



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:44 PM UTC

PDB ID : 7UEH / pdb_00007ueh
Title : Pyruvate kinase from Zymomonas mobilis
Authors : McFarlane, J.S.; Meneely, K.M.; Lamb, A.L.
Deposited on : 2022-03-21
Resolution : 2.40 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

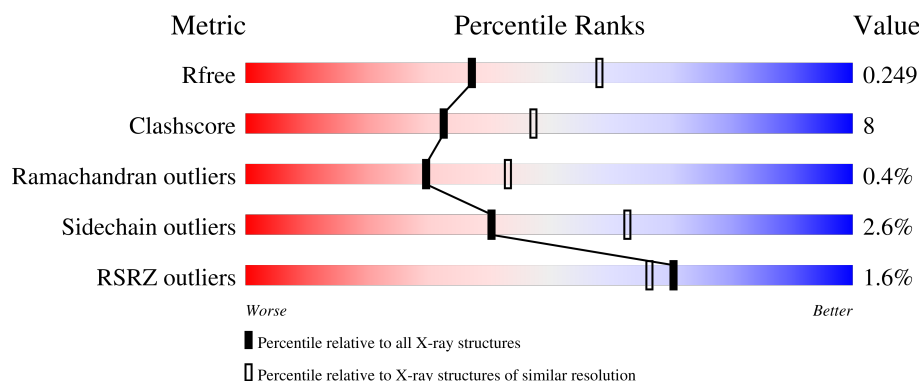
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	475	80% 18% .
1	B	475	88% 12% .
1	C	475	79% 18% ..
1	D	475	70% 26% ..
1	E	475	71% 9% 20%

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Mol	Chain	Length	Quality of chain
1	F	475	
1	G	475	
1	H	475	

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
2	GOL	E	501	-	X	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 56326 atoms, of which 28207 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 Pyruvate kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	G	473	Total	C	H	N	O	S	0	0	0
			7314	2279	3710	634	682	9			
1	A	473	Total	C	H	N	O	S	0	0	0
			7313	2279	3709	634	682	9			
1	B	472	Total	C	H	N	O	S	0	0	0
			7298	2274	3703	633	679	9			
1	H	473	Total	C	H	N	O	S	0	0	0
			7313	2279	3709	634	682	9			
1	E	382	Total	C	H	N	O	S	0	0	0
			5886	1828	2993	512	545	8			
1	F	386	Total	C	H	N	O	S	0	0	0
			5951	1854	3023	514	552	8			
1	C	468	Total	C	H	N	O	S	0	0	0
			7235	2255	3668	628	675	9			
1	D	464	Total	C	H	N	O	S	0	0	0
			7193	2239	3654	624	667	9			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	H	O	0	0
			14	3	8	3		
2	G	1	Total	C	H	O	0	0
			13	3	7	3		
2	G	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			13	3	7	3		
2	E	1	Total	C	H	O	0	0
			14	3	8	3		

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	116	Total	O	0	0
			116	116		
4	A	103	Total	O	0	0
			103	103		
4	B	125	Total	O	0	0
			125	125		
4	H	87	Total	O	0	0
			87	87		

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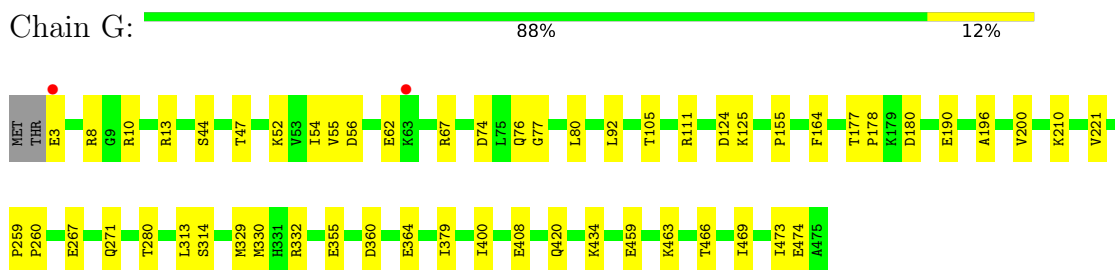
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	93	Total 93	O 93	0	0
4	F	77	Total 77	O 77	0	0
4	C	79	Total 79	O 79	0	0
4	D	35	Total 35	O 35	0	0

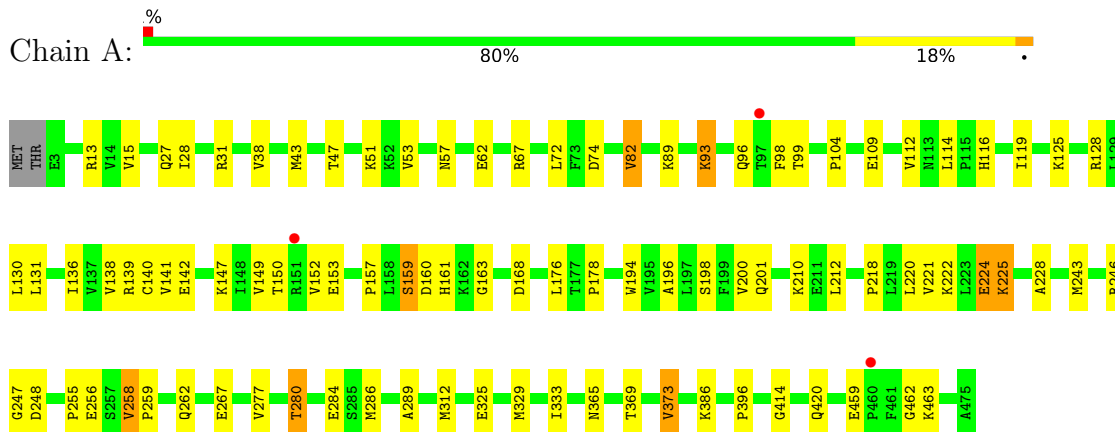
3 Residue-property plots

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.

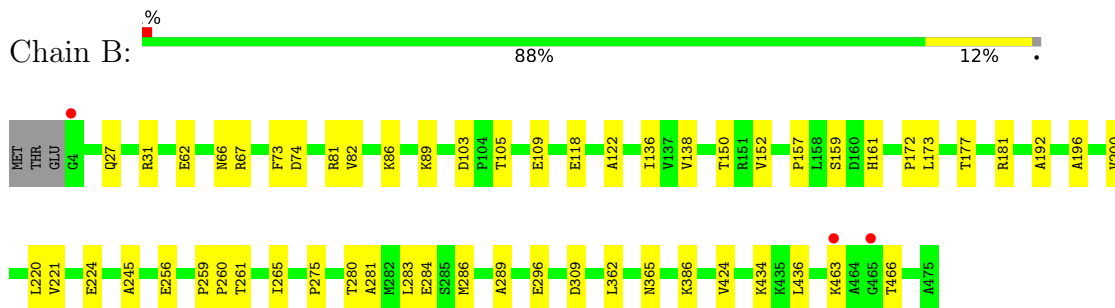
• Molecule 1: Pyruvate kinase



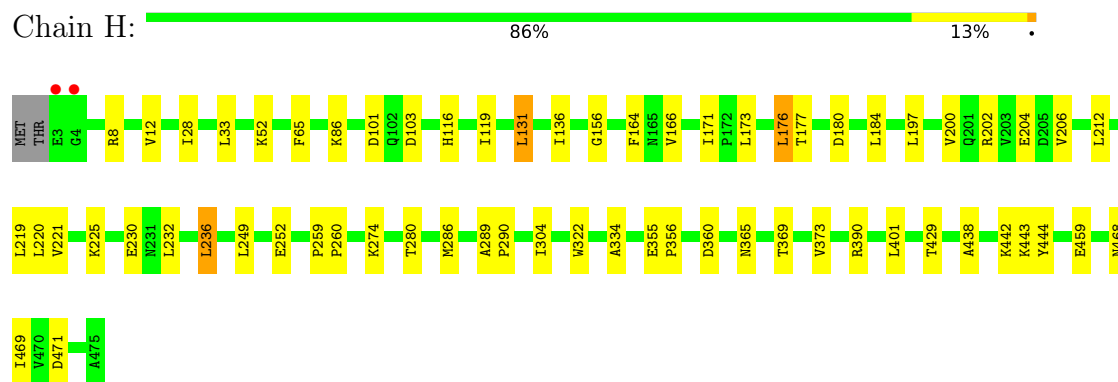
• Molecule 1: Pyruvate kinase



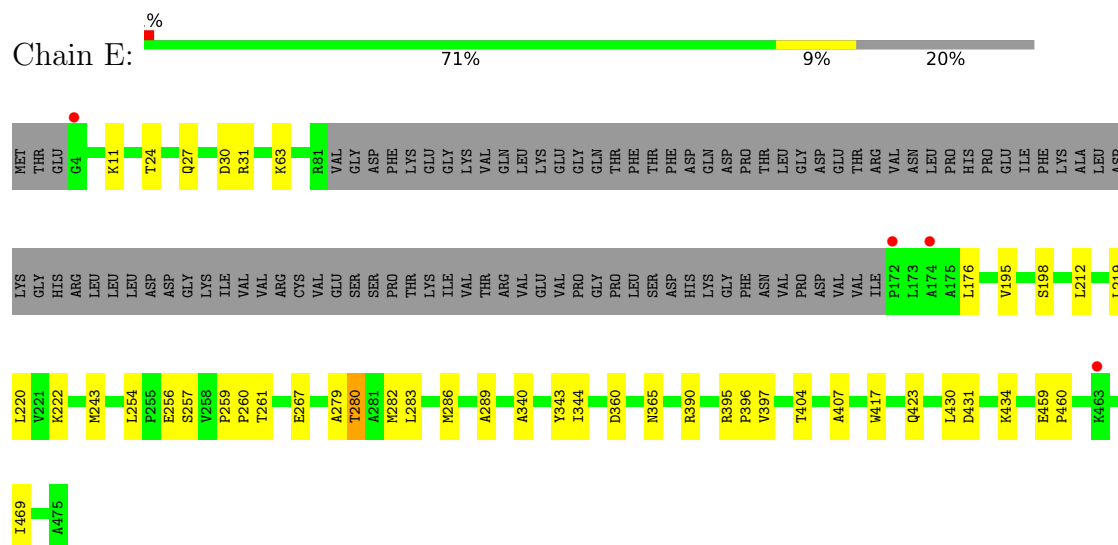
• Molecule 1: Pyruvate kinase



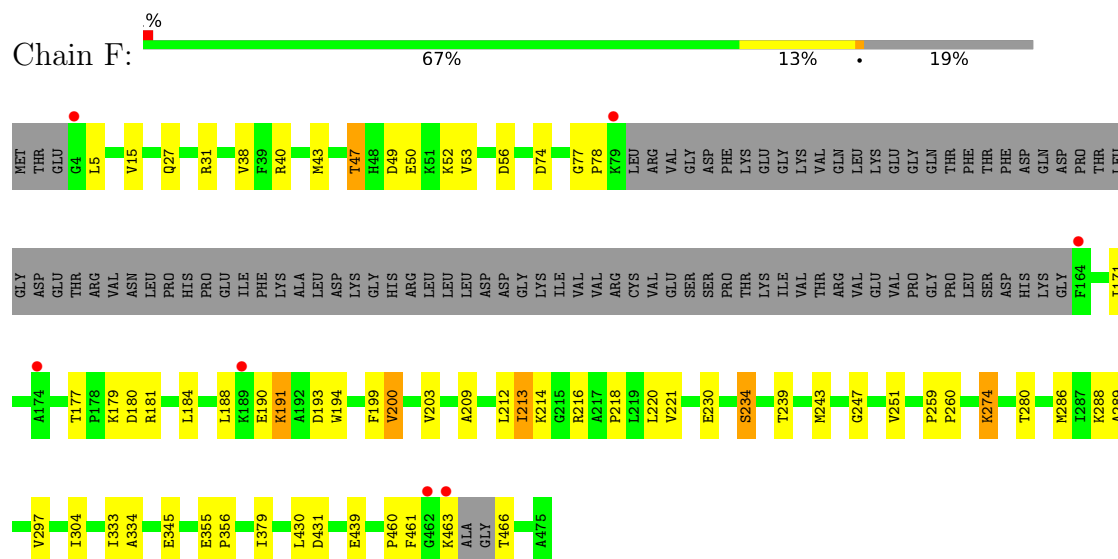
• Molecule 1: Pyruvate kinase



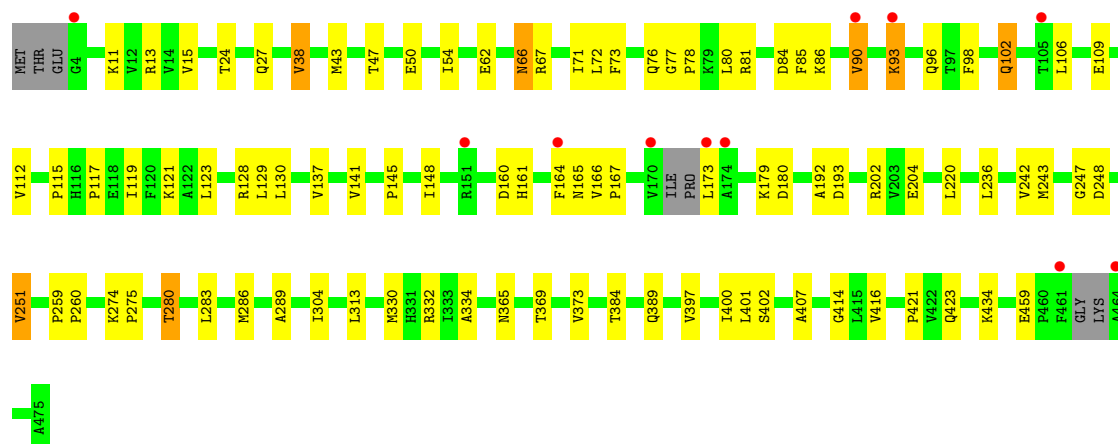
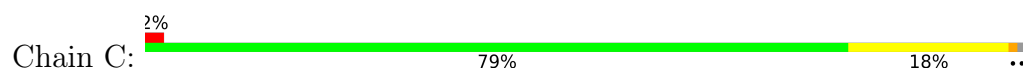
• Molecule 1: Pyruvate kinase



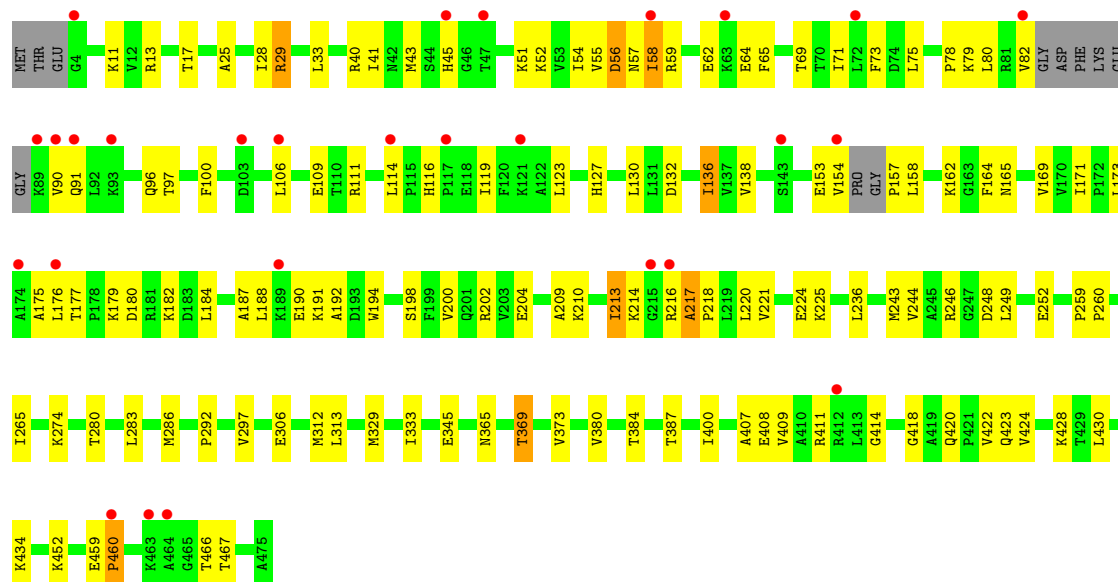
• Molecule 1: Pyruvate kinase



• Molecule 1: Pyruvate kinase



• Molecule 1: Pyruvate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	207.93Å 256.13Å 82.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.33 – 2.40 96.33 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.0 (96.33-2.40) 91.9 (96.33-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.40Å)	Xtriage
Refinement program	REFMAC 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.185 , 0.246 0.196 , 0.249	Depositor DCC
R_{free} test set	7841 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	56326	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.59	2/3667 (0.1%)	0.72	0/4977
1	B	0.58	0/3658	0.75	0/4965
1	C	0.56	0/3627	0.73	0/4920
1	D	0.55	0/3598	0.77	0/4881
1	E	0.58	0/2940	0.72	0/3988
1	F	0.55	0/2976	0.72	1/4040 (0.0%)
1	G	0.59	1/3667 (0.0%)	0.72	0/4977
1	H	0.58	0/3667	0.73	0/4977
All	All	0.57	3/27800 (0.0%)	0.73	1/37725 (0.0%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	420	GLN	C-O	-7.64	1.20	1.23
1	A	258	VAL	CA-CB	6.04	1.57	1.54
1	G	314	SER	CA-C	6.03	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	461	PHE	N-CA-C	5.17	118.72	112.93

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	217	ALA	Peptide

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	3604	3709	3709	62	0
1	B	3595	3703	3703	38	0
1	C	3567	3668	3667	72	0
1	D	3539	3654	3654	128	0
1	E	2893	2993	2993	33	0
1	F	2928	3023	3023	44	0
1	G	3604	3710	3709	34	0
1	H	3604	3709	3709	41	0
2	A	6	7	8	0	0
2	E	6	8	8	5	0
2	G	18	23	23	5	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	1	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
4	A	103	0	0	3	0
4	B	125	0	0	0	0
4	C	79	0	0	2	0
4	D	35	0	0	3	0
4	E	93	0	0	1	0
4	F	77	0	0	1	0
4	G	116	0	0	3	0
4	H	87	0	0	2	0
All	All	28119	28207	28206	439	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 (439) 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:D:213:ILE:HG21	1:D:217:ALA:HB3	1.19	1.16
1:A:243:MET:HE2	1:A:312:MET:HE1	1.17	1.11
1:D:58:ILE:HD11	1:D:71:ILE:HD11	1.31	1.10
1:C:80:LEU:HD13	1:C:119:ILE:HD11	1.37	1.05
1:D:29:ARG:NH2	1:D:64:GLU:OE2	1.93	1.01
1:D:213:ILE:HG21	1:D:217:ALA:CB	1.93	0.99
1:D:243:MET:HE2	1:D:312:MET:HE1	1.46	0.96
1:D:58:ILE:HD11	1:D:71:ILE:CD1	2.06	0.84
1:D:184:LEU:HD11	1:D:213:ILE:CD1	2.07	0.84
1:B:200:VAL:HG21	1:B:221:VAL:HG23	1.57	0.83
1:A:93:LYS:N	1:A:96:GLN:OE1	2.11	0.83
1:D:200:VAL:HG21	1:D:221:VAL:HG13	1.59	0.81
1:C:15:VAL:HG22	1:C:38:VAL:CG2	2.12	0.79
1:H:131:LEU:HD23	1:H:164:PHE:HB3	1.64	0.79
1:D:213:ILE:CG2	1:D:217:ALA:HB3	2.08	0.78
1:D:243:MET:CE	1:D:312:MET:HE1	2.13	0.78
1:D:28:ILE:HG21	1:D:58:ILE:HG22	1.64	0.78
1:C:90:VAL:HG13	1:C:109:GLU:HG3	1.66	0.77
1:H:177:THR:HG23	1:H:180:ASP:H	1.50	0.77
1:B:136:ILE:HD11	1:B:157:PRO:O	1.86	0.76
1:D:286:MET:HE2	1:D:292:PRO:HB3	1.68	0.74
1:F:463:LYS:HG2	1:F:466:THR:HG21	1.70	0.73
1:D:55:VAL:HG21	1:D:190:GLU:OE1	1.89	0.73
1:E:344:ILE:HB	2:E:501:GOL:H32	1.69	0.73
1:C:313:LEU:HG	1:C:330:MET:HE2	1.71	0.72
1:F:463:LYS:CG	1:F:466:THR:HG21	2.19	0.72
1:F:209:ALA:O	1:F:213:ILE:HG13	1.89	0.72
1:C:24:THR:HG23	1:C:27:GLN:H	1.55	0.71
1:D:184:LEU:HD11	1:D:213:ILE:HD11	1.71	0.71
1:G:200:VAL:HG21	1:G:221:VAL:HG13	1.72	0.70
1:D:43:MET:HE1	1:D:51:LYS:HG3	1.73	0.70
1:D:173:LEU:O	1:D:202:ARG:NH2	2.23	0.70
1:F:43:MET:O	1:F:179:LYS:NZ	2.25	0.69
1:C:78:PRO:HB2	1:C:173:LEU:HD23	1.72	0.69
1:C:85:PHE:CZ	1:C:112:VAL:HG21	2.27	0.69
1:C:98:PHE:HZ	1:C:112:VAL:HG23	1.57	0.69
1:A:136:ILE:HD11	1:A:157:PRO:O	1.91	0.69
1:F:230:GLU:OE2	4:F:601:HOH:O	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:THR:OG1	1:D:467:THR:HG21	1.93	0.69
1:D:25:ALA:HB2	1:D:57:ASN:ND2	2.08	0.69
1:C:102:GLN:NE2	1:C:145:PRO:O	2.26	0.68
1:D:184:LEU:HD11	1:D:213:ILE:HD13	1.75	0.68
1:D:82:VAL:HG23	1:D:164:PHE:CD1	2.29	0.67
1:H:202:ARG:HD3	4:H:681:HOH:O	1.95	0.67
1:A:243:MET:HE2	1:A:312:MET:CE	2.11	0.67
1:H:131:LEU:HD12	1:H:136:ILE:CG2	2.25	0.66
1:F:463:LYS:HE3	1:F:466:THR:HB	1.76	0.66
1:D:106:LEU:O	1:D:111:ARG:NH1	2.28	0.65
1:H:177:THR:HG21	4:H:632:HOH:O	1.97	0.65
1:C:43:MET:CE	1:C:73:PHE:HD2	2.08	0.65
1:C:365:ASN:HB3	1:D:365:ASN:HB3	1.78	0.65
1:D:90:VAL:HG11	1:D:109:GLU:HA	1.76	0.65
1:C:43:MET:HE3	1:C:73:PHE:HD2	1.61	0.65
1:G:74:ASP:HA	1:G:196:ALA:HB3	1.78	0.65
1:A:138:VAL:HG12	1:A:152:VAL:HA	1.78	0.65
1:C:15:VAL:HG22	1:C:38:VAL:HG21	1.79	0.65
1:D:171:ILE:HD12	1:D:173:LEU:HD12	1.77	0.64
1:H:200:VAL:HG21	1:H:221:VAL:HG13	1.80	0.64
1:D:171:ILE:O	1:D:173:LEU:N	2.29	0.64
1:D:13:ARG:HD3	1:D:414:GLY:O	1.98	0.63
1:C:15:VAL:HG22	1:C:38:VAL:HG22	1.80	0.63
1:D:400:ILE:O	1:D:420:GLN:NE2	2.31	0.63
1:A:15:VAL:HG22	1:A:38:VAL:HB	1.80	0.62
1:C:43:MET:CE	1:C:73:PHE:CD2	2.83	0.62
1:D:154:VAL:HG12	1:D:154:VAL:O	1.99	0.62
1:B:200:VAL:HG21	1:B:221:VAL:CG2	2.29	0.62
1:A:267:GLU:OE1	4:A:601:HOH:O	2.16	0.62
1:D:329:MET:HE3	1:D:333:ILE:HG13	1.81	0.61
1:D:28:ILE:CG2	1:D:58:ILE:HG22	2.31	0.61
1:D:460:PRO:HG2	1:D:466:THR:HB	1.83	0.61
1:H:131:LEU:HD23	1:H:164:PHE:CB	2.30	0.61
1:D:194:TRP:CZ3	1:D:218:PRO:HB2	2.36	0.60
1:D:407:ALA:HB2	1:D:423:GLN:NE2	2.16	0.60
1:B:89:LYS:HG3	1:B:159:SER:HB3	1.83	0.60
1:H:184:LEU:HD23	1:H:212:LEU:CD2	2.31	0.60
1:A:176:LEU:CD1	1:A:212:LEU:HD12	2.32	0.60
1:F:49:ASP:O	1:F:53:VAL:HG23	2.02	0.60
1:C:98:PHE:CZ	1:C:112:VAL:HG23	2.35	0.60
1:F:5:LEU:HD13	1:F:5:LEU:C	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:GLU:OE1	1:B:118:GLU:N	2.33	0.59
1:A:220:LEU:HD21	1:A:243:MET:HB2	1.84	0.59
1:F:463:LYS:HG2	1:F:466:THR:OG1	2.03	0.59
1:H:177:THR:HG22	1:H:180:ASP:CG	2.28	0.59
1:A:176:LEU:HD12	1:A:212:LEU:HD12	1.84	0.59
1:C:123:LEU:CD1	1:C:148:ILE:HD13	2.33	0.59
1:A:62:GLU:HG2	1:A:67:ARG:O	2.03	0.58
1:B:138:VAL:CG1	1:B:150:THR:OG1	2.52	0.58
1:F:200:VAL:HG21	1:F:221:VAL:HG13	1.84	0.58
1:E:459:GLU:CG	1:E:469:ILE:HD11	2.33	0.58
1:D:80:LEU:HB3	1:D:164:PHE:CZ	2.39	0.58
1:G:124:ASP:OD1	1:G:125:LYS:N	2.34	0.58
1:C:236:LEU:HD22	1:C:242:VAL:HG21	1.85	0.58
1:C:247:GLY:CA	1:C:280:THR:HG21	2.34	0.58
1:D:171:ILE:CD1	1:D:173:LEU:HD12	2.33	0.58
1:F:463:LYS:HG2	1:F:466:THR:CG2	2.33	0.58
1:D:58:ILE:HD11	1:D:71:ILE:CG1	2.34	0.58
1:F:52:LYS:HD2	1:F:190:GLU:OE1	2.04	0.57
1:H:177:THR:HG22	1:H:180:ASP:OD2	2.05	0.57
1:E:340:ALA:O	2:E:501:GOL:H12	2.05	0.57
1:C:220:LEU:HD23	1:C:220:LEU:C	2.30	0.57
1:C:459:GLU:OE2	1:D:434:LYS:HE3	2.05	0.57
1:A:325:GLU:N	1:A:325:GLU:OE1	2.36	0.57
1:C:76:GLN:OE1	1:C:179:LYS:HE3	2.04	0.57
1:G:267:GLU:HG2	4:G:638:HOH:O	2.05	0.57
1:D:90:VAL:HG13	1:D:109:GLU:HB3	1.86	0.57
1:F:15:VAL:HG22	1:F:38:VAL:HB	1.87	0.56
1:H:131:LEU:HD12	1:H:136:ILE:HG21	1.86	0.56
1:E:430:LEU:O	1:E:434:LYS:HG3	2.05	0.56
1:B:224:GLU:HG2	1:B:245:ALA:HB3	1.86	0.56
1:A:72:LEU:HD11	1:A:196:ALA:HB2	1.86	0.56
1:D:175:ALA:HB1	1:D:198:SER:O	2.06	0.56
1:H:101:ASP:HB3	1:H:103:ASP:H	1.70	0.55
1:H:459:GLU:O	1:H:459:GLU:HG2	2.06	0.55
1:C:78:PRO:CB	1:C:173:LEU:HD23	2.37	0.55
1:H:304:ILE:HD13	1:H:334:ALA:HA	1.89	0.55
1:F:193:ASP:O	1:F:218:PRO:HD2	2.06	0.55
1:D:29:ARG:HH21	1:D:64:GLU:CD	2.11	0.55
1:C:90:VAL:CG1	1:C:109:GLU:HG3	2.36	0.55
1:C:85:PHE:CE2	1:C:112:VAL:CG2	2.90	0.54
1:D:17:THR:HA	1:D:40:ARG:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:THR:O	1:D:411:ARG:HG2	2.08	0.54
1:D:80:LEU:HB3	1:D:164:PHE:CE1	2.42	0.54
1:D:224:GLU:HG2	1:D:248:ASP:HB2	1.90	0.54
1:A:139:ARG:NE	1:A:153:GLU:OE2	2.36	0.54
1:H:176:LEU:HD13	1:H:197:LEU:CD1	2.38	0.54
1:A:329:MET:HE3	1:A:333:ILE:HG13	1.90	0.54
1:B:118:GLU:HG2	1:B:173:LEU:HD13	1.89	0.54
1:D:82:VAL:HG23	1:D:164:PHE:CE1	2.42	0.54
1:A:82:VAL:O	1:A:161:HIS:HA	2.08	0.53
1:D:177:THR:OG1	1:D:180:ASP:N	2.36	0.53
1:G:332:ARG:HD2	1:E:256:GLU:OE2	2.08	0.53
1:B:138:VAL:HG12	1:B:150:THR:HB	1.90	0.53
1:D:82:VAL:HG13	1:D:114:LEU:HD12	1.90	0.53
1:E:220:LEU:HD21	1:E:243:MET:HB2	1.91	0.53
1:D:216:ARG:NE	1:D:408:GLU:OE2	2.41	0.53
1:A:47:THR:O	1:A:51:LYS:HG3	2.08	0.53
1:A:462:GLY:O	1:A:463:LYS:HD3	2.08	0.53
1:A:104:PRO:HG3	1:H:204:GLU:HB3	1.90	0.53
1:D:33:LEU:HD21	1:D:65:PHE:CZ	2.44	0.52
1:B:138:VAL:CG1	1:B:150:THR:CB	2.86	0.52
1:H:131:LEU:HD12	1:H:136:ILE:HG22	1.90	0.52
1:D:286:MET:HE2	1:D:292:PRO:CB	2.37	0.52
1:G:52:LYS:HE3	1:G:56:ASP:OD1	2.08	0.52
1:E:343:TYR:HB3	2:E:501:GOL:C1	2.40	0.52
1:F:78:PRO:HA	1:F:177:THR:HG21	1.91	0.52
1:G:379:ILE:N	1:G:379:ILE:HD12	2.25	0.52
1:A:27:GLN:O	1:A:31:ARG:HG2	2.10	0.52
1:G:13:ARG:HH12	2:G:502:GOL:C1	2.22	0.52
1:B:138:VAL:HG11	1:B:150:THR:OG1	2.08	0.52
1:C:24:THR:HG22	1:C:27:GLN:CG	2.39	0.52
1:D:96:GLN:HG2	1:D:97:THR:O	2.10	0.52
1:A:142:GLU:HB2	1:A:149:VAL:CG1	2.40	0.52
1:C:123:LEU:HD13	1:C:148:ILE:HD13	1.92	0.52
1:C:275:PRO:HG3	1:C:416:VAL:HG22	1.91	0.52
1:F:304:ILE:HD13	1:F:334:ALA:HA	1.92	0.52
1:C:62:GLU:HG2	1:C:67:ARG:O	2.10	0.52
1:C:93:LYS:HG3	1:C:96:GLN:HB3	1.90	0.52
1:D:306:GLU:OE2	4:D:601:HOH:O	2.19	0.52
1:B:220:LEU:C	1:B:220:LEU:HD23	2.34	0.51
1:C:72:LEU:HD11	1:C:220:LEU:HD13	1.92	0.51
1:C:259:PRO:HB2	1:C:260:PRO:HD3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:365:ASN:CG	1:E:365:ASN:HB3	2.34	0.51
1:D:73:PHE:CD2	1:D:187:ALA:HB1	2.45	0.51
1:E:404:THR:O	1:E:423:GLN:HA	2.10	0.51
1:G:177:THR:HG22	1:G:180:ASP:CG	2.34	0.51
1:B:74:ASP:HA	1:B:196:ALA:HB3	1.91	0.51
1:B:261:THR:HG22	1:B:265:ILE:CD1	2.40	0.51
1:A:74:ASP:HA	1:A:196:ALA:HB3	1.93	0.51
1:B:27:GLN:O	1:B:31:ARG:HG2	2.10	0.51
1:C:119:ILE:HD13	1:C:164:PHE:CE1	2.45	0.51
1:D:188:LEU:HD11	1:D:213:ILE:HD13	1.93	0.51
1:H:220:LEU:HD23	1:H:220:LEU:C	2.35	0.51
1:B:259:PRO:HB2	1:B:260:PRO:HD3	1.92	0.50
1:D:100:PHE:CD2	1:D:114:LEU:HD13	2.46	0.50
1:G:267:GLU:O	1:G:271:GLN:HG3	2.10	0.50
1:A:286:MET:HA	1:A:289:ALA:O	2.11	0.50
1:C:85:PHE:CE2	1:C:112:VAL:HG21	2.46	0.50
1:G:459:GLU:HG3	1:F:430:LEU:HD21	1.94	0.50
1:H:33:LEU:HD21	1:H:65:PHE:CZ	2.47	0.50
1:G:408:GLU:OE1	2:G:503:GOL:H2	2.11	0.50
1:B:424:VAL:HB	1:B:436:LEU:HD21	1.93	0.50
1:D:25:ALA:HB2	1:D:57:ASN:HD22	1.76	0.50
1:C:373:VAL:CG1	1:C:373:VAL:O	2.59	0.50
1:D:283:LEU:HD13	1:D:286:MET:HE3	1.94	0.50
1:G:13:ARG:HH12	2:G:502:GOL:H12	1.77	0.49
1:D:90:VAL:HG11	1:D:109:GLU:CA	2.42	0.49
1:D:13:ARG:HD2	4:D:607:HOH:O	2.12	0.49
1:D:153:GLU:O	1:D:154:VAL:HG23	2.12	0.49
1:G:364:GLU:HG2	4:G:713:HOH:O	2.11	0.49
1:A:128:ARG:HG3	1:A:168:ASP:OD2	2.13	0.49
1:C:11:LYS:NZ	1:C:397:VAL:O	2.44	0.49
1:D:179:LYS:O	1:D:182:LYS:HB2	2.12	0.49
1:C:384:THR:OG1	3:C:501:PO4:O3	2.23	0.49
1:D:90:VAL:CG1	1:D:109:GLU:HB3	2.43	0.49
1:D:225:LYS:HE2	1:D:252:GLU:OE2	2.12	0.49
1:H:438:ALA:O	1:H:442:LYS:HG3	2.13	0.49
1:A:365:ASN:ND2	1:B:365:ASN:HB3	2.28	0.48
1:B:138:VAL:CG1	1:B:150:THR:HB	2.43	0.48
1:F:47:THR:OG1	1:F:50:GLU:HG3	2.13	0.48
1:D:11:LYS:HD3	4:D:630:HOH:O	2.12	0.48
1:A:365:ASN:CG	1:B:365:ASN:HB3	2.37	0.48
1:H:206:VAL:HG13	1:H:219:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ALA:HB2	1:B:172:PRO:HD3	1.94	0.48
1:C:47:THR:OG1	1:C:50:GLU:HG3	2.12	0.48
1:D:62:GLU:O	1:D:65:PHE:O	2.32	0.48
1:A:131:LEU:O	1:A:163:GLY:O	2.31	0.48
1:D:384:THR:HA	1:D:409:VAL:HG21	1.95	0.48
1:D:82:VAL:HG22	1:D:114:LEU:HD12	1.95	0.48
1:C:24:THR:HG22	1:C:27:GLN:CD	2.38	0.48
1:C:407:ALA:HB2	1:C:423:GLN:NE2	2.29	0.48
1:B:73:PHE:CD2	1:B:192:ALA:HB2	2.49	0.48
1:H:236:LEU:O	1:H:274:LYS:HE3	2.14	0.48
1:D:119:ILE:CD1	1:D:164:PHE:CZ	2.96	0.48
1:D:259:PRO:HB2	1:D:260:PRO:HD3	1.95	0.48
1:G:329:MET:HE1	1:G:332:ARG:NH2	2.28	0.48
1:D:82:VAL:CG2	1:D:164:PHE:CD1	2.96	0.48
1:F:286:MET:HA	1:F:289:ALA:O	2.13	0.48
1:C:165:ASN:CG	1:C:251:VAL:HG11	2.38	0.48
1:C:402:SER:O	1:C:421:PRO:HA	2.13	0.48
1:D:90:VAL:CG1	1:D:109:GLU:CB	2.92	0.48
1:D:283:LEU:HB3	1:D:286:MET:HE3	1.96	0.48
1:G:44:SER:HB2	1:G:76:GLN:CD	2.39	0.47
1:F:460:PRO:HD2	1:F:463:LYS:NZ	2.29	0.47
1:D:136:ILE:CD1	1:D:157:PRO:O	2.62	0.47
1:C:86:LYS:HA	1:C:106:LEU:HD13	1.96	0.47
1:A:13:ARG:HD3	1:A:414:GLY:O	2.14	0.47
1:A:142:GLU:O	1:A:149:VAL:HG12	2.14	0.47
1:D:82:VAL:HG21	1:D:114:LEU:HD11	1.96	0.47
1:C:77:GLY:HA2	1:C:180:ASP:OD2	2.15	0.47
1:F:247:GLY:O	1:F:251:VAL:HG23	2.14	0.47
1:A:43:MET:SD	1:A:51:LYS:HD2	2.55	0.47
1:A:128:ARG:HG3	1:A:128:ARG:HH11	1.80	0.47
1:B:256:GLU:OE2	1:C:332:ARG:HD2	2.14	0.47
1:H:355:GLU:HB3	1:H:356:PRO:HD2	1.96	0.47
1:E:360:ASP:OD1	1:E:390:ARG:HD2	2.15	0.47
1:F:40:ARG:NH2	1:F:74:ASP:OD2	2.42	0.47
1:D:90:VAL:HG11	1:D:109:GLU:CB	2.45	0.47
1:D:114:LEU:O	1:D:116:HIS:N	2.48	0.47
1:G:177:THR:OG1	1:G:178:PRO:HD2	2.14	0.47
1:C:304:ILE:HD13	1:C:334:ALA:HA	1.96	0.47
1:F:463:LYS:HG2	1:F:466:THR:CB	2.45	0.46
1:D:52:LYS:HG2	1:D:190:GLU:OE2	2.15	0.46
1:D:422:VAL:HG12	1:D:424:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:THR:OG1	1:D:40:ARG:HD3	2.15	0.46
1:F:171:ILE:HD11	1:F:199:PHE:CZ	2.50	0.46
1:D:43:MET:HE2	1:D:43:MET:HA	1.98	0.46
1:D:188:LEU:HD23	1:D:188:LEU:HA	1.78	0.46
1:G:77:GLY:HA2	1:G:180:ASP:OD2	2.15	0.46
1:D:127:HIS:NE2	1:D:169:VAL:HG13	2.30	0.46
1:D:220:LEU:C	1:D:220:LEU:HD23	2.40	0.46
1:H:365:ASN:ND2	1:E:365:ASN:HB3	2.30	0.46
1:C:119:ILE:CG2	1:C:123:LEU:HD11	2.46	0.46
1:D:244:VAL:HG22	1:D:265:ILE:HG21	1.96	0.46
1:G:52:LYS:HE3	1:G:56:ASP:CG	2.40	0.46
1:G:434:LYS:HG2	1:G:473:ILE:HG21	1.98	0.46
1:F:171:ILE:HD11	1:F:199:PHE:HZ	1.81	0.46
1:F:203:VAL:HB	1:F:234:SER:OG	2.15	0.46
1:C:130:LEU:HD22	1:C:137:VAL:HG22	1.97	0.46
1:A:139:ARG:HE	1:A:153:GLU:CD	2.23	0.46
1:E:195:VAL:O	1:E:219:LEU:HD12	2.14	0.46
1:D:209:ALA:O	1:D:213:ILE:CG1	2.63	0.46
1:G:62:GLU:HG2	1:G:67:ARG:O	2.15	0.46
1:C:220:LEU:HD21	1:C:243:MET:HB2	1.97	0.46
1:D:28:ILE:HD13	1:D:58:ILE:HG23	1.98	0.46
1:C:236:LEU:O	1:C:274:LYS:HE3	2.16	0.46
1:D:132:ASP:OD1	1:D:162:LYS:HD2	2.15	0.46
1:D:176:LEU:HD23	1:D:176:LEU:HA	1.79	0.46
1:D:82:VAL:CG2	1:D:114:LEU:CD1	2.94	0.45
1:A:198:SER:OG	1:A:222:LYS:CE	2.65	0.45
1:D:224:GLU:OE2	1:D:248:ASP:OD2	2.35	0.45
1:D:380:VAL:CG1	1:D:387:THR:HG22	2.46	0.45
1:G:52:LYS:HD2	1:G:190:GLU:OE1	2.16	0.45
1:F:184:LEU:HD22	1:F:212:LEU:HD21	1.97	0.45
1:D:209:ALA:O	1:D:213:ILE:HG13	2.16	0.45
1:G:8:ARG:HD3	1:G:10:ARG:NH2	2.32	0.45
1:A:140:CYS:HA	1:A:150:THR:HG22	1.99	0.45
1:C:81:ARG:HD2	1:C:161:HIS:O	2.15	0.45
1:F:239:THR:O	1:F:274:LYS:HE2	2.17	0.45
1:D:430:LEU:O	1:D:434:LYS:HG2	2.16	0.45
1:H:171:ILE:O	1:H:173:LEU:N	2.49	0.45
1:E:395:ARG:N	1:E:396:PRO:CD	2.80	0.45
1:F:297:VAL:HG22	1:F:333:ILE:HD11	1.99	0.45
1:A:15:VAL:HG11	1:A:312:MET:HE2	1.98	0.45
1:E:198:SER:OG	1:E:222:LYS:HE3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:HIS:O	1:D:51:LYS:CE	2.65	0.45
1:D:55:VAL:O	1:D:58:ILE:HG13	2.17	0.45
1:A:277:VAL:HG11	1:A:312:MET:HE3	1.98	0.45
1:B:275:PRO:HA	1:B:309:ASP:OD1	2.17	0.45
1:H:286:MET:HA	1:H:289:ALA:O	2.17	0.45
1:D:73:PHE:HD2	1:D:192:ALA:HB2	1.81	0.45
1:D:297:VAL:HG22	1:D:333:ILE:HD11	1.98	0.45
1:A:178:PRO:HG2	1:H:230:GLU:HG2	1.98	0.45
1:A:459:GLU:OE1	1:B:434:LYS:NZ	2.50	0.45
1:C:248:ASP:OD2	4:C:601:HOH:O	2.21	0.45
1:D:82:VAL:CG2	1:D:164:PHE:CE1	3.00	0.45
1:A:255:PRO:HD2	1:A:256:GLU:OE1	2.17	0.44
1:D:73:PHE:CD2	1:D:192:ALA:HB2	2.52	0.44
1:B:82:VAL:O	1:B:161:HIS:HA	2.16	0.44
1:B:261:THR:HG22	1:B:265:ILE:HD11	1.98	0.44
1:C:84:ASP:HA	1:C:160:ASP:HB2	1.99	0.44
1:D:82:VAL:HG22	1:D:114:LEU:CD1	2.47	0.44
1:G:92:LEU:O	1:G:155:PRO:CB	2.65	0.44
1:A:246:ARG:HD3	1:A:262:GLN:OE1	2.18	0.44
1:C:202:ARG:HG3	1:C:204:GLU:HB2	1.98	0.44
1:B:138:VAL:HG22	1:B:152:VAL:HG22	1.99	0.44
1:H:136:ILE:HD11	1:H:156:GLY:HA3	1.98	0.44
1:D:90:VAL:HG12	1:D:91:GLN:N	2.32	0.44
1:A:142:GLU:HB2	1:A:149:VAL:HG11	2.00	0.44
1:A:220:LEU:C	1:A:220:LEU:HD23	2.42	0.44
1:F:184:LEU:HD11	1:F:213:ILE:HG12	2.00	0.44
1:C:166:VAL:O	1:C:166:VAL:HG12	2.18	0.44
1:D:55:VAL:O	1:D:58:ILE:N	2.51	0.44
1:A:194:TRP:CZ3	1:A:218:PRO:HB2	2.52	0.44
1:H:290:PRO:HB3	1:H:322:TRP:CD2	2.53	0.44
1:C:128:ARG:C	1:C:129:LEU:HD12	2.43	0.44
1:A:247:GLY:CA	1:A:280:THR:HG21	2.48	0.44
1:E:24:THR:OG1	1:E:27:GLN:HG3	2.18	0.44
1:E:30:ASP:OD2	1:E:31:ARG:NH1	2.51	0.44
1:C:283:LEU:HD12	1:C:313:LEU:HD21	2.00	0.43
1:E:259:PRO:HB2	1:E:260:PRO:HD3	2.00	0.43
1:F:460:PRO:O	1:F:463:LYS:HE2	2.18	0.43
1:C:117:PRO:O	1:C:121:LYS:NZ	2.50	0.43
1:A:258:VAL:HB	1:A:259:PRO:HD3	2.00	0.43
1:A:200:VAL:O	1:A:228:ALA:HB2	2.18	0.43
1:H:232:LEU:CD1	1:H:236:LEU:HD13	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:LYS:HD2	1:E:417:TRP:CZ2	2.53	0.43
1:A:159:SER:OG	1:A:160:ASP:N	2.50	0.43
1:D:130:LEU:O	1:D:165:ASN:N	2.51	0.43
1:A:224:GLU:HB2	1:A:248:ASP:HB2	1.99	0.43
1:H:471:ASP:CG	1:E:469:ILE:HD13	2.44	0.43
1:E:176:LEU:HD13	1:E:212:LEU:HD12	2.00	0.43
1:C:43:MET:HE3	1:C:73:PHE:CD2	2.47	0.43
1:G:259:PRO:HB2	1:G:260:PRO:HD3	1.99	0.43
2:G:503:GOL:H12	4:G:622:HOH:O	2.19	0.43
1:A:201:GLN:HG2	1:A:225:LYS:HD3	2.01	0.43
1:G:400:ILE:O	1:G:420:GLN:HB2	2.19	0.43
1:B:62:GLU:HG2	1:B:67:ARG:O	2.19	0.43
1:B:177:THR:O	1:B:181:ARG:HG3	2.19	0.43
1:H:116:HIS:HB2	1:H:119:ILE:HD12	2.01	0.43
1:E:267:GLU:HG2	4:E:641:HOH:O	2.19	0.43
1:D:78:PRO:HD3	1:D:175:ALA:O	2.17	0.43
1:D:127:HIS:NE2	1:D:169:VAL:CG1	2.82	0.43
1:D:380:VAL:HG11	1:D:387:THR:HG22	2.01	0.43
1:A:98:PHE:HE2	1:A:112:VAL:HG12	1.82	0.43
1:E:459:GLU:HA	1:E:460:PRO:C	2.44	0.43
1:F:77:GLY:HA2	1:F:180:ASP:OD2	2.18	0.43
1:C:13:ARG:HD3	1:C:414:GLY:O	2.18	0.43
1:D:59:ARG:HD2	1:D:411:ARG:NH2	2.34	0.43
1:D:73:PHE:HD2	1:D:192:ALA:CB	2.31	0.43
1:D:119:ILE:CD1	1:D:164:PHE:HZ	2.32	0.43
1:D:369:THR:O	1:D:373:VAL:HG22	2.19	0.43
1:G:80:LEU:HB3	1:G:164:PHE:CE1	2.54	0.43
1:F:27:GLN:O	1:F:31:ARG:HG2	2.19	0.43
1:C:13:ARG:HD2	4:C:616:HOH:O	2.19	0.43
1:A:125:LYS:HG2	1:A:141:VAL:O	2.19	0.42
1:D:286:MET:HE1	1:D:329:MET:HG2	2.01	0.42
1:D:75:LEU:HD12	1:D:176:LEU:HD21	2.01	0.42
1:H:459:GLU:HG2	1:H:468:ASN:HD21	1.84	0.42
1:D:283:LEU:HD12	1:D:313:LEU:HD21	2.00	0.42
1:F:5:LEU:HD13	1:F:5:LEU:O	2.19	0.42
1:H:360:ASP:OD1	1:H:390:ARG:HD2	2.18	0.42
1:F:47:THR:OG1	1:F:50:GLU:CD	2.62	0.42
1:F:194:TRP:CZ3	1:F:218:PRO:HB2	2.54	0.42
1:C:119:ILE:HD13	1:C:164:PHE:HE1	1.83	0.42
1:A:128:ARG:NH1	1:A:168:ASP:OD1	2.53	0.42
1:B:118:GLU:CG	1:B:173:LEU:HD13	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:343:TYR:HB3	2:E:501:GOL:H12	2.01	0.42
1:F:220:LEU:HD21	1:F:243:MET:HB2	2.00	0.42
1:D:127:HIS:CD2	1:D:169:VAL:HG13	2.54	0.42
1:A:114:LEU:C	1:A:114:LEU:HD23	2.45	0.42
1:B:286:MET:HA	1:B:289:ALA:O	2.20	0.42
1:E:279:ALA:O	1:E:280:THR:HB	2.19	0.42
1:F:5:LEU:C	1:F:5:LEU:CD1	2.93	0.42
1:D:153:GLU:C	1:D:154:VAL:HG23	2.44	0.42
1:A:28:ILE:HD12	1:A:57:ASN:CB	2.50	0.42
1:A:99:THR:HG21	1:A:147:LYS:NZ	2.35	0.42
1:B:283:LEU:HD23	1:B:296:GLU:HB3	2.01	0.42
1:D:191:LYS:HE2	1:D:408:GLU:OE2	2.20	0.42
1:B:362:LEU:HD23	1:B:362:LEU:HA	1.89	0.42
1:G:313:LEU:HG	1:G:330:MET:HE2	2.01	0.41
1:B:103:ASP:OD2	1:B:105:THR:HB	2.20	0.41
1:C:93:LYS:HG3	1:C:96:GLN:OE1	2.19	0.41
1:D:55:VAL:O	1:D:56:ASP:C	2.63	0.41
1:E:459:GLU:HG2	1:E:469:ILE:HD11	2.03	0.41
1:C:400:ILE:HG22	1:C:401:LEU:N	2.35	0.41
1:D:41:ILE:HG22	1:D:43:MET:CE	2.50	0.41
1:D:130:LEU:O	1:D:164:PHE:HA	2.20	0.41
1:C:15:VAL:HA	1:C:38:VAL:HG22	2.02	0.41
1:B:281:ALA:HB1	1:B:284:GLU:HB2	2.02	0.41
1:D:283:LEU:HD13	1:D:286:MET:CE	2.50	0.41
1:H:443:LYS:HE2	1:H:444:TYR:CZ	2.55	0.41
1:F:47:THR:HG1	1:F:50:GLU:CD	2.26	0.41
1:F:213:ILE:O	1:F:216:ARG:HG3	2.21	0.41
1:C:71:ILE:N	1:C:193:ASP:OD2	2.52	0.41
1:H:225:LYS:NZ	1:H:252:GLU:OE1	2.54	0.41
1:H:369:THR:O	1:H:373:VAL:HG22	2.20	0.41
1:C:286:MET:HA	1:C:289:ALA:O	2.20	0.41
1:D:82:VAL:CG1	1:D:114:LEU:HD12	2.49	0.41
1:D:246:ARG:HA	1:D:249:LEU:HB2	2.02	0.41
1:G:463:LYS:HB3	1:G:466:THR:HG21	2.02	0.41
1:F:190:GLU:O	1:F:191:LYS:HB2	2.21	0.41
1:C:434:LYS:HE3	1:D:459:GLU:OE1	2.21	0.41
1:G:54:ILE:O	1:G:55:VAL:C	2.64	0.41
1:A:284:GLU:OE1	1:A:284:GLU:HA	2.20	0.41
1:B:463:LYS:O	1:B:466:THR:OG1	2.27	0.41
1:E:282:MET:O	1:E:283:LEU:HD23	2.21	0.41
1:F:355:GLU:HB3	1:F:356:PRO:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:GLU:OE1	1:D:204:GLU:N	2.46	0.41
1:D:236:LEU:O	1:D:274:LYS:NZ	2.52	0.41
1:G:13:ARG:NH1	2:G:502:GOL:H12	2.36	0.41
1:A:200:VAL:HG21	1:A:221:VAL:HG13	2.03	0.41
1:A:396:PRO:HG2	4:A:602:HOH:O	2.21	0.41
1:B:136:ILE:CD1	1:B:157:PRO:O	2.63	0.41
1:E:220:LEU:C	1:E:220:LEU:HD23	2.46	0.41
1:D:213:ILE:HG22	1:D:214:LYS:N	2.35	0.41
1:G:124:ASP:CG	1:G:125:LYS:H	2.25	0.40
1:G:355:GLU:HG3	1:G:360:ASP:OD2	2.21	0.40
1:A:116:HIS:HB2	1:A:119:ILE:CD1	2.51	0.40
1:H:12:VAL:HG12	1:H:334:ALA:HB1	2.03	0.40
1:E:11:LYS:NZ	1:E:397:VAL:O	2.47	0.40
1:F:184:LEU:HD21	1:F:188:LEU:HD11	2.03	0.40
1:D:82:VAL:CG2	1:D:114:LEU:HD11	2.51	0.40
1:C:373:VAL:O	1:C:373:VAL:HG12	2.20	0.40
1:G:105:THR:O	1:G:111:ARG:NH2	2.41	0.40
1:A:28:ILE:HD12	1:A:57:ASN:HB3	2.02	0.40
1:H:259:PRO:HB2	1:H:260:PRO:HD3	2.03	0.40
1:E:254:LEU:O	1:E:257:SER:OG	2.34	0.40
1:E:286:MET:HA	1:E:289:ALA:O	2.21	0.40
1:E:344:ILE:HB	2:E:501:GOL:C3	2.47	0.40
1:C:15:VAL:HG13	1:C:38:VAL:HG23	2.03	0.40
1:C:73:PHE:CD1	1:C:192:ALA:HB2	2.56	0.40
1:A:369:THR:O	1:A:373:VAL:HB	2.21	0.40
1:F:259:PRO:HB2	1:F:260:PRO:HD3	2.04	0.40
1:D:225:LYS:CE	1:D:252:GLU:OE2	2.70	0.40
1:A:13:ARG:HD2	4:A:625:HOH:O	2.21	0.40
1:H:249:LEU:HD12	1:H:249:LEU:HA	1.98	0.40
1:E:407:ALA:HB2	1:E:423:GLN:NE2	2.37	0.40
1:E:459:GLU:HG3	1:E:469:ILE:HD11	2.03	0.40
1:C:24:THR:HG22	1:C:27:GLN:OE1	2.22	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	471/475 (99%)	458 (97%)	12 (2%)	1 (0%)	43	58
1	B	470/475 (99%)	459 (98%)	10 (2%)	1 (0%)	43	58
1	C	462/475 (97%)	447 (97%)	12 (3%)	3 (1%)	21	32
1	D	458/475 (96%)	431 (94%)	23 (5%)	4 (1%)	14	22
1	E	378/475 (80%)	369 (98%)	8 (2%)	1 (0%)	36	50
1	F	380/475 (80%)	370 (97%)	9 (2%)	1 (0%)	36	50
1	G	471/475 (99%)	461 (98%)	9 (2%)	1 (0%)	43	58
1	H	471/475 (99%)	461 (98%)	9 (2%)	1 (0%)	43	58
All	All	3561/3800 (94%)	3456 (97%)	92 (3%)	13 (0%)	30	43

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	280	THR
1	C	66	ASN
1	G	280	THR
1	H	280	THR
1	E	280	THR
1	C	280	THR
1	D	56	ASP
1	F	280	THR
1	D	460	PRO
1	D	280	THR
1	A	280	THR
1	C	115	PRO
1	D	418	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	387/389 (100%)	375 (97%)	12 (3%)	35	57
1	B	386/389 (99%)	381 (99%)	5 (1%)	61	80
1	C	383/389 (98%)	372 (97%)	11 (3%)	37	60
1	D	381/389 (98%)	367 (96%)	14 (4%)	30	51
1	E	305/389 (78%)	302 (99%)	3 (1%)	68	84
1	F	311/389 (80%)	297 (96%)	14 (4%)	24	42
1	G	387/389 (100%)	382 (99%)	5 (1%)	61	80
1	H	387/389 (100%)	376 (97%)	11 (3%)	38	60
All	All	2927/3112 (94%)	2852 (97%)	75 (3%)	40	63

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	3	GLU
1	G	47	THR
1	G	210	LYS
1	G	469	ILE
1	G	474	GLU
1	A	53	VAL
1	A	82	VAL
1	A	89	LYS
1	A	93	LYS
1	A	109	GLU
1	A	130	LEU
1	A	159	SER
1	A	210	LYS
1	A	224	GLU
1	A	225	LYS
1	A	373	VAL
1	A	386	LYS
1	B	66	ASN
1	B	81	ARG
1	B	86	LYS
1	B	109	GLU
1	B	386	LYS
1	H	8	ARG
1	H	28	ILE
1	H	52	LYS
1	H	86	LYS
1	H	131	LEU

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Mol	Chain	Res	Type
1	H	166	VAL
1	H	176	LEU
1	H	236	LEU
1	H	401	LEU
1	H	429	THR
1	H	469	ILE
1	E	63	LYS
1	E	261	THR
1	E	431	ASP
1	F	47	THR
1	F	56	ASP
1	F	181	ARG
1	F	191	LYS
1	F	200	VAL
1	F	213	ILE
1	F	214	LYS
1	F	234	SER
1	F	274	LYS
1	F	288	LYS
1	F	345	GLU
1	F	379	ILE
1	F	431	ASP
1	F	439	GLU
1	C	38	VAL
1	C	54	ILE
1	C	66	ASN
1	C	90	VAL
1	C	93	LYS
1	C	102	GLN
1	C	141	VAL
1	C	167	PRO
1	C	251	VAL
1	C	369	THR
1	C	389	GLN
1	D	29	ARG
1	D	54	ILE
1	D	58	ILE
1	D	79	LYS
1	D	123	LEU
1	D	136	ILE
1	D	138	VAL
1	D	158	LEU

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Mol	Chain	Res	Type
1	D	210	LYS
1	D	213	ILE
1	D	345	GLU
1	D	369	THR
1	D	428	LYS
1	D	452	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	102	GLN
1	G	389	GLN
1	B	423	GLN
1	H	45	HIS
1	H	113	ASN
1	E	328	ASN
1	E	423	GLN
1	F	42	ASN
1	F	45	HIS
1	F	76	GLN
1	F	201	GLN
1	F	231	ASN
1	F	328	ASN
1	F	389	GLN
1	C	231	ASN
1	C	328	ASN
1	C	365	ASN
1	D	365	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

13 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	H	501	-	4,4,4	0.89	0	6,6,6	0.99	0
2	GOL	A	501	-	5,5,5	0.99	0	5,5,5	1.15	0
3	PO4	C	501	-	4,4,4	1.20	0	6,6,6	0.96	0
2	GOL	E	501	-	5,5,5	1.60	1 (20%)	5,5,5	1.13	1 (20%)
2	GOL	G	503	-	5,5,5	2.01	3 (60%)	5,5,5	0.94	0
3	PO4	F	501	-	4,4,4	0.78	0	6,6,6	1.37	1 (16%)
2	GOL	G	502	-	5,5,5	1.62	1 (20%)	5,5,5	0.86	0
2	GOL	G	501	-	5,5,5	1.12	1 (20%)	5,5,5	1.37	1 (20%)
3	PO4	G	504	-	4,4,4	1.03	0	6,6,6	0.57	0
3	PO4	B	501	-	4,4,4	0.98	0	6,6,6	1.26	1 (16%)
3	PO4	A	502	-	4,4,4	1.14	0	6,6,6	1.27	1 (16%)
3	PO4	D	501	-	4,4,4	0.90	0	6,6,6	0.63	0
3	PO4	E	502	-	4,4,4	1.36	1 (25%)	6,6,6	0.75	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	501	-	-	2/4/4/4	-
2	GOL	E	501	-	-	4/4/4/4	-
2	GOL	G	503	-	-	2/4/4/4	-
2	GOL	G	502	-	-	3/4/4/4	-
2	GOL	G	501	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	GOL	C1-C2	3.31	1.64	1.51
2	G	503	GOL	C1-C2	2.89	1.62	1.51
2	G	502	GOL	C1-C2	2.50	1.61	1.51
2	G	501	GOL	C1-C2	2.35	1.60	1.51
2	G	503	GOL	C3-C2	2.22	1.60	1.51
3	E	502	PO4	P-O3	-2.07	1.48	1.54
2	G	503	GOL	O2-C2	2.04	1.49	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	501	PO4	O3-P-O2	2.55	115.85	107.91
2	G	501	GOL	C3-C2-C1	-2.29	103.40	111.80
3	B	501	PO4	O4-P-O2	2.29	115.04	107.91
3	A	502	PO4	O4-P-O1	-2.24	103.03	110.95
2	E	501	GOL	C3-C2-C1	-2.14	103.95	111.80

There are no chirality outliers.

All (11) torsion outliers are listed below:

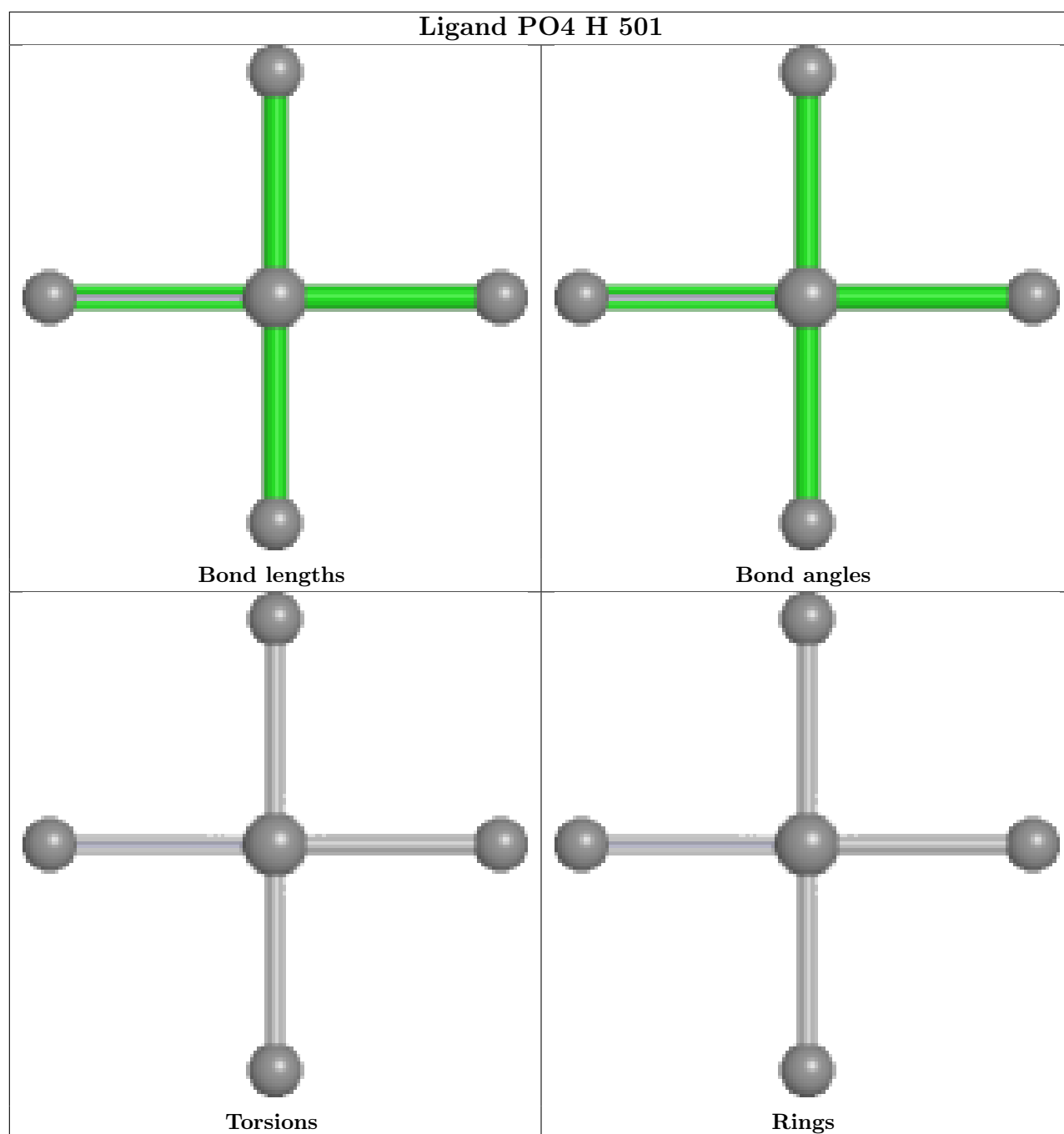
Mol	Chain	Res	Type	Atoms
2	G	502	GOL	C1-C2-C3-O3
2	A	501	GOL	C1-C2-C3-O3
2	E	501	GOL	O1-C1-C2-O2
2	G	503	GOL	C1-C2-C3-O3
2	E	501	GOL	O1-C1-C2-C3
2	G	502	GOL	O2-C2-C3-O3
2	G	503	GOL	O2-C2-C3-O3
2	A	501	GOL	O2-C2-C3-O3
2	G	502	GOL	O1-C1-C2-C3
2	E	501	GOL	O2-C2-C3-O3
2	E	501	GOL	C1-C2-C3-O3

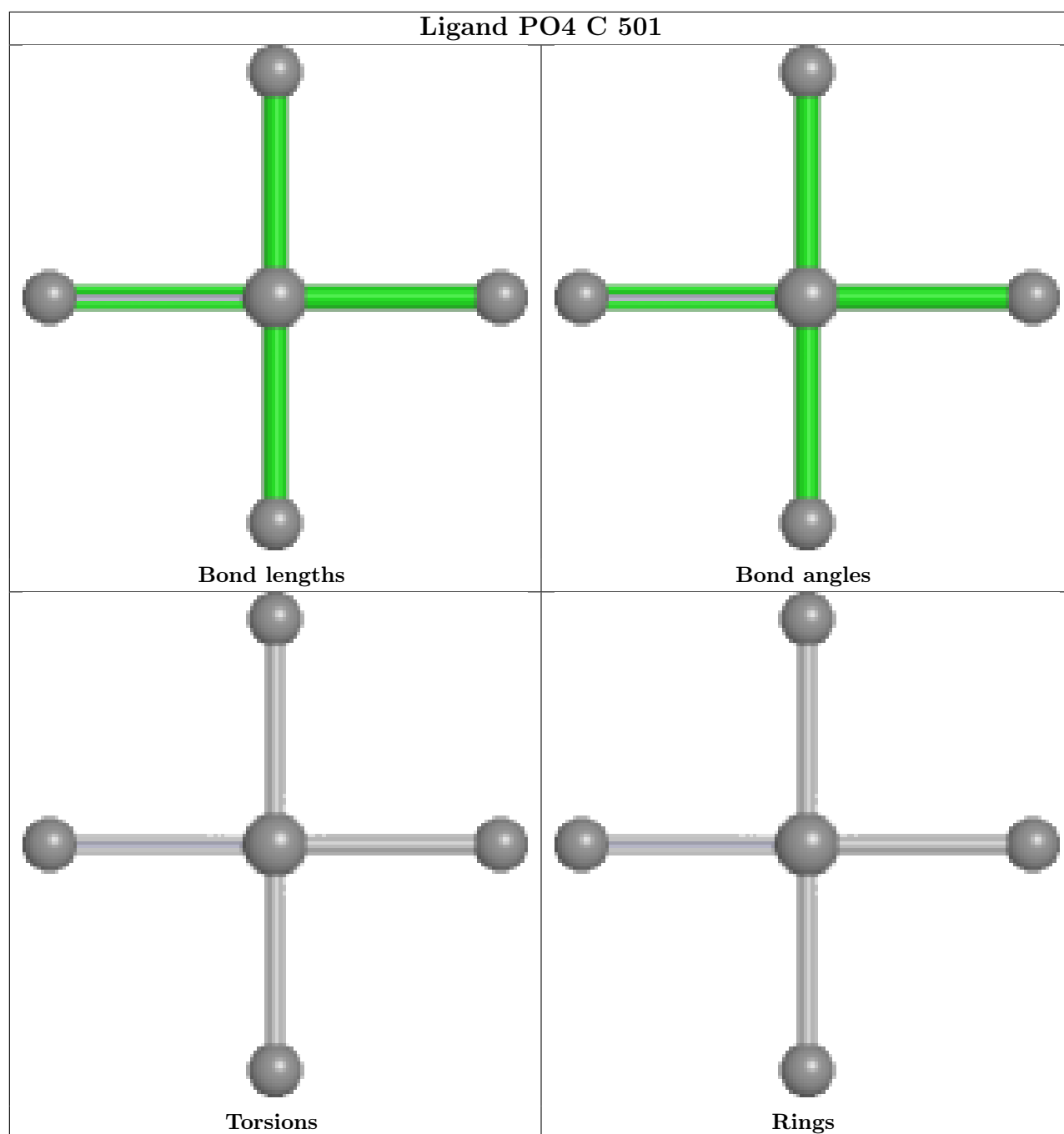
There are no ring outliers.

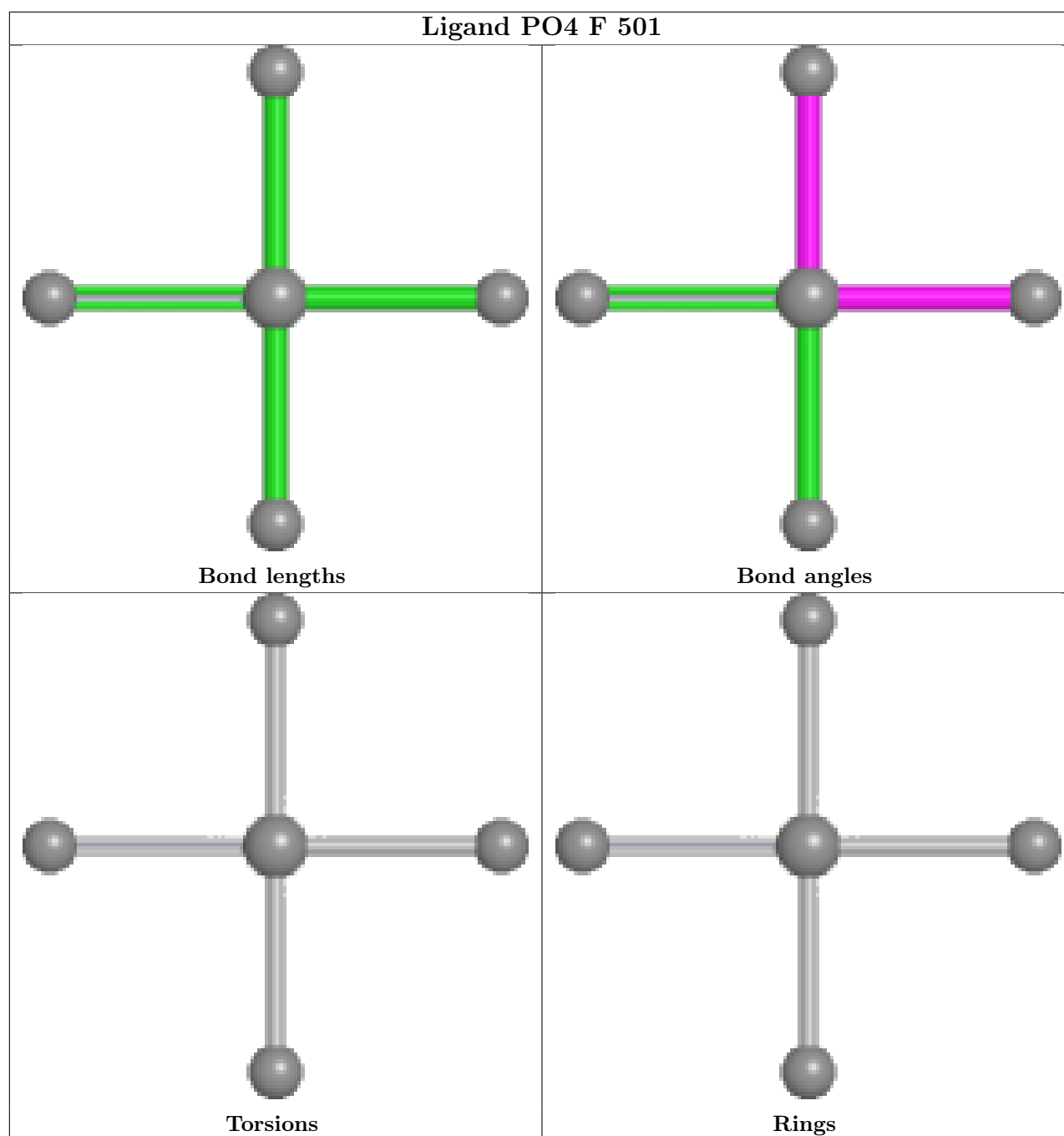
4 monomers are involved in 11 short contacts:

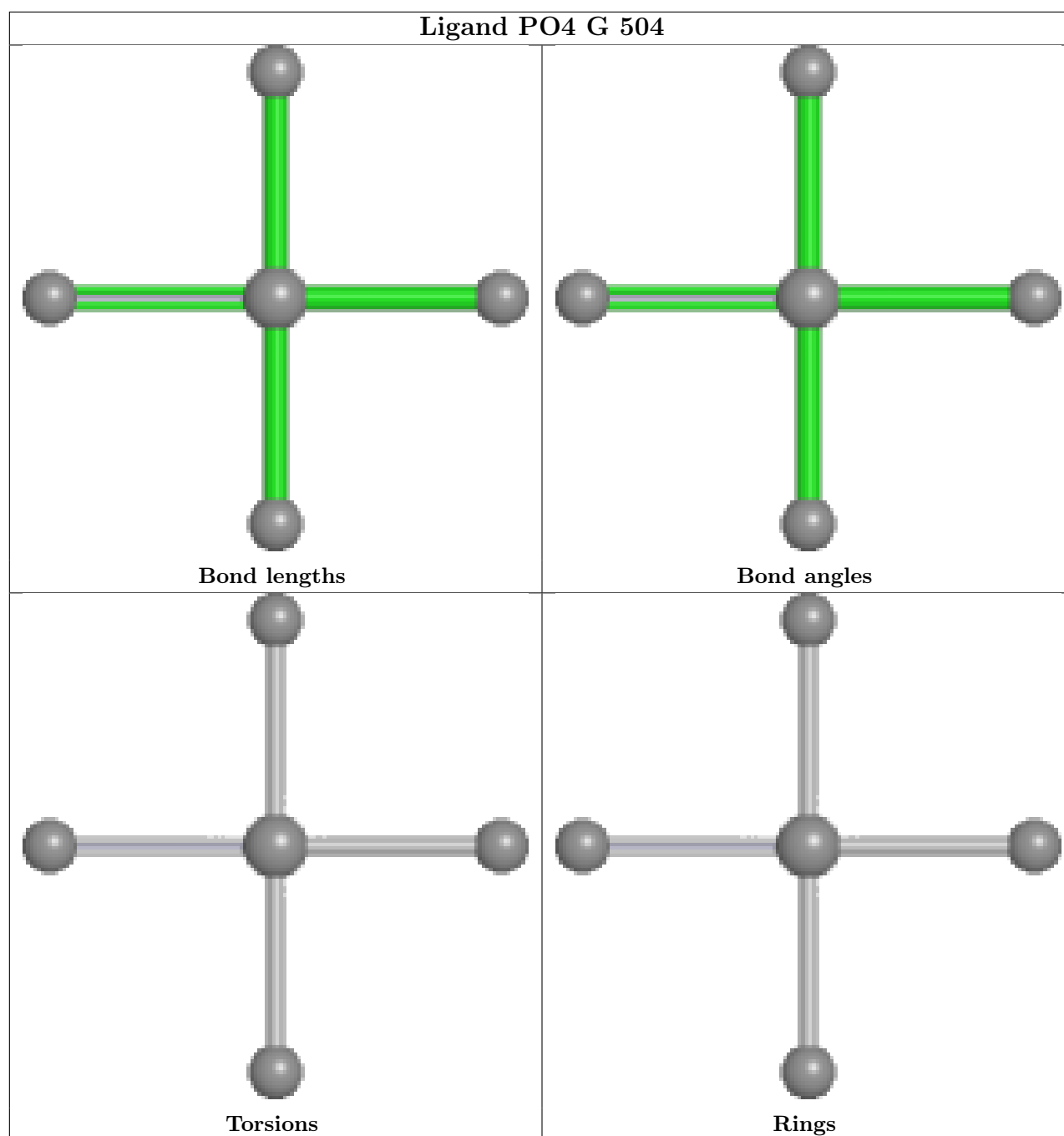
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	PO4	1	0
2	E	501	GOL	5	0
2	G	503	GOL	2	0
2	G	502	GOL	3	0

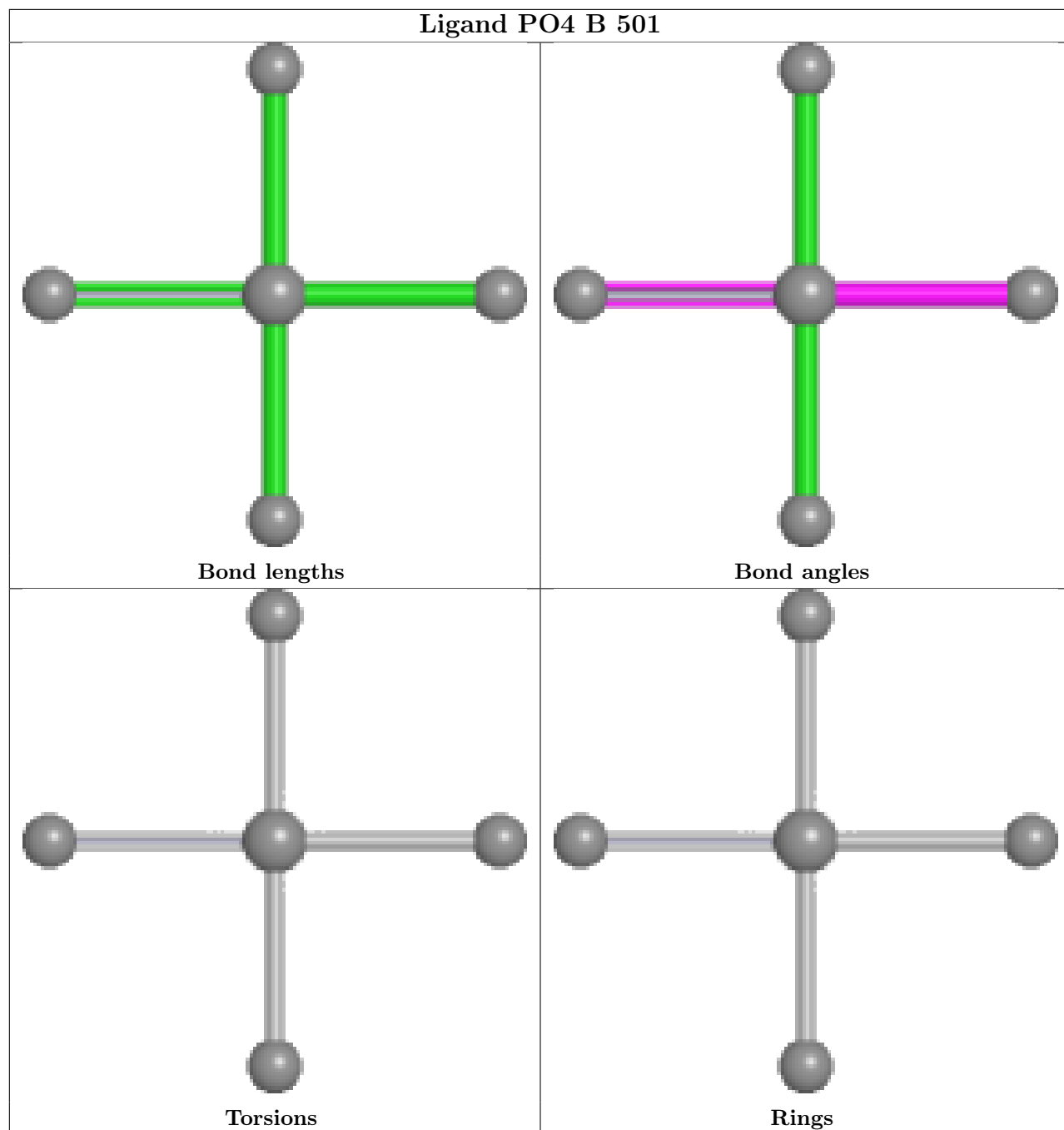
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

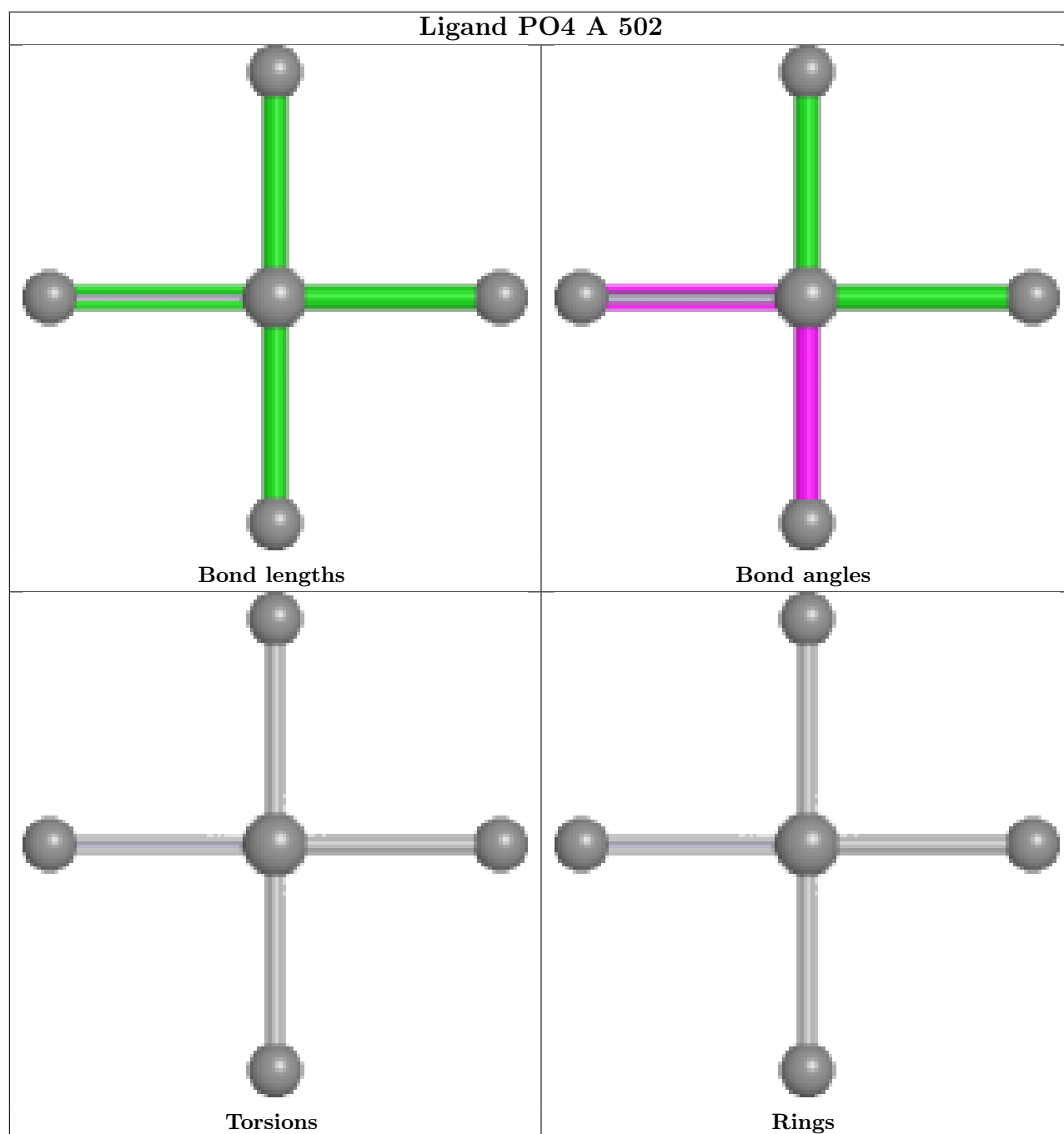


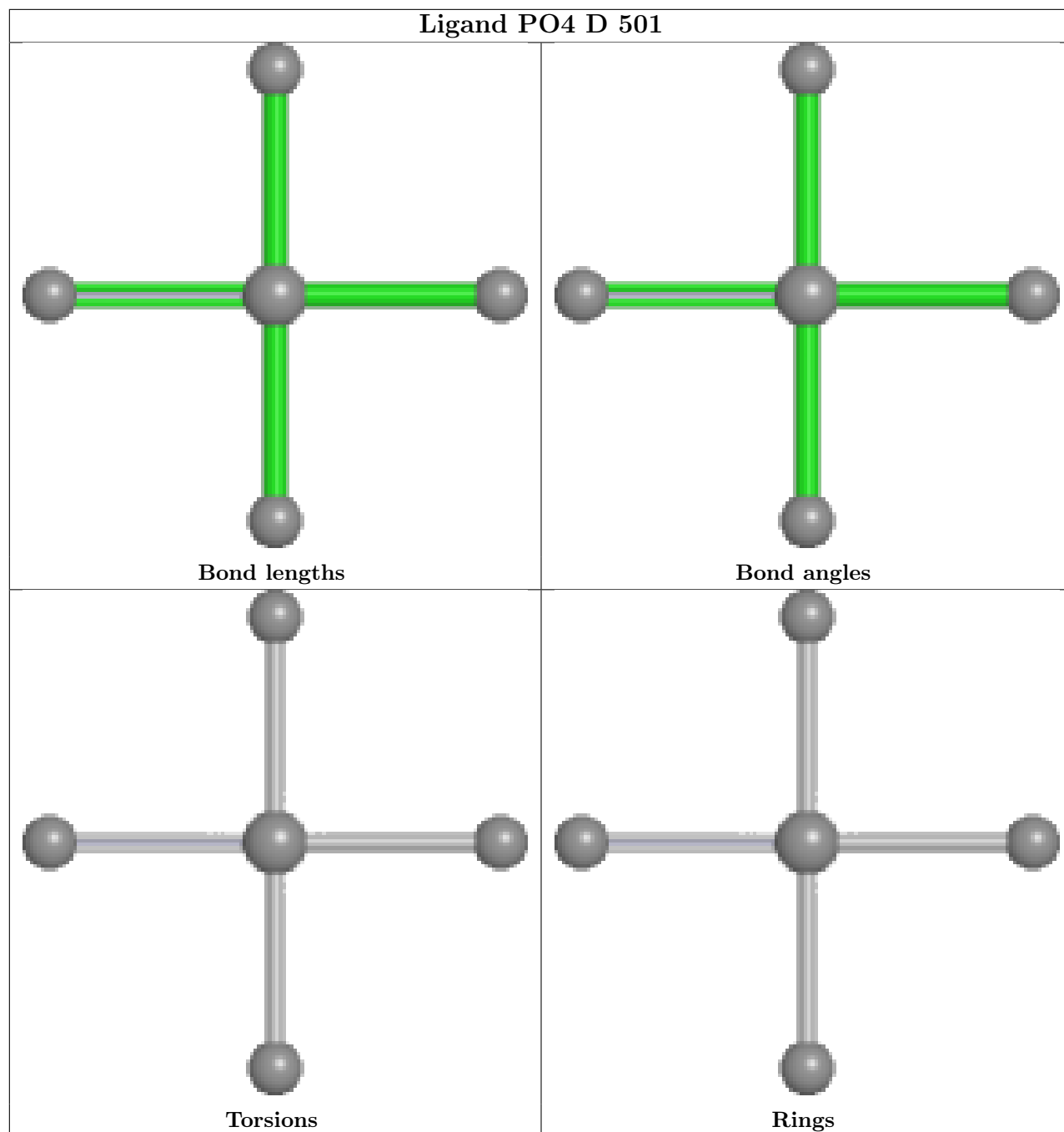


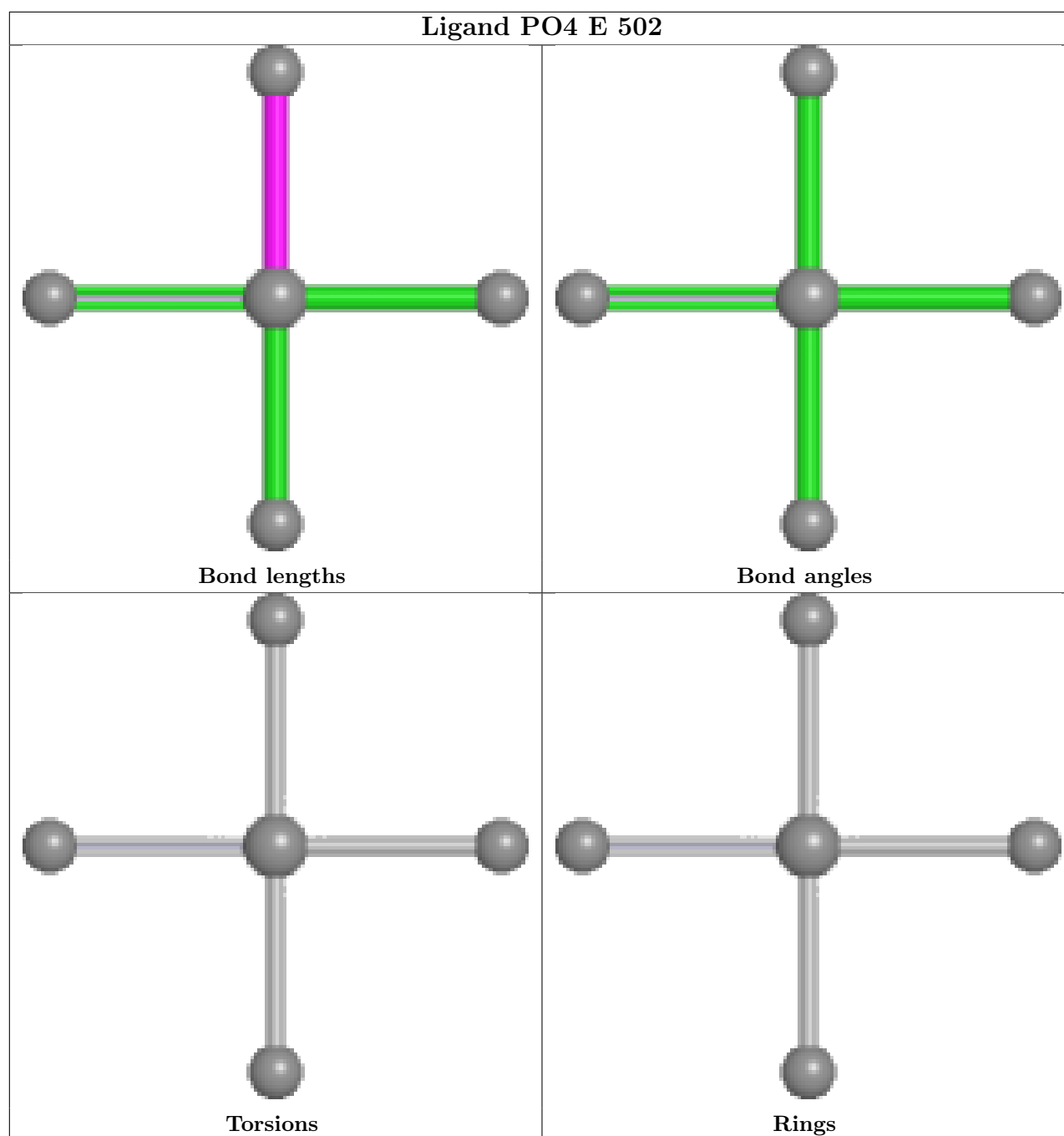












5.7 Other polymers [i](#)

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	473/475 (99%)	-0.33	3 (0%) 85 83	22, 35, 63, 85	0
1	B	472/475 (99%)	-0.55	3 (0%) 85 83	20, 32, 50, 86	0
1	C	468/475 (98%)	-0.12	11 (2%) 59 55	23, 39, 72, 83	0
1	D	464/475 (97%)	0.46	27 (5%) 29 25	27, 51, 74, 94	0
1	E	382/475 (80%)	-0.50	4 (1%) 79 76	20, 33, 53, 81	0
1	F	386/475 (81%)	-0.23	7 (1%) 67 63	23, 37, 66, 81	0
1	G	473/475 (99%)	-0.53	2 (0%) 88 86	21, 34, 50, 77	0
1	H	473/475 (99%)	-0.39	2 (0%) 88 86	22, 36, 55, 79	0
All	All	3591/3800 (94%)	-0.27	59 (1%) 70 66	20, 36, 66, 94	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	82	VAL	5.3
1	D	460	PRO	3.8
1	D	45	HIS	3.6
1	E	172	PRO	3.6
1	D	4	GLY	3.4
1	C	105	THR	3.4
1	C	4	GLY	3.3
1	D	90	VAL	3.3
1	C	170	VAL	3.1
1	D	154	VAL	3.1
1	F	462	GLY	3.1
1	D	89	LYS	3.0
1	B	4	GLY	2.8
1	D	106	LEU	2.8
1	G	3	GLU	2.8
1	C	90	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	463	LYS	2.7
1	E	463	LYS	2.7
1	F	79	LYS	2.7
1	H	3	GLU	2.6
1	C	174	ALA	2.6
1	D	121	LYS	2.6
1	A	97	THR	2.6
1	D	216	ARG	2.5
1	F	164	PHE	2.5
1	H	4	GLY	2.5
1	D	215	GLY	2.5
1	D	91	GLN	2.5
1	F	4	GLY	2.5
1	D	464	ALA	2.5
1	D	47	THR	2.4
1	C	173	LEU	2.4
1	D	114	LEU	2.4
1	E	4	GLY	2.3
1	B	463	LYS	2.3
1	D	58	ILE	2.3
1	C	464	ALA	2.3
1	A	151	ARG	2.3
1	D	93	LYS	2.3
1	C	151	ARG	2.3
1	B	465	GLY	2.3
1	C	461	PHE	2.2
1	F	174	ALA	2.2
1	D	176	LEU	2.2
1	E	174	ALA	2.2
1	D	143	SER	2.2
1	D	103	ASP	2.2
1	A	460	PRO	2.2
1	D	174	ALA	2.1
1	D	463	LYS	2.1
1	D	117	PRO	2.1
1	C	164	PHE	2.1
1	D	189	LYS	2.1
1	D	72	LEU	2.0
1	D	412	ARG	2.0
1	G	63	LYS	2.0
1	F	189	LYS	2.0
1	C	93	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	63	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

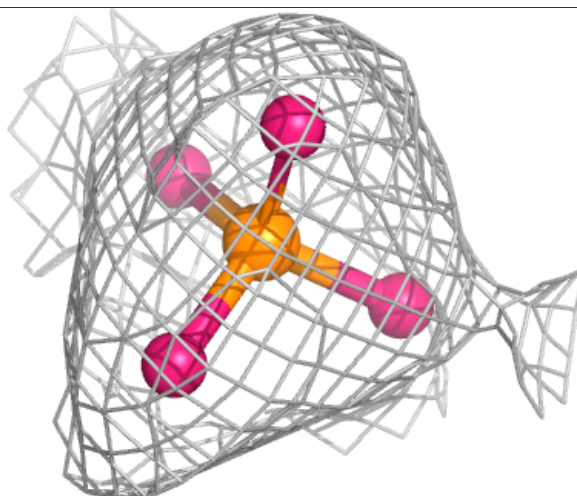
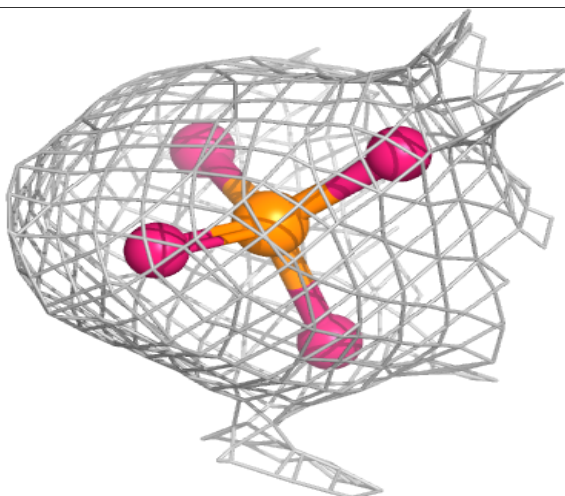
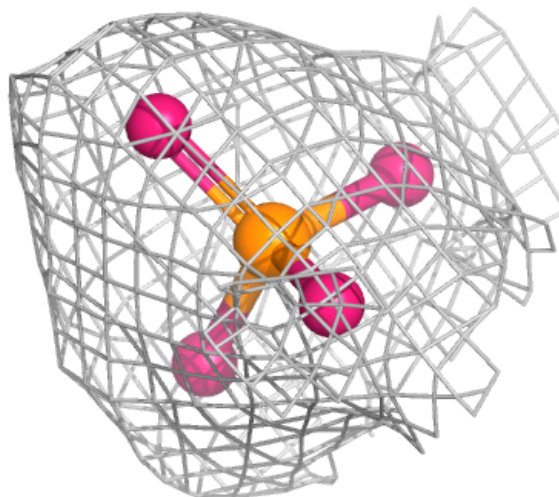
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	E	501	6/6	0.84	0.21	37,46,55,55	0
2	GOL	G	502	6/6	0.89	0.12	30,40,48,53	0
2	GOL	G	501	6/6	0.89	0.12	25,39,47,54	0
2	GOL	G	503	6/6	0.91	0.11	35,44,53,53	0
2	GOL	A	501	6/6	0.93	0.07	28,37,44,48	0
3	PO4	D	501	5/5	0.95	0.07	40,48,53,59	0
3	PO4	C	501	5/5	0.96	0.06	35,39,42,47	0
3	PO4	B	501	5/5	0.97	0.07	28,31,37,40	0
3	PO4	F	501	5/5	0.98	0.05	27,32,36,37	0
3	PO4	H	501	5/5	0.98	0.05	23,29,34,36	0
3	PO4	E	502	5/5	0.98	0.05	32,32,34,35	0
3	PO4	G	504	5/5	0.99	0.04	17,24,26,26	0
3	PO4	A	502	5/5	0.99	0.05	25,30,32,34	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.

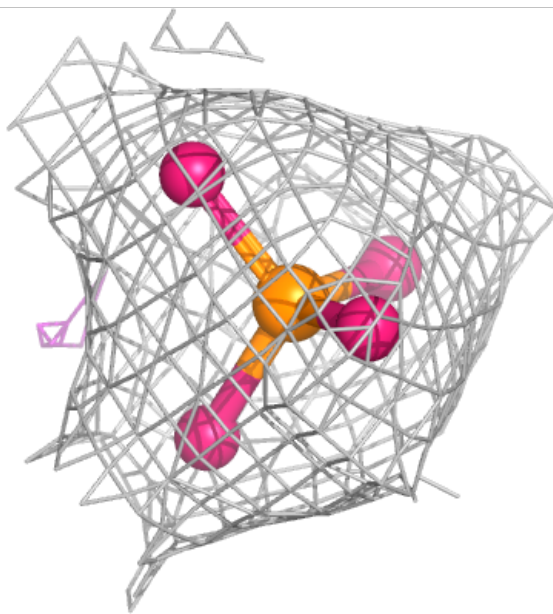
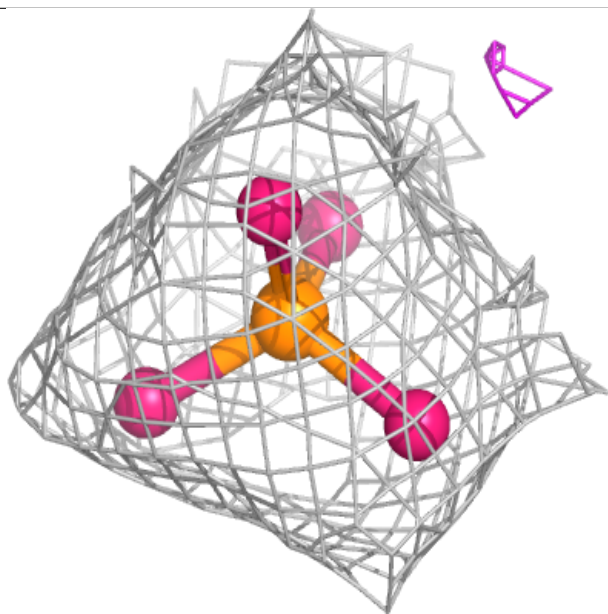
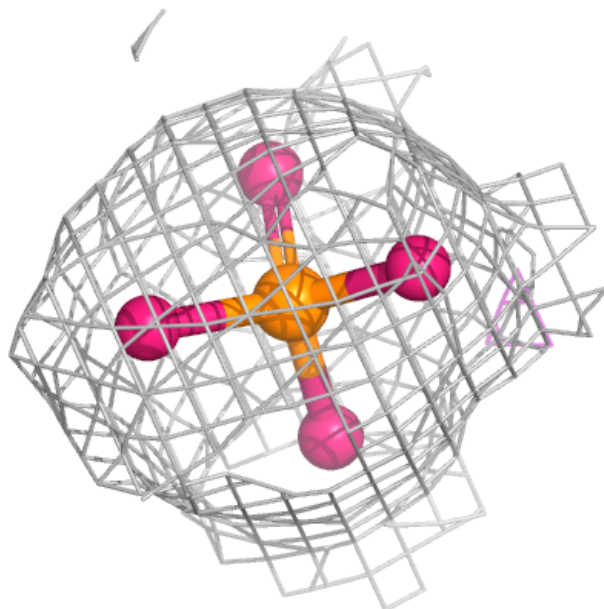
Electron density around PO4 D 501:

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



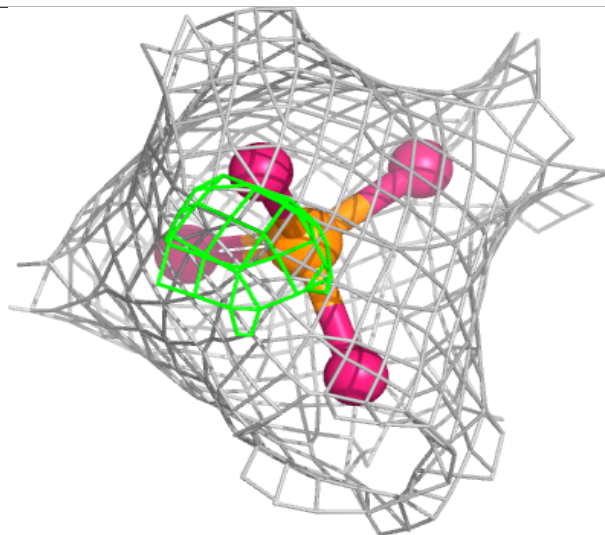
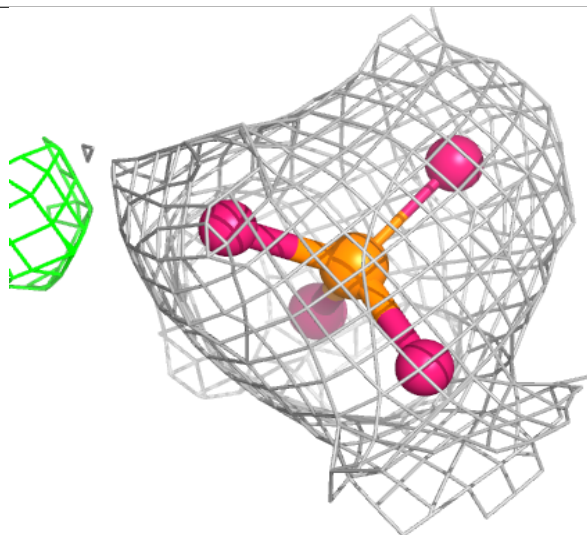
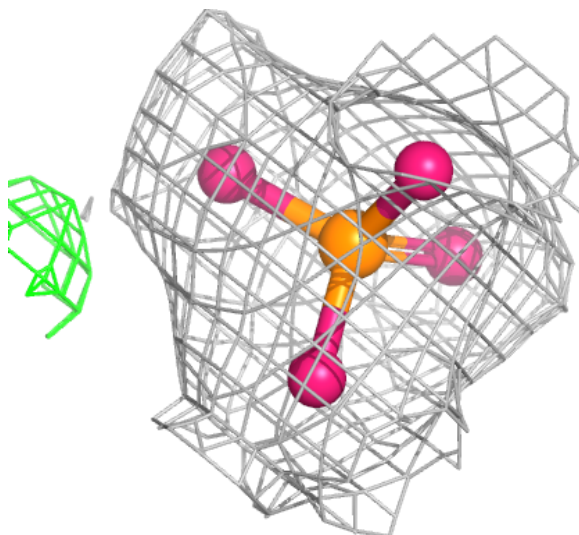
Electron density around PO4 C 501:

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



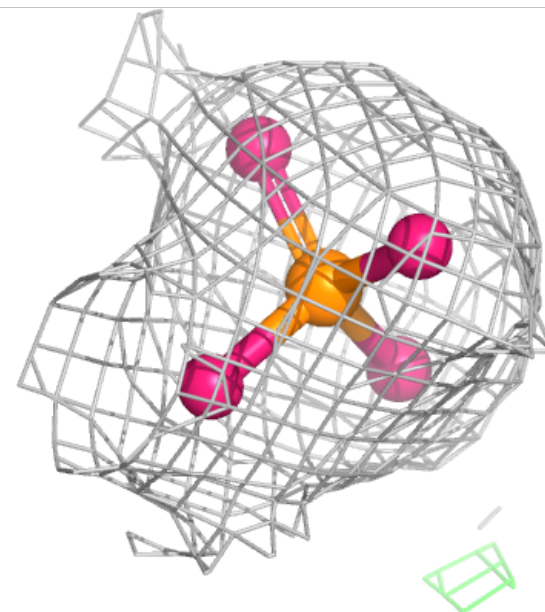
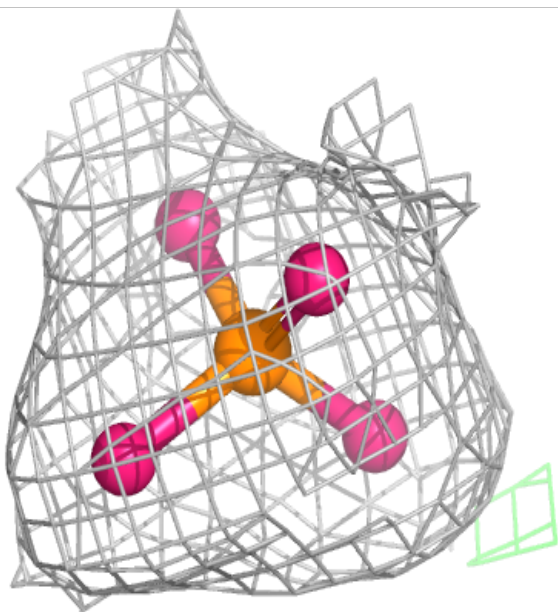
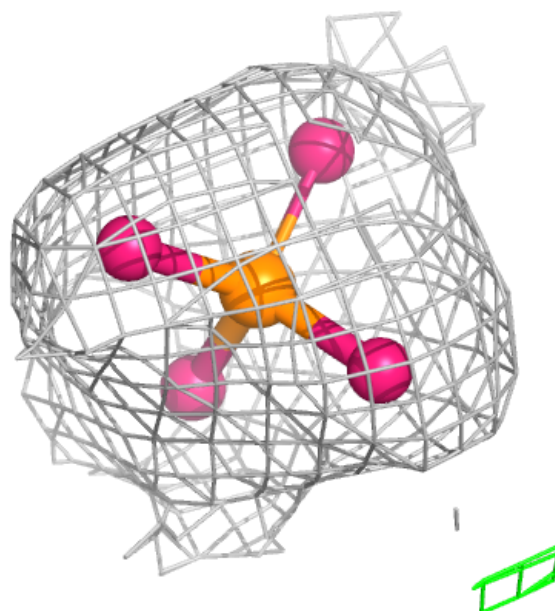
Electron density around PO4 B 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



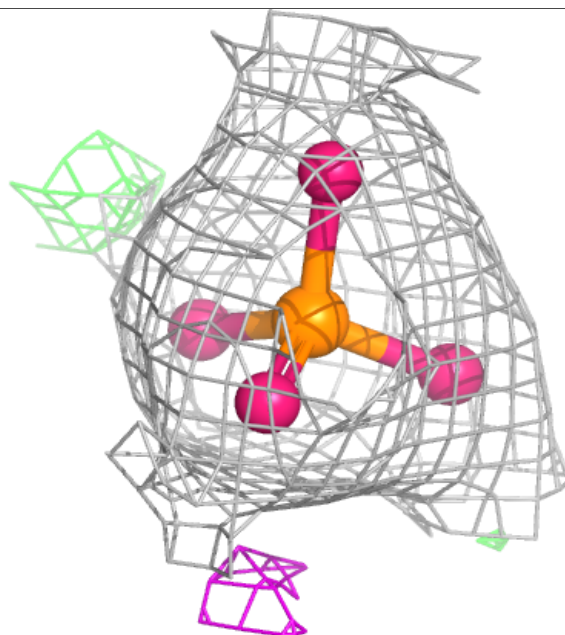
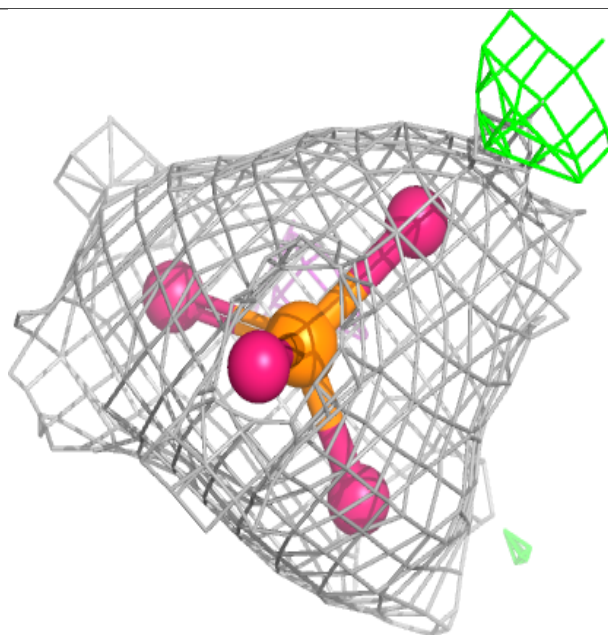
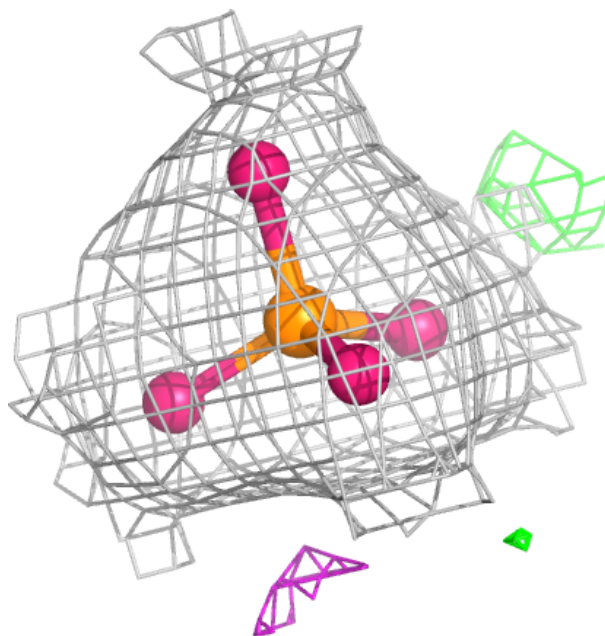
Electron density around PO4 F 501:

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



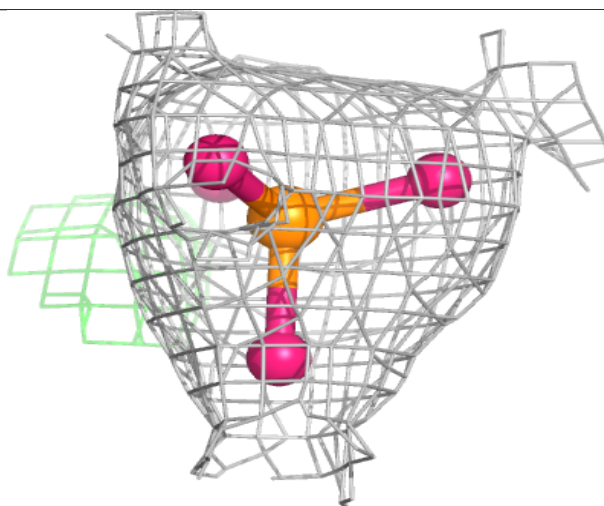
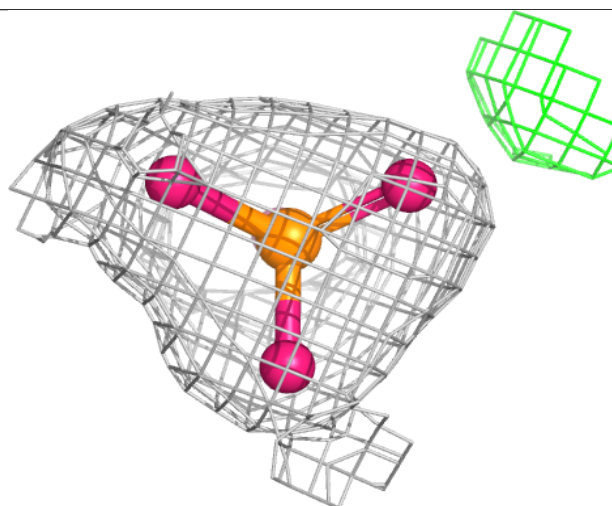
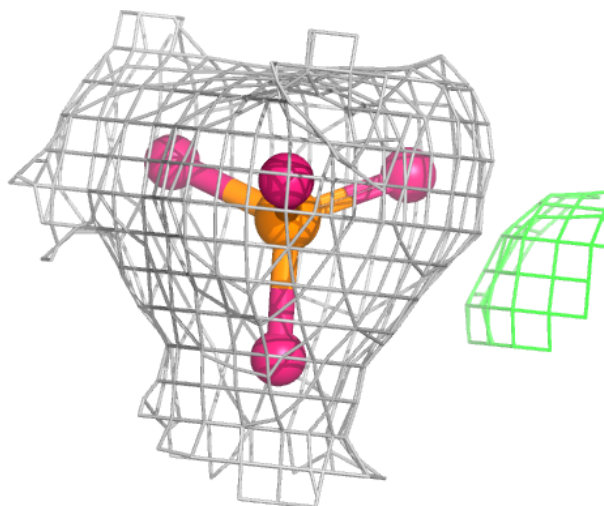
Electron density around PO4 H 501:

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



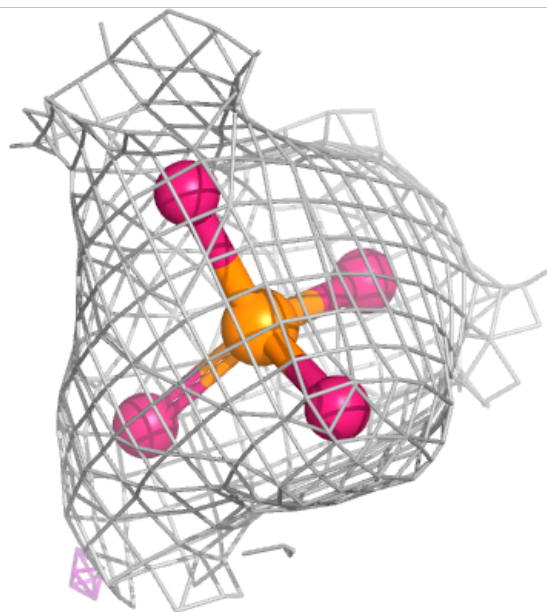
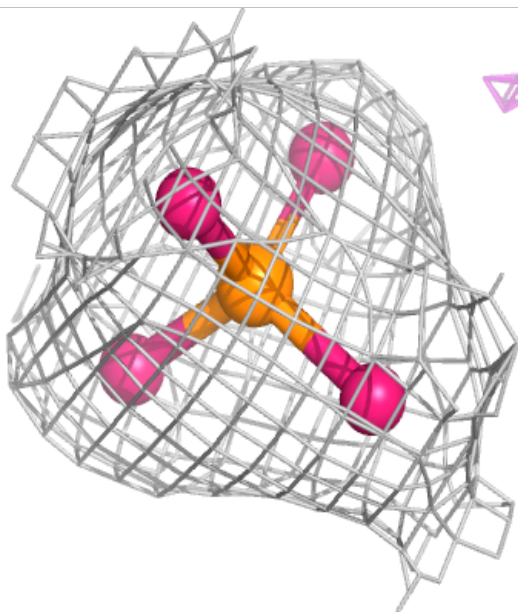
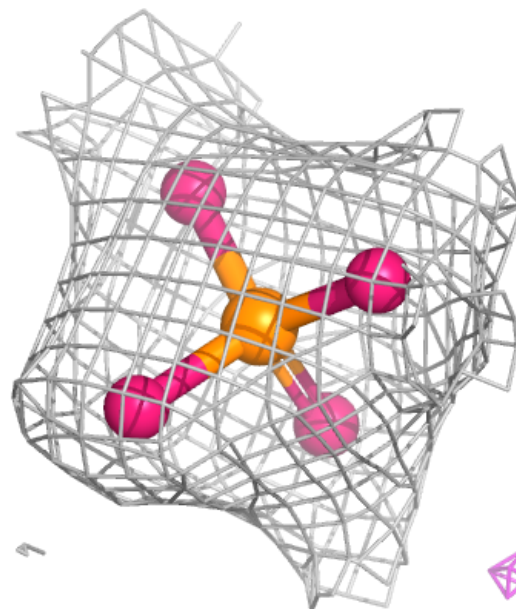
Electron density around PO4 E 502:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



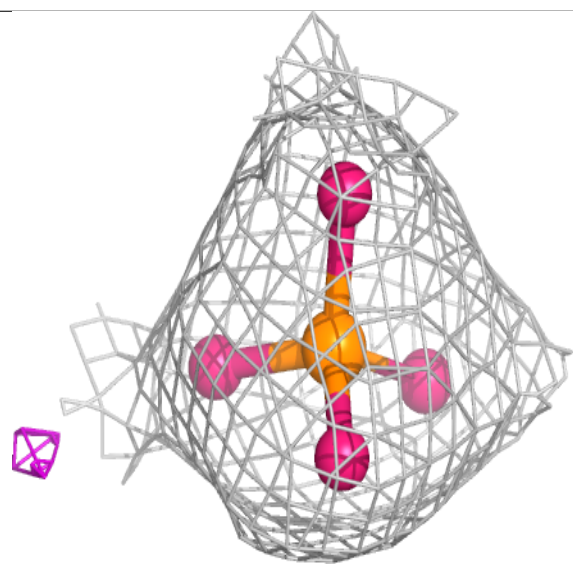
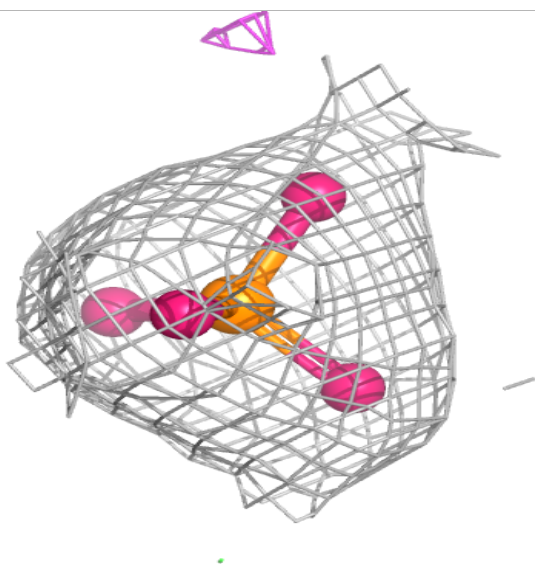
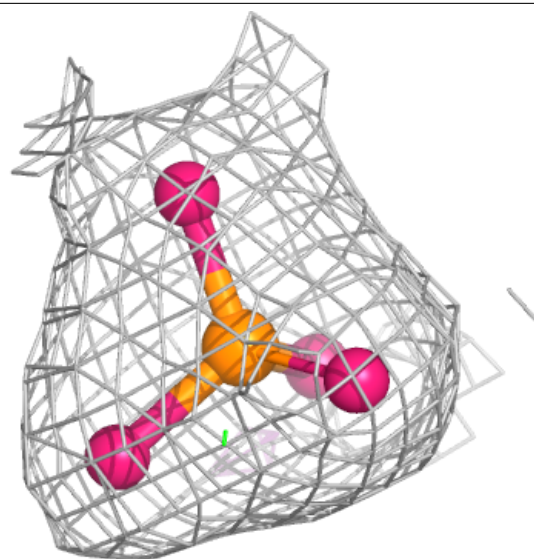
Electron density around PO4 G 504:

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



Electron density around PO4 A 502:

$2mF_o-DF_c$ (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.