



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:26 PM UTC

PDB ID : 8Q3J / pdb_00008q3j
Title : Crystal structure of mIL-38 in complex with a neutralizing Fab e04 fragment
Authors : Garcia-Pardo, J.; Da Silva, P.; Mora, J.; Wiechmann, S.; Putyrski, M.; You, X.; Kannt, A.; Ernst, A.; Brune, B.; Weigert, A.
Deposited on : 2023-08-04
Resolution : 2.50 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

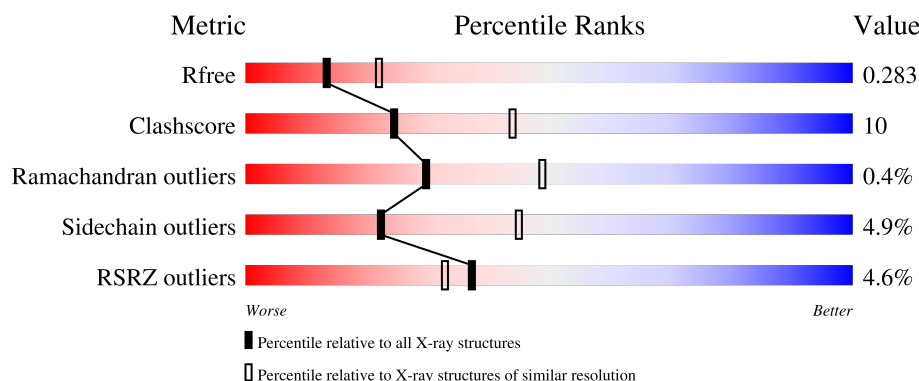
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 ≥ 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	152	7% 65% 28% • 5%
1	D	152	9% 63% 31% • •
2	B	223	0% 79% 14% • 6%
2	E	223	4% 69% 23% • 6%
3	C	241	3% 68% 21% • 9%

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Mol	Chain	Length	Quality of chain
3	F	241	4% 75% 15% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8922 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 Interleukin-1 family member 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	0	0	0
			1131	719	192	211	9			
1	D	148	Total	C	N	O	S	0	0	0
			1161	736	197	218	10			

- Molecule 2 is a protein called Fab e04 Light Chain (e04 LC).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1619	1020	270	324	5			
2	E	209	Total	C	N	O	S	0	0	0
			1609	1012	269	323	5			

- Molecule 3 is a protein called Fab e04 Heavy Chain (e04 HC).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	219	Total	C	N	O	S	0	0	0
			1647	1045	277	319	6			
3	F	216	Total	C	N	O	S	0	0	0
			1626	1034	273	313	6			

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		

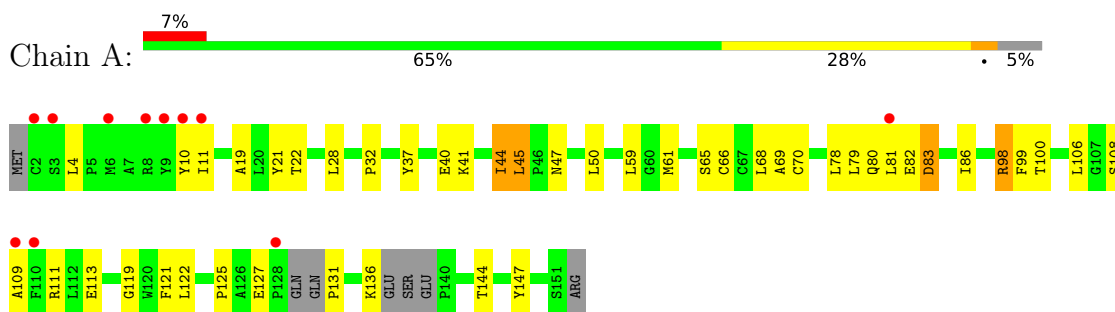
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	21	Total	O	0	0
			21	21		
5	B	19	Total	O	0	0
			19	19		
5	C	21	Total	O	0	0
			21	21		
5	D	16	Total	O	0	0
			16	16		
5	E	18	Total	O	0	0
			18	18		
5	F	14	Total	O	0	0
			14	14		

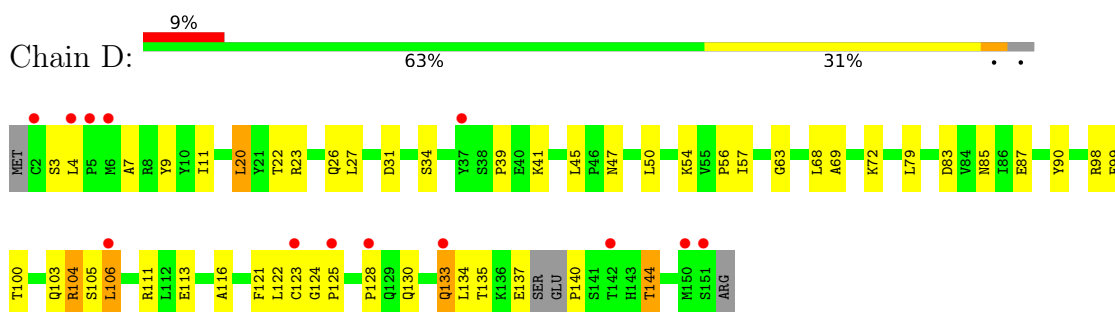
3 Residue-property plots [i](#)

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.

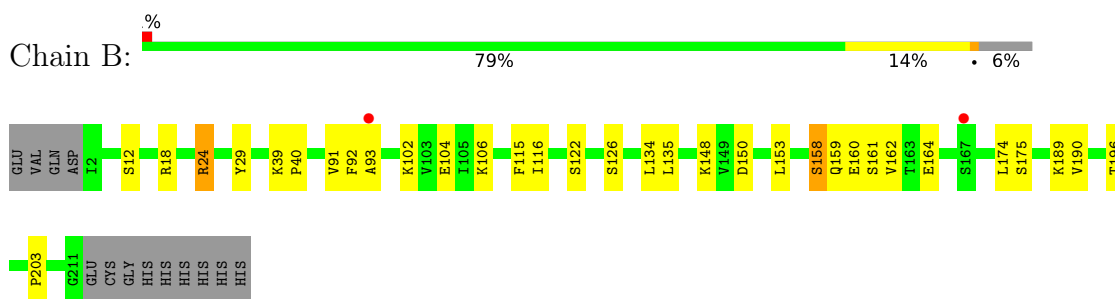
- Molecule 1: Interleukin-1 family member 10



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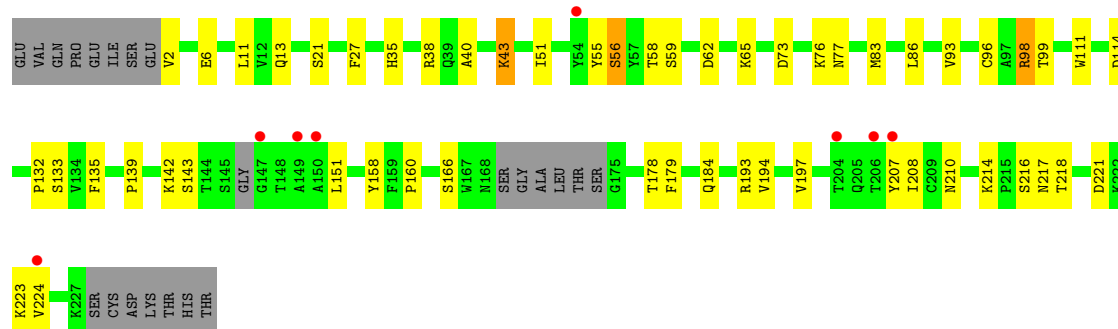
- Molecule 2: Fab e04 Light Chain (e04 LC)



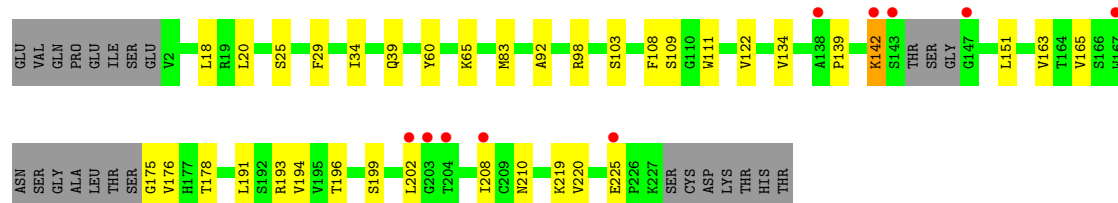
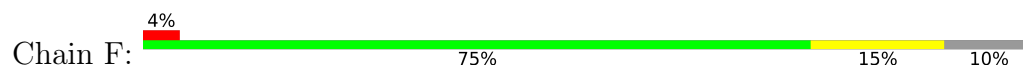
- Molecule 2: Fab e04 Light Chain (e04 LC)



- Molecule 3: Fab e04 Heavy Chain (e04 HC)



- Molecule 3: Fab e04 Heavy Chain (e04 HC)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.80Å 66.94Å 129.05Å 90.00° 104.73° 90.00°	Depositor
Resolution (Å)	70.11 – 2.50 70.11 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (70.11-2.50) 99.3 (70.11-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.227 , 0.283 0.227 , 0.283	Depositor DCC
R_{free} test set	5068 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	54.1	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8922	wwPDB-VP
Average B, all atoms (Å ²)	62.0	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 41.28 % 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 2.4178e-04. 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 [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	0.40	0/1157	0.65	0/1562
1	D	0.45	0/1188	0.68	0/1605
2	B	0.37	0/1656	0.61	0/2249
2	E	0.35	0/1645	0.63	0/2235
3	C	0.40	0/1689	0.58	0/2298
3	F	0.41	0/1668	0.59	0/2269
All	All	0.40	0/9003	0.62	0/12218

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	104	ARG	Sidechain

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	1131	0	1103	37	0
1	D	1161	0	1132	40	0
2	B	1619	0	1580	21	0
2	E	1609	0	1570	34	0
3	C	1647	0	1613	36	0
3	F	1626	0	1595	21	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
5	A	21	0	0	2	0
5	B	19	0	0	1	0
5	C	21	0	0	1	0
5	D	16	0	0	1	0
5	E	18	0	0	1	0
5	F	14	0	0	1	0
All	All	8922	0	8593	172	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 10.

All (172) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:175:GLY:N	3:F:196:THR:HG1	1.59	1.00
3:C:139:PRO:HG3	3:C:151:LEU:HB3	1.59	0.85
3:C:98:ARG:NH2	3:C:114:ASP:OD2	2.16	0.79
2:E:2:ILE:HD12	2:E:27:GLN:HG2	1.65	0.78
3:C:208:ILE:HG22	3:C:223:LYS:HG2	1.68	0.76
1:A:111:ARG:NH1	1:A:144:THR:OG1	2.19	0.76
2:B:40:PRO:HB3	2:B:164:GLU:HG3	1.69	0.75
2:E:149:VAL:H	2:E:154:GLN:HE22	1.33	0.74
3:F:175:GLY:N	3:F:196:THR:OG1	2.21	0.73
2:B:162:VAL:HG22	2:B:174:LEU:HD23	1.70	0.73
2:E:132:VAL:HG22	2:E:177:THR:HG22	1.70	0.72
1:D:125:PRO:HB2	1:D:130:GLN:HB3	1.71	0.72
1:A:41:LYS:HE2	2:B:29:TYR:HA	1.73	0.71
1:D:105:SER:O	5:D:201:HOH:O	2.09	0.70
2:E:191:TYR:HE2	2:E:210:ARG:HB2	1.57	0.70
1:D:123:CYS:HB3	1:D:133:GLN:HG2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:THR:HG22	2:B:203:PRO:HB3	1.73	0.69
2:B:135:LEU:HD13	2:B:174:LEU:HD12	1.76	0.66
2:E:196:THR:HG22	2:E:203:PRO:HB3	1.77	0.65
2:B:159:GLN:HE22	3:C:184:GLN:HA	1.61	0.65
2:E:80:PRO:HA	2:E:105:ILE:HG13	1.79	0.65
1:D:9:TYR:HE1	1:D:63:GLY:HA2	1.62	0.64
2:E:20:THR:HG22	2:E:74:THR:OG1	1.98	0.64
1:D:144:THR:O	1:D:144:THR:OG1	2.14	0.64
3:F:60:TYR:O	3:F:65:LYS:NZ	2.32	0.63
3:C:151:LEU:HD13	3:C:224:VAL:HG21	1.80	0.63
1:D:83:ASP:HB3	3:F:111:TRP:CD1	2.34	0.63
2:E:141:ARG:HB2	2:E:172:TYR:CE2	2.35	0.62
1:D:20:LEU:HD21	1:D:27:LEU:HG	1.80	0.62
2:E:134:LEU:HD11	3:F:194:VAL:HG11	1.81	0.62
3:C:40:ALA:HB3	3:C:43:LYS:HD3	1.82	0.61
3:F:134:VAL:HG21	3:F:220:VAL:HG21	1.82	0.61
1:A:98:ARG:NH1	3:C:55:TYR:OH	2.24	0.60
1:D:85:ASN:ND2	1:D:87:GLU:HB2	2.16	0.60
1:D:41:LYS:HD3	2:E:29:TYR:HB3	1.84	0.59
2:E:185:TYR:O	2:E:191:TYR:OH	2.21	0.58
1:A:70:CYS:O	1:A:98:ARG:HD3	2.04	0.58
1:A:98:ARG:HH12	3:C:55:TYR:HH	1.50	0.57
2:E:37:GLN:HB2	2:E:47:LEU:HD11	1.86	0.57
2:E:119:PRO:HD3	2:E:131:VAL:HG22	1.87	0.57
3:C:210:ASN:ND2	3:C:221:ASP:OD1	2.37	0.57
3:F:208:ILE:HD12	3:F:210:ASN:HD21	1.69	0.57
2:E:197:HIS:HB3	2:E:200:LEU:HD13	1.86	0.57
1:D:125:PRO:CB	1:D:130:GLN:HB3	2.35	0.56
1:A:11:ILE:HG22	5:A:306:HOH:O	2.05	0.55
1:A:41:LYS:CE	2:B:29:TYR:HA	2.37	0.55
2:E:112:PRO:HD2	2:E:200:LEU:HD11	1.89	0.55
1:D:54:LYS:HG2	1:D:104:ARG:HH21	1.72	0.55
1:A:136:LYS:NZ	5:A:305:HOH:O	2.39	0.55
2:E:93:ALA:HB3	2:E:94:PRO:HD3	1.88	0.55
2:E:38:GLN:OE1	5:E:401:HOH:O	2.18	0.54
1:D:68:LEU:HD11	1:D:79:LEU:HD22	1.90	0.54
1:A:109:ALA:HB2	1:A:147:TYR:CZ	2.43	0.54
3:C:73:ASP:OD2	3:C:76:LYS:HB2	2.09	0.53
1:A:28:LEU:HD23	1:A:131:PRO:HA	1.90	0.53
2:E:115:PHE:HE2	2:E:136:ASN:HD22	1.53	0.53
3:F:199:SER:O	3:F:202:LEU:HD12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLU:HB2	1:A:121:PHE:CE2	2.44	0.53
1:D:45:LEU:HG	1:D:90:TYR:CD1	2.44	0.52
1:A:83:ASP:HB2	3:C:111:TRP:CD1	2.44	0.52
1:A:106:LEU:HD22	1:A:111:ARG:HH21	1.74	0.52
3:C:51:ILE:HG13	3:C:58:THR:HG22	1.91	0.52
2:E:141:ARG:HB2	2:E:172:TYR:CD2	2.44	0.52
3:C:132:PRO:HB3	3:C:158:TYR:HB3	1.92	0.52
1:A:80:GLN:HG2	1:A:82:GLU:HG3	1.91	0.51
1:D:85:ASN:HD21	1:D:87:GLU:HB2	1.74	0.51
3:C:216:SER:HG	3:C:218:THR:HG1	1.57	0.51
1:A:19:ALA:HB2	1:A:32:PRO:HG3	1.91	0.51
1:A:125:PRO:HB2	1:A:127:GLU:O	2.11	0.51
3:C:83:MET:HB3	3:C:86:LEU:HD21	1.93	0.51
1:D:4:LEU:H	1:D:7:ALA:HB3	1.75	0.50
3:F:165:VAL:HB	3:F:193:ARG:HD2	1.93	0.50
2:B:115:PHE:HB3	3:C:143:SER:HA	1.94	0.50
2:B:158:SER:OG	5:B:301:HOH:O	2.20	0.50
1:D:128:PRO:C	1:D:130:GLN:H	2.19	0.50
1:D:4:LEU:HD21	1:D:87:GLU:CG	2.42	0.50
1:D:4:LEU:HD21	1:D:87:GLU:OE2	2.11	0.50
2:E:139:TYR:CD1	2:E:140:PRO:HA	2.47	0.50
3:C:98:ARG:HG2	3:C:99:THR:N	2.27	0.49
3:F:103:SER:HA	3:F:108:PHE:CD1	2.46	0.49
1:A:106:LEU:HD22	1:A:111:ARG:NH2	2.28	0.49
3:F:20:LEU:HG	3:F:83:MET:HE2	1.95	0.48
1:D:98:ARG:HA	1:D:116:ALA:HB2	1.95	0.48
3:C:178:THR:HG23	3:C:193:ARG:CZ	2.43	0.48
3:F:139:PRO:HD3	3:F:151:LEU:HB2	1.96	0.48
1:D:20:LEU:HD21	1:D:27:LEU:CG	2.42	0.48
2:E:39:LYS:O	2:E:42:LYS:HB2	2.14	0.48
1:A:50:LEU:HD12	1:A:100:THR:HG21	1.95	0.48
1:A:61:MET:HG3	1:A:81:LEU:HD11	1.96	0.48
1:A:10:TYR:CD2	1:A:44:ILE:HG13	2.49	0.48
2:E:91:VAL:HG11	3:F:111:TRP:HB2	1.95	0.47
1:A:111:ARG:HG2	1:A:121:PHE:CD2	2.50	0.47
1:D:72:LYS:HE2	1:D:116:ALA:O	2.15	0.47
1:D:104:ARG:HD2	1:D:113:GLU:OE1	2.13	0.47
2:B:12:SER:HA	2:B:104:GLU:O	2.13	0.47
1:A:44:ILE:HD13	1:A:59:LEU:HD23	1.96	0.47
3:C:6:GLU:HA	3:C:21:SER:O	2.14	0.47
1:A:45:LEU:HD22	1:A:86:ILE:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:ALA:HB2	1:D:99:PHE:CE1	2.50	0.47
2:E:166:ASP:O	2:E:170:SER:HA	2.15	0.47
3:F:109:SER:OG	5:F:401:HOH:O	2.15	0.47
2:B:160:GLU:HB3	2:B:174:LEU:HD21	1.97	0.46
1:D:50:LEU:HD12	1:D:100:THR:HG21	1.97	0.46
3:F:18:LEU:HB3	3:F:83:MET:HE3	1.97	0.46
1:D:41:LYS:CD	2:E:29:TYR:HB3	2.45	0.46
1:D:54:LYS:HG2	1:D:104:ARG:NH2	2.30	0.46
1:A:69:ALA:HB2	1:A:99:PHE:CE1	2.50	0.46
2:E:5:THR:HA	2:E:99:GLN:HE22	1.79	0.46
2:E:107:ARG:HD2	2:E:170:SER:HB3	1.98	0.46
2:E:106:LYS:HA	2:E:139:TYR:OH	2.16	0.45
1:A:4:LEU:HD12	1:A:45:LEU:HD21	1.97	0.45
1:A:65:SER:HB3	2:B:92:PHE:HB3	1.99	0.45
3:C:62:ASP:O	3:C:65:LYS:HG2	2.16	0.45
2:E:112:PRO:HD2	2:E:200:LEU:CD1	2.46	0.45
3:C:56:SER:O	3:C:56:SER:OG	2.26	0.45
1:D:9:TYR:CG	1:D:41:LYS:HE2	2.51	0.45
2:E:2:ILE:HG13	2:E:3:GLN:N	2.31	0.45
3:C:132:PRO:HD2	3:C:218:THR:HG21	1.99	0.45
1:A:69:ALA:HB2	1:A:99:PHE:CD1	2.51	0.45
1:D:57:ILE:HD13	1:D:103:GLN:HE21	1.81	0.45
1:D:106:LEU:HD21	1:D:140:PRO:HB3	1.98	0.45
3:F:39:GLN:C	3:F:92:ALA:HB1	2.42	0.45
1:D:79:LEU:HG	1:D:134:LEU:HG	1.99	0.45
1:A:41:LYS:N	1:A:41:LYS:HD3	2.32	0.44
1:D:113:GLU:HB2	1:D:121:PHE:CE2	2.52	0.44
2:E:140:PRO:HG3	2:E:198:GLN:NE2	2.31	0.44
2:E:206:LYS:HE3	3:F:142:LYS:NZ	2.31	0.44
3:C:133:SER:HB3	3:C:135:PHE:CZ	2.53	0.44
2:B:102:LYS:HE3	2:B:102:LYS:HB2	1.75	0.44
1:A:66:CYS:SG	1:A:81:LEU:HD12	2.58	0.44
3:C:193:ARG:HA	3:C:193:ARG:HD3	1.67	0.44
2:B:150:ASP:OD1	2:B:189:LYS:HG2	2.17	0.43
3:C:13:GLN:NE2	5:C:404:HOH:O	2.46	0.43
1:D:9:TYR:CE1	1:D:63:GLY:HA2	2.49	0.43
1:D:47:ASN:HB3	1:D:56:PRO:HB2	2.01	0.43
3:F:34:ILE:HD13	3:F:34:ILE:HA	1.85	0.43
3:C:11:LEU:HB2	3:C:160:PRO:HG3	2.00	0.43
2:E:104:GLU:OE2	2:E:165:GLN:NE2	2.52	0.43
3:C:35:HIS:O	3:C:96:CYS:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:GLY:O	1:D:133:GLN:NE2	2.52	0.43
3:C:2:VAL:HG13	3:C:27:PHE:HD1	1.83	0.42
2:B:148:LYS:HG3	2:B:153:LEU:HA	2.01	0.42
1:A:79:LEU:HA	1:A:79:LEU:HD23	1.74	0.42
2:B:116:ILE:HG22	3:C:142:LYS:HB3	2.02	0.42
3:C:73:ASP:OD2	3:C:76:LYS:HE3	2.19	0.42
1:D:11:ILE:HD13	1:D:39:PRO:HB2	2.02	0.42
2:B:24:ARG:HH11	2:B:24:ARG:HD2	1.74	0.42
1:D:135:THR:HG22	1:D:137:GLU:H	1.84	0.42
3:F:83:MET:HE1	3:F:122:VAL:HG21	2.02	0.42
1:D:123:CYS:N	1:D:133:GLN:O	2.52	0.41
2:E:104:GLU:HG3	2:E:165:GLN:HE22	1.85	0.41
1:A:45:LEU:HD12	1:A:45:LEU:HA	1.92	0.41
1:A:22:THR:OG1	1:A:40:GLU:OE2	2.22	0.41
1:A:47:ASN:C	1:A:47:ASN:HD22	2.27	0.41
2:B:91:VAL:HG13	3:C:111:TRP:O	2.21	0.41
3:C:224:VAL:O	3:C:224:VAL:HG23	2.19	0.41
1:A:111:ARG:NH1	1:A:144:THR:HG1	2.15	0.41
2:B:12:SER:OG	2:B:106:LYS:HE2	2.20	0.41
3:F:139:PRO:HD3	3:F:151:LEU:CB	2.50	0.41
2:B:40:PRO:CB	2:B:164:GLU:HG3	2.45	0.41
2:B:161:SER:OG	3:C:179:PHE:HB3	2.20	0.41
1:A:68:LEU:HD11	1:A:79:LEU:HD22	2.01	0.41
1:A:119:GLY:O	1:A:136:LYS:HG2	2.20	0.41
3:C:179:PHE:HE2	3:C:194:VAL:HG23	1.85	0.41
1:D:106:LEU:HD13	1:D:111:ARG:HD2	2.03	0.41
2:E:109:VAL:HG22	2:E:140:PRO:HD3	2.02	0.41
1:A:21:TYR:CZ	1:A:37:TYR:CD1	3.09	0.40
3:F:178:THR:HG23	3:F:193:ARG:NH2	2.36	0.40
3:C:38:ARG:HA	3:C:93:VAL:O	2.21	0.40
3:C:197:VAL:HG11	3:C:207:TYR:CZ	2.56	0.40
1:D:22:THR:HA	1:D:26:GLN:O	2.21	0.40
1:D:31:ASP:HB3	1:D:34:SER:H	1.85	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	139/152 (91%)	132 (95%)	6 (4%)	1 (1%)	18	34
1	D	144/152 (95%)	133 (92%)	10 (7%)	1 (1%)	18	34
2	B	208/223 (93%)	201 (97%)	6 (3%)	1 (0%)	24	43
2	E	207/223 (93%)	192 (93%)	14 (7%)	1 (0%)	24	43
3	C	213/241 (88%)	203 (95%)	10 (5%)	0	100	100
3	F	210/241 (87%)	208 (99%)	2 (1%)	0	100	100
All	All	1121/1232 (91%)	1069 (95%)	48 (4%)	4 (0%)	30	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	ASP
2	B	93	ALA
2	E	93	ALA
1	D	3	SER

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	123/131 (94%)	117 (95%)	6 (5%)	22	45
1	D	127/131 (97%)	121 (95%)	6 (5%)	23	47
2	B	185/197 (94%)	176 (95%)	9 (5%)	22	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	184/197 (93%)	174 (95%)	10 (5%)	20	41
3	C	184/203 (91%)	176 (96%)	8 (4%)	26	51
3	F	181/203 (89%)	172 (95%)	9 (5%)	22	44
All	All	984/1062 (93%)	936 (95%)	48 (5%)	22	45

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ILE
1	A	45	LEU
1	A	78	LEU
1	A	98	ARG
1	A	108	SER
1	A	122	LEU
2	B	18	ARG
2	B	24	ARG
2	B	39	LYS
2	B	122	SER
2	B	126	SER
2	B	134	LEU
2	B	158	SER
2	B	175	SER
2	B	190	VAL
3	C	43	LYS
3	C	56	SER
3	C	59	SER
3	C	77	ASN
3	C	98	ARG
3	C	166	SER
3	C	214	LYS
3	C	217	ASN
1	D	20	LEU
1	D	23	ARG
1	D	106	LEU
1	D	122	LEU
1	D	133	GLN
1	D	144	THR
2	E	2	ILE
2	E	12	SER
2	E	45	LYS
2	E	72	THR

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Mol	Chain	Res	Type
2	E	74	THR
2	E	91	VAL
2	E	108	THR
2	E	184	ASP
2	E	205	THR
2	E	209	ASN
3	F	25	SER
3	F	29	PHE
3	F	98	ARG
3	F	142	LYS
3	F	163	VAL
3	F	176	VAL
3	F	191	LEU
3	F	219	LYS
3	F	225	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	47	ASN
2	B	146	GLN
2	B	159	GLN
3	C	210	ASN
1	D	26	GLN
1	D	85	ASN
1	D	103	GLN
1	D	133	GLN
2	E	79	GLN
2	E	99	GLN
2	E	154	GLN
3	F	13	GLN
3	F	210	ASN

5.3.3 RNA ⓘ

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](#)

4 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	PO4	A	201	-	4,4,4	0.55	0	6,6,6	0.95	0
4	PO4	E	301	-	4,4,4	0.66	0	6,6,6	0.52	0
4	PO4	F	301	-	4,4,4	0.64	0	6,6,6	0.54	0
4	PO4	C	301	-	4,4,4	0.80	0	6,6,6	0.51	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

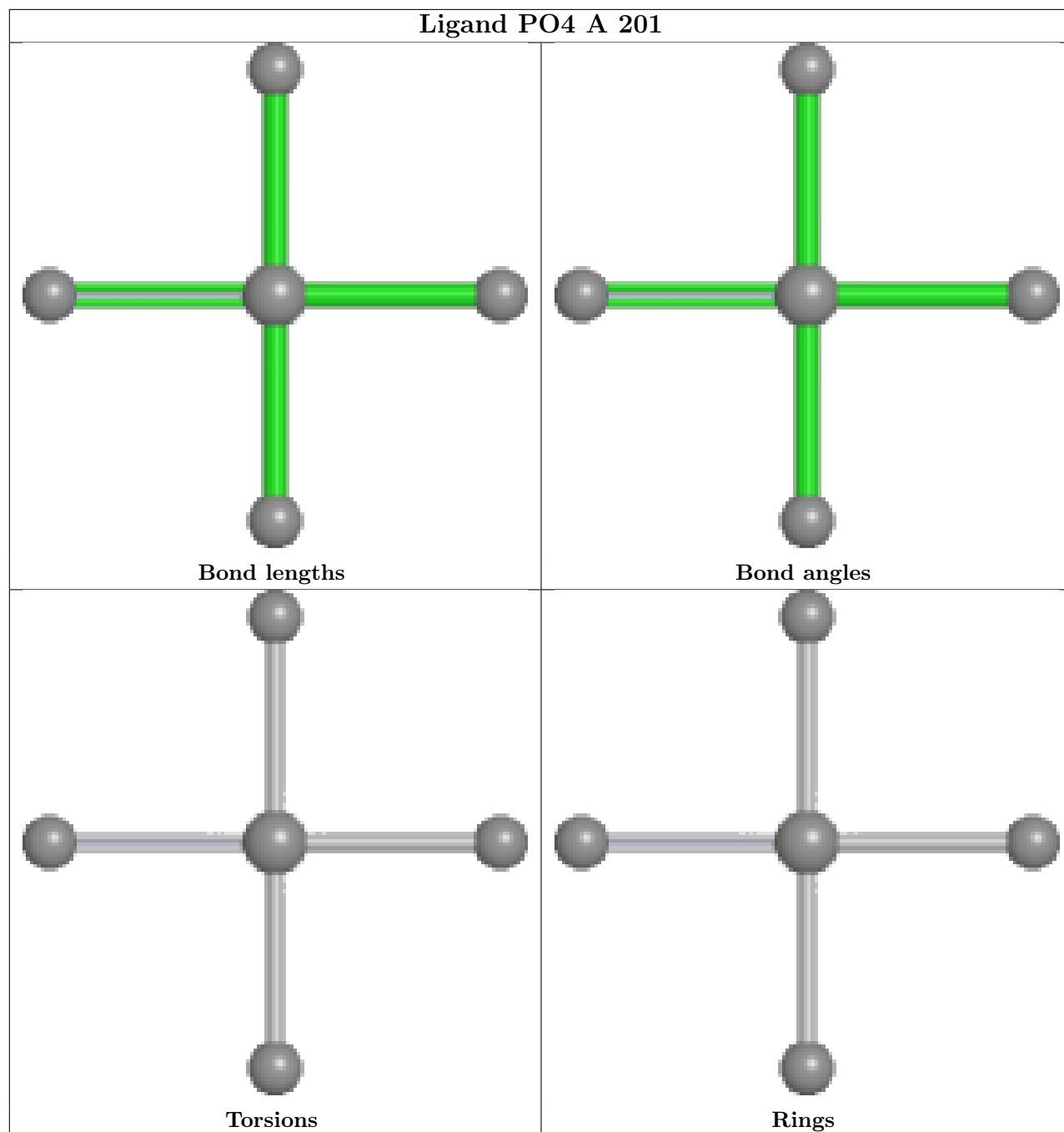
There are no torsion outliers.

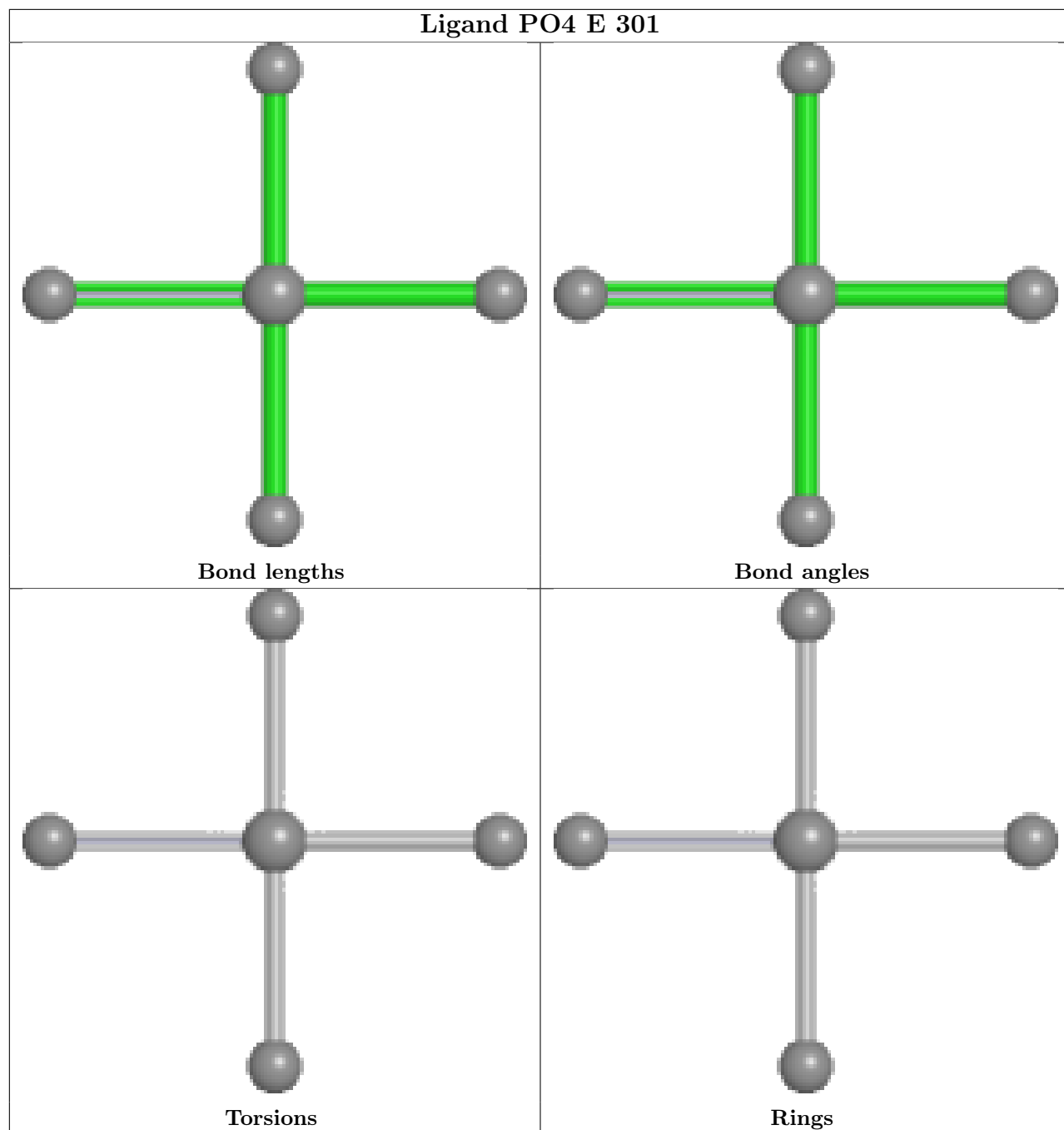
There are no ring outliers.

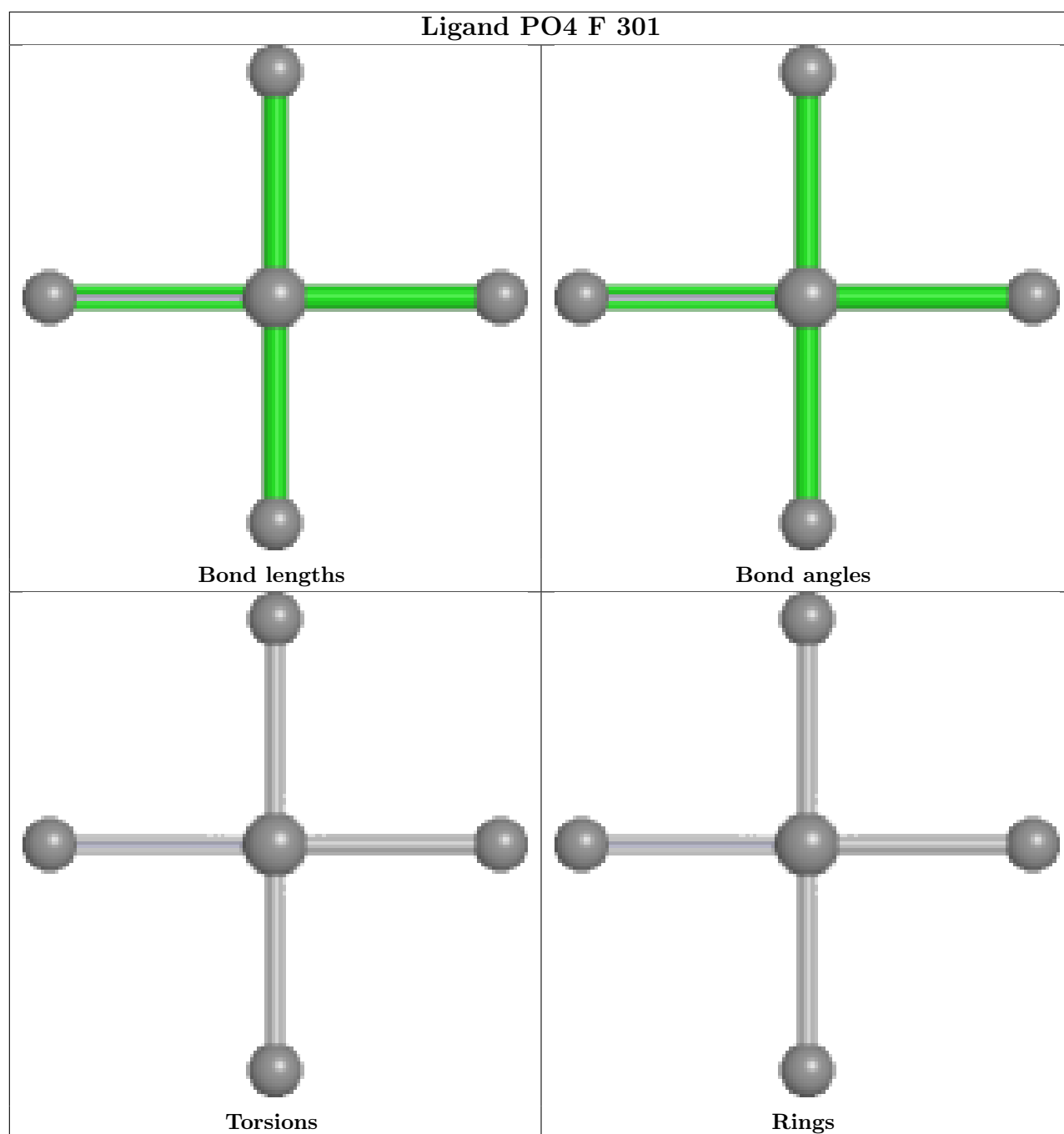
No monomer is involved in short contacts.

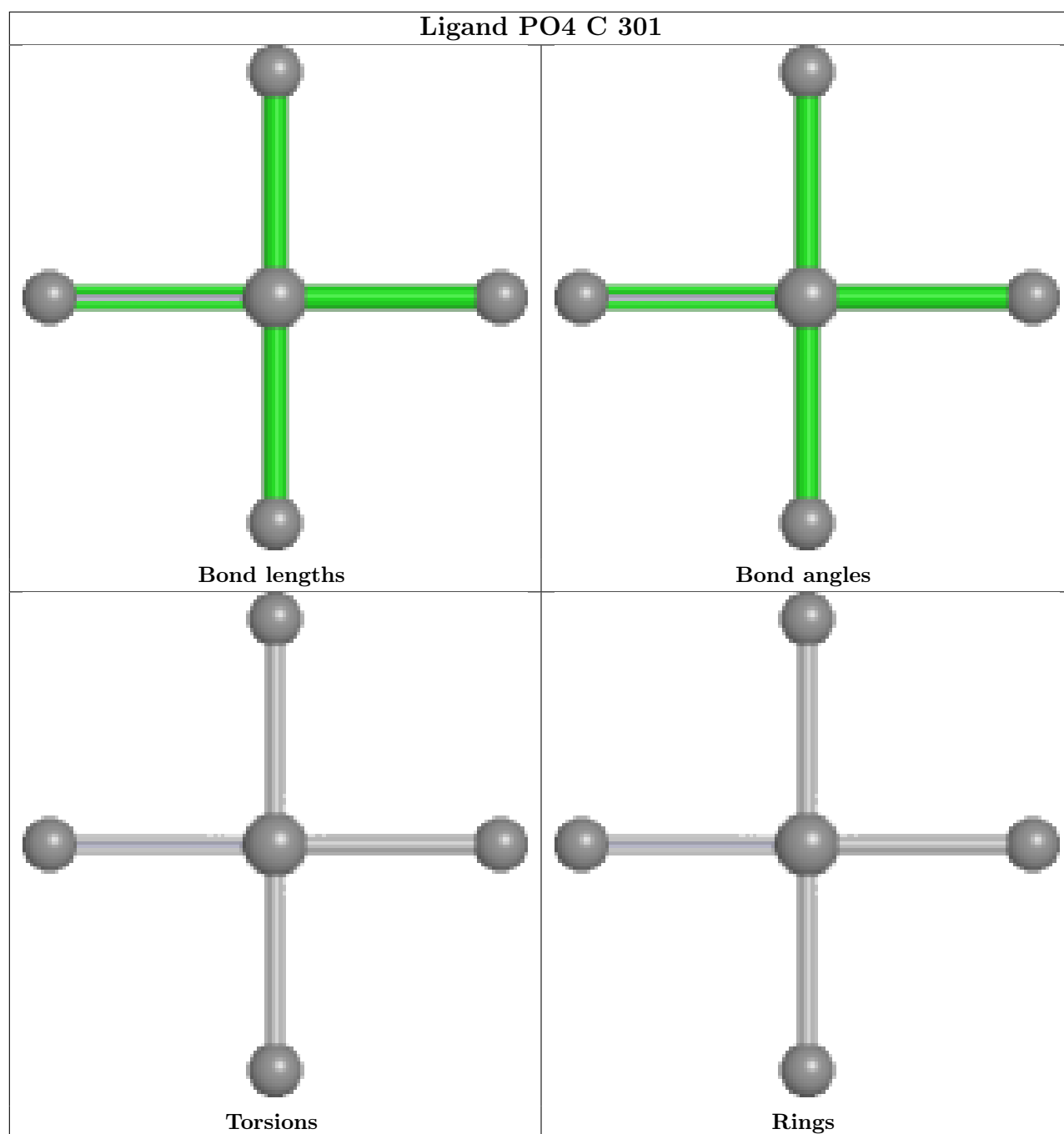
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 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	145/152 (95%)	0.79	11 (7%)	20 17	30, 59, 94, 101	0
1	D	148/152 (97%)	0.81	13 (8%)	15 14	45, 62, 94, 97	0
2	B	210/223 (94%)	0.40	2 (0%)	79 76	40, 58, 80, 89	0
2	E	209/223 (93%)	0.76	9 (4%)	40 35	45, 67, 94, 109	0
3	C	219/241 (90%)	0.54	8 (3%)	45 40	39, 56, 83, 106	0
3	F	216/241 (89%)	0.44	10 (4%)	37 33	37, 55, 87, 98	0
All	All	1147/1232 (93%)	0.60	53 (4%)	37 33	30, 60, 91, 109	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	TYR	5.2
2	E	93	ALA	4.5
1	A	2	CYS	3.9
3	F	203	GLY	3.8
1	A	128	PRO	3.7
3	C	206	THR	3.7
2	B	93	ALA	3.6
1	A	109	ALA	3.5
1	A	6	MET	3.3
1	D	6	MET	3.3
3	F	208	ILE	3.1
2	E	191	TYR	3.0
2	E	168	LYS	3.0
3	F	202	LEU	3.0
1	D	2	CYS	3.0
1	D	4	LEU	2.9
1	D	106	LEU	2.9
3	C	207	TYR	2.9
3	F	147	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	125	PRO	2.8
3	C	147	GLY	2.8
1	D	5	PRO	2.8
1	D	37	TYR	2.7
3	F	167	TRP	2.7
1	D	133	GLN	2.7
3	F	204	THR	2.6
3	F	225	GLU	2.6
2	E	192	ALA	2.6
1	D	150	MET	2.6
3	C	149	ALA	2.5
3	C	204	THR	2.5
2	E	208	PHE	2.4
2	E	190	VAL	2.4
1	D	151	SER	2.4
2	E	167	SER	2.4
1	D	142	THR	2.3
1	D	123	CYS	2.3
3	C	150	ALA	2.2
3	F	138	ALA	2.2
2	E	141	ARG	2.2
1	A	110	PHE	2.2
1	A	8	ARG	2.1
2	B	167	SER	2.1
1	A	81	LEU	2.1
3	F	142	LYS	2.1
3	C	54	TYR	2.1
3	C	224	VAL	2.1
1	A	11	ILE	2.1
1	A	10	TYR	2.1
1	A	3	SER	2.1
1	D	128	PRO	2.1
2	E	193	CYS	2.1
3	F	143	SER	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

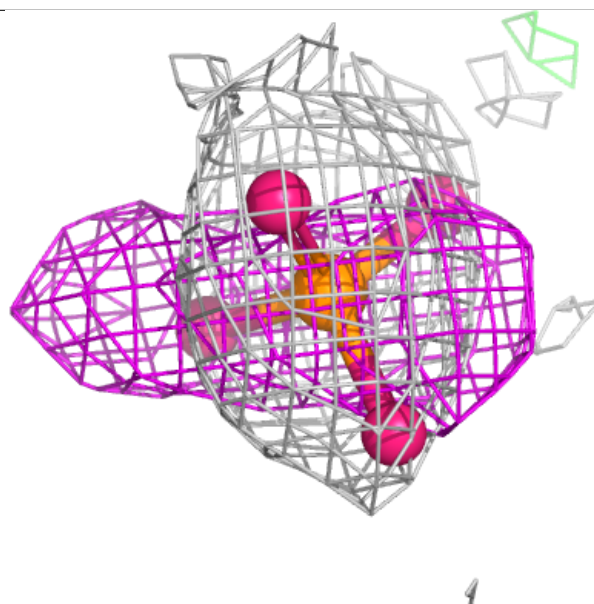
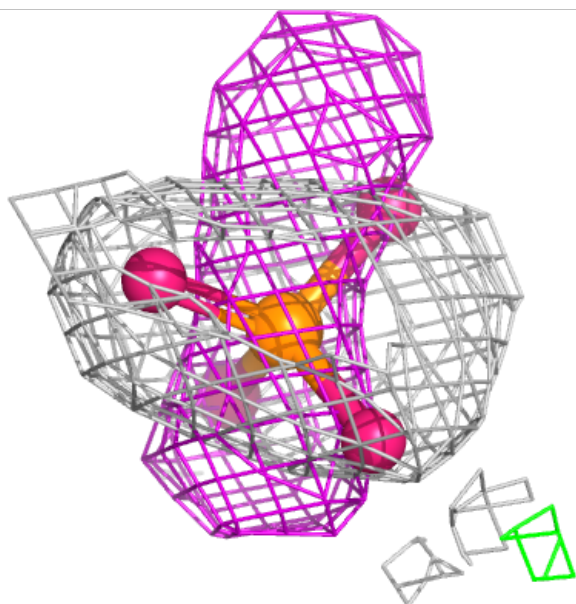
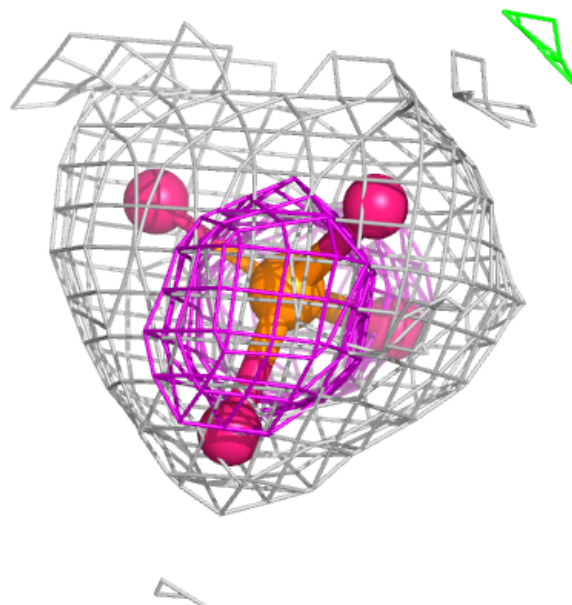
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PO4	A	201	5/5	0.81	0.21	60,69,74,82	0
4	PO4	F	301	5/5	0.81	0.19	58,74,77,83	0
4	PO4	C	301	5/5	0.84	0.24	62,78,82,89	0
4	PO4	E	301	5/5	0.85	0.23	58,65,78,78	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.

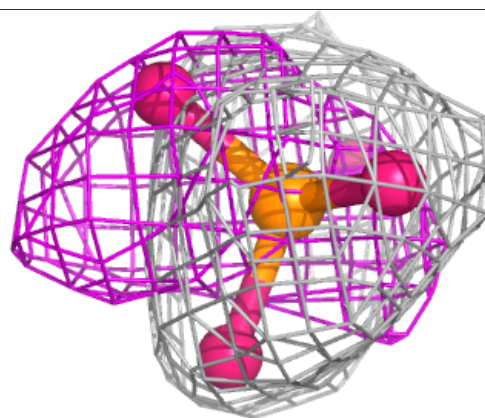
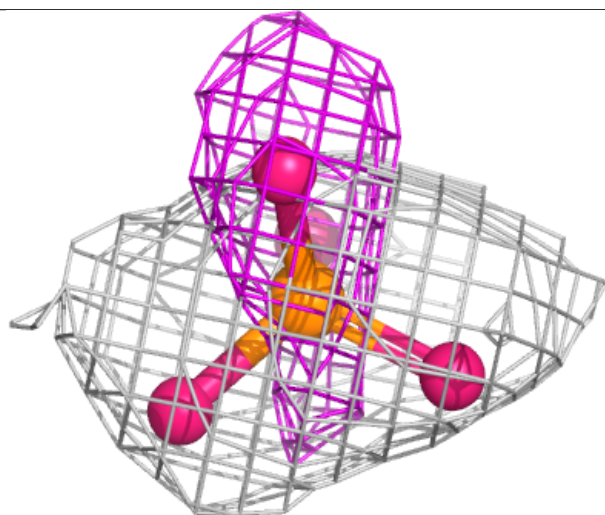
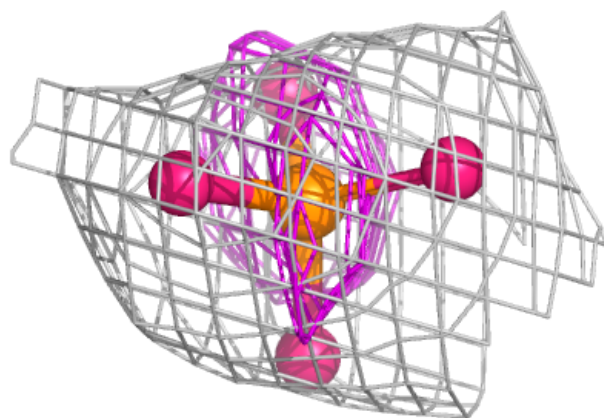
Electron density around PO4 A 201:

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



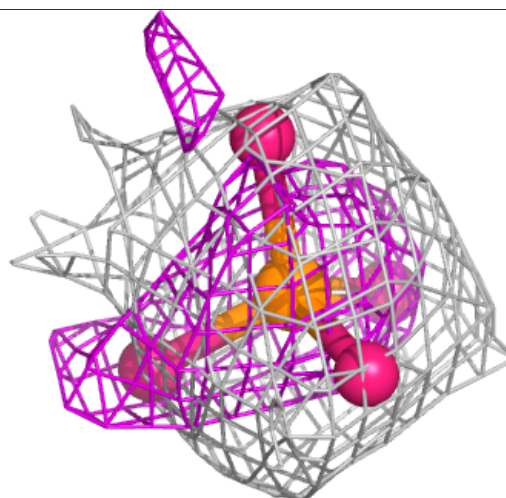
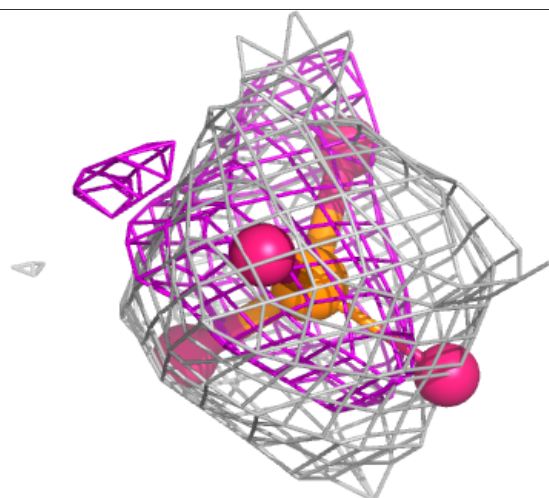
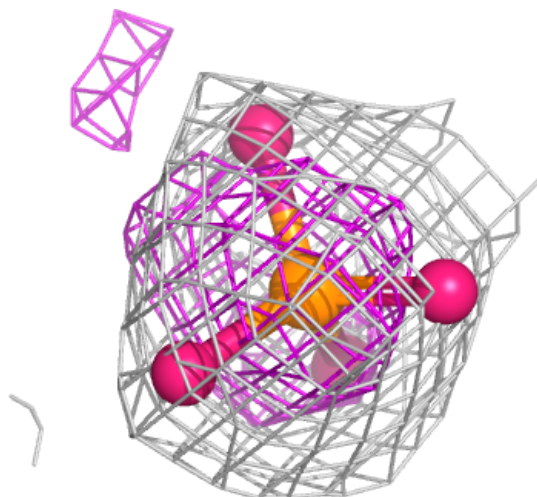
Electron density around PO4 F 301:

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



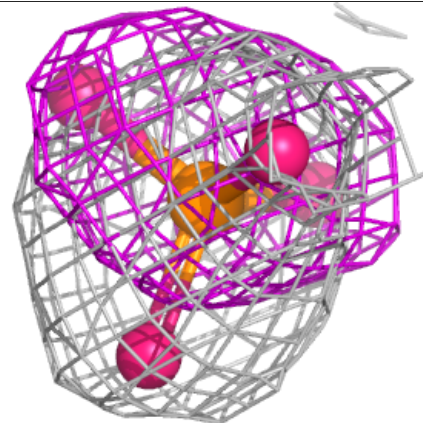
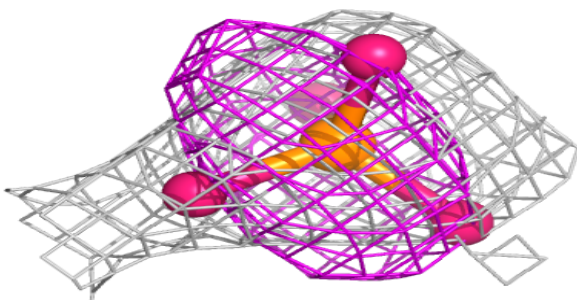
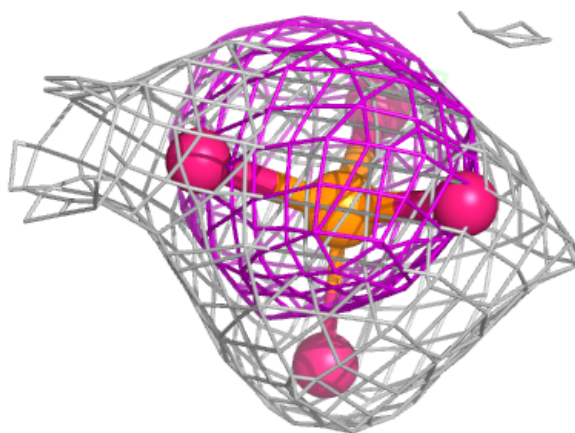
Electron density around PO4 C 301:

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



Electron density around PO4 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.