



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:48 PM UTC

PDB ID : 7CF8 / pdb_00007cf8
Title : PfkB(Mycobacterium marinum)
Authors : Li, J.; Gao, B.; Ji, R.
Deposited on : 2020-06-24
Resolution : 2.21 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:

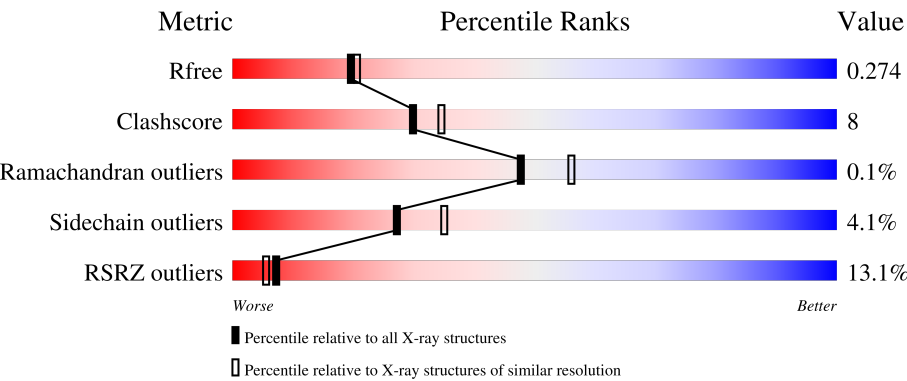
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	303	8% 81%10%8%
1	B	303	15% 70%18%10%
1	C	303	14% 76%14%10%
1	D	303	10% 81%12%7%
1	E	303	8% 80%10%8%

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Mol	Chain	Length	Quality of chain
1	F	303	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	402	-	X	-	-

2 Entry composition [i](#)

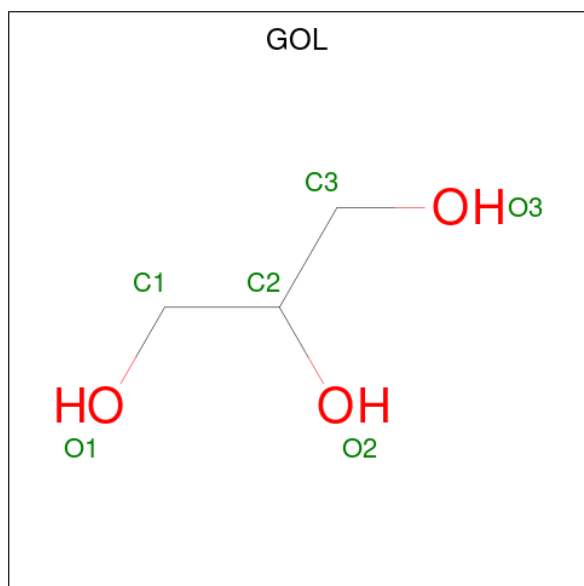
There are 4 unique types of molecules in this entry. The entry contains 11872 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fructokinase, PfkB.

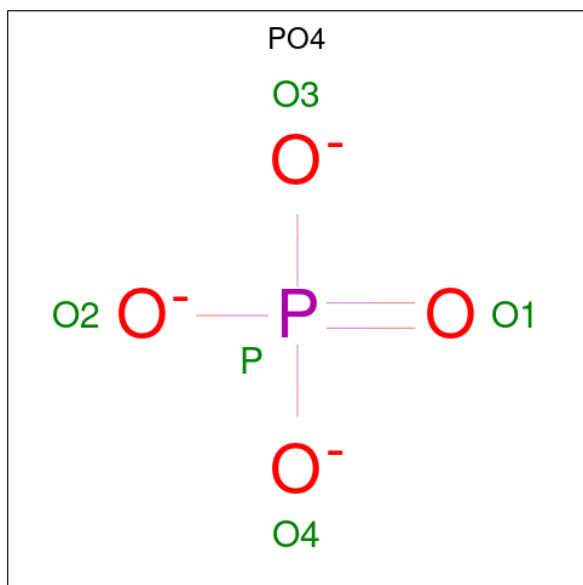
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			1967	1238	353	371	5			
1	B	272	Total	C	N	O	S	0	0	0
			1924	1209	340	371	4			
1	C	273	Total	C	N	O	S	0	0	0
			1918	1207	341	366	4			
1	D	282	Total	C	N	O	S	0	0	0
			1990	1249	354	383	4			
1	E	278	Total	C	N	O	S	0	0	0
			1960	1233	349	374	4			
1	F	271	Total	C	N	O	S	0	0	0
			1914	1207	342	362	3			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	46	Total O 46 46	0	0

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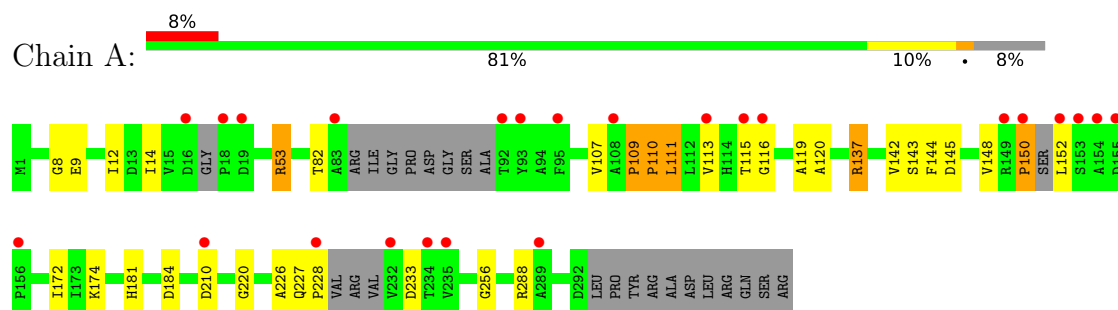
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	22	Total 22	O 22	0	0
4	C	19	Total 19	O 19	0	0
4	D	41	Total 41	O 41	0	0
4	E	15	Total 15	O 15	0	0
4	F	13	Total 13	O 13	0	0

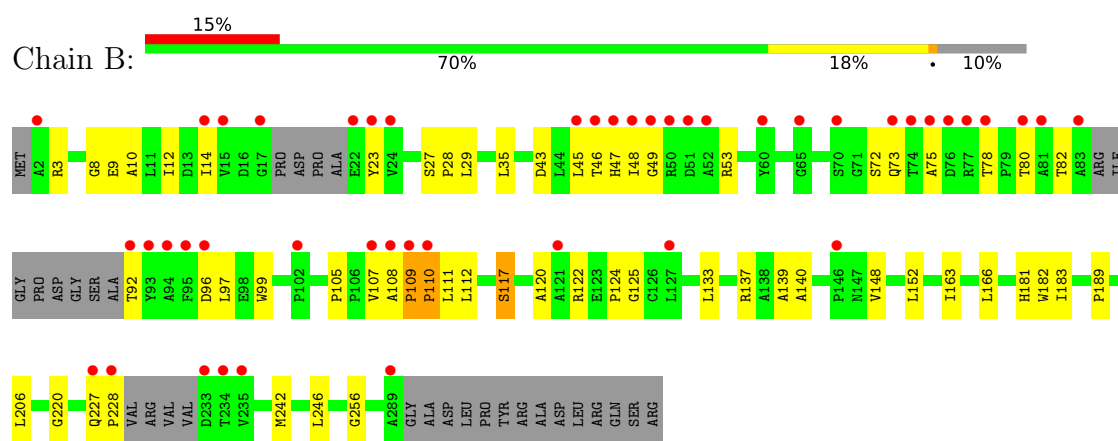
3 Residue-property plots [i](#)

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.

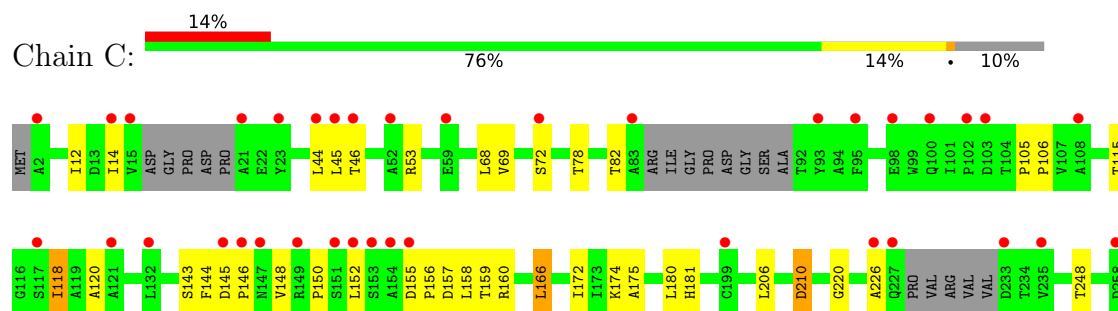
• Molecule 1: Fructokinase, PfkB

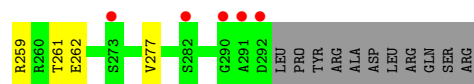


• Molecule 1: Fructokinase, PfkB

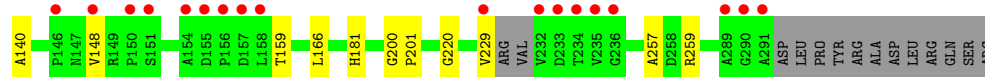
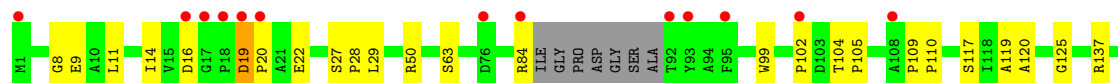
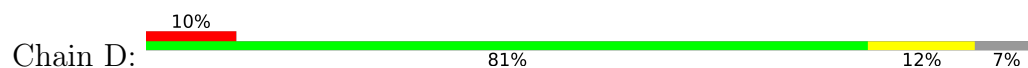


• Molecule 1: Fructokinase, PfkB

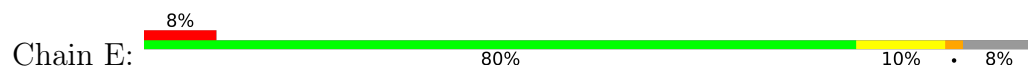




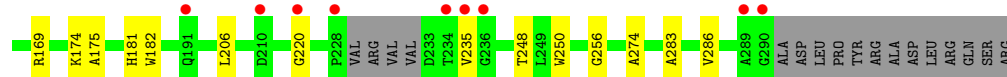
• Molecule 1: Fructokinase, PfkB



• Molecule 1: Fructokinase, PfkB



• Molecule 1: Fructokinase, PfkB



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.41Å 125.41Å 137.52Å 90.00° 106.83° 90.00°	Depositor
Resolution (Å)	66.92 – 2.21 66.92 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.8 (66.92-2.21) 99.8 (66.92-2.21)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.13_2998, PHENIX 1.13_2998	Depositor
R, R_{free}	0.218 , 0.247 (Not available) , 0.274	Depositor DCC
R_{free} test set	5126 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	55.0	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11872	wwPDB-VP
Average B, all atoms (Å ²)	63.0	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 39.62 % 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 3.0880e-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: GOL, 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	1.18	4/1999 (0.2%)	1.42	4/2738 (0.1%)
1	B	1.13	0/1954	1.47	7/2677 (0.3%)
1	C	1.17	2/1948 (0.1%)	1.56	8/2671 (0.3%)
1	D	1.18	3/2024 (0.1%)	1.50	6/2777 (0.2%)
1	E	1.10	1/1992 (0.1%)	1.40	2/2732 (0.1%)
1	F	1.19	3/1946 (0.2%)	1.52	10/2669 (0.4%)
All	All	1.16	13/11863 (0.1%)	1.48	37/16264 (0.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	155	ASP	C-N	13.08	1.50	1.33
1	D	19	ASP	C-N	12.55	1.50	1.33
1	A	109	PRO	C-O	-8.48	1.15	1.24
1	F	145	ASP	C-O	-7.00	1.18	1.24
1	A	110	PRO	C-O	-6.82	1.14	1.23
1	D	105	PRO	C-O	-6.38	1.19	1.24
1	E	145	ASP	C-O	-6.27	1.20	1.25
1	A	107	VAL	C-O	-6.08	1.17	1.24
1	A	9	GLU	C-O	6.06	1.31	1.23
1	F	129	VAL	C-O	-5.86	1.17	1.24
1	D	109	PRO	C-O	-5.69	1.18	1.24
1	F	146	PRO	C-O	-5.53	1.17	1.24
1	C	105	PRO	C-O	-5.22	1.18	1.24

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	19	ASP	CA-C-N	18.05	138.38	119.78
1	D	19	ASP	C-N-CA	18.05	138.38	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	155	ASP	CA-C-N	17.36	138.37	119.28
1	C	155	ASP	C-N-CA	17.36	138.37	119.28
1	F	81	ALA	N-CA-C	-11.63	86.03	110.80
1	B	109	PRO	N-CA-C	-11.20	97.03	110.70
1	B	110	PRO	N-CA-CB	9.42	113.14	103.25
1	B	109	PRO	CB-CA-C	7.90	120.55	110.92
1	B	110	PRO	N-CA-C	-6.82	98.43	112.47
1	C	146	PRO	N-CA-CB	6.34	109.91	103.25
1	D	102	PRO	N-CA-CB	6.28	108.92	103.27
1	A	233	ASP	CA-CB-CG	6.22	118.82	112.60
1	F	256	GLY	CA-C-O	-6.14	117.09	121.88
1	F	82	THR	N-CA-C	-6.11	93.90	111.00
1	D	257	ALA	CA-C-N	6.02	128.62	120.38
1	D	257	ALA	C-N-CA	6.02	128.62	120.38
1	E	179	ASP	CA-CB-CG	5.98	118.58	112.60
1	C	157	ASP	CB-CA-C	5.84	120.00	110.95
1	B	228	PRO	N-CA-CB	5.84	109.42	103.00
1	F	68	LEU	CA-C-N	-5.83	115.44	122.90
1	F	68	LEU	C-N-CA	-5.83	115.44	122.90
1	A	150	PRO	N-CD-CG	-5.71	94.64	103.20
1	F	250	TRP	CA-C-N	5.44	127.57	120.28
1	F	250	TRP	C-N-CA	5.44	127.57	120.28
1	F	81	ALA	CB-CA-C	-5.36	99.75	110.42
1	A	109	PRO	N-CA-C	5.35	117.22	110.70
1	A	233	ASP	CB-CA-C	5.31	118.18	109.90
1	C	118	ILE	CA-C-N	5.25	127.31	120.28
1	C	118	ILE	C-N-CA	5.25	127.31	120.28
1	C	159	THR	CB-CA-C	5.23	121.05	110.38
1	D	105	PRO	N-CA-C	5.21	116.16	110.58
1	B	105	PRO	CB-CA-C	-5.19	106.30	111.17
1	B	256	GLY	CA-C-O	-5.14	117.87	121.88
1	F	60	TYR	CA-C-N	5.12	127.74	120.53
1	F	60	TYR	C-N-CA	5.12	127.74	120.53
1	C	78	THR	CA-CB-OG1	-5.09	101.97	109.60
1	E	148	VAL	N-CA-C	5.09	115.97	109.30

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	1967	0	1939	28	0
1	B	1924	0	1864	43	0
1	C	1918	0	1885	28	0
1	D	1990	0	1943	20	0
1	E	1960	0	1927	25	0
1	F	1914	0	1887	59	0
2	A	6	0	8	0	0
2	D	6	0	8	0	0
2	E	6	0	8	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	46	0	0	1	0
4	B	22	0	0	0	0
4	C	19	0	0	0	0
4	D	41	0	0	0	0
4	E	15	0	0	1	0
4	F	13	0	0	0	0
All	All	11872	0	11469	197	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 8.

All (197) 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:F:79:PRO:HB3	1:F:97:LEU:CB	1.62	1.25
1:F:79:PRO:HB3	1:F:97:LEU:HB3	1.29	1.10
1:B:110:PRO:O	1:B:140:ALA:HB2	1.53	1.06
1:F:79:PRO:HB3	1:F:97:LEU:HB2	1.38	1.05
1:F:122:ARG:HG3	1:F:122:ARG:HH21	1.31	0.96
1:F:149:ARG:HG2	1:F:149:ARG:HH11	1.42	0.85
1:F:13:ASP:HA	1:F:81:ALA:HB3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:ILE:O	1:F:82:THR:HA	1.79	0.82
1:B:47:HIS:NE2	1:B:75:ALA:HA	1.96	0.79
1:B:80:THR:HG22	1:B:96:ASP:HB3	1.63	0.79
1:F:79:PRO:CB	1:F:97:LEU:HB2	2.13	0.77
1:C:145:ASP:OD2	1:C:174:LYS:HE2	1.87	0.74
1:C:46:THR:O	1:C:72:SER:HA	1.89	0.72
1:D:16:ASP:HB3	1:D:84:ARG:HA	1.70	0.72
1:F:130:ALA:HB1	1:F:169:ARG:NH2	2.04	0.72
1:E:27:SER:HB3	1:E:28:PRO:HD3	1.71	0.71
1:B:80:THR:CG2	1:B:96:ASP:HB3	2.21	0.71
1:B:110:PRO:O	1:B:140:ALA:CB	2.36	0.70
1:C:12:ILE:HG13	1:C:53:ARG:HG2	1.71	0.70
1:B:97:LEU:O	1:B:122:ARG:NH1	2.25	0.70
1:A:210:ASP:O	1:A:226:ALA:HB2	1.92	0.69
1:C:45:LEU:HD12	1:C:69:VAL:HG11	1.73	0.69
1:F:137:ARG:HG2	1:F:137:ARG:NH1	2.06	0.69
1:A:116:GLY:HA2	1:A:120:ALA:HB2	1.74	0.69
1:C:45:LEU:HD12	1:C:106:PRO:HG3	1.75	0.69
1:C:148:VAL:HG12	1:C:150:PRO:HG3	1.75	0.68
1:B:148:VAL:HG21	1:B:182:TRP:CE3	2.28	0.68
1:B:99:TRP:CD1	1:B:125:GLY:HA3	2.28	0.68
1:E:14:ILE:HB	1:E:82:THR:HG22	1.77	0.67
1:B:49:GLY:HA2	1:B:75:ALA:HB3	1.77	0.67
1:F:149:ARG:NH2	1:F:235:VAL:HG11	2.10	0.67
1:A:181:HIS:CD2	1:C:220:GLY:HA2	2.31	0.66
1:F:79:PRO:CB	1:F:97:LEU:HB3	2.19	0.65
1:B:3:ARG:NH1	1:B:43:ASP:OD1	2.29	0.65
1:A:210:ASP:O	1:A:226:ALA:CB	2.45	0.65
1:C:118:ILE:HG12	1:C:152:LEU:HD22	1.79	0.64
1:B:45:LEU:HG	1:B:45:LEU:O	1.98	0.63
1:D:11:LEU:C	1:D:11:LEU:HD12	2.23	0.63
1:E:40:ARG:HD2	1:E:247:ASP:OD1	1.99	0.63
1:E:40:ARG:HD3	1:E:250:TRP:CE3	2.34	0.63
1:E:11:LEU:C	1:E:11:LEU:HD12	2.25	0.62
1:E:123:GLU:H	1:E:123:GLU:CD	2.06	0.62
1:F:122:ARG:HH21	1:F:122:ARG:CG	2.09	0.62
1:E:179:ASP:O	1:E:183:ILE:HG12	1.99	0.62
1:F:79:PRO:CB	1:F:97:LEU:CB	2.57	0.62
1:E:12:ILE:HG13	1:E:53:ARG:HB3	1.80	0.62
1:D:27:SER:HB3	1:D:28:PRO:HD3	1.81	0.61
1:F:122:ARG:HD2	1:F:152:LEU:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ALA:HB1	1:D:166:LEU:HD12	1.83	0.60
1:B:109:PRO:HB3	1:B:139:ALA:HB3	1.82	0.60
1:A:150:PRO:HB2	1:A:152:LEU:HA	1.82	0.60
1:B:120:ALA:HB1	1:B:166:LEU:HD12	1.84	0.59
1:B:46:THR:O	1:B:72:SER:HB2	2.02	0.59
1:F:122:ARG:HG3	1:F:122:ARG:NH2	2.08	0.59
1:B:108:ALA:O	1:B:109:PRO:C	2.45	0.59
1:F:56:ARG:CG	1:F:56:ARG:HH11	2.15	0.59
1:B:9:GLU:OE1	1:B:117:SER:HB3	2.03	0.58
1:F:149:ARG:HH11	1:F:149:ARG:CG	2.14	0.58
1:C:180:LEU:HD22	1:C:206:LEU:HD13	1.86	0.58
1:A:113:VAL:CG1	1:A:142:VAL:HG22	2.34	0.58
1:F:49:GLY:HA2	1:F:75:ALA:O	2.03	0.58
1:B:12:ILE:HD12	1:B:12:ILE:O	2.03	0.58
1:E:104:THR:O	1:E:104:THR:HG23	2.04	0.57
1:F:120:ALA:HB1	1:F:166:LEU:HD12	1.87	0.57
1:B:14:ILE:O	1:B:82:THR:HA	2.05	0.56
1:A:14:ILE:HB	1:A:82:THR:HG22	1.87	0.56
1:E:29:LEU:HD13	1:E:29:LEU:C	2.31	0.56
1:F:149:ARG:HH22	1:F:235:VAL:HG11	1.70	0.56
1:E:8:GLY:HA2	1:E:119:ALA:HB2	1.88	0.55
1:F:156:PRO:HB2	1:F:160:ARG:HH12	1.72	0.55
1:F:149:ARG:HG2	1:F:149:ARG:NH1	2.18	0.55
1:D:120:ALA:HB1	1:D:166:LEU:CD1	2.38	0.54
1:F:283:ALA:O	1:F:286:VAL:HG22	2.07	0.54
1:A:137:ARG:HG3	1:A:137:ARG:NH1	2.21	0.54
1:B:48:ILE:C	1:B:75:ALA:HB3	2.33	0.53
1:F:10:ALA:HB1	1:F:29:LEU:HD13	1.90	0.53
1:D:104:THR:O	1:D:104:THR:OG1	2.23	0.53
1:B:49:GLY:CA	1:B:75:ALA:HB3	2.39	0.53
1:C:14:ILE:O	1:C:82:THR:HA	2.08	0.53
1:F:76:ASP:OD1	1:F:76:ASP:N	2.30	0.53
1:A:137:ARG:HG3	1:A:137:ARG:HH11	1.75	0.52
1:A:148:VAL:HG23	1:A:148:VAL:O	2.09	0.52
1:C:120:ALA:HB1	1:C:166:LEU:HD12	1.92	0.51
1:C:45:LEU:CD1	1:C:69:VAL:HG11	2.41	0.51
1:E:181:HIS:CE1	1:F:220:GLY:HA2	2.44	0.51
1:C:210:ASP:O	1:C:226:ALA:CB	2.58	0.51
1:E:29:LEU:C	1:E:29:LEU:CD1	2.84	0.51
1:A:227:GLN:HB3	1:A:228:PRO:HD2	1.92	0.51
1:B:8:GLY:O	1:B:46:THR:HB	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:TRP:CD1	1:D:125:GLY:HA3	2.46	0.51
1:B:242:MET:HE3	1:B:242:MET:HA	1.93	0.50
1:C:248:THR:OG1	1:C:277:VAL:HG11	2.12	0.50
1:E:8:GLY:HA2	1:E:119:ALA:CB	2.42	0.50
1:B:48:ILE:O	1:B:73:GLN:HA	2.11	0.50
1:F:137:ARG:HG2	1:F:137:ARG:HH11	1.76	0.50
1:E:14:ILE:HD12	1:E:82:THR:HG22	1.92	0.50
1:A:111:LEU:HD22	1:A:256:GLY:CA	2.43	0.49
1:A:143:SER:HA	1:A:172:ILE:O	2.13	0.49
1:B:47:HIS:NE2	1:B:75:ALA:CA	2.71	0.49
1:F:80:THR:OG1	1:F:96:ASP:HB3	2.12	0.49
1:A:53:ARG:HG3	4:A:532:HOH:O	2.13	0.49
1:E:51:ASP:OD1	1:E:51:ASP:N	2.43	0.49
1:D:181:HIS:CD2	1:E:220:GLY:HA2	2.48	0.49
1:B:12:ILE:HA	1:B:23:TYR:O	2.13	0.49
1:C:259:ARG:HA	1:C:262:GLU:OE1	2.13	0.49
1:F:107:VAL:HG12	1:F:108:ALA:O	2.13	0.48
1:F:47:HIS:HD2	1:F:100:GLN:H	1.61	0.48
1:F:149:ARG:CG	1:F:149:ARG:NH1	2.73	0.48
1:D:14:ILE:HG12	1:D:22:GLU:HG2	1.96	0.48
1:C:44:LEU:O	1:C:68:LEU:HD12	2.14	0.47
1:C:45:LEU:CD1	1:C:106:PRO:HG3	2.42	0.47
1:F:47:HIS:ND1	1:F:75:ALA:HB2	2.29	0.47
1:B:122:ARG:HD3	1:B:152:LEU:HD21	1.96	0.47
1:A:109:PRO:HA	1:A:110:PRO:HD3	1.80	0.47
1:F:56:ARG:HH11	1:F:56:ARG:HG3	1.79	0.47
1:B:163:ILE:HD13	1:B:183:ILE:HD11	1.97	0.47
1:B:47:HIS:CE1	1:B:75:ALA:HA	2.51	0.46
1:C:156:PRO:HB2	1:C:160:ARG:HH12	1.80	0.46
1:C:45:LEU:HG	1:C:69:VAL:HB	1.98	0.46
1:B:120:ALA:HB1	1:B:166:LEU:CD1	2.45	0.46
1:B:53:ARG:CB	1:B:78:THR:HG21	2.47	0.46
1:E:8:GLY:HA3	1:E:28:PRO:HG2	1.98	0.45
1:B:47:HIS:CD2	1:B:75:ALA:HB2	2.52	0.45
1:E:11:LEU:C	1:E:11:LEU:CD1	2.90	0.45
1:E:15:VAL:HG12	1:E:20:PRO:HB2	1.97	0.45
1:B:27:SER:HB3	1:B:28:PRO:HD3	1.99	0.45
1:D:220:GLY:HA2	1:F:181:HIS:CD2	2.51	0.45
1:D:19:ASP:HA	1:D:20:PRO:HD2	1.86	0.44
1:D:99:TRP:CZ2	1:D:119:ALA:HB1	2.53	0.44
1:F:120:ALA:HB1	1:F:166:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:ALA:HB1	1:F:169:ARG:HH22	1.81	0.44
1:D:50:ARG:HH11	1:D:50:ARG:HG2	1.82	0.44
1:F:97:LEU:C	1:F:97:LEU:HD12	2.42	0.44
1:C:145:ASP:HA	1:C:174:LYS:O	2.18	0.44
1:B:99:TRP:O	1:B:124:PRO:HD2	2.18	0.44
1:F:118:ILE:HG12	1:F:152:LEU:HD13	1.99	0.44
1:B:8:GLY:O	1:B:46:THR:CB	2.66	0.44
1:D:8:GLY:HA3	1:D:28:PRO:CB	2.48	0.44
1:D:11:LEU:C	1:D:11:LEU:CD1	2.89	0.43
1:B:133:LEU:HD12	1:B:166:LEU:HD22	2.00	0.43
1:A:137:ARG:HH11	1:A:137:ARG:CG	2.31	0.43
1:F:122:ARG:CG	1:F:122:ARG:NH2	2.72	0.43
1:A:8:GLY:HA2	1:A:119:ALA:CB	2.49	0.43
1:F:48:ILE:HG22	1:F:73:GLN:HG2	2.00	0.43
1:F:156:PRO:HB2	1:F:160:ARG:NH1	2.33	0.43
1:A:220:GLY:HA2	1:B:181:HIS:CD2	2.53	0.43
1:D:9:GLU:O	1:D:9:GLU:HG2	2.18	0.43
1:E:9:GLU:O	1:E:9:GLU:HG2	2.19	0.43
1:A:8:GLY:HA2	1:A:119:ALA:HB2	2.01	0.43
1:C:143:SER:HA	1:C:172:ILE:O	2.19	0.42
1:F:11:LEU:HD12	1:F:11:LEU:C	2.43	0.42
1:E:12:ILE:CG2	1:E:22:GLU:HB3	2.49	0.42
1:B:10:ALA:HB1	1:B:29:LEU:HD12	2.02	0.42
1:F:48:ILE:C	1:F:75:ALA:HB3	2.44	0.42
1:A:12:ILE:HG13	1:A:53:ARG:HB3	2.00	0.42
1:A:150:PRO:HB2	1:A:152:LEU:CA	2.48	0.42
1:C:115:THR:O	1:C:144:PHE:HA	2.19	0.42
1:F:47:HIS:CD2	1:F:100:GLN:HB3	2.55	0.42
1:B:49:GLY:N	1:B:75:ALA:HB3	2.34	0.42
1:F:44:LEU:O	1:F:69:VAL:N	2.52	0.42
1:D:200:GLY:N	1:D:201:PRO:CD	2.82	0.42
1:F:148:VAL:HG11	1:F:182:TRP:HB3	2.01	0.42
1:A:113:VAL:O	1:A:113:VAL:HG13	2.20	0.42
1:F:175:ALA:O	1:F:206:LEU:HA	2.20	0.42
1:E:8:GLY:HA3	1:E:28:PRO:CB	2.50	0.42
1:F:24:VAL:HG11	1:F:60:TYR:CD1	2.55	0.42
1:F:49:GLY:O	1:F:54:GLY:HA3	2.20	0.42
1:F:137:ARG:HH11	1:F:137:ARG:CG	2.31	0.42
1:D:110:PRO:O	1:D:140:ALA:HB2	2.20	0.42
1:F:248:THR:HG21	1:F:274:ALA:HA	2.02	0.41
1:A:116:GLY:CA	1:A:120:ALA:HB2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:LEU:O	1:F:113:VAL:HA	2.20	0.41
1:F:12:ILE:O	1:F:81:ALA:N	2.50	0.41
1:B:189:PRO:HB2	1:B:206:LEU:HD21	2.01	0.41
1:E:174:LYS:NZ	4:E:502:HOH:O	2.43	0.41
1:E:115:THR:O	1:E:144:PHE:HA	2.20	0.41
1:A:145:ASP:OD2	1:A:174:LYS:HE2	2.21	0.41
1:B:10:ALA:CB	1:B:29:LEU:HD12	2.51	0.41
1:F:110:PRO:O	1:F:140:ALA:HB2	2.21	0.41
1:B:242:MET:HE2	1:B:246:LEU:HG	2.02	0.41
1:D:8:GLY:HA2	1:D:119:ALA:CB	2.50	0.41
1:B:35:LEU:HD23	1:B:35:LEU:HA	1.93	0.41
1:F:125:GLY:C	1:F:127:LEU:N	2.78	0.41
1:A:115:THR:O	1:A:144:PHE:HA	2.21	0.41
1:A:184:ASP:C	1:A:184:ASP:OD1	2.63	0.41
1:A:111:LEU:HD22	1:A:256:GLY:HA2	2.03	0.40
1:F:10:ALA:HB1	1:F:29:LEU:CD1	2.51	0.40
1:C:118:ILE:HG12	1:C:152:LEU:CD2	2.47	0.40
1:C:158:LEU:HD12	1:C:158:LEU:HA	1.92	0.40
1:C:175:ALA:HB1	1:C:180:LEU:HD13	2.03	0.40
1:F:47:HIS:HD2	1:F:100:GLN:N	2.19	0.40
1:C:210:ASP:O	1:C:226:ALA:HB2	2.20	0.40
1:C:210:ASP:O	1:C:226:ALA:HB1	2.22	0.40
1:F:47:HIS:CE1	1:F:75:ALA:HB2	2.56	0.40
1:B:220:GLY:HA2	1:C:181:HIS:CE1	2.56	0.40
1:D:19:ASP:N	1:D:20:PRO:CD	2.84	0.40
1:A:14:ILE:O	1:A:82:THR:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	269/303 (89%)	260 (97%)	9 (3%)	0	100	100
1	B	264/303 (87%)	252 (96%)	11 (4%)	1 (0%)	30	33
1	C	265/303 (88%)	253 (96%)	12 (4%)	0	100	100
1	D	276/303 (91%)	268 (97%)	8 (3%)	0	100	100
1	E	270/303 (89%)	264 (98%)	6 (2%)	0	100	100
1	F	263/303 (87%)	254 (97%)	9 (3%)	0	100	100
All	All	1607/1818 (88%)	1551 (96%)	55 (3%)	1 (0%)	48	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	227	GLN

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	187/227 (82%)	183 (98%)	4 (2%)	47	61
1	B	181/227 (80%)	175 (97%)	6 (3%)	33	44
1	C	182/227 (80%)	179 (98%)	3 (2%)	55	70
1	D	190/227 (84%)	182 (96%)	8 (4%)	26	34
1	E	187/227 (82%)	174 (93%)	13 (7%)	14	15
1	F	182/227 (80%)	170 (93%)	12 (7%)	15	17
All	All	1109/1362 (81%)	1063 (96%)	46 (4%)	27	35

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	111	LEU
1	A	137	ARG
1	A	288	ARG

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Mol	Chain	Res	Type
1	B	92	THR
1	B	107	VAL
1	B	111	LEU
1	B	112	LEU
1	B	117	SER
1	B	137	ARG
1	C	166	LEU
1	C	210	ASP
1	C	261	THR
1	D	29	LEU
1	D	63	SER
1	D	117	SER
1	D	137	ARG
1	D	148	VAL
1	D	159	THR
1	D	229	VAL
1	D	259	ARG
1	E	3	ARG
1	E	15	VAL
1	E	29	LEU
1	E	40	ARG
1	E	53	ARG
1	E	63	SER
1	E	73	GLN
1	E	80	THR
1	E	101	ILE
1	E	103	ASP
1	E	123	GLU
1	E	191	GLN
1	E	234	THR
1	F	14	ILE
1	F	48	ILE
1	F	56	ARG
1	F	64	SER
1	F	74	THR
1	F	76	ASP
1	F	103	ASP
1	F	127	LEU
1	F	148	VAL
1	F	149	ARG
1	F	151	SER
1	F	174	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	164	GLN
1	B	191	GLN
1	C	191	GLN
1	D	191	GLN
1	D	252	GLN
1	E	191	GLN
1	F	47	HIS

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](#)

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	PO4	A	402	-	4,4,4	2.71	4 (100%)	6,6,6	0.63	0
3	PO4	B	401	-	4,4,4	1.40	0	6,6,6	0.47	0
3	PO4	D	402	-	4,4,4	1.44	0	6,6,6	0.48	0
3	PO4	F	401	-	4,4,4	1.56	0	6,6,6	0.50	0
3	PO4	E	402	-	4,4,4	1.32	0	6,6,6	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	401	-	5,5,5	0.20	0	5,5,5	0.41	0
2	GOL	E	401	-	5,5,5	0.18	0	5,5,5	0.36	0
2	GOL	D	401	-	5,5,5	0.12	0	5,5,5	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	401	-	-	2/4/4/4	-
2	GOL	E	401	-	-	2/4/4/4	-
2	GOL	D	401	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	PO4	P-O4	-3.09	1.45	1.54
3	A	402	PO4	P-O3	-2.86	1.46	1.54
3	A	402	PO4	P-O2	-2.73	1.46	1.54
3	A	402	PO4	P-O1	-2.07	1.45	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

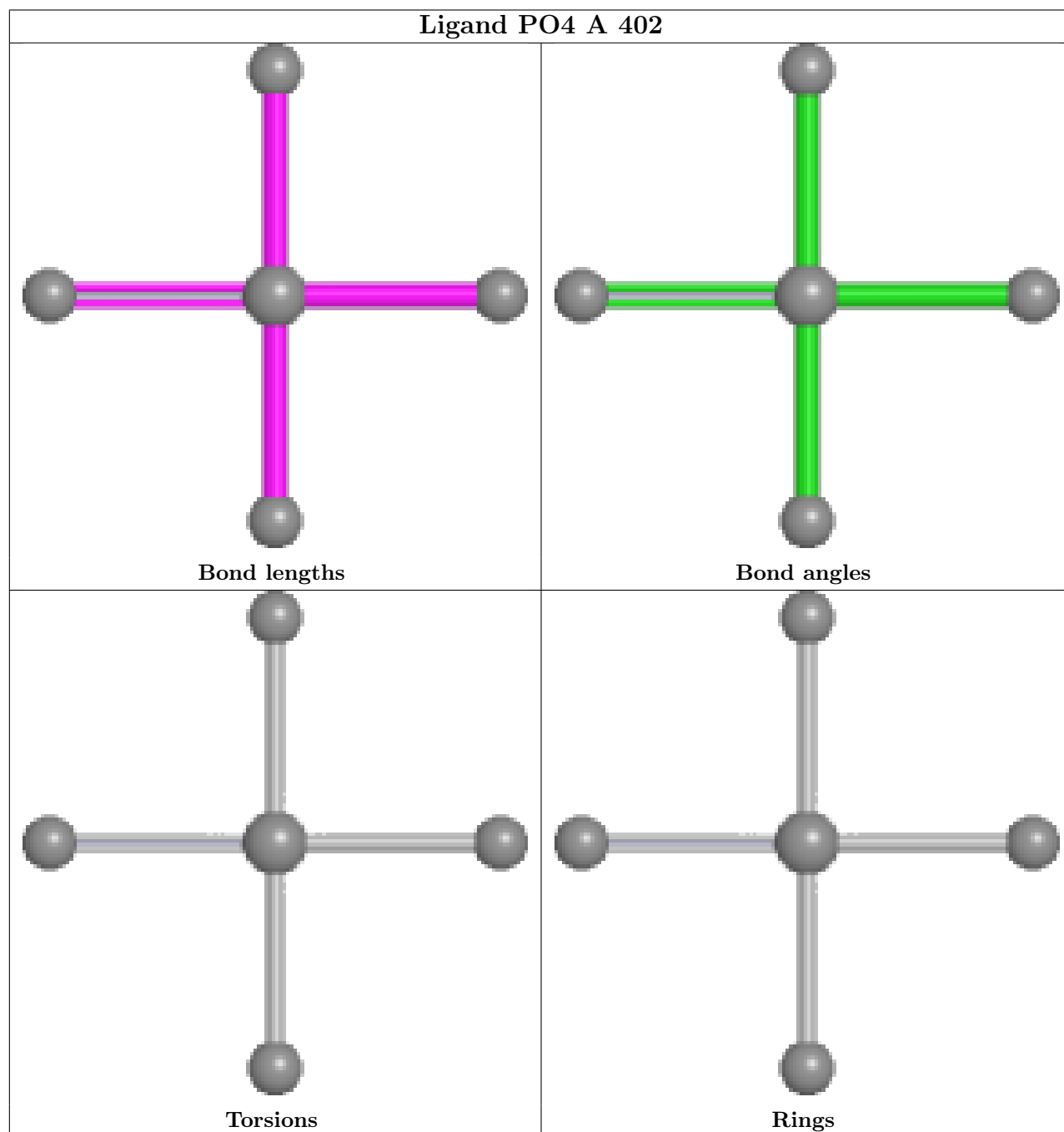
Mol	Chain	Res	Type	Atoms
2	A	401	GOL	C1-C2-C3-O3
2	A	401	GOL	O2-C2-C3-O3
2	E	401	GOL	O1-C1-C2-C3
2	E	401	GOL	O1-C1-C2-O2
2	D	401	GOL	O1-C1-C2-C3
2	D	401	GOL	O1-C1-C2-O2

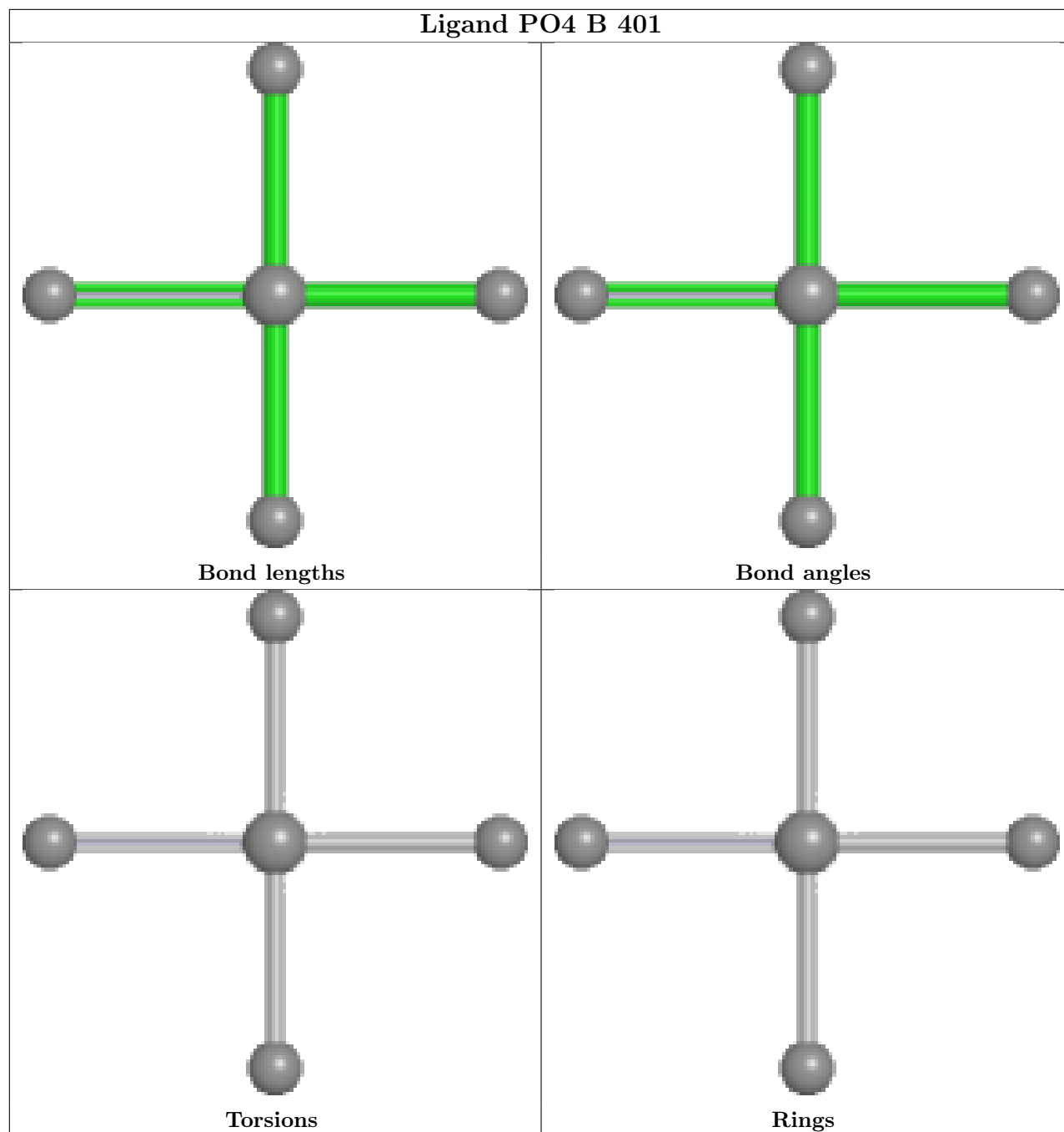
There are no ring outliers.

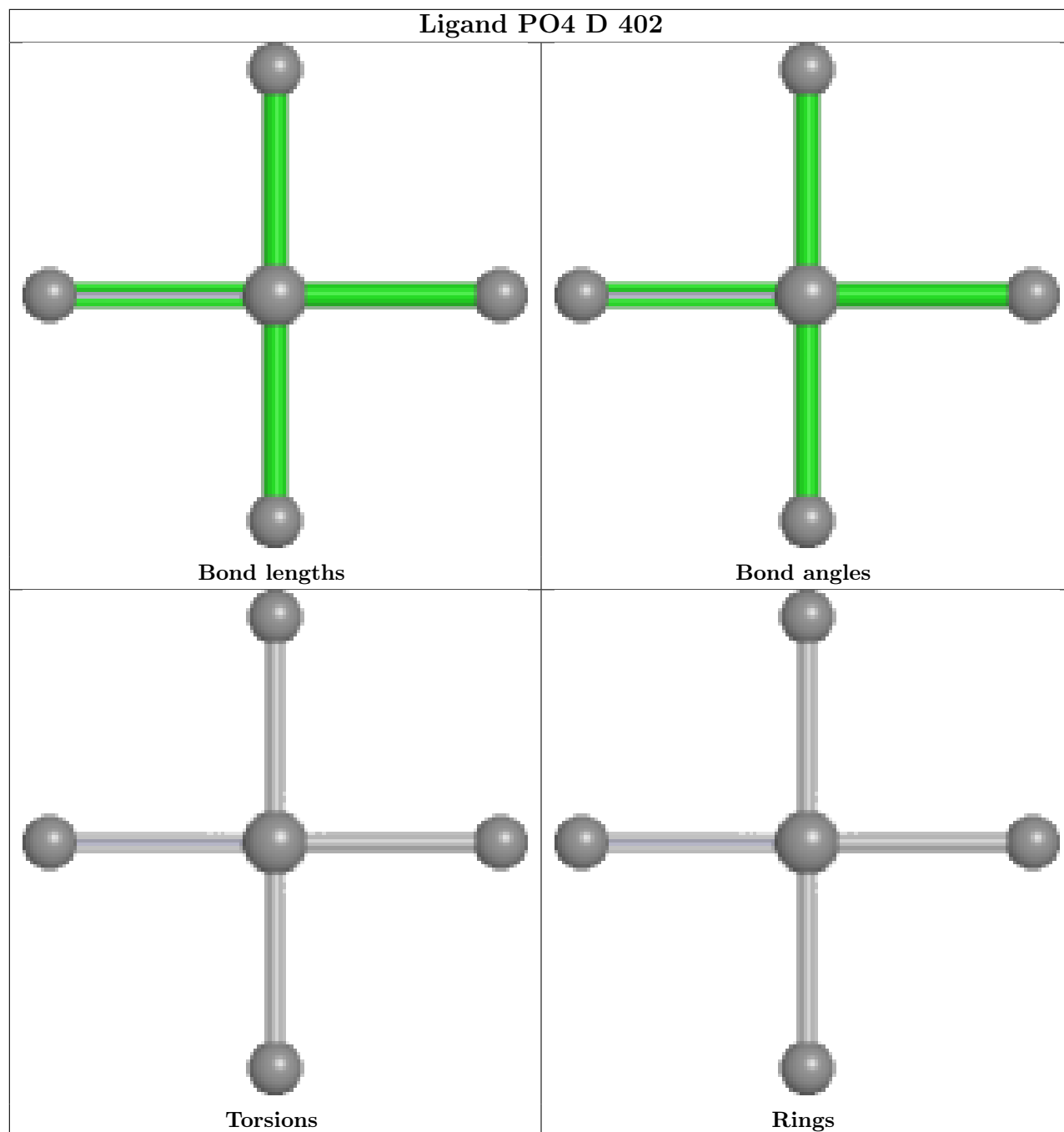
No monomer is involved in short contacts.

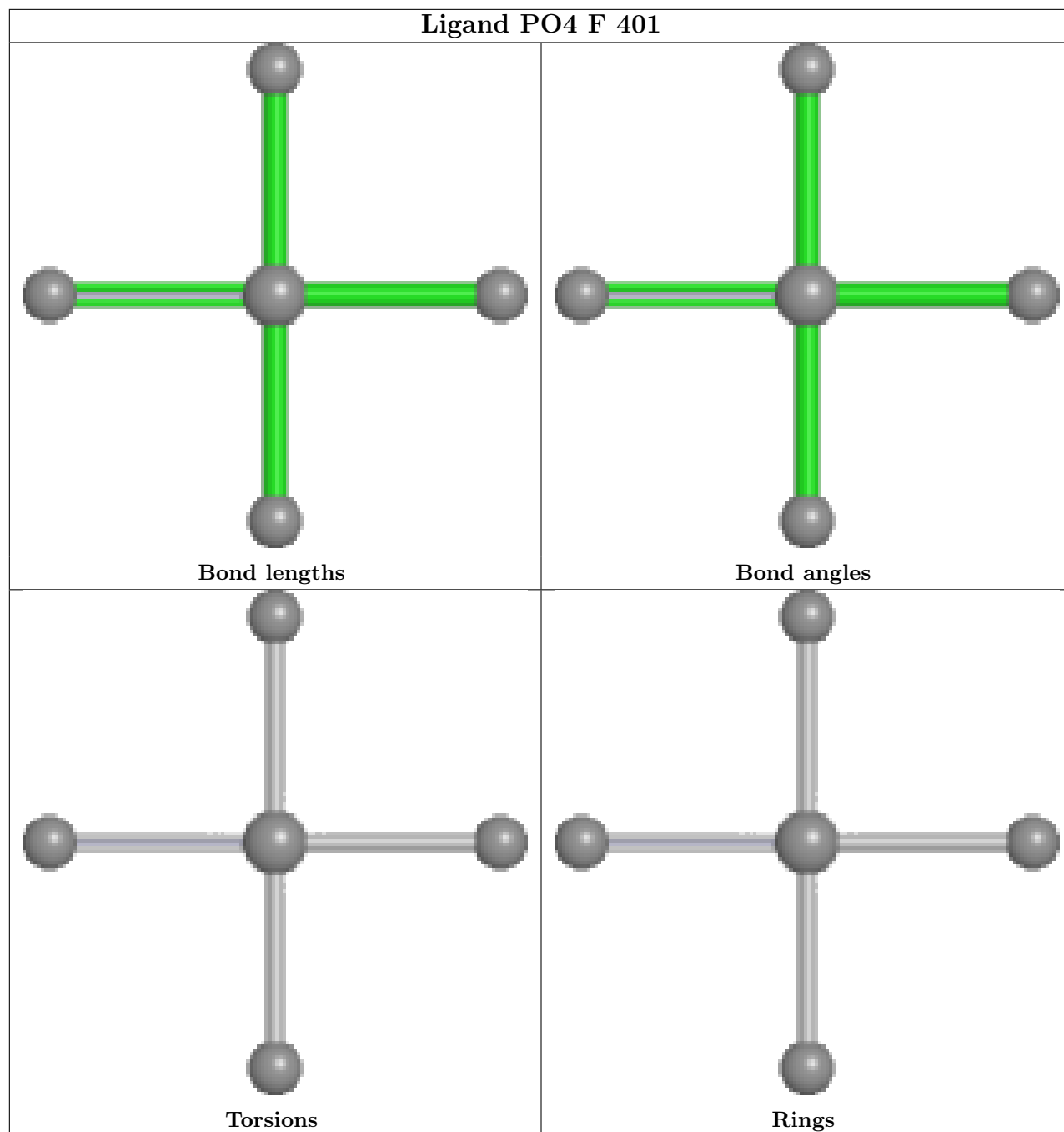
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

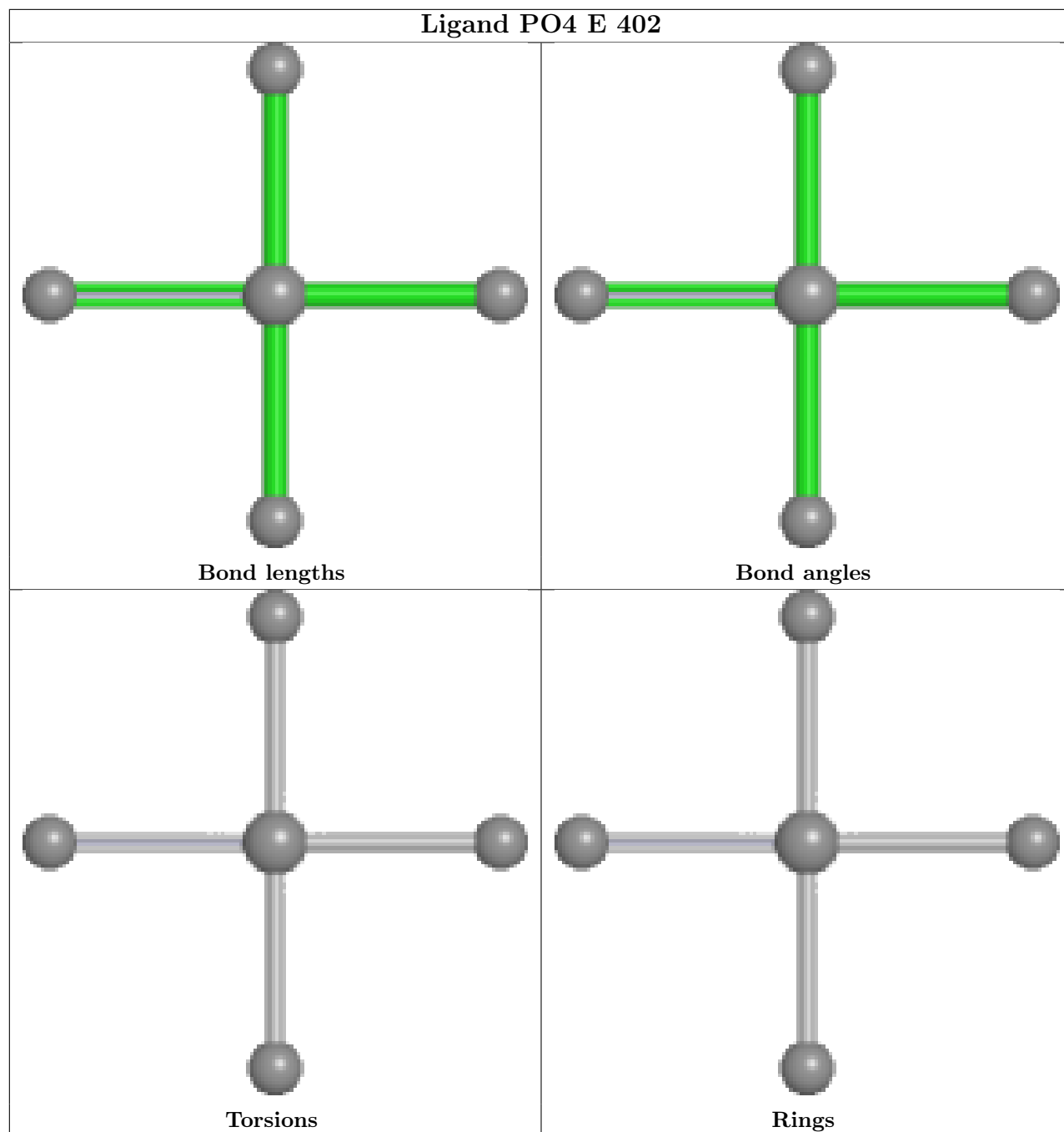
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

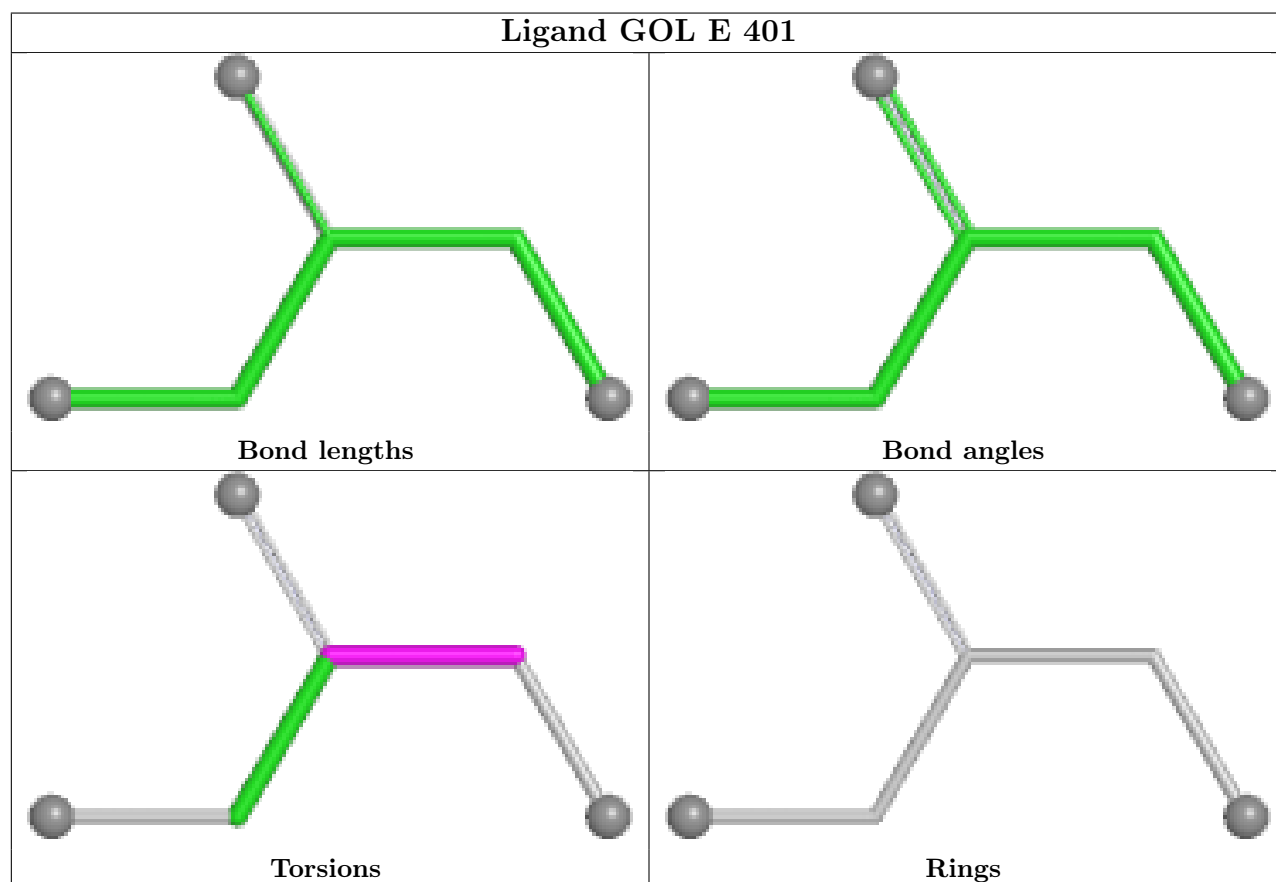
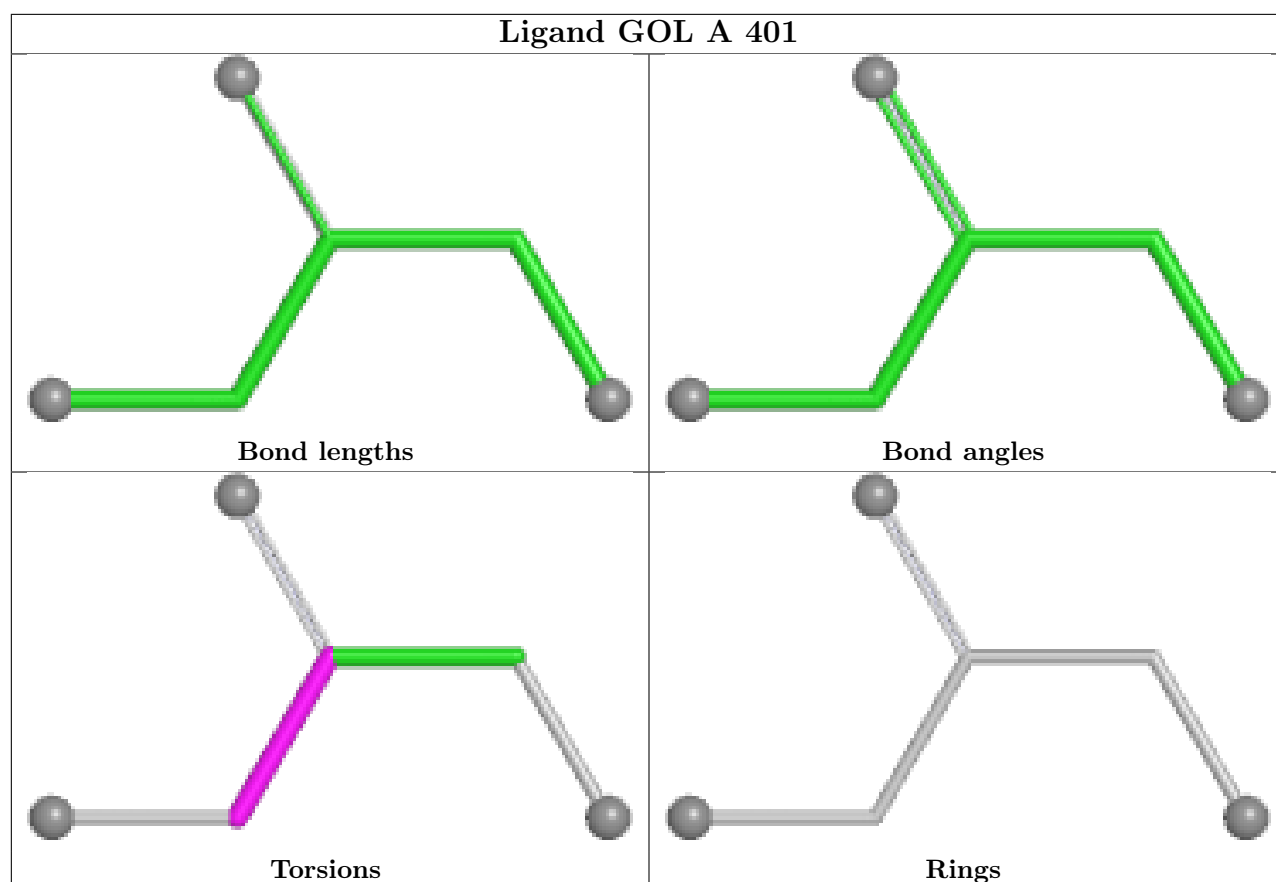


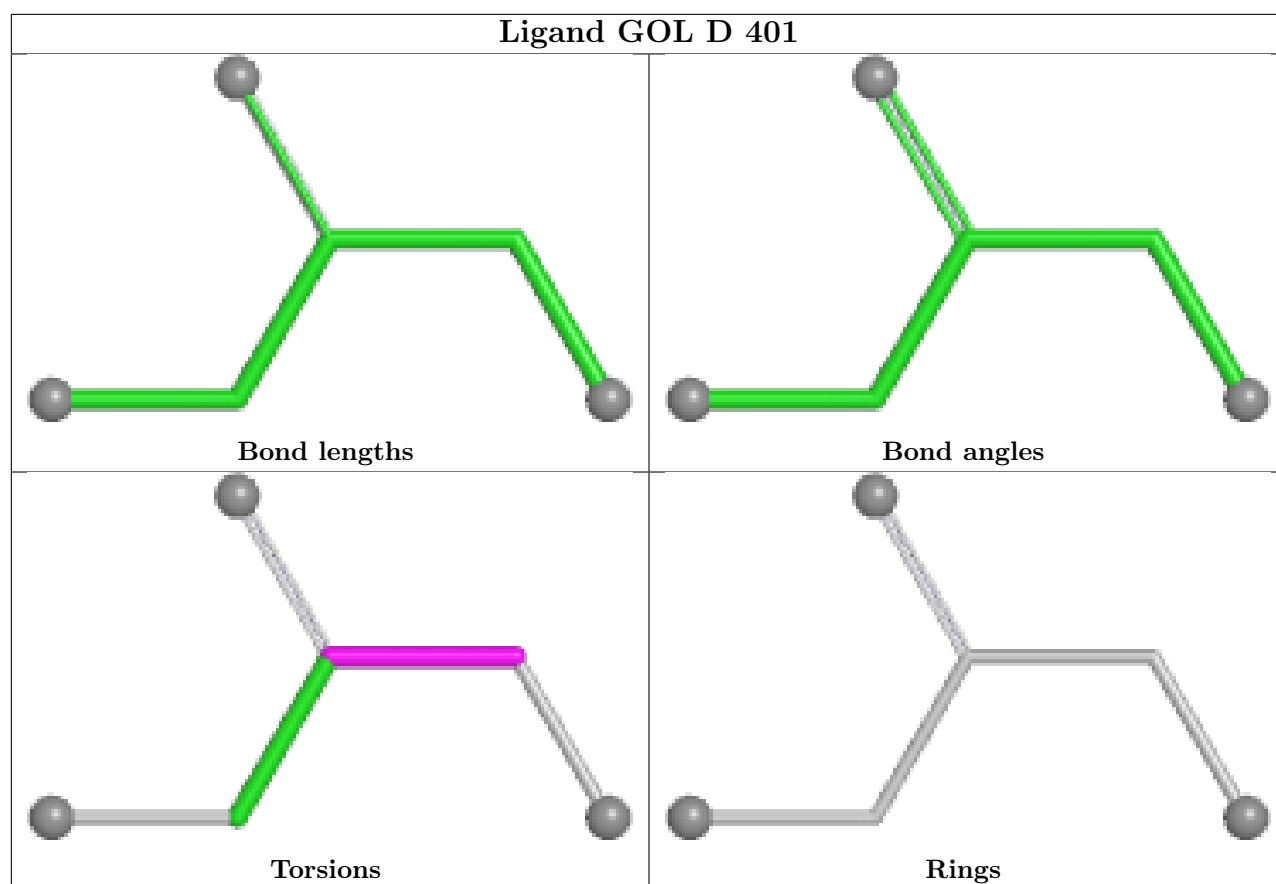












5.7 Other polymers [i](#)

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	279/303 (92%)	0.64	24 (8%)	16 14	30, 50, 85, 107	0
1	B	272/303 (89%)	1.00	46 (16%)	4 3	43, 62, 94, 107	0
1	C	273/303 (90%)	1.04	42 (15%)	5 4	30, 67, 96, 117	0
1	D	282/303 (93%)	0.64	31 (10%)	10 8	38, 54, 87, 122	0
1	E	278/303 (91%)	0.75	23 (8%)	17 15	46, 63, 92, 115	0
1	F	271/303 (89%)	1.15	50 (18%)	3 2	30, 65, 103, 110	0
All	All	1655/1818 (91%)	0.86	216 (13%)	7 5	30, 60, 96, 122	0

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	153	SER	9.5
1	F	235	VAL	7.0
1	F	125	GLY	7.0
1	A	153	SER	6.6
1	F	82	THR	6.5
1	A	154	ALA	6.2
1	A	93	TYR	6.2
1	C	154	ALA	6.1
1	C	146	PRO	6.0
1	A	152	LEU	5.8
1	C	45	LEU	5.8
1	A	150	PRO	5.7
1	B	108	ALA	5.6
1	A	116	GLY	5.6
1	D	1	MET	5.5
1	B	110	PRO	5.3
1	A	16	ASP	5.2
1	F	68	LEU	5.2
1	D	229	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	232	VAL	5.2
1	D	235	VAL	5.1
1	A	18	PRO	5.0
1	B	109	PRO	5.0
1	D	157	ASP	5.0
1	F	81	ALA	4.9
1	B	235	VAL	4.8
1	A	115	THR	4.6
1	F	50	ARG	4.5
1	F	126	CYS	4.4
1	C	83	ALA	4.4
1	B	74	THR	4.3
1	A	92	THR	4.3
1	B	75	ALA	4.3
1	B	76	ASP	4.2
1	D	291	ALA	4.2
1	C	155	ASP	4.1
1	B	228	PRO	4.1
1	A	235	VAL	4.0
1	E	17	GLY	4.0
1	F	49	GLY	4.0
1	C	145	ASP	4.0
1	C	121	ALA	3.9
1	D	154	ALA	3.9
1	B	227	GLN	3.9
1	B	46	THR	3.8
1	E	20	PRO	3.8
1	B	83	ALA	3.7
1	F	228	PRO	3.7
1	B	47	HIS	3.7
1	B	45	LEU	3.6
1	D	158	LEU	3.6
1	B	234	THR	3.6
1	D	236	GLY	3.5
1	F	75	ALA	3.5
1	A	149	ARG	3.5
1	D	84	ARG	3.5
1	C	23	TYR	3.4
1	D	155	ASP	3.4
1	B	92	THR	3.4
1	E	229	VAL	3.4
1	B	49	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	48	ILE	3.4
1	A	234	THR	3.4
1	C	44	LEU	3.3
1	D	102	PRO	3.3
1	B	24	VAL	3.3
1	E	19	ASP	3.3
1	C	46	THR	3.3
1	D	234	THR	3.3
1	F	236	GLY	3.2
1	C	21	ALA	3.2
1	F	11	LEU	3.2
1	A	228	PRO	3.2
1	A	155	ASP	3.2
1	F	14	ILE	3.2
1	B	50	ARG	3.1
1	F	210	ASP	3.1
1	F	93	TYR	3.1
1	B	77	ARG	3.1
1	B	95	PHE	3.1
1	D	108	ALA	3.0
1	C	72	SER	3.0
1	F	158	LEU	3.0
1	A	232	VAL	2.9
1	F	95	PHE	2.9
1	F	10	ALA	2.9
1	F	23	TYR	2.9
1	B	289	ALA	2.9
1	D	92	THR	2.9
1	E	83	ALA	2.9
1	F	94	ALA	2.9
1	B	146	PRO	2.8
1	F	220	GLY	2.8
1	C	102	PRO	2.8
1	E	146	PRO	2.8
1	A	108	ALA	2.8
1	B	15	VAL	2.8
1	B	80	THR	2.8
1	F	15	VAL	2.8
1	F	234	THR	2.8
1	C	258	ASP	2.8
1	F	153	SER	2.8
1	C	108	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	149	ARG	2.8
1	C	235	VAL	2.8
1	E	76	ASP	2.7
1	C	117	SER	2.7
1	F	124	PRO	2.7
1	C	132	LEU	2.7
1	A	83	ALA	2.7
1	D	289	ALA	2.7
1	A	113	VAL	2.7
1	C	103	ASP	2.7
1	D	233	ASP	2.7
1	C	282	SER	2.7
1	B	52	ALA	2.6
1	B	94	ALA	2.6
1	E	104	THR	2.6
1	F	69	VAL	2.6
1	B	102	PRO	2.6
1	D	20	PRO	2.6
1	F	121	ALA	2.6
1	D	156	PRO	2.6
1	F	290	GLY	2.6
1	B	2	ALA	2.5
1	C	52	ALA	2.5
1	C	199	CYS	2.5
1	D	16	ASP	2.5
1	D	18	PRO	2.5
1	D	150	PRO	2.5
1	C	152	LEU	2.5
1	E	72	SER	2.5
1	B	14	ILE	2.5
1	B	60	TYR	2.5
1	E	52	ALA	2.5
1	B	73	GLN	2.5
1	B	48	ILE	2.5
1	F	60	TYR	2.4
1	D	76	ASP	2.4
1	B	107	VAL	2.4
1	F	1	MET	2.4
1	C	59	GLU	2.4
1	F	74	THR	2.4
1	D	95	PHE	2.4
1	C	227	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	98	GLU	2.4
1	C	233	ASP	2.4
1	C	2	ALA	2.4
1	E	36	ALA	2.4
1	E	121	ALA	2.4
1	F	21	ALA	2.4
1	C	14	ILE	2.4
1	C	15	VAL	2.4
1	B	23	TYR	2.3
1	B	93	TYR	2.3
1	B	17	GLY	2.3
1	F	289	ALA	2.3
1	C	273	SER	2.3
1	F	24	VAL	2.3
1	B	233	ASP	2.3
1	C	147	ASN	2.3
1	F	58	ALA	2.3
1	B	78	THR	2.3
1	E	234	THR	2.3
1	F	72	SER	2.3
1	D	19	ASP	2.3
1	E	108	ALA	2.3
1	C	100	GLN	2.3
1	E	23	TYR	2.3
1	C	291	ALA	2.3
1	A	95	PHE	2.2
1	A	210	ASP	2.2
1	D	146	PRO	2.2
1	E	228	PRO	2.2
1	F	102	PRO	2.2
1	F	191	GLN	2.2
1	B	127	LEU	2.2
1	F	148	VAL	2.2
1	F	22	GLU	2.2
1	A	289	ALA	2.2
1	B	81	ALA	2.2
1	B	121	ALA	2.2
1	E	226	ALA	2.2
1	F	131	ALA	2.2
1	E	12	ILE	2.2
1	E	210	ASP	2.2
1	D	290	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	151	SER	2.2
1	D	93	TYR	2.2
1	B	65	GLY	2.2
1	C	290	GLY	2.2
1	D	17	GLY	2.2
1	F	73	GLN	2.2
1	E	151	SER	2.2
1	F	46	THR	2.2
1	C	93	TYR	2.1
1	A	156	PRO	2.1
1	B	22	GLU	2.1
1	F	130	ALA	2.1
1	B	70	SER	2.1
1	D	151	SER	2.1
1	F	97	LEU	2.1
1	F	129	VAL	2.1
1	C	95	PHE	2.1
1	C	226	ALA	2.1
1	F	62	GLU	2.1
1	E	152	LEU	2.1
1	A	19	ASP	2.1
1	B	51	ASP	2.1
1	C	292	ASP	2.1
1	E	15	VAL	2.1
1	B	96	ASP	2.0
1	E	258	ASP	2.0
1	F	79	PRO	2.0
1	D	148	VAL	2.0
1	F	117	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 ⓘ

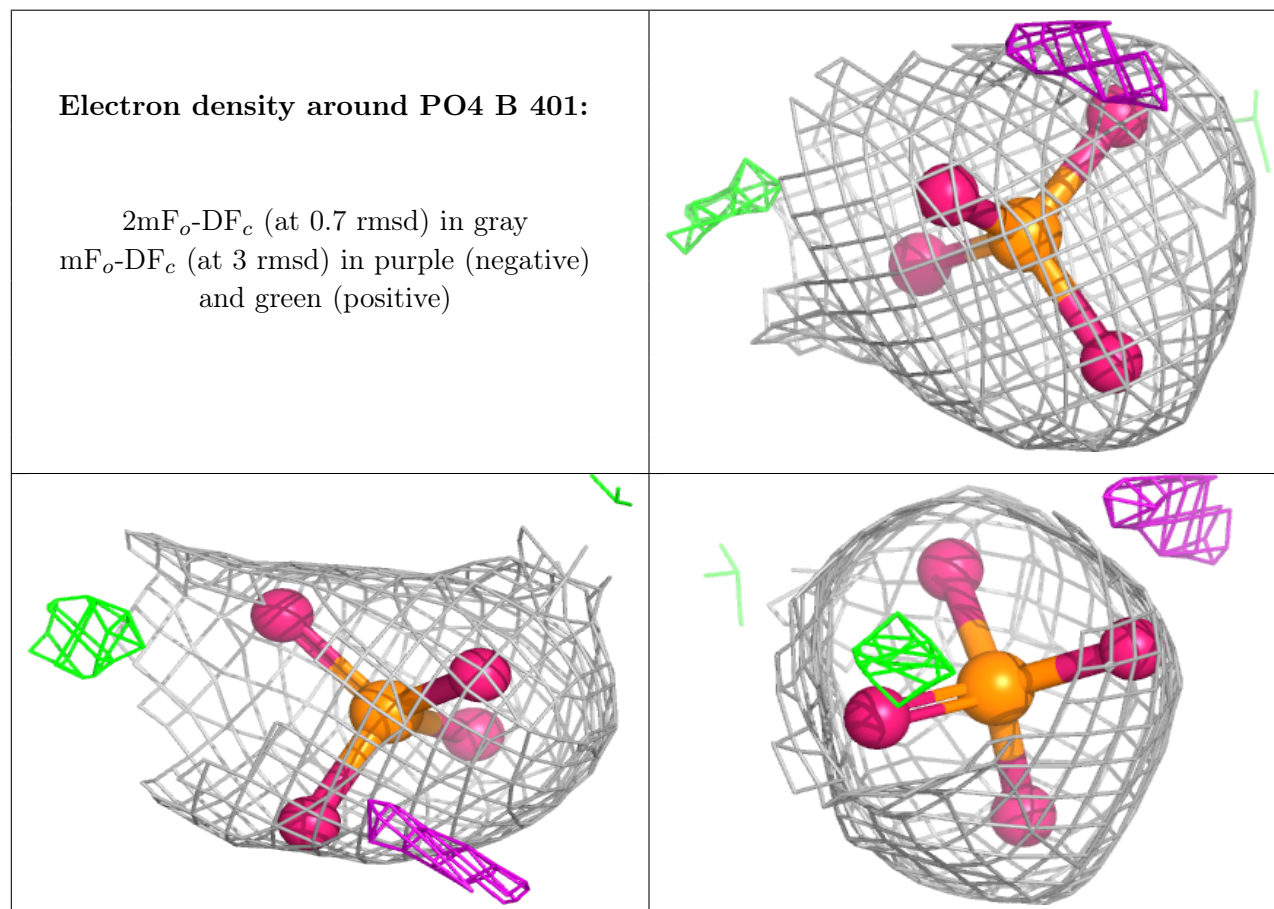
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

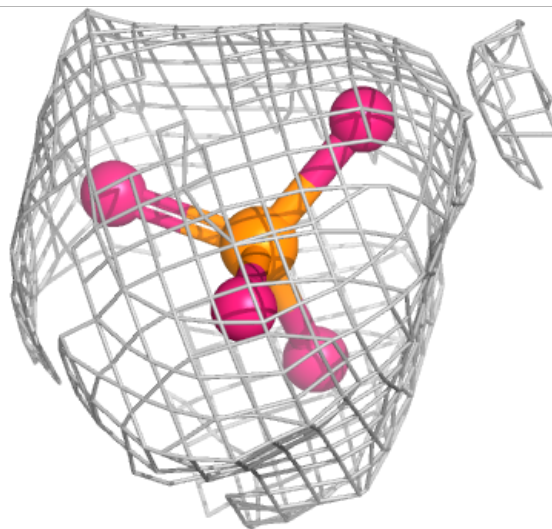
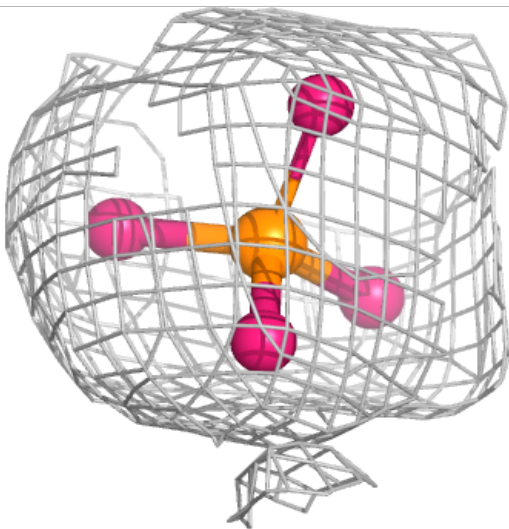
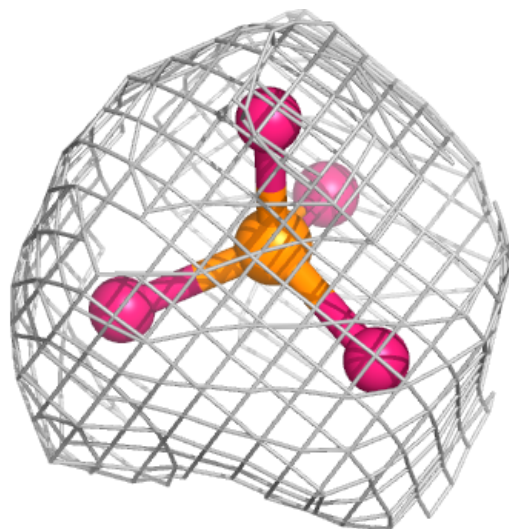
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PO4	B	401	5/5	0.70	0.11	88,99,104,105	0
3	PO4	F	401	5/5	0.73	0.08	107,110,112,122	0
2	GOL	A	401	6/6	0.78	0.19	52,70,75,78	0
2	GOL	D	401	6/6	0.80	0.18	50,68,74,77	0
3	PO4	D	402	5/5	0.83	0.10	80,81,88,96	0
3	PO4	A	402	5/5	0.83	0.09	73,75,84,84	0
3	PO4	E	402	5/5	0.86	0.08	84,87,93,96	0
2	GOL	E	401	6/6	0.86	0.19	74,76,80,87	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.



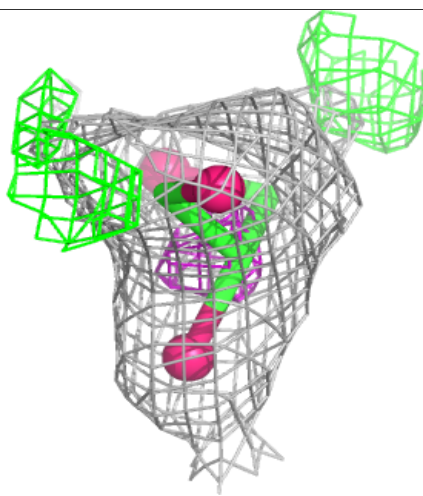
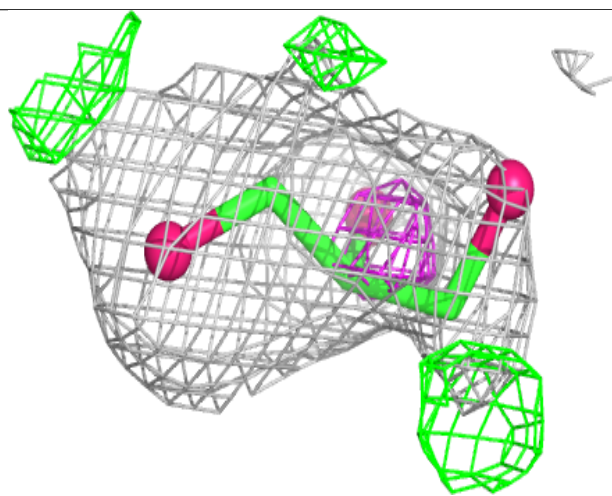
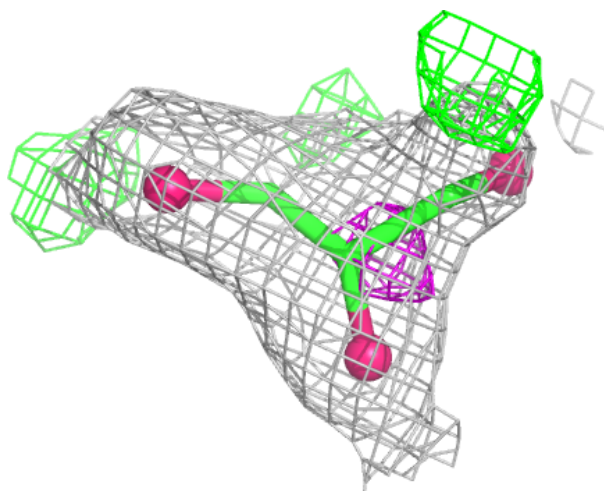
Electron density around PO4 F 401:

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



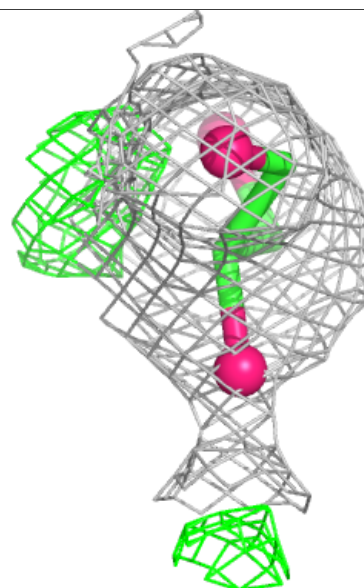
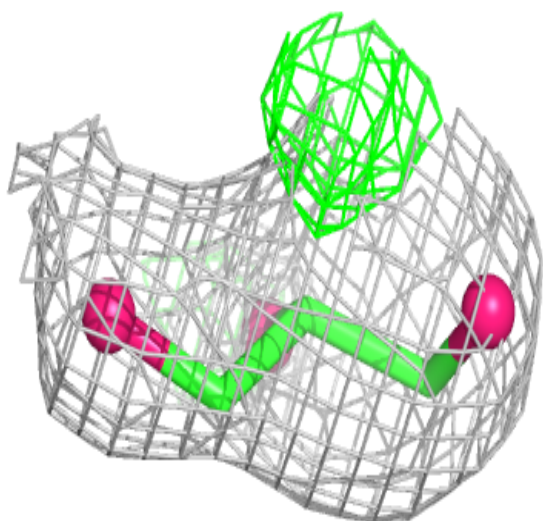
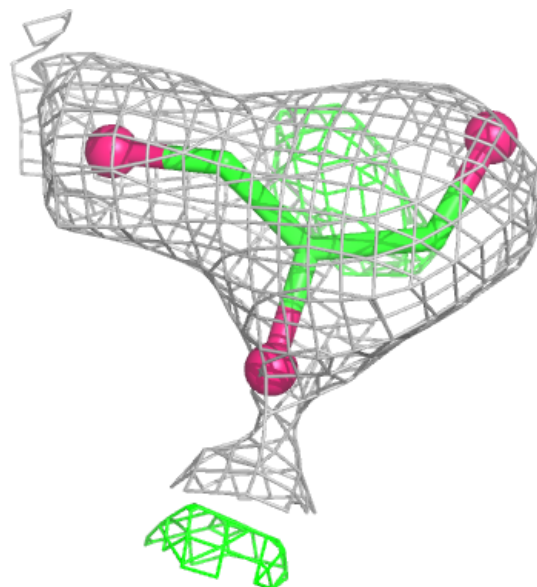
Electron density around GOL A 401:

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



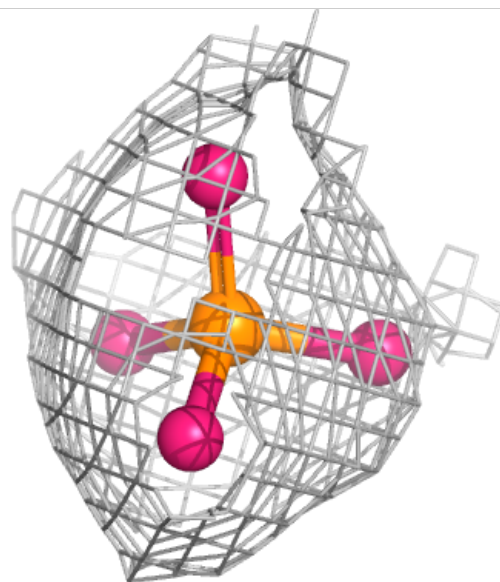
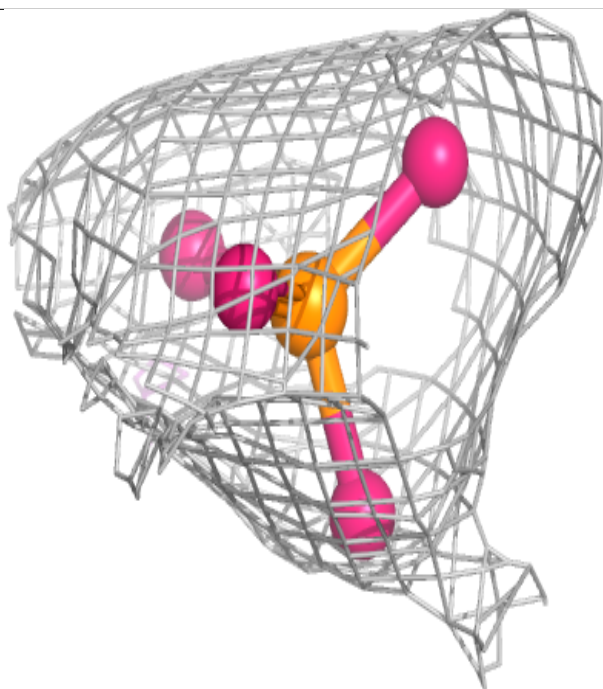
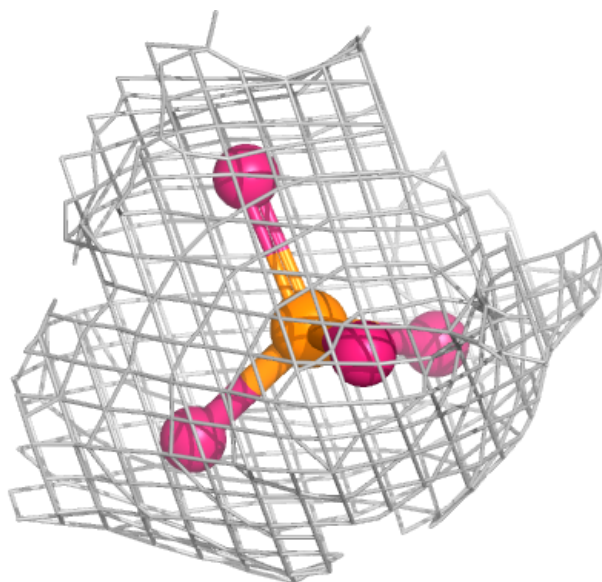
Electron density around GOL D 401:

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



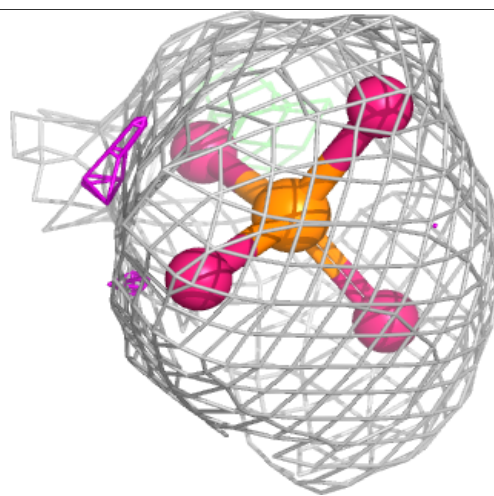
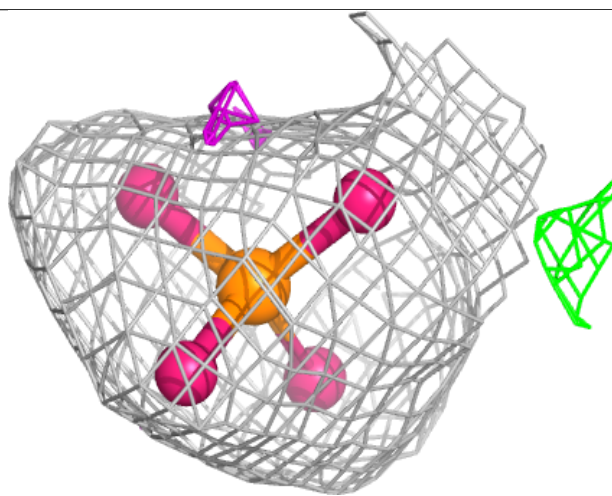
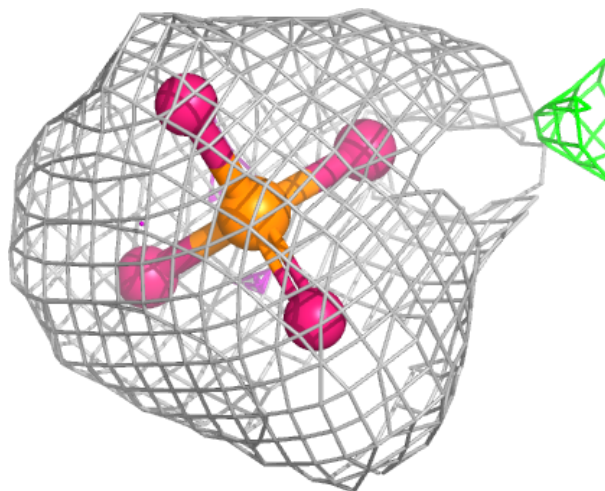
Electron density around PO4 D 402:

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



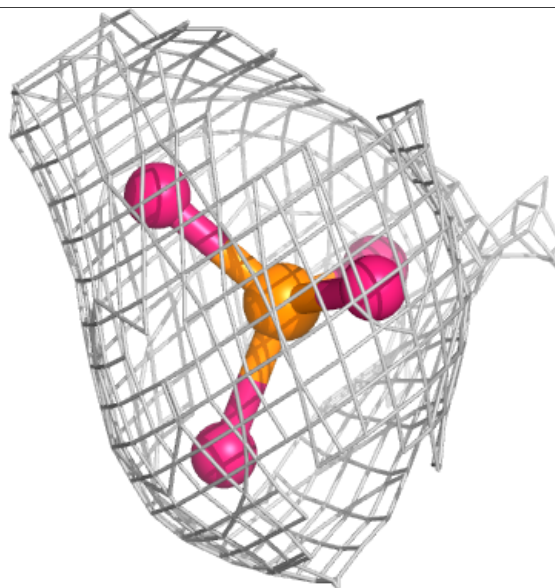
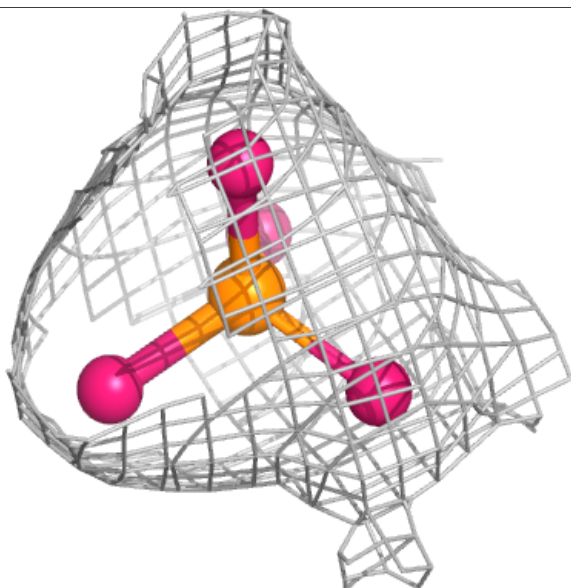
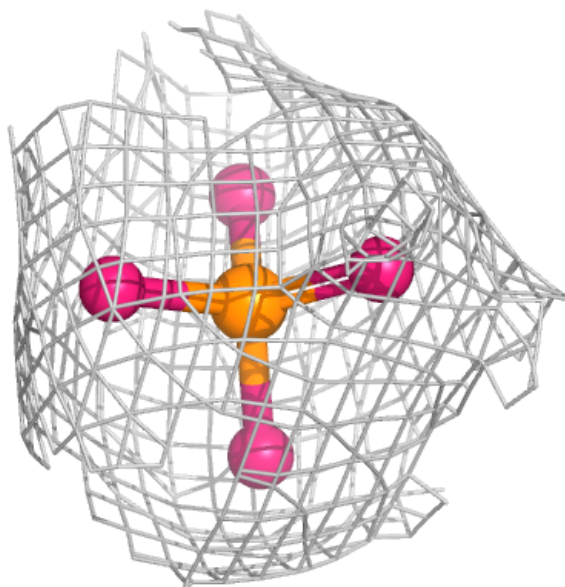
Electron density around PO4 A 402:

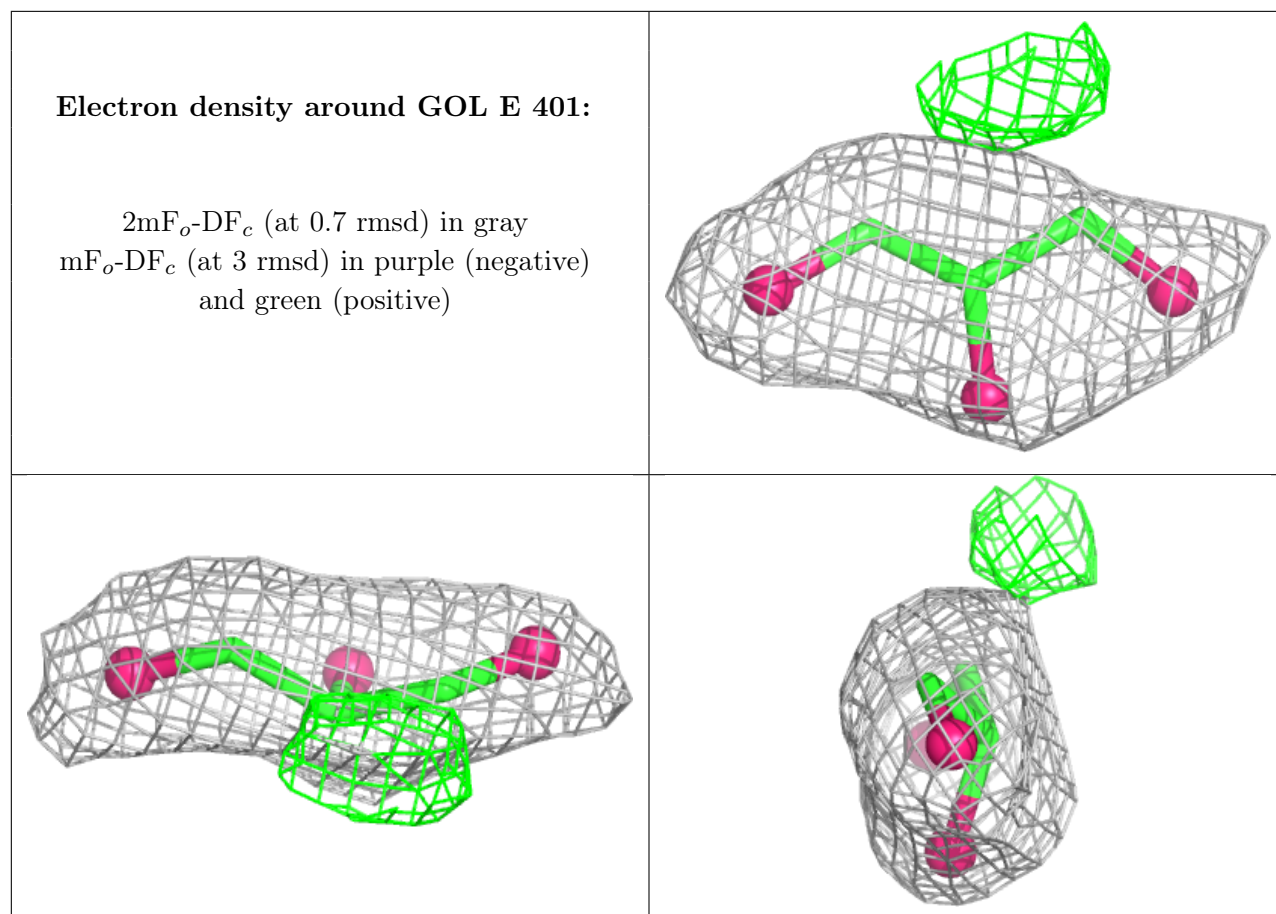
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PO4 E 402:

$2mF_o-DF_c$ (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.