



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2020 – 06:09 PM JST

PDB ID : 6LFN
Title : Crystal structure of LpCGTb
Authors : Gao, H.M.; Yun, C.H.
Deposited on : 2019-12-03
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

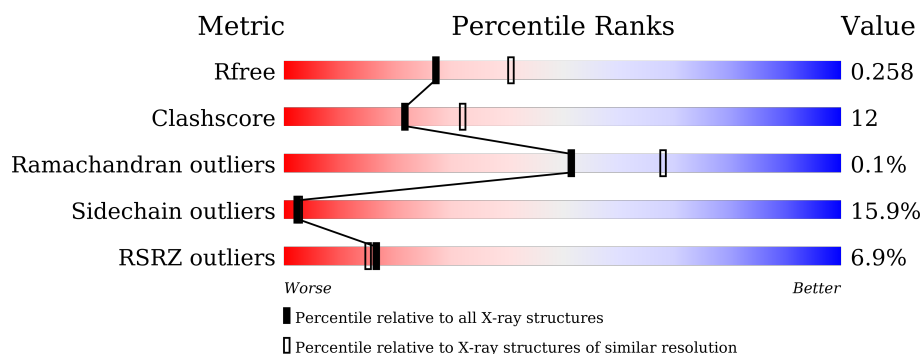
1 Overall quality at a glance

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 on 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	469	<div> <div>6%</div> <div> <div></div> <div>66%</div> <div>24%</div> <div>•</div> <div>6%</div> </div> </div>
1	B	469	<div> <div>7%</div> <div> <div></div> <div>67%</div> <div>21%</div> <div>6%</div> <div>6%</div> </div> </div>

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	PO4	A	501	-	-	X	-

2 Entry composition [i](#)

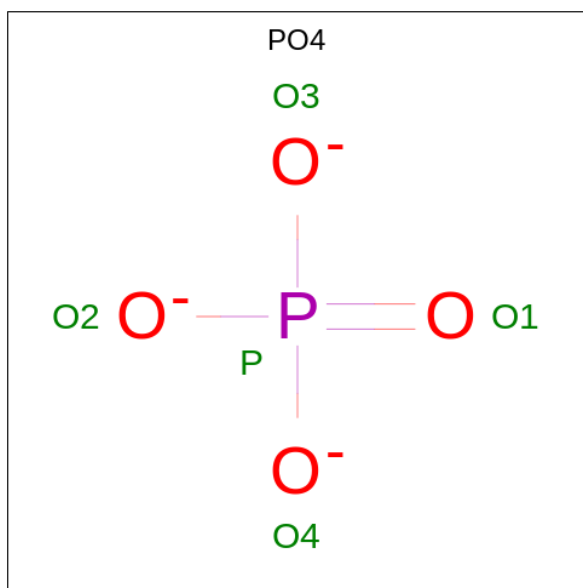
There are 2 unique types of molecules in this entry. The entry contains 6552 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LpCGTb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	1	0
			3299	2121	574	587	17			
1	B	441	Total	C	N	O	S	0	0	0
			3243	2083	565	577	18			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by author).

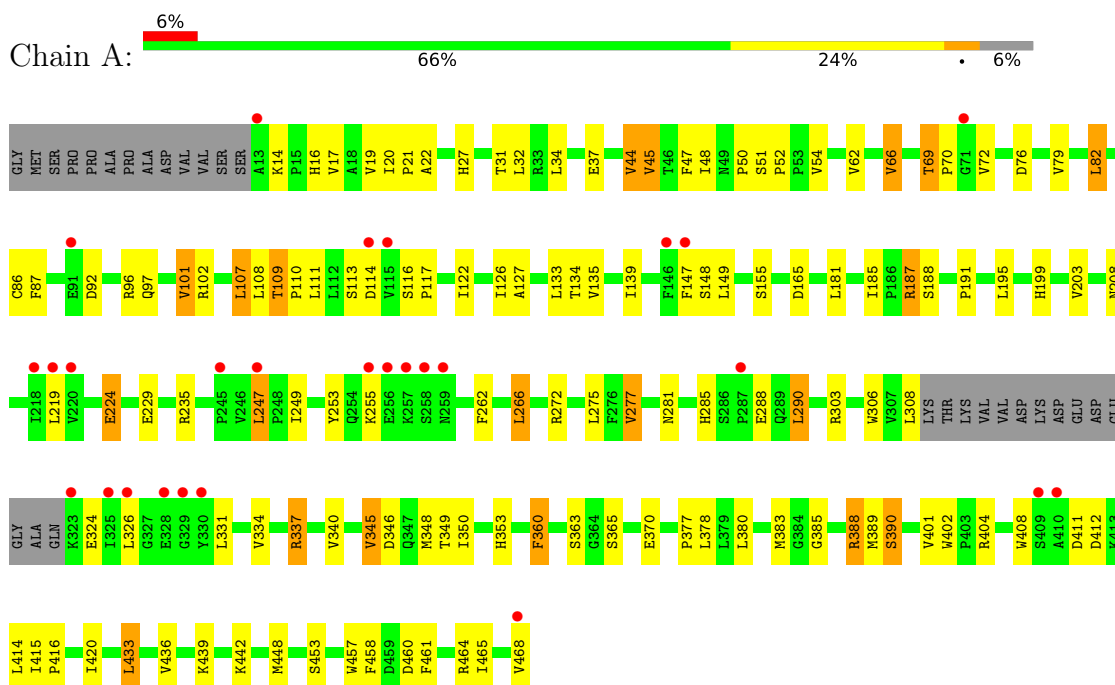


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

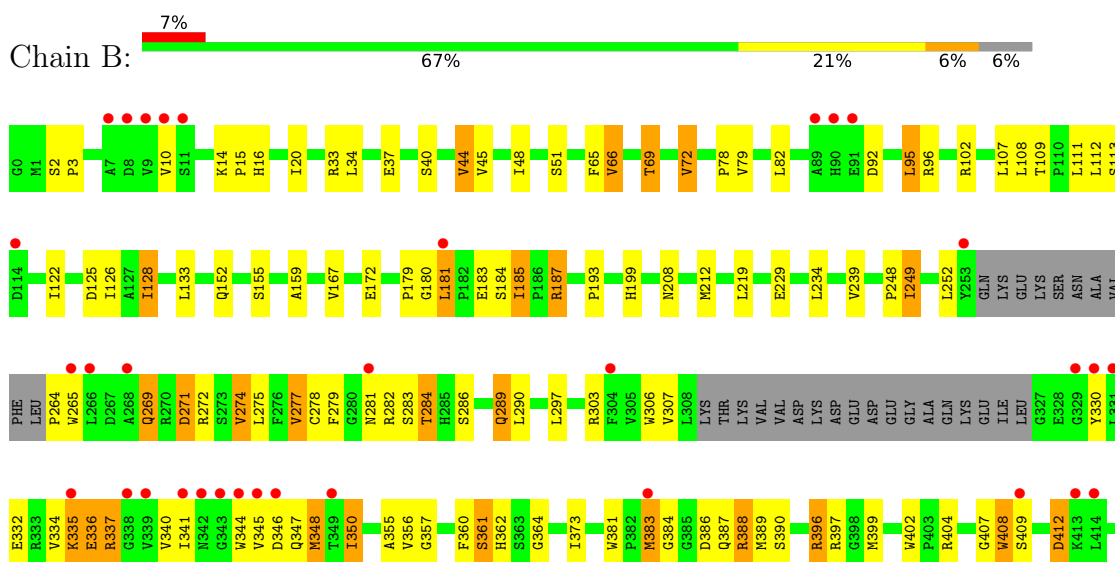
3 Residue-property plots

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: LpCGTb



• Molecule 1: LpCGTb





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.34Å 87.82Å 134.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.60 – 2.40 33.60 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (33.60-2.40) 99.0 (33.60-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.211 , 0.256 0.215 , 0.258	Depositor DCC
R_{free} test set	1764 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6552	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.71% 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

5.1 Standard geometry

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	0.55	0/3392	0.69	0/4632
1	B	0.50	0/3331	0.71	0/4551
All	All	0.53	0/6723	0.70	0/9183

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3299	0	3251	69	0
1	B	3243	0	3191	86	0
2	A	10	0	0	2	0
All	All	6552	0	6442	155	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 12.

All (155) 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:A:363:SER:HB2	1:A:380:LEU:HD22	1.48	0.95
1:B:279:PHE:O	1:B:362:HIS:HD2	1.52	0.93
1:A:54:VAL:HG23	1:A:97:GLN:HG3	1.63	0.81
1:B:332:GLU:O	1:B:335:LYS:HG2	1.81	0.80
1:B:279:PHE:O	1:B:362:HIS:CD2	2.39	0.73
1:B:277:VAL:HB	1:B:360:PHE:HB3	1.71	0.72
1:B:271:ASP:N	1:B:271:ASP:OD1	2.23	0.71
1:B:126:ILE:HD11	1:B:208:ASN:HB3	1.72	0.70
1:B:159:ALA:HB1	1:B:179:PRO:HD2	1.73	0.69
1:B:275:LEU:HD11	1:B:360:PHE:HB2	1.77	0.67
1:A:266:LEU:HD13	1:A:353:HIS:CD2	2.30	0.66
1:B:336:GLU:OE1	1:B:336:GLU:HA	1.95	0.66
1:B:269:GLN:HG3	1:B:303:ARG:CZ	2.26	0.66
1:B:20:ILE:HD11	1:B:122:ILE:HD11	1.78	0.65
1:B:167:VAL:O	1:B:187:ARG:NH2	2.29	0.65
1:B:384:GLY:HA2	1:B:408:TRP:CE3	2.32	0.65
1:B:412:ASP:OD1	1:B:412:ASP:N	2.30	0.65
1:A:402:TRP:O	1:A:404:ARG:NH1	2.31	0.64
1:A:20:ILE:HD11	1:A:122:ILE:HD11	1.80	0.63
1:B:82:LEU:O	1:B:96:ARG:NH2	2.31	0.63
1:A:86:CYS:O	1:A:96:ARG:NH1	2.28	0.62
1:A:363:SER:HB2	1:A:380:LEU:CD2	2.26	0.61
1:B:388:ARG:HD3	1:B:408:TRP:CZ3	2.35	0.61
1:B:65:PHE:O	1:B:69:THR:HG23	2.02	0.60
1:B:92:ASP:HB3	1:B:95:LEU:HD22	1.82	0.59
1:A:109:THR:HG22	1:A:135:VAL:HG13	1.84	0.59
1:A:363:SER:O	1:A:363:SER:OG	2.18	0.58
1:A:348:MET:SD	1:A:370:GLU:HG2	2.43	0.58
1:A:461:PHE:CZ	1:A:465:ILE:HD11	2.39	0.58
1:A:460:ASP:OD1	1:A:464:ARG:NH1	2.36	0.58
1:B:362:HIS:HA	1:B:381:TRP:O	2.04	0.58
1:A:303:ARG:HD3	1:A:337:ARG:HA	1.86	0.57
1:B:20:ILE:HG12	1:B:48:ILE:HG13	1.85	0.57
1:B:388:ARG:HH22	1:B:408:TRP:H	1.52	0.57
1:A:102:ARG:NH1	1:A:127:ALA:O	2.34	0.57
1:B:16:HIS:CD2	1:B:44:VAL:HG22	2.40	0.56
1:B:334:VAL:HG23	1:B:334:VAL:O	2.05	0.56
1:B:274:VAL:HG22	1:B:356:VAL:HA	1.88	0.56
1:A:345:VAL:HG13	1:A:350:ILE:HD12	1.88	0.56
1:A:275:LEU:HD11	1:A:360:PHE:HB2	1.88	0.56
1:A:92:ASP:O	1:A:96:ARG:HG3	2.07	0.55
1:A:199:HIS:O	1:A:203:VAL:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:PHE:CE1	1:A:149:LEU:HB2	2.42	0.54
1:B:306:TRP:HB3	1:B:340:VAL:HG22	1.89	0.54
1:B:125:ASP:O	1:B:128:ILE:HD13	2.08	0.53
1:B:3:PRO:HD3	1:B:457:TRP:CH2	2.44	0.53
1:B:155:SER:HB3	1:B:181:LEU:HD21	1.91	0.53
1:B:397:ARG:HD3	1:B:440:MET:HE1	1.91	0.52
1:A:50:PRO:HB3	1:A:79:VAL:HG11	1.92	0.52
1:B:265:TRP:HZ2	1:B:337:ARG:O	1.93	0.52
1:A:345:VAL:CG1	1:A:350:ILE:HD12	2.39	0.52
1:A:97:GLN:O	1:A:101:VAL:HG13	2.10	0.52
1:B:172:GLU:HA	1:B:187:ARG:HD2	1.91	0.52
1:B:332:GLU:O	1:B:335:LYS:CG	2.57	0.52
1:B:152:GLN:OE1	1:B:396:ARG:NH2	2.43	0.51
1:A:16:HIS:CD2	1:A:44:VAL:HG22	2.45	0.51
1:A:346:ASP:OD2	1:A:349:THR:CB	2.60	0.50
1:B:234:LEU:HD23	1:B:239:VAL:HG21	1.94	0.50
1:A:324:GLU:HG3	1:A:326:LEU:H	1.77	0.50
1:B:347:GLN:O	1:B:350:ILE:HG12	2.12	0.50
1:A:48:ILE:HD13	1:A:108:LEU:HD11	1.94	0.49
1:B:37:GLU:HG2	1:B:458:PHE:CE2	2.47	0.49
1:A:277:VAL:HB	1:A:360:PHE:HB3	1.95	0.49
1:A:247:LEU:HD23	1:A:247:LEU:N	2.28	0.49
1:B:271:ASP:HA	1:B:355:ALA:HA	1.94	0.49
1:B:383:MET:HB2	1:B:387:GLN:OE1	2.13	0.49
1:A:62:VAL:O	1:A:66:VAL:HG12	2.14	0.48
1:A:107:LEU:O	1:A:110:PRO:HD2	2.13	0.48
1:A:126:ILE:HD11	1:A:208:ASN:HB3	1.94	0.48
1:B:281:ASN:OD1	1:B:282:ARG:N	2.47	0.48
1:A:277:VAL:HG22	1:A:306:TRP:CD1	2.49	0.48
1:A:37:GLU:HG2	1:A:458:PHE:CZ	2.49	0.48
1:B:102:ARG:HD2	1:B:128:ILE:HA	1.96	0.48
1:B:388:ARG:HG3	1:B:402:TRP:CH2	2.49	0.48
1:A:107:LEU:O	1:A:111:LEU:HD23	2.14	0.48
1:A:187:ARG:NH1	1:A:195:LEU:HD13	2.29	0.47
1:B:388:ARG:HH22	1:B:407:GLY:HA2	1.78	0.47
1:A:416:PRO:O	1:A:420:ILE:HG13	2.14	0.47
1:B:279:PHE:C	1:B:362:HIS:HD2	2.15	0.47
1:B:284:THR:CG2	1:B:383:MET:HG3	2.45	0.47
1:B:33:ARG:HD3	1:B:252:LEU:O	2.14	0.47
1:A:185:ILE:HD12	1:A:389:MET:HE1	1.97	0.47
1:A:285:HIS:NE2	1:A:383:MET:CE	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ILE:CD1	1:B:208:ASN:HB3	2.44	0.47
1:B:344:TRP:O	1:B:344:TRP:CE3	2.68	0.47
1:A:155:SER:HB2	1:A:181:LEU:HD21	1.98	0.46
1:A:388:ARG:HD3	1:A:408:TRP:CH2	2.50	0.46
1:B:397:ARG:CZ	1:B:397:ARG:HA	2.45	0.46
1:B:69:THR:O	1:B:72:VAL:HG13	2.15	0.46
1:B:183:GLU:O	1:B:185:ILE:HG22	2.15	0.46
1:B:397:ARG:HD3	1:B:440:MET:CE	2.45	0.46
1:A:147:PHE:HE1	1:A:149:LEU:HB2	1.80	0.46
1:B:180:GLY:C	1:B:181:LEU:HD23	2.37	0.45
1:B:193:PRO:HB3	1:B:199:HIS:CE1	2.51	0.45
1:B:399:MET:HB3	1:B:436:VAL:HG22	1.98	0.45
1:A:235:ARG:HH22	2:A:501:PO4:P	2.38	0.45
1:B:388:ARG:HH22	1:B:408:TRP:N	2.15	0.45
1:A:401:VAL:HG23	1:A:433:LEU:HD11	1.99	0.45
1:A:266:LEU:O	1:A:266:LEU:HD22	2.16	0.45
1:B:335:LYS:HB2	1:B:335:LYS:HE3	1.35	0.45
1:A:465:ILE:HG21	1:A:465:ILE:HD13	1.57	0.45
1:B:348:MET:HE1	1:B:373:ILE:HB	1.98	0.44
1:A:306:TRP:CZ2	1:A:308:LEU:HD21	2.52	0.44
1:A:288:GLU:H	1:A:288:GLU:CD	2.19	0.44
1:A:187:ARG:HG3	1:A:188:SER:N	2.32	0.44
1:A:116:SER:HA	1:A:117:PRO:C	2.38	0.44
1:A:224:GLU:H	1:A:224:GLU:HG2	1.45	0.44
1:B:249:ILE:HG13	1:B:458:PHE:CZ	2.53	0.44
1:B:265:TRP:CZ2	1:B:337:ARG:O	2.70	0.43
1:B:344:TRP:O	1:B:344:TRP:HE3	2.00	0.43
1:B:126:ILE:HD13	1:B:212:MET:SD	2.58	0.43
1:B:386:ASP:N	1:B:386:ASP:OD1	2.50	0.43
1:A:402:TRP:C	1:A:402:TRP:CD1	2.91	0.43
1:B:384:GLY:O	1:B:387:GLN:HG3	2.19	0.43
1:A:32:LEU:HD23	1:A:32:LEU:HA	1.81	0.43
1:B:361:SER:OG	1:B:362:HIS:N	2.51	0.43
1:B:277:VAL:HA	1:B:360:PHE:O	2.18	0.43
1:B:249:ILE:HA	1:B:249:ILE:HD12	1.50	0.43
1:B:335:LYS:O	1:B:335:LYS:HE3	2.19	0.42
1:A:87:PHE:O	1:A:96:ARG:NH1	2.53	0.42
1:B:284:THR:HG22	1:B:383:MET:HG3	2.01	0.42
1:B:297:LEU:HD23	1:B:297:LEU:HA	1.77	0.42
1:A:69:THR:HA	1:A:70:PRO:HD3	1.87	0.42
1:B:108:LEU:HD21	1:B:112:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:HA	1:A:111:LEU:HD13	1.85	0.42
1:A:191:PRO:HB3	1:A:385:GLY:HA2	2.01	0.42
1:A:21:PRO:HB3	1:A:31:THR:HG21	2.02	0.41
1:A:21:PRO:HG3	1:A:47:PHE:CZ	2.55	0.41
1:A:365:SER:HA	1:A:390:SER:OG	2.19	0.41
1:A:247:LEU:HB3	1:A:457:TRP:CE3	2.55	0.41
1:B:348:MET:CE	1:B:373:ILE:HB	2.51	0.41
1:B:364:GLY:H	1:B:390:SER:HB2	1.85	0.41
1:A:290:LEU:HD12	1:A:290:LEU:HA	1.81	0.41
1:B:289:GLN:NE2	1:B:289:GLN:HA	2.35	0.41
1:B:347:GLN:HA	1:B:350:ILE:HD11	2.02	0.41
1:A:377:PRO:HB3	1:A:433:LEU:HD22	2.02	0.41
1:B:66:VAL:HB	1:B:72:VAL:HG22	2.01	0.41
1:A:464:ARG:NH2	2:A:501:PO4:O2	2.54	0.41
1:B:152:GLN:HE21	1:B:389:MET:HE3	1.85	0.41
1:A:415:ILE:HA	1:A:416:PRO:HD3	1.89	0.41
1:A:51:SER:HA	1:A:52:PRO:HA	1.54	0.41
1:B:14:LYS:HD3	1:B:14:LYS:HA	1.90	0.41
1:B:51:SER:O	1:B:78:PRO:HA	2.21	0.41
1:B:126:ILE:HD13	1:B:212:MET:HG3	2.03	0.40
1:B:264:PRO:HB2	1:B:265:TRP:H	1.59	0.40
1:B:15:PRO:HD3	1:B:466:ASN:ND2	2.36	0.40
1:A:22:ALA:HB3	1:A:27:HIS:HB3	2.04	0.40
1:A:249:ILE:HD12	1:A:249:ILE:HA	1.89	0.40
1:B:335:LYS:O	1:B:335:LYS:CD	2.69	0.40
1:B:335:LYS:O	1:B:335:LYS:CE	2.69	0.40
1:B:388:ARG:NH2	1:B:407:GLY:HA2	2.35	0.40
1:B:357:GLY:O	1:B:434:ARG:NH1	2.55	0.40
1:B:248:PRO:HD2	1:B:457:TRP:CD2	2.57	0.40
1:A:17:VAL:O	1:A:45:VAL:HA	2.22	0.40
1:A:82:LEU:HA	1:A:82:LEU:HD23	1.72	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	439/469 (94%)	431 (98%)	8 (2%)	0	100	100
1	B	435/469 (93%)	421 (97%)	13 (3%)	1 (0%)	47	62
All	All	874/938 (93%)	852 (98%)	21 (2%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	330	TYR

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	336/374 (90%)	284 (84%)	52 (16%)	2	3
1	B	327/374 (87%)	274 (84%)	53 (16%)	2	3
All	All	663/748 (89%)	558 (84%)	105 (16%)	2	3

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	19	VAL
1	A	34	LEU
1	A	44	VAL
1	A	45	VAL
1	A	66	VAL
1	A	69	THR
1	A	72	VAL
1	A	76	ASP
1	A	82	LEU
1	A	101	VAL
1	A	107	LEU

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Mol	Chain	Res	Type
1	A	109	THR
1	A	113	SER
1	A	114	ASP
1	A	133	LEU
1	A	134	THR
1	A	139	ILE
1	A	148	SER
1	A	165	ASP
1	A	187	ARG
1	A	219	LEU
1	A	224	GLU
1	A	229	GLU
1	A	247	LEU
1	A	253	TYR
1	A	255	LYS
1	A	262	PHE
1	A	266	LEU
1	A	272	ARG
1	A	277	VAL
1	A	281	ASN
1	A	290	LEU
1	A	331	LEU
1	A	334	VAL
1	A	337	ARG
1	A	340	VAL
1	A	345	VAL
1	A	360	PHE
1	A	378	LEU
1	A	388	ARG
1	A	390	SER
1	A	411	ASP
1	A	412	ASP
1	A	414	LEU
1	A	433	LEU
1	A	436	VAL
1	A	439	LYS
1	A	442	LYS
1	A	448	MET
1	A	453	SER
1	A	468	VAL
1	B	2	SER
1	B	10	VAL

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Mol	Chain	Res	Type
1	B	34	LEU
1	B	40	SER
1	B	44	VAL
1	B	45	VAL
1	B	66	VAL
1	B	69	THR
1	B	72	VAL
1	B	79	VAL
1	B	95	LEU
1	B	107	LEU
1	B	109	THR
1	B	111	LEU
1	B	113	SER
1	B	128	ILE
1	B	133	LEU
1	B	181	LEU
1	B	184	SER
1	B	185	ILE
1	B	187	ARG
1	B	219	LEU
1	B	229	GLU
1	B	249	ILE
1	B	269	GLN
1	B	271	ASP
1	B	272	ARG
1	B	274	VAL
1	B	277	VAL
1	B	278	CYS
1	B	283	SER
1	B	284	THR
1	B	286	SER
1	B	289	GLN
1	B	290	LEU
1	B	307	VAL
1	B	335	LYS
1	B	336	GLU
1	B	337	ARG
1	B	341	ILE
1	B	345	VAL
1	B	346	ASP
1	B	348	MET
1	B	350	ILE

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Mol	Chain	Res	Type
1	B	361	SER
1	B	383	MET
1	B	388	ARG
1	B	396	ARG
1	B	404	ARG
1	B	408	TRP
1	B	409	SER
1	B	412	ASP
1	B	453	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	362	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	A	501	-	4,4,4	0.93	0	6,6,6	0.57	0
2	PO4	A	502	-	4,4,4	0.86	0	6,6,6	0.63	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

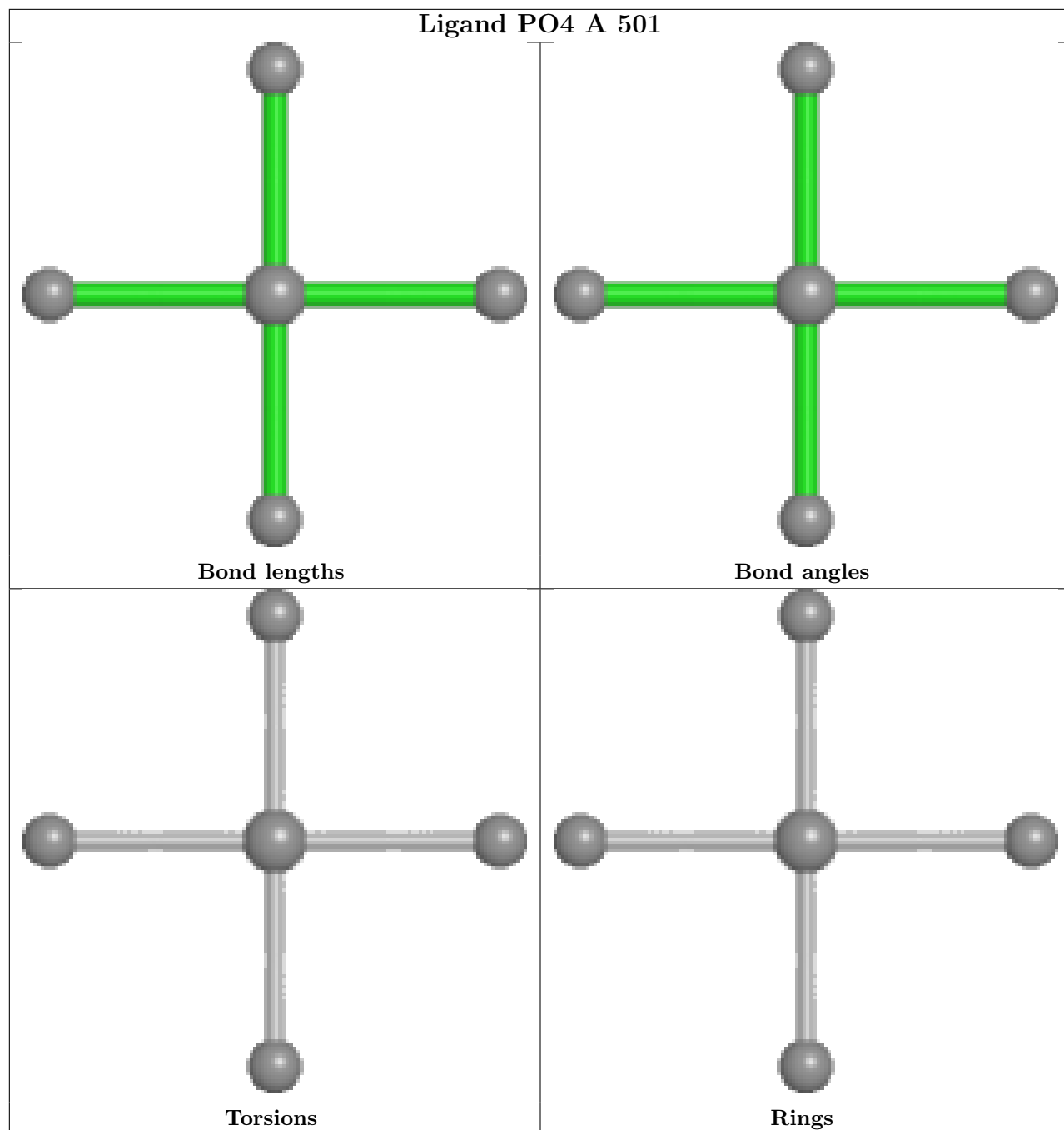
There are no torsion outliers.

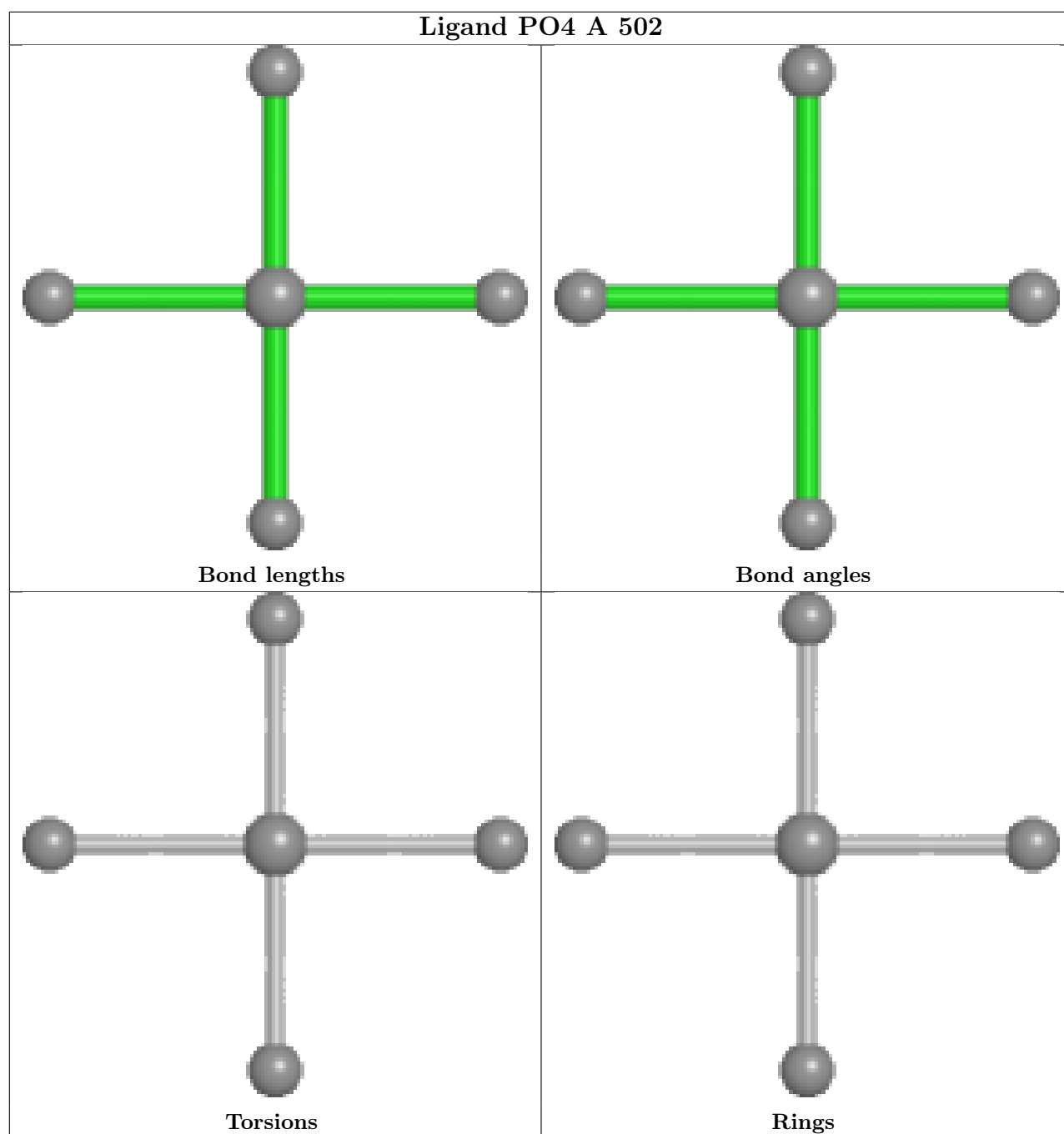
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PO4	2	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	442/469 (94%)	0.27	27 (6%) 21 20	30, 49, 71, 102	0
1	B	441/469 (94%)	0.36	34 (7%) 13 12	30, 48, 87, 109	0
All	All	883/938 (94%)	0.32	61 (6%) 16 15	30, 48, 81, 109	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	SER	13.2
1	B	11	SER	11.7
1	B	10	VAL	10.4
1	A	257	LYS	6.6
1	B	345	VAL	5.9
1	A	323	LYS	5.8
1	B	9	VAL	5.6
1	B	7	ALA	5.3
1	B	339	VAL	5.3
1	A	326	LEU	5.2
1	B	330	TYR	5.1
1	A	325	ILE	5.1
1	B	331	LEU	4.7
1	B	8	ASP	4.5
1	B	344	TRP	4.4
1	B	89	ALA	4.2
1	B	265	TRP	4.2
1	A	256	GLU	4.1
1	A	468	VAL	4.0
1	A	219	LEU	4.0
1	A	410	ALA	3.9
1	B	414	LEU	3.6
1	B	90	HIS	3.6
1	B	349	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	255	LYS	3.4
1	B	409	SER	3.4
1	A	409	SER	3.4
1	B	281	ASN	3.3
1	B	468	VAL	3.1
1	B	341	ILE	3.1
1	A	330	TYR	3.1
1	B	343	GLY	3.1
1	A	329	GLY	3.1
1	A	328	GLU	3.0
1	A	114	ASP	2.9
1	A	247	LEU	2.9
1	A	115	VAL	2.8
1	A	220	VAL	2.7
1	A	287	PRO	2.6
1	B	383	MET	2.6
1	A	13	ALA	2.6
1	B	342	ASN	2.6
1	B	266	LEU	2.5
1	B	91	GLU	2.5
1	B	114	ASP	2.5
1	A	218	ILE	2.4
1	A	147	PHE	2.4
1	B	181	LEU	2.4
1	B	346	ASP	2.4
1	A	245	PRO	2.4
1	A	259	ASN	2.3
1	B	268	ALA	2.3
1	A	71	GLY	2.2
1	A	91	GLU	2.2
1	B	253	TYR	2.2
1	B	413	LYS	2.1
1	B	335	LYS	2.1
1	B	338	GLY	2.1
1	A	146	PHE	2.1
1	B	304	PHE	2.1
1	B	329	GLY	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 monosaccharides in this entry.

6.4 Ligands [i](#)

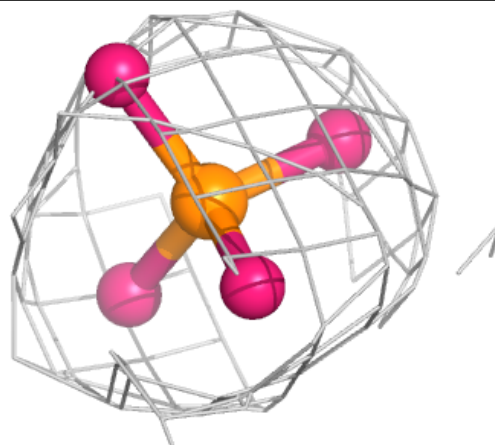
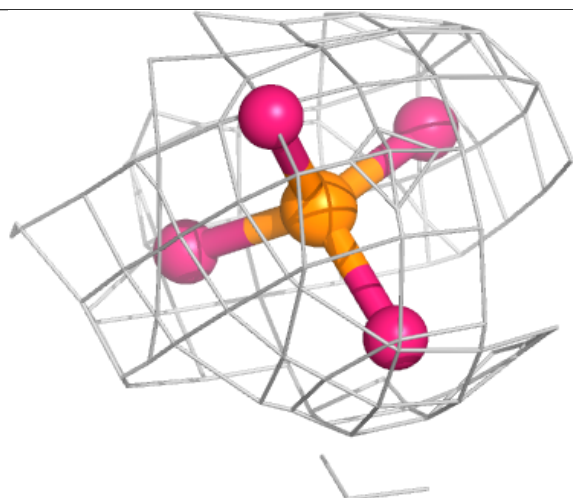
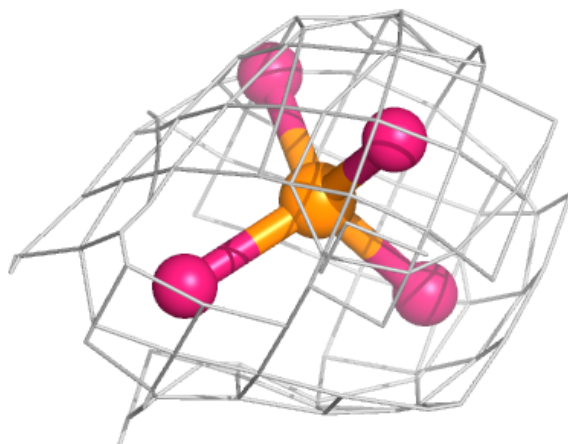
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO4	A	502	5/5	0.93	0.19	68,75,82,83	0
2	PO4	A	501	5/5	0.99	0.19	29,36,37,38	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.

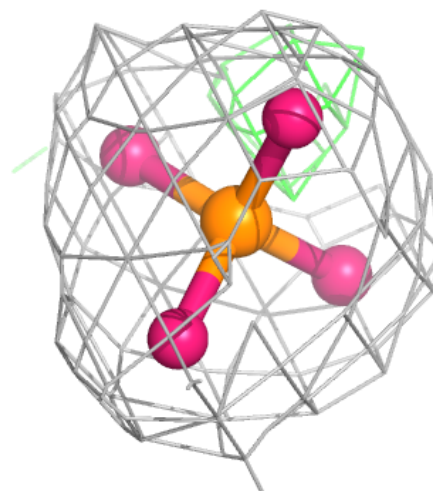
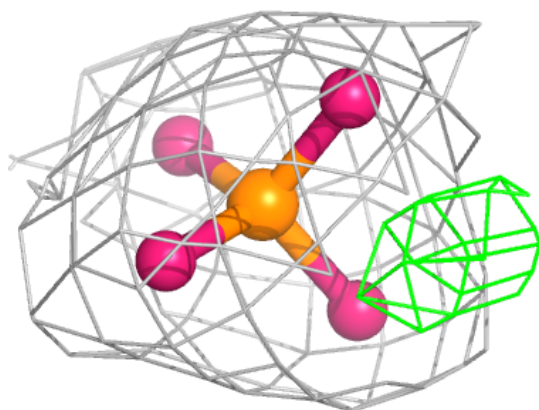
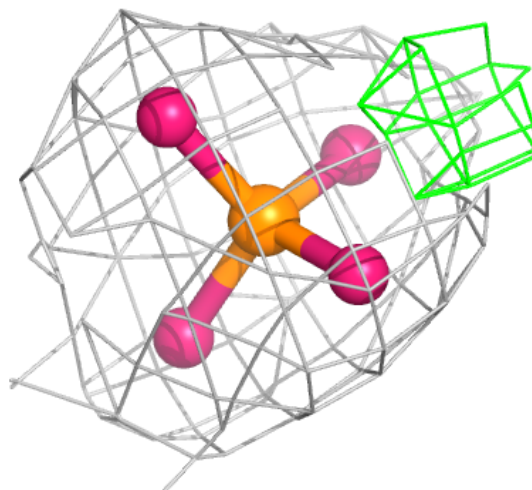
Electron density around PO4 A 502:

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



Electron density around PO4 A 501:

$2mF_o-DF_c$ (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.