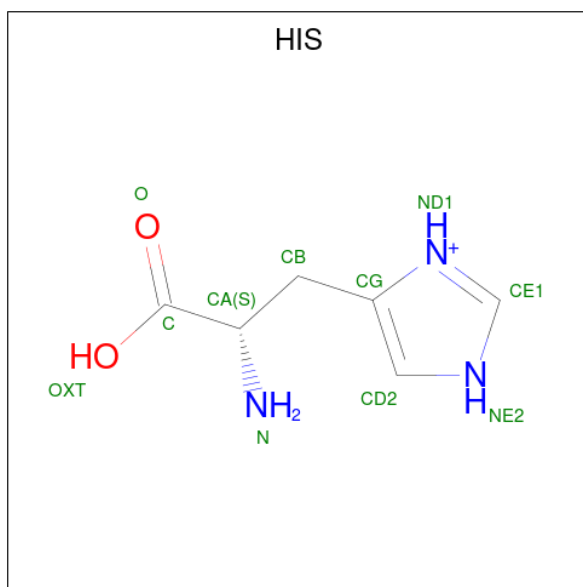
- Molecule 2 is a protein called ATP phosphoribosyltransferase.

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:

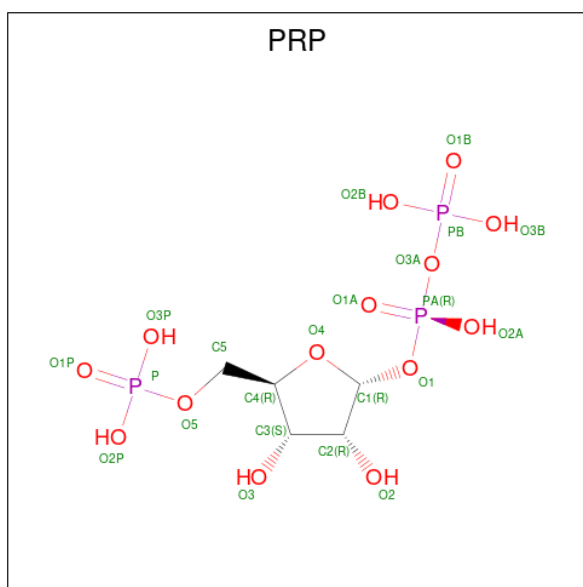
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	GLY	-	expression tag	UNP Q4FQF7
F	0	GLY	-	expression tag	UNP Q4FQF7
G	0	GLY	-	expression tag	UNP Q4FQF7
H	0	GLY	-	expression tag	UNP Q4FQF7

- Molecule 3 is HISTIDINE (CCD ID: 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 (CCD ID: 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		

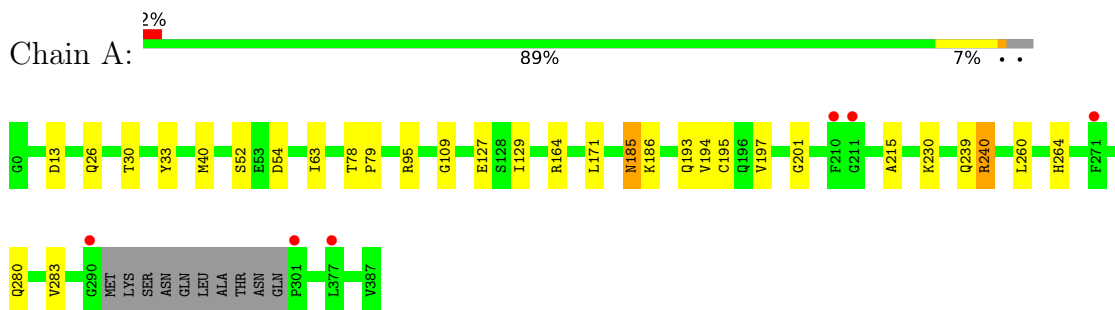
- Molecule 5 is water.

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		

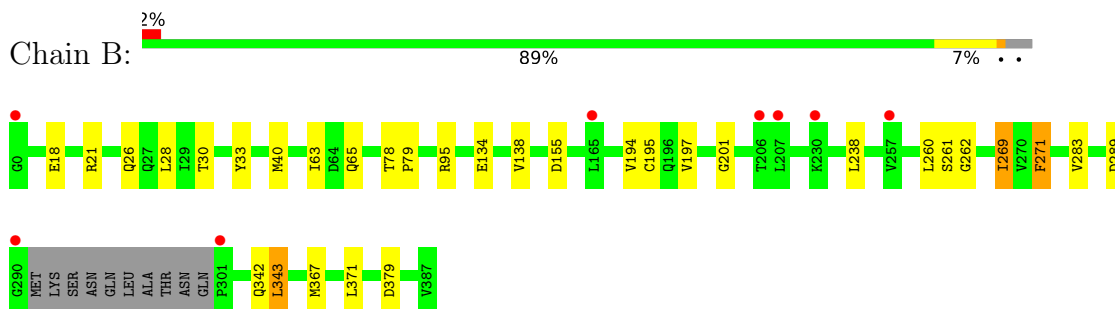
3 Residue-property plots [i](#)

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.

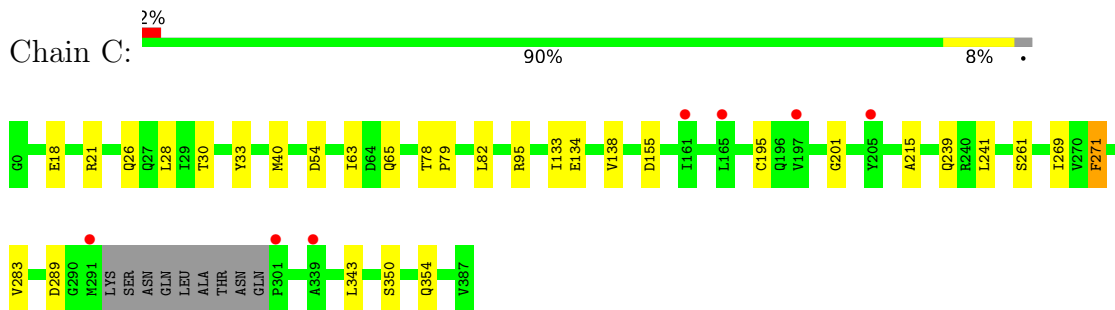
- Molecule 1: ATP phosphoribosyltransferase regulatory subunit



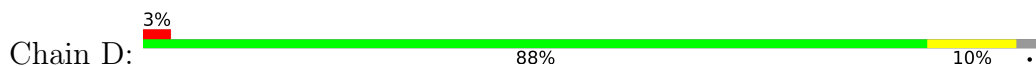
- Molecule 1: ATP phosphoribosyltransferase regulatory subunit

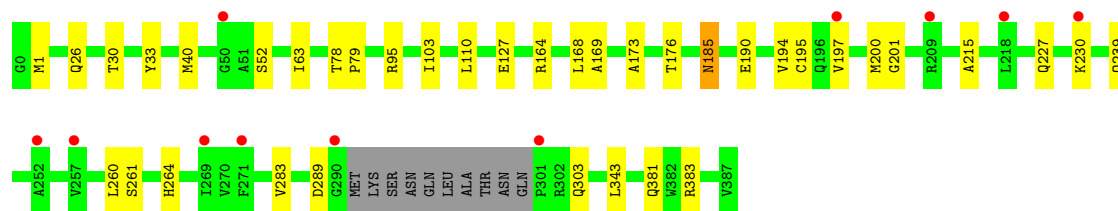


- Molecule 1: ATP phosphoribosyltransferase regulatory subunit

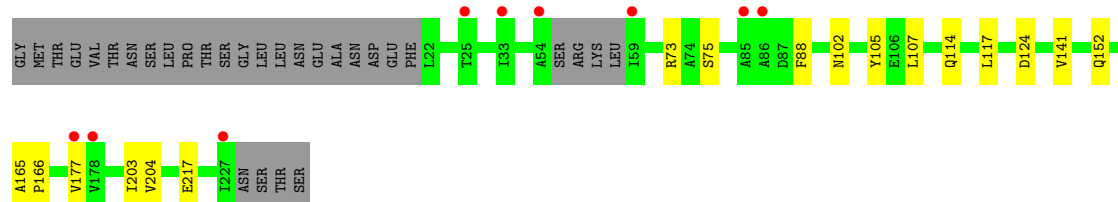
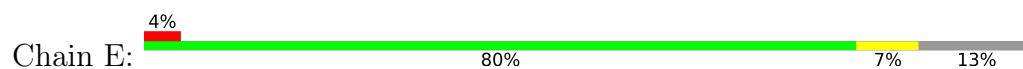


- Molecule 1: ATP phosphoribosyltransferase regulatory subunit

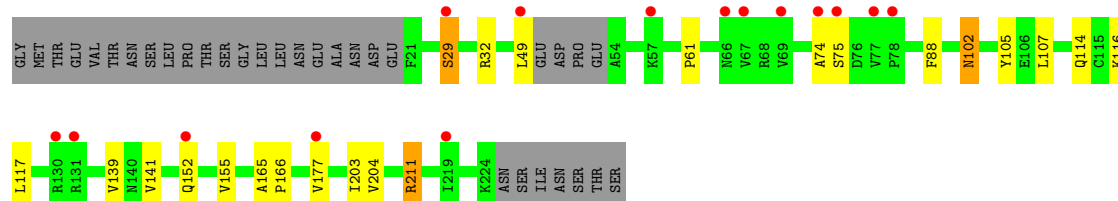
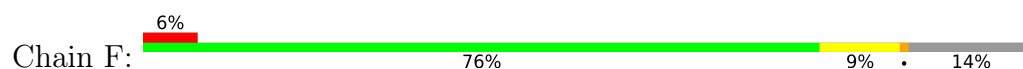




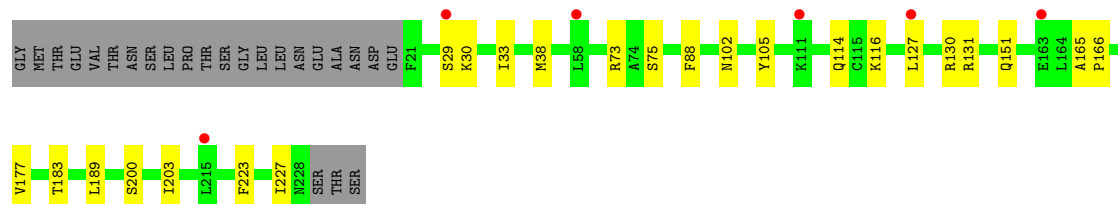
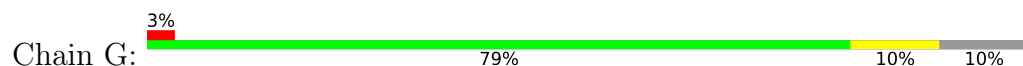
• Molecule 2: ATP phosphoribosyltransferase



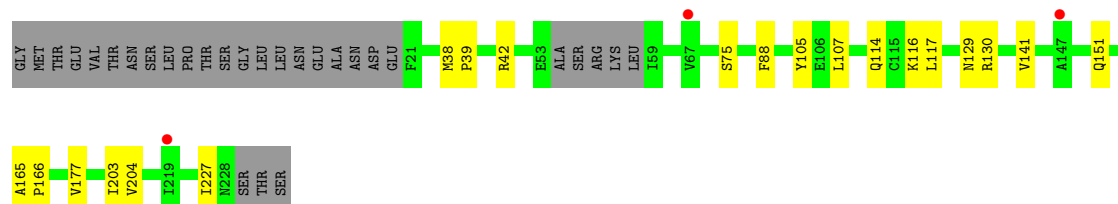
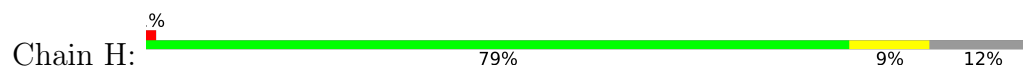
• Molecule 2: ATP phosphoribosyltransferase



• 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, α , β , γ	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) 99.8 (77.31-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (3.16%)	wwPDB-VP
Wilson B-factor (Å ²)	60.9	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 24.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	1.00	0/2992	1.44	0/4062
1	B	1.00	0/2997	1.45	2/4066 (0.0%)
1	C	0.99	0/3001	1.45	1/4071 (0.0%)
1	D	1.00	0/2972	1.46	0/4037
2	E	1.04	0/1554	1.47	0/2110
2	F	1.07	0/1502	1.47	0/2045
2	G	1.05	0/1609	1.47	0/2183
2	H	1.05	0/1551	1.47	0/2110
All	All	1.02	0/18178	1.46	3/24684 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	262	GLY	CA-C-O	-5.79	117.41	122.16
1	C	271	PHE	CA-CB-CG	5.25	119.05	113.80
1	B	271	PHE	CA-CB-CG	5.19	118.99	113.80

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	2935	0	2904	18	0
1	B	2943	0	2925	14	0
1	C	2947	0	2929	19	0
1	D	2918	0	2876	20	0
2	E	1532	0	1569	5	0
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	0	0
3	B	11	0	6	0	0
3	C	11	0	6	0	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	90	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 3.

All (90) 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:40:MET:HE2	1:B:40:MET:HE2	1.70	0.74
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:C:40:MET:HE2	1:D:40:MET:HE2	1.74	0.69
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
1:D:168:LEU:HB3	1:D:200:MET:HE1	1.77	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:D:168:LEU:CB	1:D:200:MET:HE1	2.42	0.49
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: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:109:GLY:HA3	1:A:280[B]:GLN:CD	2.39	0.47
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: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:367:MET:HE1	1:B:371:LEU:HD22	1.99	0.45
1:B:238:LEU:HD23	1:B:269:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HA	2:F:211:ARG:HD3	1.89	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
1:D:169:ALA:HB2	1:D:200:MET:HE3	2.02	0.42
2:F:105:TYR:O	2:F:203:ILE:HA	2.20	0.42
1:D:1:MET:HE2	1:D:1:MET:HB3	1.94	0.41
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:186:LYS:CB	2:G:105:TYR:CD1	3.04	0.40
1:A:215:ALA:HA	1:A:239:GLN:NE2	2.35	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%)	36	52
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%)	309 (98%)	7 (2%)	45	67
1	B	318/329 (97%)	308 (97%)	10 (3%)	35	56
1	C	318/329 (97%)	309 (97%)	9 (3%)	38	60
1	D	312/329 (95%)	304 (97%)	8 (3%)	40	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	164/195 (84%)	155 (94%)	9 (6%)	19	33
2	F	153/195 (78%)	143 (94%)	10 (6%)	15	27
2	G	170/195 (87%)	155 (91%)	15 (9%)	9	15
2	H	163/195 (84%)	154 (94%)	9 (6%)	19	33
All	All	1914/2096 (91%)	1837 (96%)	77 (4%)	28	47

All (77) 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	193	GLN
1	A	240	ARG
1	A	260	LEU
1	A	283	VAL
1	B	155	ASP
1	B	260	LEU
1	B	261	SER
1	B	269	ILE
1	B	271	PHE
1	B	283	VAL
1	B	289	ASP
1	B	342	GLN
1	B	343	LEU
1	B	379	ASP
1	C	54	ASP
1	C	82	LEU
1	C	133	ILE
1	C	155	ASP
1	C	261	SER
1	C	271	PHE
1	C	283	VAL
1	C	289	ASP
1	C	343	LEU
1	D	185	ASN
1	D	190	GLU
1	D	227	GLN
1	D	260	LEU
1	D	261	SER
1	D	283	VAL

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Mol	Chain	Res	Type
1	D	289	ASP
1	D	343	LEU
2	E	73	ARG
2	E	75	SER
2	E	88	PHE
2	E	102	ASN
2	E	114	GLN
2	E	124	ASP
2	E	152	GLN
2	E	177	VAL
2	E	217	GLU
2	F	29	SER
2	F	32	ARG
2	F	75	SER
2	F	88	PHE
2	F	102	ASN
2	F	114	GLN
2	F	116	LYS
2	F	152	GLN
2	F	177	VAL
2	F	211	ARG
2	G	29	SER
2	G	30	LYS
2	G	38	MET
2	G	73	ARG
2	G	75	SER
2	G	88	PHE
2	G	102	ASN
2	G	114	GLN
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	114	GLN
2	H	116	LYS
2	H	130	ARG

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Mol	Chain	Res	Type
2	H	151	GLN
2	H	177	VAL
2	H	227	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	GLN
1	A	239	GLN
1	A	303	GLN
1	A	353	GLN
1	B	212	HIS
1	B	216	ASN
1	B	226	GLN
1	B	250	GLN
1	B	266	HIS
1	B	272	ASN
1	B	280	GLN
1	B	346	GLN
1	B	380	ASN
1	C	196	GLN
1	C	212	HIS
1	C	239	GLN
1	C	250	GLN
1	C	266	HIS
1	C	272	ASN
1	C	334	ASN
1	D	88	HIS
1	D	239	GLN
1	D	250	GLN
1	D	303	GLN
1	D	353	GLN
1	D	381	GLN
2	E	66	ASN
2	E	83	HIS
2	F	66	ASN
2	F	102	ASN
2	F	152	GLN
2	G	151	GLN
2	H	99	HIS
2	H	129	ASN
2	H	151	GLN

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Mol	Chain	Res	Type
2	H	194	HIS
2	H	206	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
3	HIS	B	401	-	10,11,11	0.73	1 (10%)	10,14,14	1.26	1 (10%)
3	HIS	C	401	-	10,11,11	0.74	1 (10%)	10,14,14	1.23	1 (10%)
4	PRP	E	301	-	20,22,22	0.85	1 (5%)	32,35,35	0.93	0
4	PRP	F	301	-	20,22,22	0.84	1 (5%)	32,35,35	0.98	1 (3%)
4	PRP	H	301	-	20,22,22	0.88	1 (5%)	32,35,35	1.06	2 (6%)
3	HIS	D	401	-	10,11,11	0.76	1 (10%)	10,14,14	1.28	1 (10%)
4	PRP	G	301	-	20,22,22	0.96	1 (5%)	32,35,35	1.09	2 (6%)
3	HIS	A	401	-	10,11,11	0.73	1 (10%)	10,14,14	1.21	1 (10%)

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
3	HIS	B	401	-	-	0/8/8/8	0/1/1/1
3	HIS	C	401	-	-	1/8/8/8	0/1/1/1
4	PRP	E	301	-	-	2/16/33/33	0/1/1/1
4	PRP	F	301	-	-	7/16/33/33	0/1/1/1
4	PRP	H	301	-	-	4/16/33/33	0/1/1/1
3	HIS	D	401	-	-	0/8/8/8	0/1/1/1
4	PRP	G	301	-	-	8/16/33/33	0/1/1/1
3	HIS	A	401	-	-	1/8/8/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	301	PRP	PA-O3A	3.19	1.62	1.59
4	H	301	PRP	PA-O3A	2.84	1.62	1.59
4	E	301	PRP	PA-O3A	2.59	1.62	1.59
4	F	301	PRP	PA-O3A	2.50	1.62	1.59
3	D	401	HIS	OXT-C	-2.18	1.23	1.30
3	B	401	HIS	OXT-C	-2.17	1.23	1.30
3	A	401	HIS	OXT-C	-2.16	1.23	1.30
3	C	401	HIS	OXT-C	-2.14	1.23	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	HIS	OXT-C-O	-2.94	117.42	124.08
4	G	301	PRP	C1-C2-C3	2.90	105.90	102.29
4	G	301	PRP	O1-C1-C2	2.90	111.35	106.65
4	H	301	PRP	C1-C2-C3	2.86	105.85	102.29
3	B	401	HIS	OXT-C-O	-2.76	117.82	124.08
3	C	401	HIS	OXT-C-O	-2.69	117.98	124.08
3	A	401	HIS	OXT-C-O	-2.60	118.19	124.08
4	H	301	PRP	O1-C1-C2	2.24	110.28	106.65
4	F	301	PRP	O1-C1-C2	2.24	110.28	106.65

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	301	PRP	C5-O5-P-O2P
4	E	301	PRP	C5-O5-P-O3P
4	F	301	PRP	C1-O1-PA-O1A
4	F	301	PRP	C1-O1-PA-O3A
4	F	301	PRP	C5-O5-P-O1P
4	F	301	PRP	C5-O5-P-O2P
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	H	301	PRP	C1-O1-PA-O3A
4	F	301	PRP	C3-C4-C5-O5
4	F	301	PRP	O4-C4-C5-O5
4	G	301	PRP	C5-O5-P-O1P
4	G	301	PRP	C1-O1-PA-O1A
4	H	301	PRP	C1-O1-PA-O1A
4	G	301	PRP	PA-O3A-PB-O1B
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	H	301	PRP	O4-C4-C5-O5
3	A	401	HIS	OXT-C-CA-N
3	C	401	HIS	O-C-CA-N

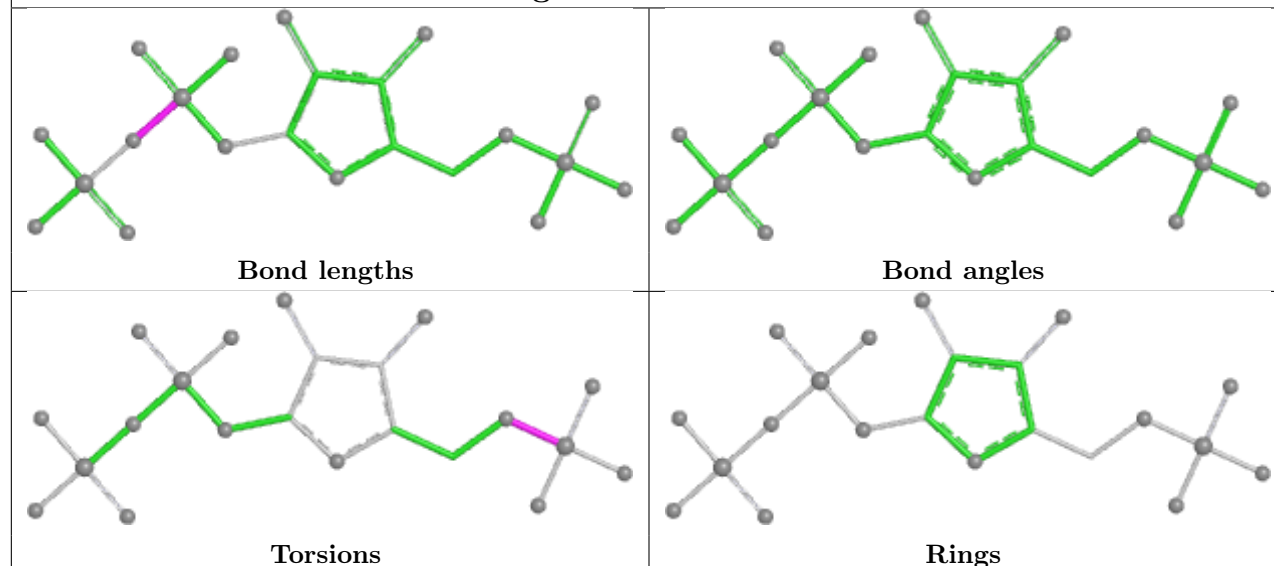
There are no ring outliers.

1 monomer is involved in 1 short contact:

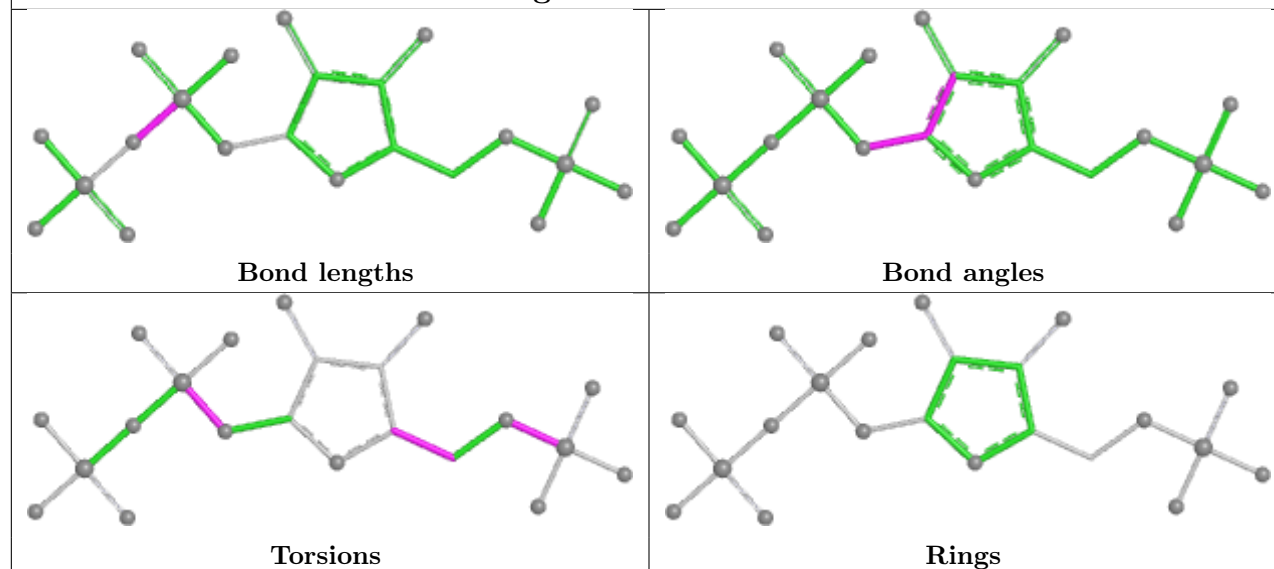
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	301	PRP	1	0

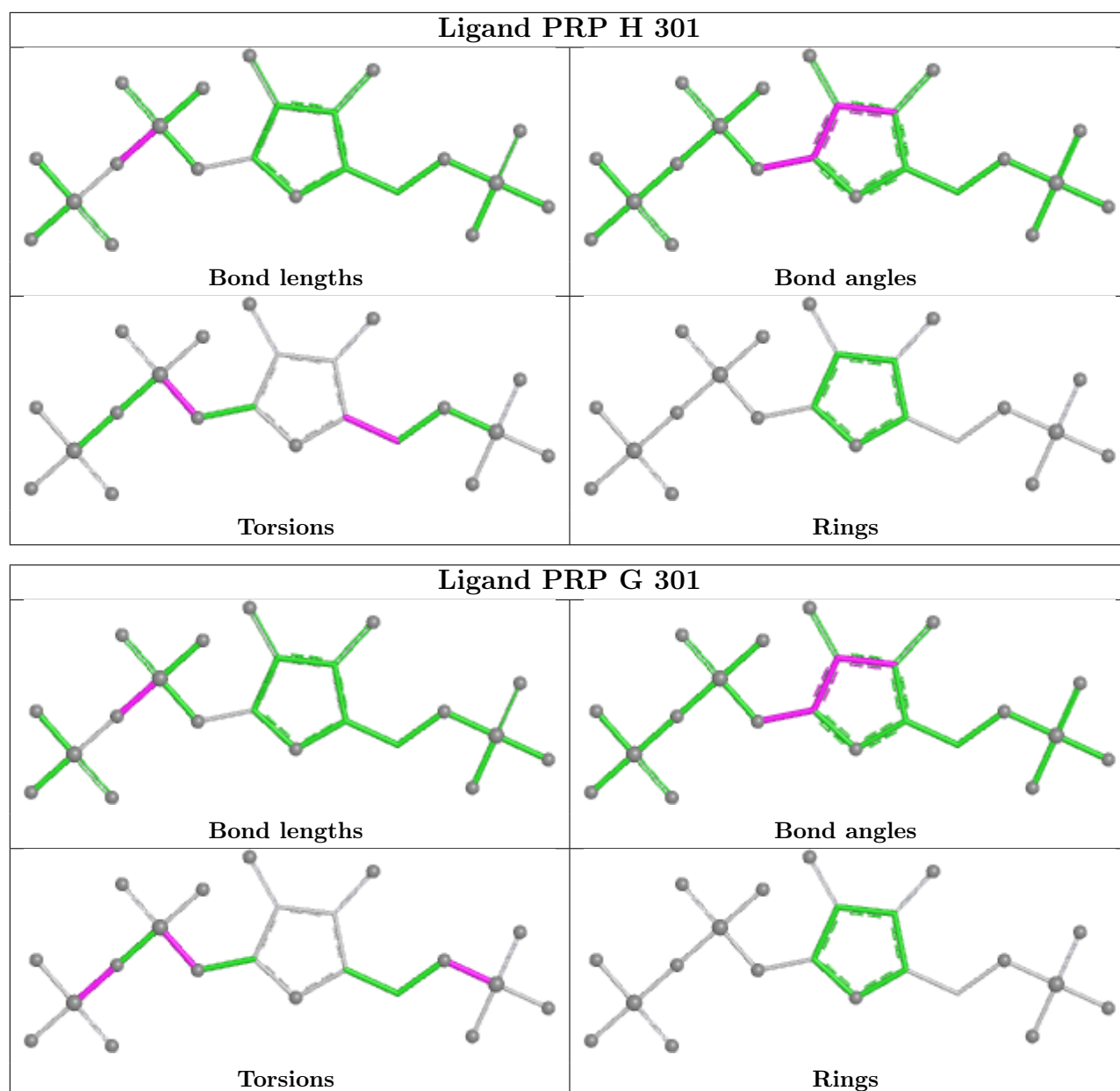
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 E 301



Ligand PRP F 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, 95th 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 ²)	Q < 0.9
1	A	378/388 (97%)	0.21	6 (1%)	70	66	44, 77, 115, 124	1 (0%)
1	B	378/388 (97%)	0.10	8 (2%)	63	57	45, 70, 101, 124	0
1	C	379/388 (97%)	0.09	7 (1%)	67	63	44, 71, 111, 133	0
1	D	378/388 (97%)	0.25	11 (2%)	53	46	53, 80, 132, 158	0
2	E	202/232 (87%)	0.47	9 (4%)	38	31	73, 98, 127, 146	0
2	F	200/232 (86%)	0.56	15 (7%)	20	15	67, 96, 132, 141	0
2	G	208/232 (89%)	0.27	6 (2%)	53	46	66, 85, 111, 126	0
2	H	203/232 (87%)	0.26	3 (1%)	72	67	59, 87, 118, 141	0
All	All	2326/2480 (93%)	0.24	65 (2%)	55	48	44, 81, 120, 158	1 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	301	PRO	5.7
2	F	74	ALA	5.6
1	D	290	GLY	4.5
1	C	339	ALA	4.4
2	F	69	VAL	4.1
2	F	78	PRO	3.7
1	A	271	PHE	3.6
2	E	85	ALA	3.5
1	D	209	ARG	3.4
2	F	49	LEU	3.1
1	A	301	PRO	3.1
1	A	211	GLY	3.1
1	D	271	PHE	3.1
1	D	269	ILE	3.0
2	G	127	LEU	3.0
1	B	207	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	206	THR	2.9
1	D	252	ALA	2.8
1	B	301	PRO	2.7
1	C	291	MET	2.7
1	B	257	VAL	2.7
1	C	301	PRO	2.7
2	F	177	VAL	2.6
2	E	59	ILE	2.6
1	B	290	GLY	2.6
1	C	161	ILE	2.6
2	E	177	VAL	2.5
1	C	165	LEU	2.4
1	D	218	LEU	2.4
2	E	178	VAL	2.4
2	F	67	VAL	2.4
2	F	57	LYS	2.4
1	A	290	GLY	2.4
1	C	197	VAL	2.4
2	F	152	GLN	2.3
2	E	54	ALA	2.3
1	D	50	GLY	2.3
1	B	165	LEU	2.3
2	F	130	ARG	2.3
2	F	77	VAL	2.3
1	B	230	LYS	2.2
2	F	219	ILE	2.2
2	F	29	SER	2.2
2	E	25	THR	2.2
2	E	33	ILE	2.2
2	E	227	ILE	2.2
2	H	219	ILE	2.2
2	F	131	ARG	2.1
2	G	215	LEU	2.1
2	F	66	ASN	2.1
1	B	0	GLY	2.1
1	D	257	VAL	2.1
2	F	75	SER	2.1
2	G	163	GLU	2.1
2	G	111	LYS	2.1
2	H	147	ALA	2.1
1	D	230	LYS	2.1
1	C	205	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	86	ALA	2.0
1	A	377	LEU	2.0
2	H	67	VAL	2.0
1	A	210	PHE	2.0
2	G	29	SER	2.0
2	G	58	LEU	2.0
1	D	197	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

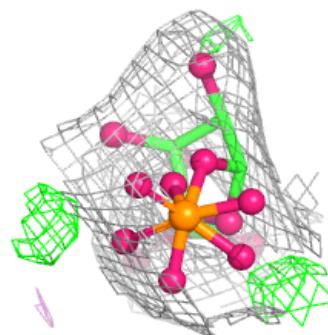
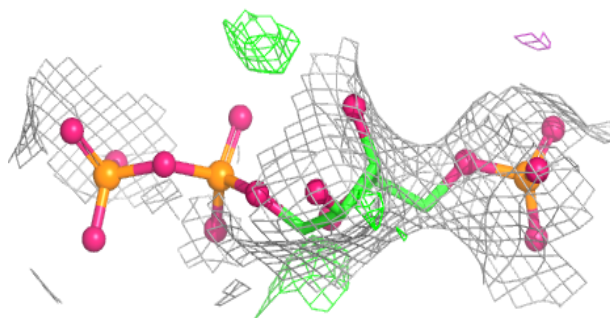
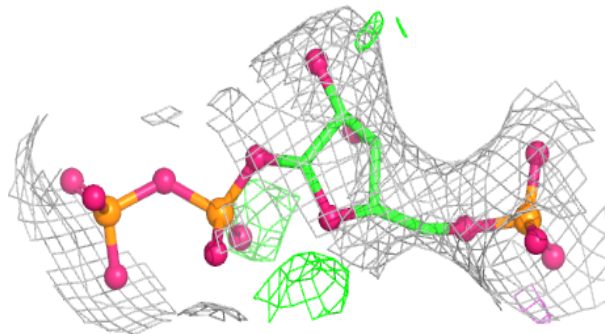
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PRP	E	301	22/22	0.62	0.11	118,131,161,163	0
4	PRP	F	301	22/22	0.72	0.09	122,151,171,175	0
4	PRP	H	301	22/22	0.73	0.09	117,123,148,149	0
4	PRP	G	301	22/22	0.78	0.10	100,120,142,143	0
3	HIS	C	401	11/11	0.79	0.12	65,70,74,75	0
3	HIS	D	401	11/11	0.81	0.11	70,72,73,73	0
3	HIS	B	401	11/11	0.87	0.10	73,76,85,85	0
3	HIS	A	401	11/11	0.88	0.09	70,73,77,79	0

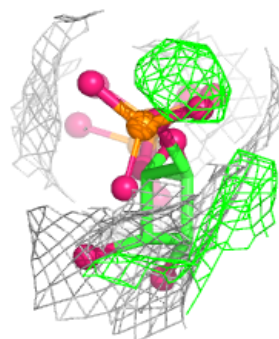
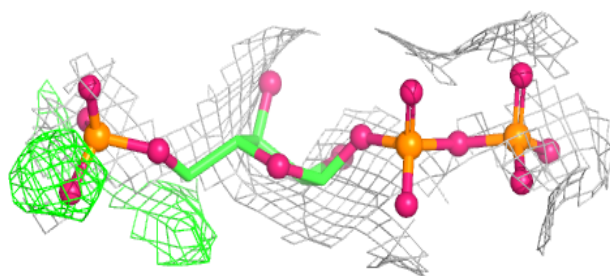
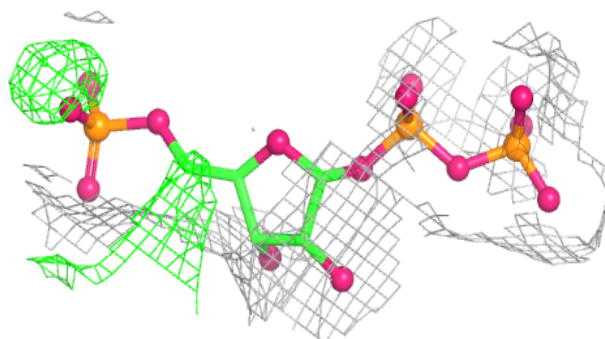
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PRP E 301:

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

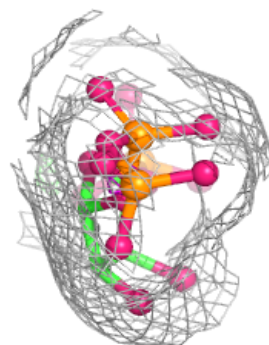
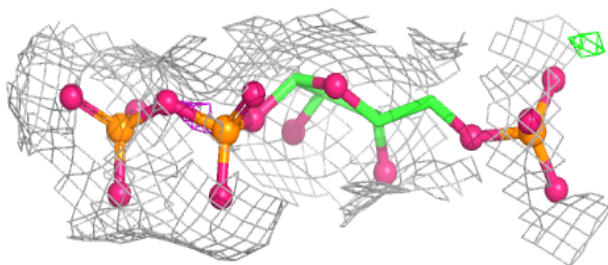
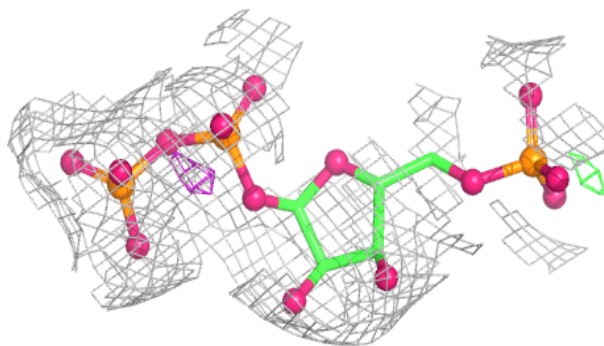
**Electron density around PRP F 301:**

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

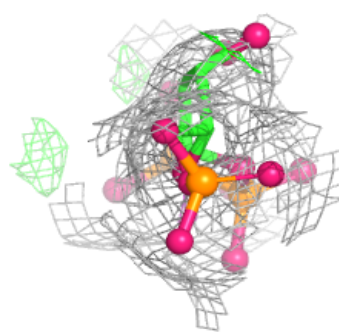
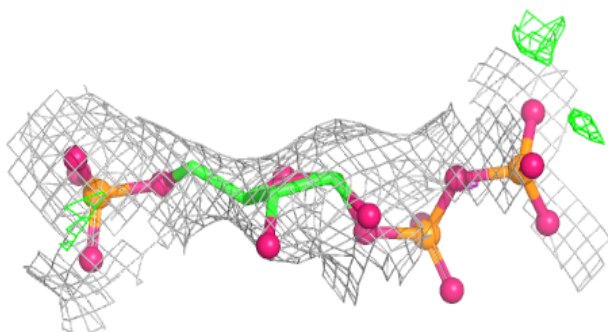
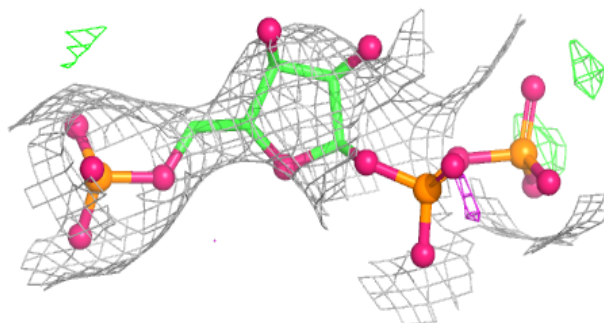


Electron density around PRP H 301:

$2mF_o-DF_c$ (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.