



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2025 – 04:55 PM EST

PDB ID : 9CR6  
Title : Crystal structure of histidine racemase (HisR) of *Fusobacterium nucleatum* (C209S)  
Authors : Chen, P.; Lamer, T.; Vederas, J.C.; Lemieux, M.J.  
Deposited on : 2024-07-20  
Resolution : 2.49 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.

The types of validation reports are described at

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

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

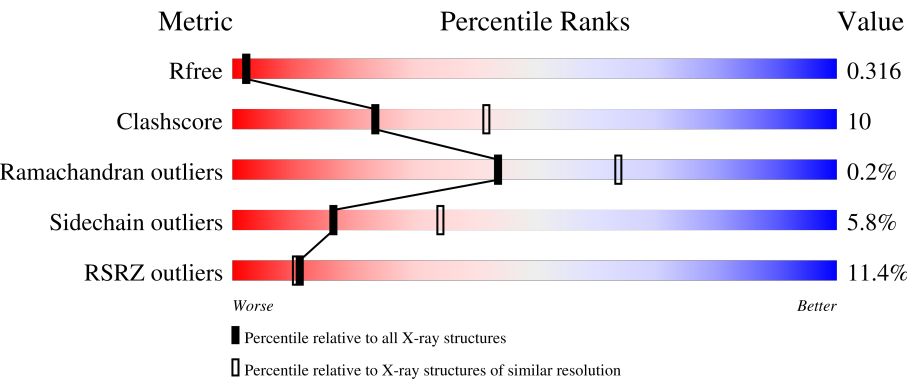
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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))
$R_{free}$	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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 of 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	271	<div><div>10%</div><div><div></div><div></div><div></div><div></div></div><div>75%</div><div>21%</div><div>..</div></div>
1	B	271	<div><div>10%</div><div><div></div><div></div><div></div><div></div></div><div>78%</div><div>18%</div><div>..</div></div>
1	C	271	<div><div>8%</div><div><div></div><div></div><div></div><div></div></div><div>71%</div><div>24%</div><div>..</div></div>
1	D	271	<div><div>15%</div><div><div></div><div></div><div></div><div></div></div><div>68%</div><div>21%</div><div>11%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16453 atoms, of which 8195 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 Histidine racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	260	Total	C	H	N	O	S	0	0	0
			4165	1343	2079	333	400	10			
1	B	262	Total	C	H	N	O	S	0	0	0
			4194	1351	2095	336	402	10			
1	C	262	Total	C	H	N	O	S	0	0	0
			4195	1351	2094	338	402	10			
1	D	242	Total	C	H	N	O	S	0	0	0
			3862	1248	1927	310	367	10			

There are 28 discrepancies between the modelled and reference sequences:

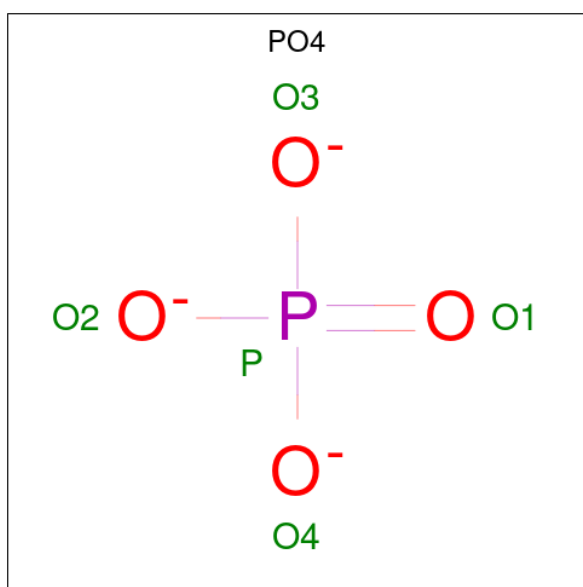
Chain	Residue	Modelled	Actual	Comment	Reference
A	209	SER	CYS	engineered mutation	UNP Q8RI81
A	266	HIS	-	expression tag	UNP Q8RI81
A	267	HIS	-	expression tag	UNP Q8RI81
A	268	HIS	-	expression tag	UNP Q8RI81
A	269	HIS	-	expression tag	UNP Q8RI81
A	270	HIS	-	expression tag	UNP Q8RI81
A	271	HIS	-	expression tag	UNP Q8RI81
B	209	SER	CYS	engineered mutation	UNP Q8RI81
B	266	HIS	-	expression tag	UNP Q8RI81
B	267	HIS	-	expression tag	UNP Q8RI81
B	268	HIS	-	expression tag	UNP Q8RI81
B	269	HIS	-	expression tag	UNP Q8RI81
B	270	HIS	-	expression tag	UNP Q8RI81
B	271	HIS	-	expression tag	UNP Q8RI81
C	209	SER	CYS	engineered mutation	UNP Q8RI81
C	266	HIS	-	expression tag	UNP Q8RI81
C	267	HIS	-	expression tag	UNP Q8RI81
C	268	HIS	-	expression tag	UNP Q8RI81
C	269	HIS	-	expression tag	UNP Q8RI81
C	270	HIS	-	expression tag	UNP Q8RI81
C	271	HIS	-	expression tag	UNP Q8RI81

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Chain	Residue	Modelled	Actual	Comment	Reference
D	209	SER	CYS	engineered mutation	UNP Q8RI81
D	266	HIS	-	expression tag	UNP Q8RI81
D	267	HIS	-	expression tag	UNP Q8RI81
D	268	HIS	-	expression tag	UNP Q8RI81
D	269	HIS	-	expression tag	UNP Q8RI81
D	270	HIS	-	expression tag	UNP Q8RI81
D	271	HIS	-	expression tag	UNP Q8RI81

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0

- Molecule 3 is water.

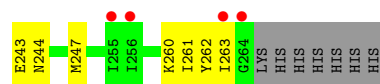
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	B	3	Total O 3 3	0	0

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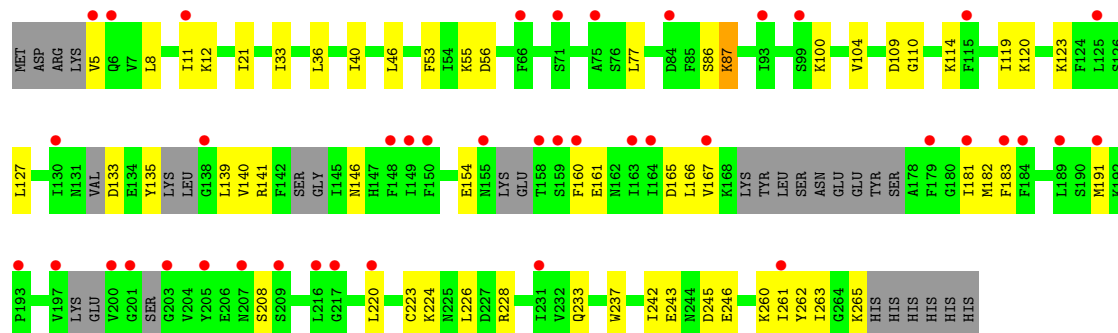
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	5	Total	O	0	0
			5	5		
3	D	9	Total	O	0	0
			9	9		





● Molecule 1: Histidine racemase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.84Å 89.12Å 100.33Å 90.00° 100.91° 90.00°	Depositor
Resolution (Å)	35.86 – 2.49 35.86 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.6 (35.86-2.49) 98.3 (35.86-2.49)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.261 , 0.313 0.266 , 0.316	Depositor DCC
$R_{free}$ test set	2220 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.2	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 32.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	16453	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	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 38.26 % 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 3.7884e-04. 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: PO4

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	0.27	0/2124	0.47	0/2854
1	B	0.27	0/2138	0.46	0/2873
1	C	0.27	0/2140	0.47	0/2876
1	D	0.27	0/1965	0.47	0/2633
All	All	0.27	0/8367	0.47	0/11236

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	2086	2079	2077	42	0
1	B	2099	2095	2094	36	1
1	C	2101	2094	2094	46	1
1	D	1935	1927	1920	43	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	5	0	0	9	0
3	B	3	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	5	0	0	11	0
3	D	9	0	0	14	0
All	All	8258	8195	8185	164	1

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 10.

All (164) 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:47:TYR:N	3:C:401:HOH:O	1.88	1.06
1:A:53:PHE:HB2	3:A:401:HOH:O	1.53	1.04
1:D:135:TYR:N	3:D:301:HOH:O	1.80	1.02
1:C:46:LEU:CA	3:C:401:HOH:O	2.08	1.02
1:A:28:ILE:HG22	3:A:401:HOH:O	1.62	0.98
1:A:53:PHE:CB	3:A:401:HOH:O	2.08	0.98
1:C:46:LEU:HA	3:C:401:HOH:O	1.62	0.98
1:C:46:LEU:C	3:C:401:HOH:O	2.01	0.98
1:A:53:PHE:C	3:A:401:HOH:O	2.03	0.95
1:B:113:ASN:OD1	3:B:401:HOH:O	1.86	0.94
1:D:87:LYS:N	3:D:302:HOH:O	1.83	0.92
1:A:53:PHE:O	3:A:401:HOH:O	1.90	0.88
1:B:111:ALA:CB	3:B:401:HOH:O	2.24	0.85
1:D:182:MET:HA	3:D:305:HOH:O	1.77	0.84
1:D:237:TRP:NE1	3:D:303:HOH:O	1.92	0.84
1:C:26:PHE:N	3:C:403:HOH:O	2.13	0.81
1:D:56:ASP:OD1	3:D:304:HOH:O	1.97	0.81
1:B:261:ILE:HD13	1:B:263:ILE:HD11	1.63	0.81
1:B:113:ASN:N	3:B:401:HOH:O	1.90	0.79
1:D:139:LEU:HD11	1:D:141:ARG:HG2	1.63	0.79
1:B:102:LEU:HD11	3:B:403:HOH:O	1.80	0.79
1:D:181:ILE:O	3:D:305:HOH:O	1.99	0.78
1:A:34:PRO:O	3:A:402:HOH:O	2.02	0.77
1:B:111:ALA:HB3	3:B:401:HOH:O	1.80	0.77
1:D:86:SER:HB3	3:D:302:HOH:O	1.87	0.74
1:A:164:ILE:HD13	1:A:194:TYR:CE2	2.24	0.73
1:A:132:VAL:HG11	1:A:166:LEU:HD21	1.71	0.72
1:D:100:LYS:O	3:D:306:HOH:O	2.07	0.72
1:D:127:LEU:CD2	1:D:140:VAL:HG22	2.20	0.71
1:A:11:ILE:HG21	1:A:77:LEU:HD13	1.72	0.71
1:D:120:LYS:NZ	1:D:246:GLU:OE2	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ASN:OD1	3:B:402:HOH:O	2.10	0.69
1:C:128:GLU:OE2	1:C:141:ARG:NH1	2.26	0.68
1:C:65:GLU:OE1	1:C:65:GLU:N	2.20	0.68
1:A:154:GLU:HA	1:A:154:GLU:OE1	1.95	0.66
1:C:150:PHE:HE1	1:C:152:ILE:HG22	1.60	0.65
1:D:127:LEU:HD22	1:D:140:VAL:HG22	1.78	0.65
1:B:128:GLU:OE2	1:B:141:ARG:NE	2.29	0.64
1:A:60:GLN:HB3	3:A:401:HOH:O	1.98	0.63
1:D:182:MET:CA	3:D:305:HOH:O	2.40	0.63
1:B:134:GLU:N	1:B:134:GLU:OE1	2.33	0.62
1:C:130:ILE:CD1	1:C:132:VAL:HG23	2.30	0.62
1:C:24:ASP:C	3:C:403:HOH:O	2.38	0.61
1:C:127:LEU:HD13	1:C:140:VAL:HG22	1.83	0.61
1:A:39:GLU:HA	1:A:42:LYS:HE2	1.82	0.60
1:C:150:PHE:CE1	1:C:152:ILE:HG22	2.36	0.60
1:D:167:VAL:HG21	1:D:181:ILE:HD11	1.82	0.60
1:C:182:MET:HE2	1:C:212:GLY:HA3	1.84	0.59
1:A:59:LEU:HD11	1:A:61:MET:CE	2.33	0.59
1:D:262:TYR:C	1:D:263:ILE:HD13	2.23	0.59
1:A:53:PHE:CA	3:A:401:HOH:O	2.30	0.58
1:A:164:ILE:HD13	1:A:194:TYR:CZ	2.37	0.58
1:C:69:ASN:OD1	1:C:72:ARG:NH1	2.37	0.58
1:A:130:ILE:HG22	1:B:128:GLU:HG2	1.86	0.57
1:D:161:GLU:N	1:D:161:GLU:OE1	2.34	0.57
1:D:11:ILE:HG21	1:D:77:LEU:HD13	1.87	0.57
1:D:55:LYS:CE	3:D:304:HOH:O	2.53	0.56
1:C:26:PHE:CB	3:C:403:HOH:O	2.53	0.56
1:C:214:THR:HG23	1:C:247:MET:HG2	1.88	0.56
1:B:12:LYS:NZ	1:B:47:TYR:O	2.37	0.55
1:A:13:ILE:CD1	1:A:22:LEU:HD12	2.37	0.55
1:D:260:LYS:N	1:D:260:LYS:HD3	2.23	0.53
1:B:120:LYS:HE2	1:B:246:GLU:OE2	2.08	0.53
1:C:130:ILE:O	1:C:131:ASN:ND2	2.39	0.53
1:D:123:LYS:NZ	1:D:245:ASP:O	2.40	0.52
1:C:182:MET:CE	1:C:212:GLY:HA3	2.40	0.52
1:A:14:ASN:HB2	1:A:256:ILE:HD11	1.91	0.51
1:D:183:PHE:N	3:D:305:HOH:O	2.37	0.51
1:B:12:LYS:HD2	1:B:21:ILE:HD11	1.92	0.50
1:D:33:ILE:HG23	1:D:53:PHE:CE1	2.46	0.50
1:A:28:ILE:CG2	3:A:401:HOH:O	2.40	0.50
1:B:32:ASN:HB3	1:B:35:LYS:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:SER:HA	1:D:233:GLN:OE1	2.13	0.48
1:D:242:ILE:O	1:D:243:GLU:OE1	2.31	0.48
1:B:133:ASP:HB3	1:B:134:GLU:OE1	2.13	0.48
1:C:150:PHE:CE1	1:C:152:ILE:HA	2.49	0.48
1:C:82:ASP:HA	3:C:402:HOH:O	2.13	0.48
1:D:160:PHE:CD1	1:D:183:PHE:CD2	3.02	0.48
1:A:90:ASN:ND2	1:A:103:ASP:OD1	2.46	0.47
1:A:134:GLU:O	1:A:134:GLU:CG	2.62	0.47
1:C:179:PHE:CD1	1:C:179:PHE:C	2.88	0.47
1:B:58:HIS:HD2	1:B:94:THR:OG1	1.98	0.47
1:B:102:LEU:CD1	3:B:403:HOH:O	2.48	0.47
1:C:39:GLU:CD	1:C:42:LYS:HZ3	2.18	0.47
1:C:130:ILE:C	1:C:130:ILE:HD12	2.35	0.47
1:B:6:GLN:HG2	1:B:8:LEU:HD21	1.97	0.47
1:A:50:GLN:HA	1:A:62:MET:HE1	1.97	0.46
1:C:243:GLU:O	1:C:244:ASN:OD1	2.33	0.46
1:C:182:MET:HE2	1:C:212:GLY:CA	2.46	0.46
1:D:40:ILE:O	1:D:46:LEU:O	2.34	0.46
1:B:11:ILE:HG21	1:B:77:LEU:HD13	1.97	0.46
1:A:197:VAL:O	1:A:201:GLY:N	2.48	0.46
1:C:36:LEU:O	1:C:40:ILE:HG12	2.16	0.46
1:C:39:GLU:OE2	1:C:42:LYS:NZ	2.49	0.46
1:A:21:ILE:HG12	1:A:48:ALA:HB2	1.97	0.46
1:D:8:LEU:HD21	1:D:36:LEU:HD21	1.97	0.46
1:C:100:LYS:NZ	1:C:123:LYS:NZ	2.65	0.45
1:D:12:LYS:HA	1:D:21:ILE:HD13	1.97	0.45
1:A:50:GLN:NE2	1:A:62:MET:HE1	2.32	0.45
1:A:130:ILE:HG22	1:B:128:GLU:CG	2.45	0.45
1:D:133:ASP:OD2	1:D:166:LEU:CD2	2.65	0.45
1:C:39:GLU:OE1	1:C:42:LYS:HD2	2.16	0.45
1:B:36:LEU:O	1:B:40:ILE:HG13	2.17	0.45
1:C:83:LYS:N	3:C:402:HOH:O	2.03	0.45
1:D:5:VAL:HG13	1:D:5:VAL:O	2.17	0.45
1:B:127:LEU:HD13	1:B:140:VAL:HG22	1.97	0.44
1:C:33:ILE:HG23	1:C:53:PHE:CE1	2.52	0.44
1:D:5:VAL:HG23	1:D:263:ILE:O	2.18	0.44
1:B:214:THR:HG23	1:B:247:MET:HG2	1.99	0.44
1:C:153:LYS:O	3:C:404:HOH:O	2.21	0.44
1:A:166:LEU:C	1:A:166:LEU:HD23	2.37	0.44
1:D:261:ILE:CD1	1:D:263:ILE:HD11	2.48	0.44
1:B:139:LEU:HD23	1:B:140:VAL:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:LYS:HE3	3:D:304:HOH:O	2.14	0.43
1:C:26:PHE:HB2	3:C:403:HOH:O	2.16	0.43
1:C:152:ILE:HD11	1:C:185:ASP:HB3	1.99	0.43
1:D:55:LYS:HE2	3:D:304:HOH:O	2.16	0.43
1:A:33:ILE:HG23	1:A:53:PHE:CE1	2.54	0.43
1:A:50:GLN:HE22	1:A:62:MET:HE2	1.84	0.43
1:A:134:GLU:O	1:A:134:GLU:HG3	2.18	0.43
1:B:114:LYS:N	3:B:401:HOH:O	2.45	0.43
1:B:153:LYS:N	1:B:153:LYS:HD2	2.33	0.43
1:D:261:ILE:HD13	1:D:263:ILE:HD11	2.01	0.43
1:A:22:LEU:HD13	1:A:54:ILE:HD11	2.00	0.43
1:A:227:ASP:N	1:A:227:ASP:OD1	2.52	0.43
1:D:220:LEU:O	1:D:224:LYS:N	2.43	0.42
1:A:242:ILE:HG12	1:A:247:MET:CE	2.49	0.42
1:B:12:LYS:HA	1:B:21:ILE:HD13	2.01	0.42
1:C:4:LYS:N	1:C:4:LYS:HD2	2.34	0.42
1:C:22:LEU:HD13	1:C:54:ILE:HD11	2.00	0.42
1:C:40:ILE:CD1	1:C:261:ILE:HD13	2.49	0.42
1:C:196:TYR:HD1	1:C:197:VAL:N	2.17	0.42
1:D:109:ASP:HB3	1:D:114:LYS:HB3	2.02	0.42
1:B:228:ARG:HH21	1:B:241:ILE:HD13	1.83	0.42
1:D:226:LEU:HD21	1:D:228:ARG:O	2.20	0.42
1:D:263:ILE:HD13	1:D:263:ILE:N	2.34	0.42
1:B:111:ALA:HB1	3:B:401:HOH:O	2.04	0.42
1:C:233:GLN:HB3	1:C:234:PRO:HD2	2.01	0.42
1:A:46:LEU:O	1:A:47:TYR:CB	2.68	0.42
1:C:5:VAL:HG11	1:C:262:TYR:HB3	2.01	0.42
1:D:104:VAL:HG22	1:D:119:ILE:HD12	2.01	0.42
1:C:170:TYR:HD1	1:C:171:LEU:CD1	2.33	0.42
1:A:50:GLN:NE2	1:A:62:MET:CE	2.83	0.42
1:C:263:ILE:HD12	1:C:263:ILE:N	2.35	0.42
1:D:56:ASP:CG	3:D:304:HOH:O	2.52	0.42
1:A:30:ASP:HB3	1:A:33:ILE:HG13	2.02	0.42
1:A:116:LEU:HD23	1:A:252:PRO:HA	2.01	0.41
1:B:157:GLU:N	1:B:157:GLU:OE1	2.53	0.41
1:B:35:LYS:HD2	1:B:36:LEU:N	2.35	0.41
1:A:13:ILE:HG22	1:A:14:ASN:N	2.34	0.41
1:C:130:ILE:HD13	1:C:132:VAL:HG23	1.99	0.41
1:C:213:THR:HG22	1:C:240:TYR:HB3	2.03	0.41
1:A:141:ARG:NH2	1:A:174:GLU:OE2	2.54	0.41
1:C:165:ASP:HA	1:C:168:LYS:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ASN:OD1	1:D:224:LYS:HD2	2.21	0.41
1:D:36:LEU:O	1:D:40:ILE:HG12	2.21	0.41
1:A:35:LYS:HG3	1:A:36:LEU:N	2.35	0.41
1:A:152:ILE:HD11	1:A:183:PHE:HB3	2.02	0.40
1:B:8:LEU:HD11	1:B:36:LEU:HD21	2.03	0.40
1:B:111:ALA:C	3:B:401:HOH:O	2.59	0.40
1:C:182:MET:HB3	1:C:191:MET:HE3	2.04	0.40
1:A:46:LEU:O	1:A:47:TYR:HB3	2.22	0.40
1:B:196:TYR:CD1	1:B:197:VAL:N	2.89	0.40
1:B:130:ILE:HG13	1:B:132:VAL:HG23	2.04	0.40

All (1) 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)
1:B:47:TYR:OH	1:C:43:GLU:OE2[1_455]	1.81	0.39

## 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	256/271 (94%)	245 (96%)	10 (4%)	1 (0%)	30	49
1	B	260/271 (96%)	244 (94%)	16 (6%)	0	100	100
1	C	260/271 (96%)	246 (95%)	14 (5%)	0	100	100
1	D	226/271 (83%)	216 (96%)	9 (4%)	1 (0%)	30	49
All	All	1002/1084 (92%)	951 (95%)	49 (5%)	2 (0%)	44	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	TYR
1	D	110	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	230/240 (96%)	216 (94%)	14 (6%)	15	32
1	B	231/240 (96%)	219 (95%)	12 (5%)	19	39
1	C	231/240 (96%)	212 (92%)	19 (8%)	9	19
1	D	212/240 (88%)	205 (97%)	7 (3%)	33	59
All	All	904/960 (94%)	852 (94%)	52 (6%)	17	34

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	TYR
1	A	55	LYS
1	A	57	SER
1	A	94	THR
1	A	96	SER
1	A	98	GLU
1	A	107	ARG
1	A	112	LYS
1	A	123	LYS
1	A	159	SER
1	A	173	ASN
1	A	188	ASN
1	A	227	ASP
1	A	233	GLN
1	B	4	LYS
1	B	35	LYS
1	B	67	CYS
1	B	99	SER
1	B	123	LYS
1	B	124	PHE

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Mol	Chain	Res	Type
1	B	169	LYS
1	B	208	SER
1	B	220	LEU
1	B	222	LYS
1	B	230	LYS
1	B	246	GLU
1	C	3	ARG
1	C	4	LYS
1	C	31	LYS
1	C	57	SER
1	C	86	SER
1	C	98	GLU
1	C	108	ASN
1	C	114	LYS
1	C	136	LYS
1	C	146	ASN
1	C	179	PHE
1	C	182	MET
1	C	187	ASP
1	C	196	TYR
1	C	202	SER
1	C	222	LYS
1	C	224	LYS
1	C	227	ASP
1	C	260	LYS
1	D	87	LYS
1	D	146	ASN
1	D	154	GLU
1	D	165	ASP
1	D	191	MET
1	D	223	CYS
1	D	265	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	B	58	HIS
1	D	58	HIS
1	D	60	GLN



### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 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	$\# Z  > 2$
2	PO4	C	301	-	4,4,4	0.95	0	6,6,6	0.45	0
2	PO4	B	301	-	4,4,4	0.93	0	6,6,6	0.48	0
2	PO4	A	301	-	4,4,4	0.94	0	6,6,6	0.42	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

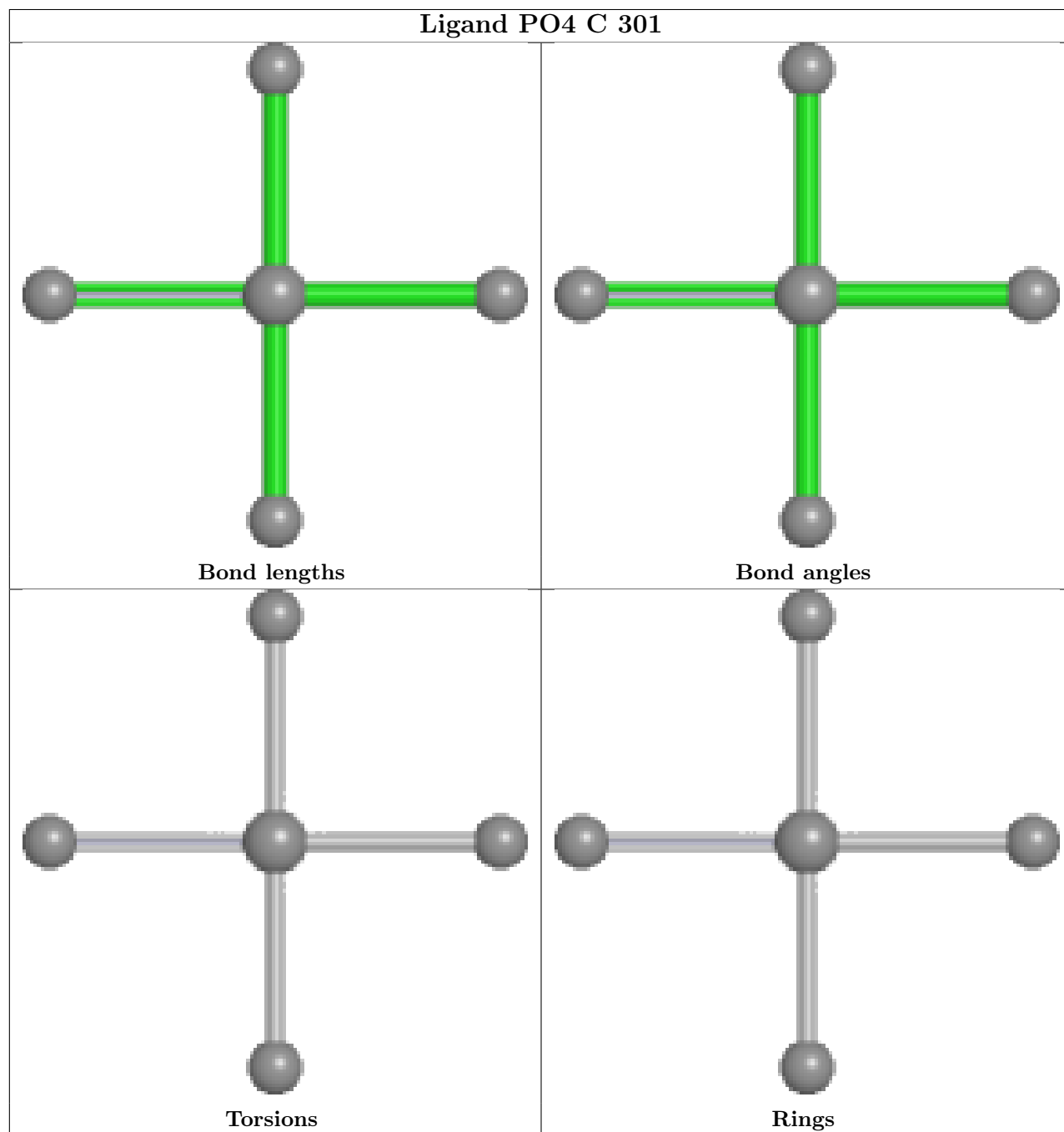
There are no torsion outliers.

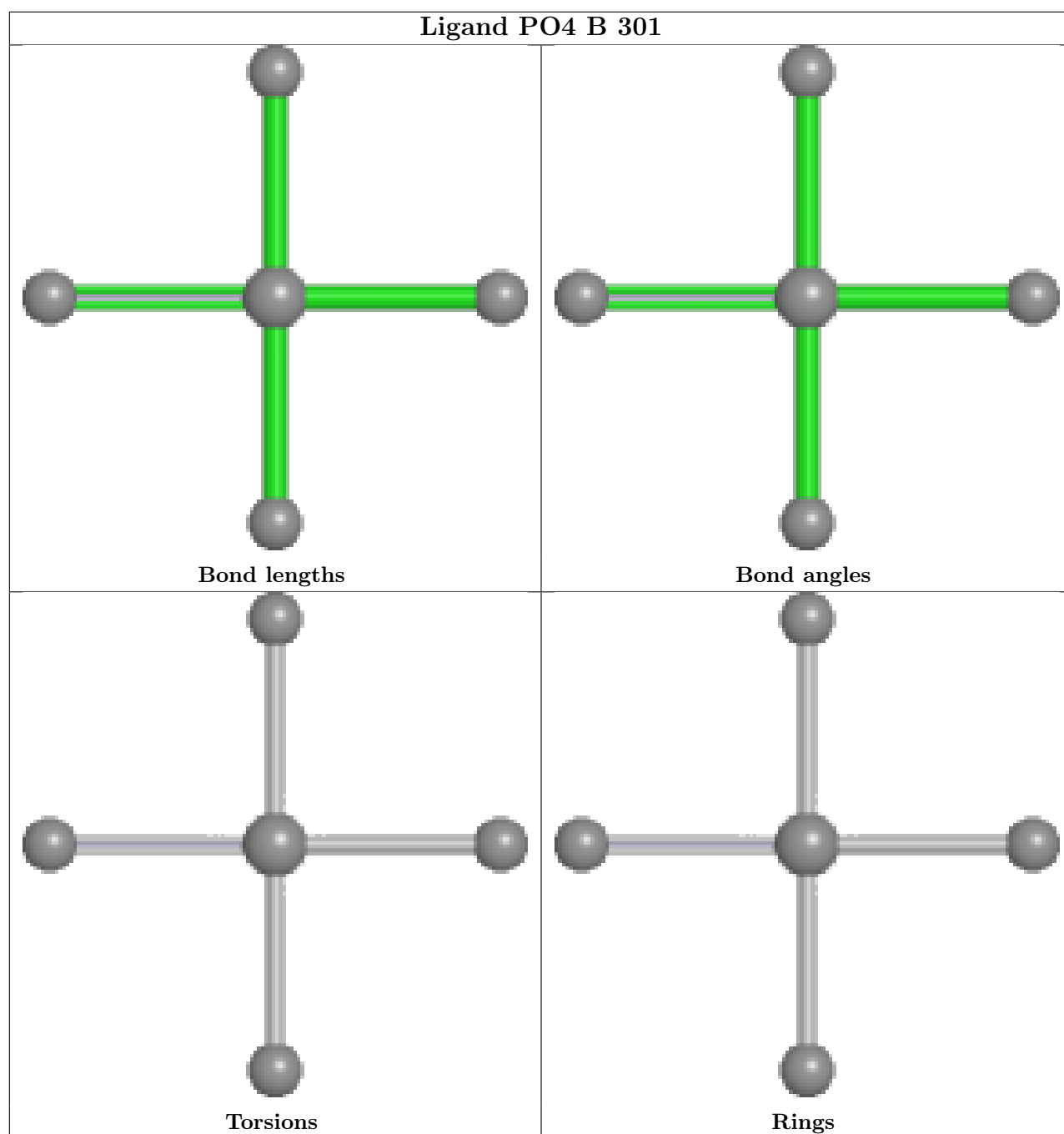
There are no ring outliers.

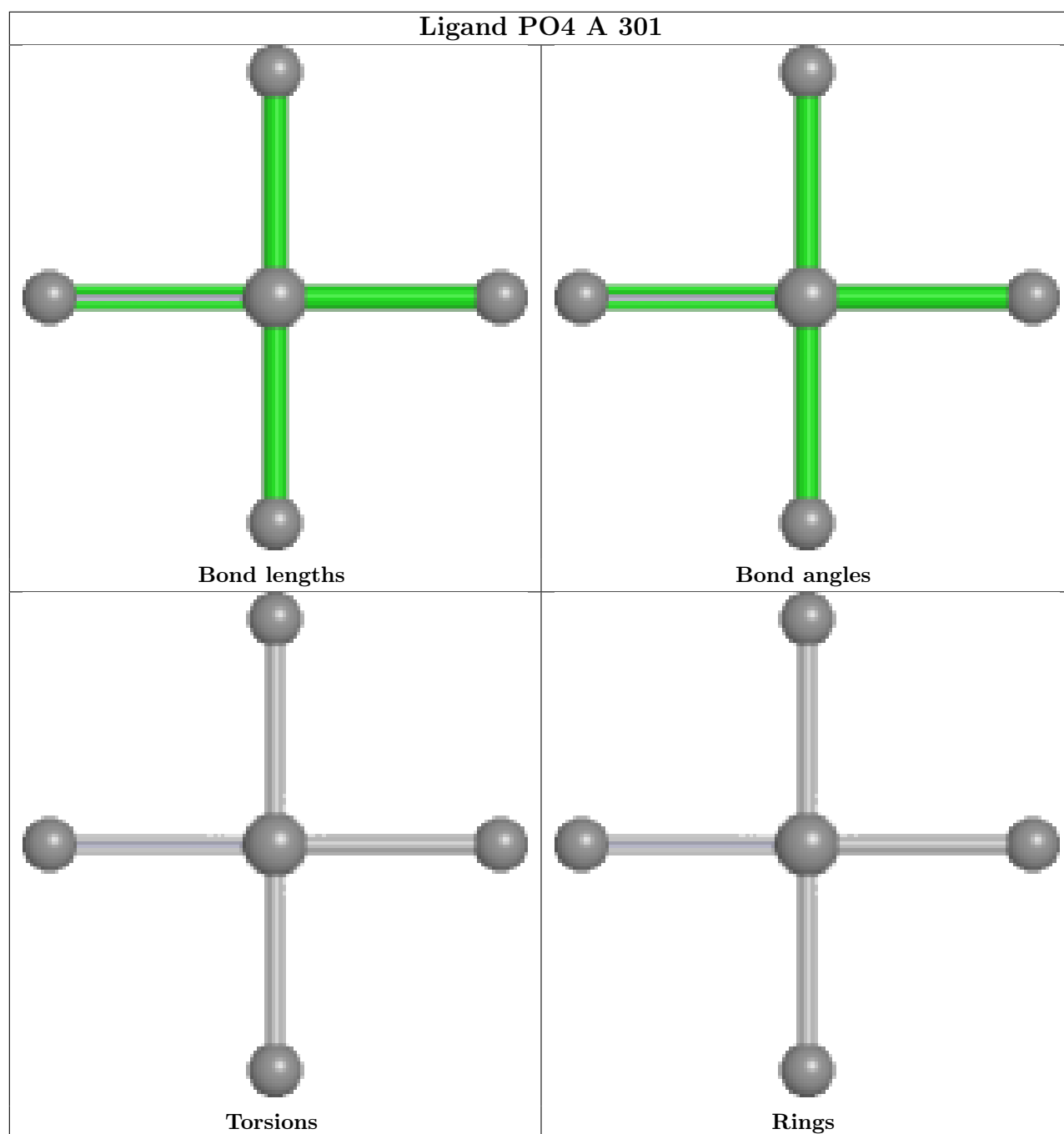
No monomer is involved in short contacts.

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.







## 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	260/271 (95%)	0.88	27 (10%) 13 12	51, 75, 117, 147	0
1	B	262/271 (96%)	0.80	26 (9%) 14 13	50, 72, 105, 148	0
1	C	262/271 (96%)	0.74	22 (8%) 18 17	49, 72, 118, 154	0
1	D	242/271 (89%)	0.99	42 (17%) 5 5	44, 79, 134, 153	0
All	All	1026/1084 (94%)	0.85	117 (11%) 11 10	44, 74, 124, 154	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	189	LEU	7.7
1	A	226	LEU	7.5
1	C	5	VAL	6.5
1	D	150	PHE	6.3
1	D	167	VAL	5.1
1	C	4	LYS	5.0
1	B	261	ILE	4.1
1	A	80	PHE	4.0
1	B	179	PHE	4.0
1	A	36	LEU	3.9
1	D	163	ILE	3.9
1	D	71	SER	3.9
1	A	147	HIS	3.8
1	B	263	ILE	3.8
1	C	144	GLY	3.7
1	C	33	ILE	3.7
1	D	184	PHE	3.7
1	D	203	GLY	3.6
1	D	231	ILE	3.5
1	C	256	ILE	3.5
1	D	216	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	47	TYR	3.3
1	D	93	ILE	3.3
1	C	137	LEU	3.3
1	B	245	ASP	3.3
1	B	186	SER	3.3
1	A	179	PHE	3.3
1	C	177	SER	3.2
1	B	242	ILE	3.2
1	C	130	ILE	3.2
1	D	193	PRO	3.1
1	C	80	PHE	3.1
1	D	217	GLY	3.1
1	A	86	SER	3.1
1	D	181	ILE	3.0
1	A	140	VAL	3.0
1	D	183	PHE	2.9
1	D	6	GLN	2.9
1	B	214	THR	2.9
1	D	205	TYR	2.9
1	D	11	ILE	2.9
1	D	261	ILE	2.9
1	D	125	LEU	2.9
1	B	111	ALA	2.9
1	A	164	ILE	2.9
1	B	189	LEU	2.8
1	A	199	GLU	2.8
1	B	6	GLN	2.8
1	D	201	GLY	2.7
1	B	5	VAL	2.7
1	D	130	ILE	2.7
1	A	109	ASP	2.7
1	D	148	PHE	2.7
1	A	163	ILE	2.6
1	A	130	ILE	2.6
1	C	132	VAL	2.6
1	B	29	TYR	2.6
1	D	191	MET	2.6
1	A	85	PHE	2.5
1	A	237	TRP	2.5
1	D	149	ILE	2.5
1	C	109	ASP	2.5
1	B	8	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	28	ILE	2.5
1	B	231	ILE	2.5
1	D	164	ILE	2.5
1	D	138	GLY	2.5
1	B	112	LYS	2.5
1	A	204	VAL	2.5
1	D	209	SER	2.5
1	A	256	ILE	2.5
1	D	115	PHE	2.5
1	D	160	PHE	2.5
1	A	115	PHE	2.4
1	D	179	PHE	2.4
1	B	253	VAL	2.4
1	B	23	ILE	2.4
1	A	217	GLY	2.4
1	A	53	PHE	2.3
1	C	179	PHE	2.3
1	A	262	TYR	2.3
1	D	220	LEU	2.3
1	C	263	ILE	2.3
1	D	207	ASN	2.3
1	B	193	PRO	2.3
1	C	7	VAL	2.3
1	A	144	GLY	2.3
1	B	265	LYS	2.3
1	B	127	LEU	2.2
1	A	205	TYR	2.2
1	C	178	ALA	2.2
1	D	200	VAL	2.2
1	A	137	LEU	2.2
1	C	114	LYS	2.2
1	D	99	SER	2.2
1	C	255	ILE	2.2
1	C	149	ILE	2.2
1	B	184	PHE	2.1
1	A	145	ILE	2.1
1	B	75	ALA	2.1
1	D	75	ALA	2.1
1	B	247	MET	2.1
1	B	117	ALA	2.1
1	A	26	PHE	2.1
1	D	159	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	181	ILE	2.1
1	C	264	GLY	2.1
1	D	66	PHE	2.1
1	D	84	ASP	2.1
1	D	155	ASN	2.1
1	C	36	LEU	2.0
1	C	54	ILE	2.0
1	D	5	VAL	2.0
1	D	197	VAL	2.0
1	A	257	ALA	2.0
1	D	158	THR	2.0
1	C	146	ASN	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 monosaccharides 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, 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.

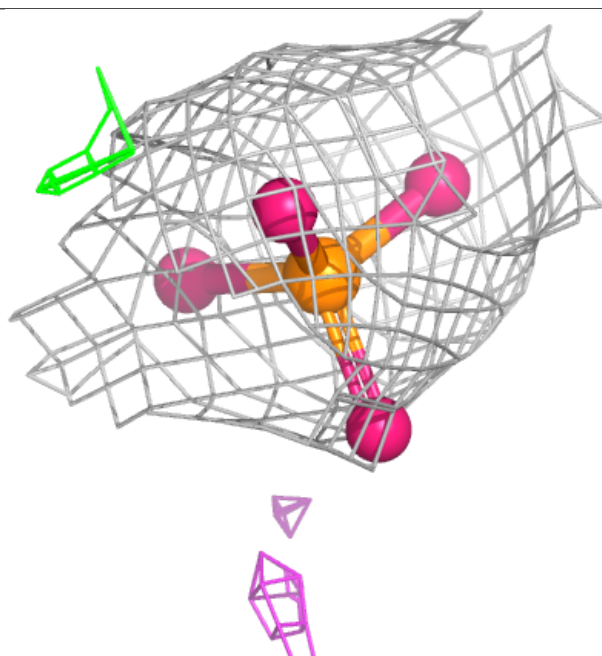
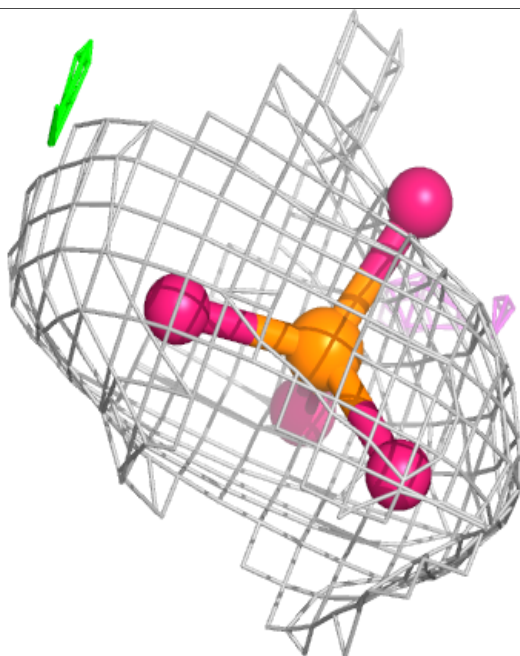
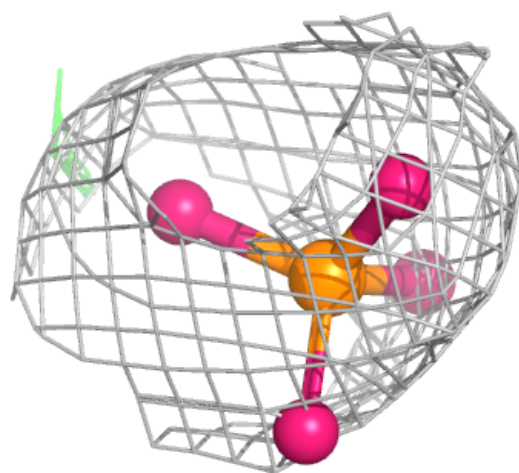
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	B	301	5/5	0.64	0.13	67,70,123,129	0
2	PO4	A	301	5/5	0.74	0.12	78,87,169,178	0
2	PO4	C	301	5/5	0.75	0.14	66,67,99,134	0

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.



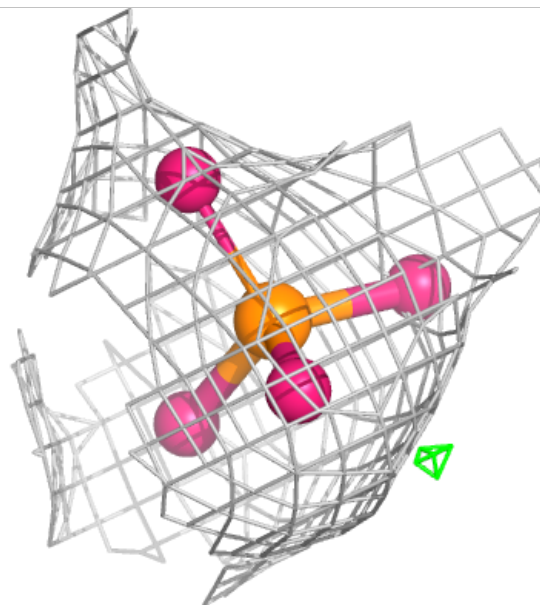
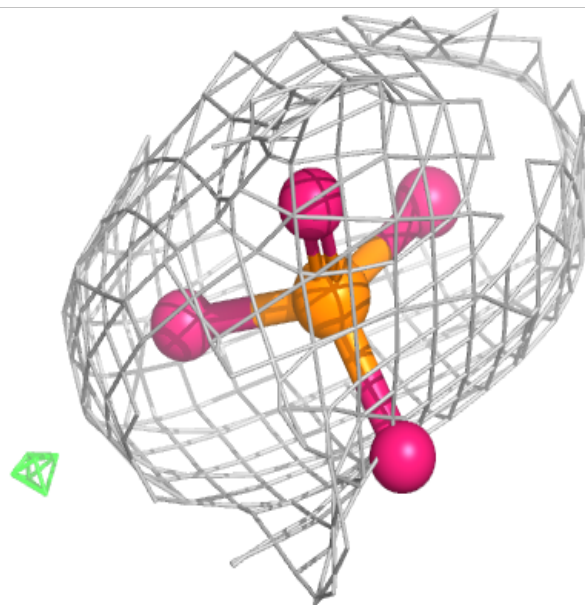
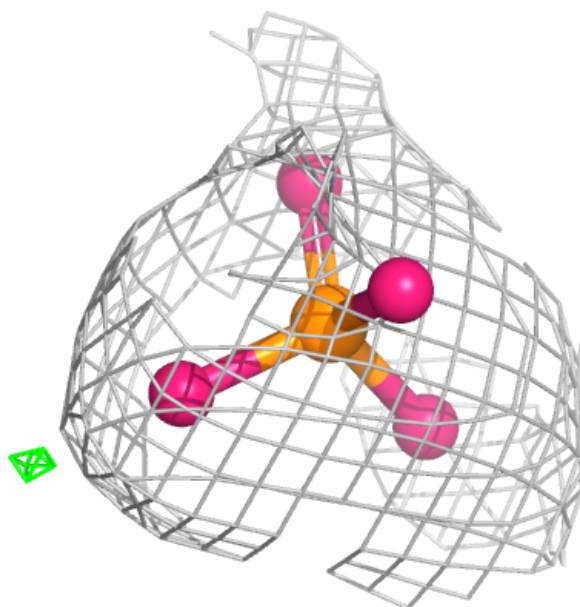
**Electron density around PO4 B 301:**

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



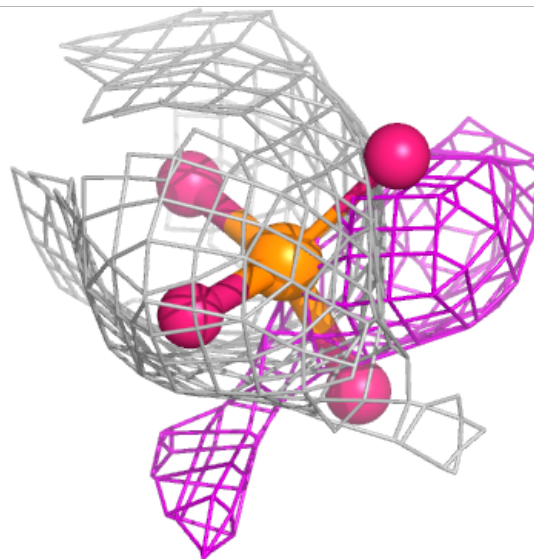
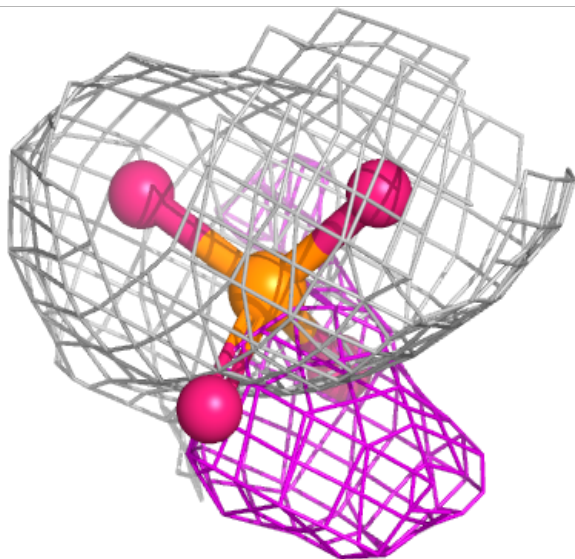
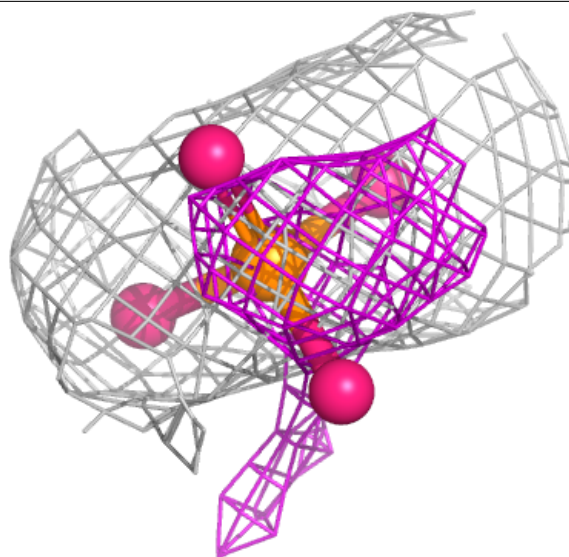
**Electron density around PO4 A 301:**

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



**Electron density around PO4 C 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.