



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:00 AM UTC

PDB ID : 8OJF / pdb_00008ojf
Title : Arabidopsis thaliana Phosphoenolpyruvate carboxylase PPC1 with bound phosphate
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Deposited on : 2023-03-24
Resolution : 3.04 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

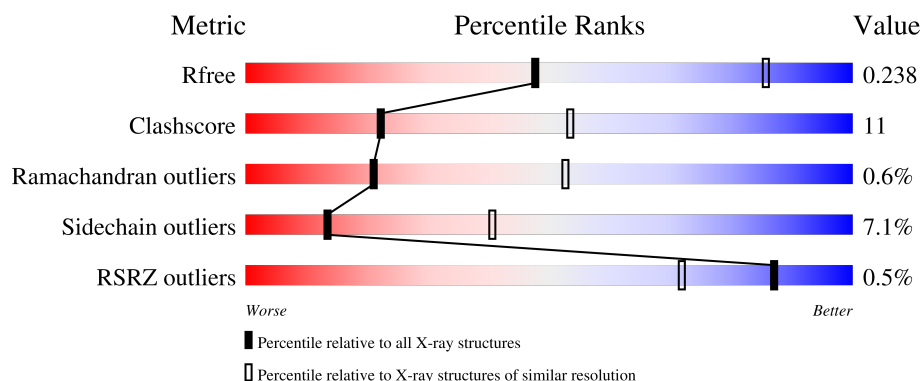
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	974	 66% 24% • 7%
1	B	974	 66% 22% • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14393 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.

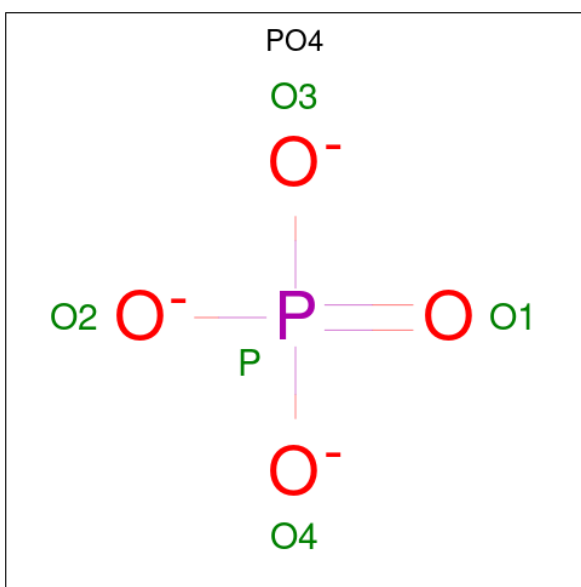
- Molecule 1 is a protein called Phosphoenolpyruvate carboxylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	906	Total	C	N	O	S	0	3	0
			7252	4604	1268	1351	29			
1	B	888	Total	C	N	O	S	0	0	0
			7106	4512	1232	1333	29			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q9MAH0
A	-5	HIS	-	expression tag	UNP Q9MAH0
A	-4	HIS	-	expression tag	UNP Q9MAH0
A	-3	HIS	-	expression tag	UNP Q9MAH0
A	-2	HIS	-	expression tag	UNP Q9MAH0
A	-1	HIS	-	expression tag	UNP Q9MAH0
A	0	HIS	-	expression tag	UNP Q9MAH0
B	-6	MET	-	initiating methionine	UNP Q9MAH0
B	-5	HIS	-	expression tag	UNP Q9MAH0
B	-4	HIS	-	expression tag	UNP Q9MAH0
B	-3	HIS	-	expression tag	UNP Q9MAH0
B	-2	HIS	-	expression tag	UNP Q9MAH0
B	-1	HIS	-	expression tag	UNP Q9MAH0
B	0	HIS	-	expression tag	UNP Q9MAH0

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



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		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		

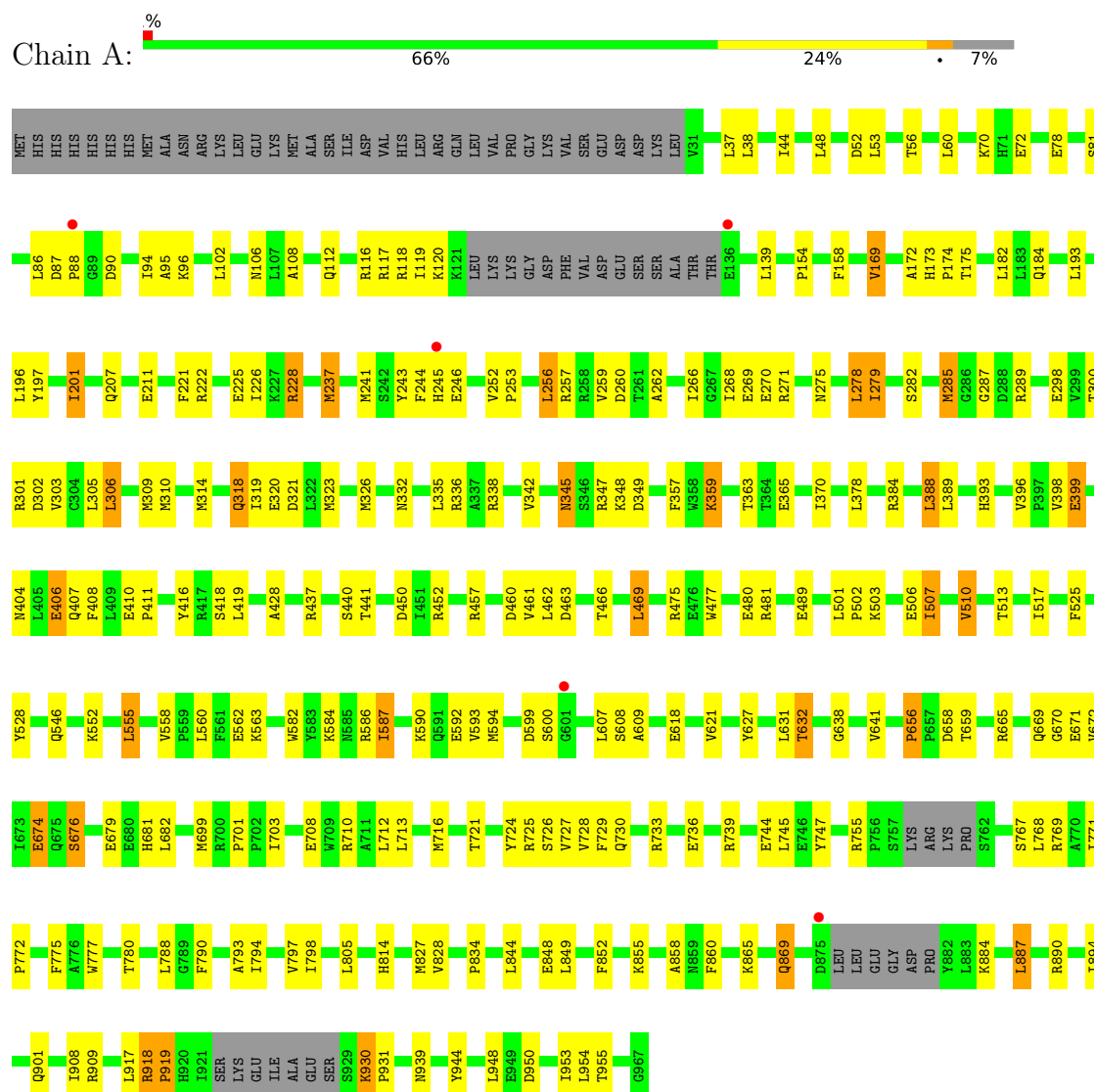
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	5	Total	O	0	0
			5	5		

3 Residue-property plots

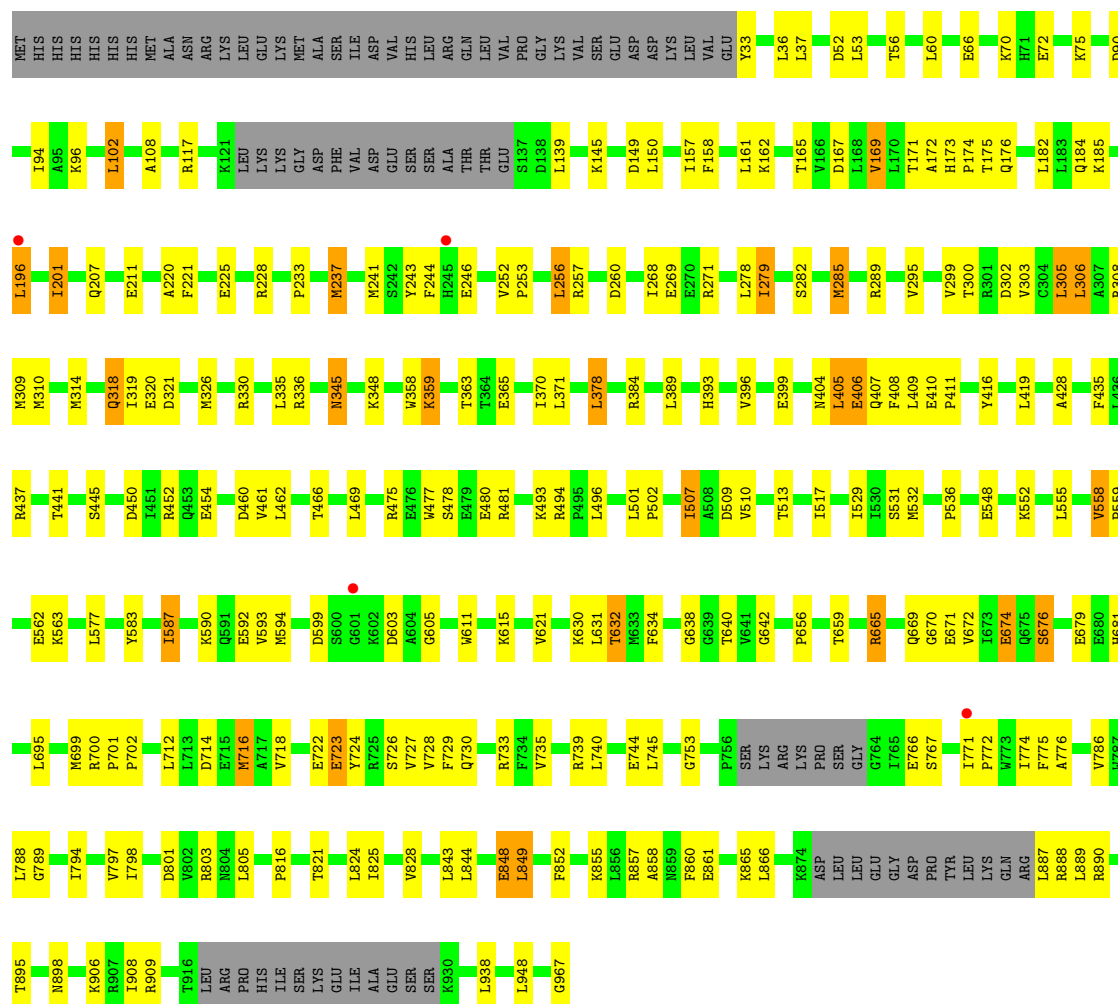
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Phosphoenolpyruvate carboxylase 1



• Molecule 1: Phosphoenolpyruvate carboxylase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	127.22Å 158.17Å 141.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.71 – 3.04 48.71 – 3.04	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.71-3.04) 90.3 (48.71-3.04)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.15 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.203 , 0.243 (Not available) , 0.238	Depositor DCC
R_{free} test set	2774 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	100.3	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 86.0	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	0.95	EDS
Total number of atoms	14393	wwPDB-VP
Average B, all atoms (Å ²)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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, CL

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	0.35	1/7418 (0.0%)	0.58	0/10048
1	B	0.22	0/7259	0.43	0/9833
All	All	0.29	1/14677 (0.0%)	0.51	0/19881

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	656	PRO	CA-C	-5.51	1.48	1.51

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	7252	0	7166	159	0
1	B	7106	0	7025	147	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	A	2	0	0	0	0
4	A	13	0	0	0	0
4	B	5	0	0	0	0
All	All	14393	0	14191	304	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 11.

All (304) 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:B:638:GLY:HA2	1:B:669:GLN:HG3	1.50	0.92
1:A:618:GLU:OE1	1:A:710:ARG:NH2	2.08	0.86
1:A:679:GLU:HB3	1:A:682:LEU:HG	1.61	0.83
1:A:175:THR:HG23	1:A:671:GLU:H	1.43	0.82
1:B:888:ARG:O	1:B:890:ARG:N	2.16	0.79
1:A:712:LEU:HG	1:A:716:MET:HE2	1.64	0.79
1:B:723:GLU:HG2	1:B:789:GLY:HA2	1.64	0.79
1:A:638:GLY:HA2	1:A:669:GLN:HG3	1.65	0.77
1:A:169:VAL:HB	1:A:282:SER:HB2	1.66	0.76
1:A:237:MET:HG2	1:A:303:VAL:HG12	1.71	0.72
1:B:173:HIS:ND1	1:B:669:GLN:OE1	2.23	0.71
1:A:641:VAL:HG21	1:A:828:VAL:HG21	1.72	0.70
1:A:884:LYS:HA	1:A:887:LEU:HB3	1.73	0.70
1:A:289:ARG:NH2	1:A:300:THR:OG1	2.24	0.70
1:A:593:VAL:HG12	1:A:631:LEU:HD11	1.74	0.70
1:B:702:PRO:HB3	1:B:816:PRO:HG2	1.75	0.69
1:B:384:ARG:HD2	1:B:396:VAL:HB	1.75	0.69
1:B:656:PRO:HG2	1:B:659:THR:HG21	1.74	0.69
1:B:326:MET:HE1	1:B:419:LEU:HD11	1.74	0.69
1:A:739:ARG:NH1	1:A:744:GLU:OE1	2.26	0.68
1:A:237:MET:HA	1:A:285:MET:HE3	1.77	0.66
1:A:237:MET:HE3	1:A:303:VAL:HB	1.78	0.66
1:A:528:TYR:HB2	1:A:555:LEU:HD13	1.78	0.66
1:B:461:VAL:HG22	1:B:507:ILE:HG23	1.78	0.66
1:A:679:GLU:HG3	1:A:681:HIS:H	1.60	0.66
1:A:908:ILE:HD11	1:A:948:LEU:HB3	1.78	0.65
1:A:106:ASN:OD1	1:A:890:ARG:NH2	2.29	0.65
1:B:175:THR:HG23	1:B:671:GLU:H	1.60	0.65
1:A:345:ASN:OD1	1:A:345:ASN:N	2.26	0.65
1:A:326:MET:HE1	1:A:419:LEU:HD11	1.78	0.64
1:B:563:LYS:NZ	1:B:766:GLU:OE2	2.31	0.63
1:B:404:ASN:HB2	1:B:407:GLN:HB2	1.81	0.63
1:A:298:GLU:OE1	1:A:301[A]:ARG:NH1	2.31	0.63
1:B:228:ARG:HH12	1:B:938:LEU:HB3	1.62	0.63
1:B:861:GLU:HG3	1:B:865:LYS:HE3	1.81	0.62
1:B:237:MET:HE3	1:B:303:VAL:HB	1.80	0.62
1:A:726:SER:HA	1:A:730:GLN:CG	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:ARG:NH1	1:B:744:GLU:OE1	2.32	0.62
1:A:656:PRO:HG2	1:A:659:THR:HG21	1.82	0.62
1:A:48:LEU:HD22	1:A:222:ARG:NH1	2.15	0.61
1:A:173:HIS:ND1	1:A:669:GLN:OE1	2.34	0.61
1:B:733:ARG:NH2	1:B:848:GLU:OE1	2.22	0.60
1:A:306:LEU:O	1:A:310:MET:HG3	2.00	0.60
1:B:306:LEU:O	1:B:310:MET:HG3	2.00	0.60
1:B:460:ASP:OD1	1:B:475:ARG:NH1	2.34	0.60
1:A:726:SER:HA	1:A:730:GLN:HG3	1.83	0.60
1:A:158:PHE:HB2	1:A:268:ILE:HD13	1.84	0.59
1:B:852:PHE:O	1:B:855:LYS:HB2	2.03	0.59
1:B:477:TRP:CG	1:B:481:ARG:HD2	2.37	0.59
1:B:849:LEU:H	1:B:849:LEU:HD23	1.68	0.59
1:A:90:ASP:O	1:A:94:ILE:HG12	2.02	0.58
1:A:96:LYS:HE2	1:A:225:GLU:OE2	2.03	0.58
1:B:722:GLU:O	1:B:726:SER:HB3	2.04	0.58
1:A:918:ARG:HB2	1:A:919:PRO:HD3	1.85	0.58
1:B:642:GLY:HA3	1:B:774:ILE:HD12	1.85	0.58
1:B:562:GLU:HG2	1:B:599:ASP:HB2	1.86	0.57
1:B:477:TRP:HA	1:B:481:ARG:HH11	1.69	0.57
1:A:563:LYS:HE3	1:A:599:ASP:HB3	1.87	0.57
1:B:593:VAL:HG12	1:B:631:LEU:HD11	1.85	0.57
1:B:169:VAL:HB	1:B:282:SER:HB2	1.86	0.57
1:B:244:PHE:C	1:B:246:GLU:H	2.13	0.57
1:A:618:GLU:CD	1:A:710:ARG:HH22	2.12	0.56
1:B:345:ASN:N	1:B:345:ASN:OD1	2.38	0.56
1:A:48:LEU:HD22	1:A:222:ARG:HH12	1.71	0.56
1:A:855:LYS:O	1:A:858:ALA:HB3	2.05	0.56
1:B:302:ASP:O	1:B:306:LEU:HB2	2.04	0.56
1:B:406:GLU:HA	1:B:409:LEU:HB2	1.87	0.56
1:B:558:VAL:HG23	1:B:593:VAL:HA	1.88	0.56
1:B:306:LEU:HD22	1:B:389:LEU:HD11	1.88	0.56
1:B:844:LEU:HD22	1:B:909:ARG:HH21	1.71	0.55
1:A:302:ASP:O	1:A:306:LEU:HB2	2.07	0.55
1:B:740:LEU:HA	1:B:909:ARG:HH12	1.70	0.55
1:B:358:TRP:CD1	1:B:359:LYS:HD2	2.42	0.55
1:A:237:MET:O	1:A:241:MET:HG2	2.07	0.55
1:A:228:ARG:NH2	1:A:950:ASP:OD1	2.40	0.55
1:B:37:LEU:HD11	1:B:108:ALA:HB2	1.89	0.55
1:B:336:ARG:NH2	1:B:363:THR:O	2.40	0.54
1:A:174:PRO:O	1:A:747:TYR:OH	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:MET:HA	1:B:634:PHE:HB3	1.88	0.54
1:B:237:MET:HG2	1:B:303:VAL:HG12	1.88	0.54
1:B:260:ASP:CG	1:B:271:ARG:HG2	2.32	0.54
1:B:679:GLU:HG3	1:B:681:HIS:H	1.73	0.54
1:A:716:MET:HG3	1:A:797:VAL:HG21	1.90	0.54
1:A:728:VAL:HG23	1:A:729:PHE:CD2	2.43	0.54
1:B:253:PRO:O	1:B:257:ARG:HG3	2.07	0.54
1:A:462:LEU:O	1:A:466:THR:HG23	2.08	0.53
1:A:546:GLN:OE1	1:A:555:LEU:HD12	2.08	0.53
1:B:308:ARG:HG3	1:B:445:SER:HB3	1.90	0.53
1:A:336:ARG:NH2	1:A:363:THR:O	2.41	0.53
1:B:201:ILE:HD13	1:B:201:ILE:H	1.74	0.53
1:B:824:LEU:O	1:B:828:VAL:HG23	2.09	0.53
1:A:256:LEU:HD23	1:A:437:ARG:HD3	1.90	0.53
1:A:310:MET:O	1:A:314:MET:HG3	2.08	0.53
1:B:437:ARG:O	1:B:441:THR:HB	2.09	0.53
1:A:86:LEU:HD22	1:A:90:ASP:HB3	1.90	0.52
1:B:728:VAL:HG23	1:B:729:PHE:CD2	2.43	0.52
1:B:478:SER:H	1:B:481:ARG:NH1	2.06	0.52
1:A:562:GLU:HG2	1:A:599:ASP:HB2	1.92	0.52
1:A:306:LEU:HD22	1:A:389:LEU:HD11	1.91	0.52
1:A:37:LEU:HD21	1:A:193:LEU:HD21	1.92	0.52
1:A:243:TYR:OH	1:A:674:GLU:HG2	2.10	0.52
1:B:621:VAL:HG21	1:B:659:THR:HA	1.91	0.52
1:A:724:TYR:CD1	1:A:788:LEU:HD23	2.45	0.52
1:A:461:VAL:HA	1:A:507:ILE:HD13	1.91	0.52
1:B:169:VAL:HG11	1:B:634:PHE:CZ	2.45	0.52
1:B:167:ASP:HB3	1:B:665:ARG:HG3	1.92	0.52
1:B:358:TRP:HD1	1:B:359:LYS:HD2	1.73	0.52
1:A:772:PRO:HA	1:A:775:PHE:HB3	1.92	0.51
1:B:289:ARG:NH2	1:B:300:THR:OG1	2.44	0.51
1:B:185:LYS:HD2	1:B:220:ALA:HA	1.92	0.51
1:B:462:LEU:O	1:B:466:THR:HG23	2.10	0.51
1:B:150:LEU:HD11	1:B:700:ARG:HB2	1.92	0.51
1:A:335:LEU:HG	1:A:370:ILE:HD12	1.93	0.51
1:A:112:GLN:O	1:A:116:ARG:HB2	2.11	0.50
1:A:592:GLU:HA	1:A:632:THR:O	2.11	0.50
1:B:908:ILE:HD11	1:B:948:LEU:HB3	1.93	0.50
1:A:226:ILE:HG23	1:A:953:ILE:HG21	1.93	0.50
1:B:90:ASP:O	1:B:94:ILE:HG12	2.12	0.50
1:A:930:LYS:HG2	1:A:931:PRO:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ASP:O	1:B:56:THR:HG23	2.12	0.50
1:B:745:LEU:HD12	1:B:745:LEU:H	1.77	0.50
1:B:477:TRP:CD1	1:B:481:ARG:HD2	2.47	0.49
1:A:244:PHE:C	1:A:246:GLU:H	2.20	0.49
1:B:405:LEU:HD12	1:B:405:LEU:H	1.76	0.49
1:B:454:GLU:HA	1:B:531:SER:HB2	1.93	0.49
1:B:158:PHE:HB2	1:B:268:ILE:HD13	1.93	0.49
1:A:260:ASP:CG	1:A:271:ARG:HG2	2.37	0.49
1:A:844:LEU:HD13	1:A:909:ARG:NH2	2.27	0.49
1:A:404:ASN:HB2	1:A:407:GLN:HB2	1.95	0.48
1:B:477:TRP:HA	1:B:481:ARG:NH1	2.28	0.48
1:A:408:PHE:O	1:A:411:PRO:HD2	2.13	0.48
1:B:726:SER:HA	1:B:730:GLN:HG3	1.94	0.48
1:A:641:VAL:HG21	1:A:828:VAL:CG2	2.41	0.48
1:A:745:LEU:HD12	1:A:745:LEU:H	1.77	0.48
1:A:95:ALA:HB1	1:A:954:LEU:HB3	1.95	0.48
1:A:621:VAL:HG21	1:A:659:THR:HG22	1.95	0.48
1:B:256:LEU:HD23	1:B:437:ARG:HD3	1.96	0.48
1:A:584:LYS:HE2	1:A:627:TYR:O	2.14	0.47
1:B:786:VAL:HG11	1:B:828:VAL:HG21	1.95	0.47
1:B:724:TYR:O	1:B:728:VAL:HG22	2.14	0.47
1:A:755:ARG:HD3	1:A:769:ARG:NH2	2.29	0.47
1:A:460:ASP:OD1	1:A:475:ARG:NH1	2.48	0.47
1:B:310:MET:O	1:B:314:MET:HG3	2.14	0.47
1:B:592:GLU:HA	1:B:632:THR:O	2.15	0.47
1:A:96:LYS:NZ	1:A:221:PHE:O	2.46	0.47
1:A:461:VAL:HG21	1:A:510:VAL:CG2	2.45	0.47
1:A:457:ARG:NE	1:A:506:GLU:HB3	2.30	0.47
1:A:712:LEU:HG	1:A:716:MET:CE	2.39	0.47
1:B:158:PHE:CE2	1:B:162:LYS:HD2	2.50	0.47
1:B:724:TYR:CD1	1:B:788:LEU:HD23	2.50	0.46
1:A:721:THR:O	1:A:725:ARG:HG3	2.14	0.46
1:B:237:MET:O	1:B:241:MET:HG2	2.16	0.46
1:B:408:PHE:O	1:B:411:PRO:HD2	2.14	0.46
1:B:513:THR:O	1:B:517:ILE:HG13	2.15	0.46
1:A:154:PRO:HB3	1:A:266:ILE:HG22	1.97	0.46
1:B:794:ILE:O	1:B:798:ILE:HG12	2.15	0.46
1:A:279:ILE:HD13	1:A:279:ILE:H	1.81	0.46
1:A:289:ARG:HG2	1:A:452:ARG:O	2.16	0.46
1:A:301[B]:ARG:NH2	1:A:388:LEU:O	2.48	0.46
1:B:172:ALA:HB2	1:B:285:MET:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:716:MET:SD	1:B:797:VAL:HG21	2.56	0.46
1:B:857:ARG:O	1:B:860:PHE:HB3	2.16	0.46
1:A:716:MET:HG2	1:A:793:ALA:HB1	1.97	0.46
1:B:794:ILE:HB	1:B:866:LEU:HD13	1.98	0.46
1:A:87:ASP:HB3	1:A:88:PRO:HD2	1.97	0.46
1:A:285:MET:HB2	1:A:285:MET:HE2	1.67	0.46
1:A:338:ARG:O	1:A:342:VAL:HG23	2.15	0.46
1:B:53:LEU:HD12	1:B:53:LEU:HA	1.70	0.46
1:B:174:PRO:HB3	1:B:753:GLY:HA3	1.98	0.46
1:B:583:TYR:CZ	1:B:587:ILE:HG12	2.50	0.46
1:A:399:GLU:CD	1:A:399:GLU:H	2.23	0.46
1:B:96:LYS:HB3	1:B:221:PHE:CZ	2.50	0.46
1:A:794:ILE:O	1:A:798:ILE:HG12	2.16	0.45
1:B:33:TYR:HE1	1:B:36:LEU:HD22	1.81	0.45
1:B:672:VAL:O	1:B:676:SER:OG	2.33	0.45
1:A:252:VAL:HB	1:A:253:PRO:HD3	1.98	0.45
1:A:461:VAL:HG22	1:A:507:ILE:HG23	1.97	0.45
1:A:679:GLU:HG3	1:A:681:HIS:N	2.29	0.45
1:B:279:ILE:HD13	1:B:279:ILE:H	1.81	0.45
1:B:552:LYS:H	1:B:552:LYS:HG2	1.53	0.45
1:B:157:ILE:O	1:B:161:LEU:HB2	2.16	0.45
1:B:318:GLN:HB3	1:B:435:PHE:HE1	1.82	0.45
1:A:256:LEU:HB3	1:A:437:ARG:CZ	2.47	0.45
1:A:517:ILE:HA	1:A:525:PHE:CZ	2.51	0.45
1:B:450:ASP:OD2	1:B:665:ARG:NH2	2.47	0.45
1:B:821:THR:O	1:B:825:ILE:HG12	2.15	0.45
1:A:332:ASN:ND2	1:A:418:SER:HA	2.32	0.45
1:A:724:TYR:HD1	1:A:788:LEU:HB3	1.82	0.45
1:A:37:LEU:HD11	1:A:108:ALA:HB2	1.98	0.45
1:B:252:VAL:HB	1:B:253:PRO:HD3	1.99	0.45
1:B:536:PRO:HB3	1:B:577:LEU:HD13	1.99	0.45
1:B:712:LEU:O	1:B:716:MET:HB2	2.16	0.45
1:A:410:GLU:HB3	1:A:411:PRO:HD3	1.99	0.45
1:A:901:GLN:HB2	1:A:955:THR:HB	1.99	0.45
1:A:908:ILE:HD12	1:A:944:TYR:CD2	2.52	0.44
1:A:384:ARG:HD2	1:A:396:VAL:HB	1.99	0.44
1:A:855:LYS:HE2	1:A:855:LYS:HB3	1.86	0.44
1:A:52:ASP:O	1:A:56:THR:HG23	2.17	0.44
1:A:546:GLN:OE1	1:A:555:LEU:N	2.50	0.44
1:B:416:TYR:CD2	1:B:428:ALA:HB1	2.53	0.44
1:A:607:LEU:HB2	1:A:790:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:GLU:OE2	1:B:494:ARG:NH2	2.39	0.44
1:B:66:GLU:HB2	1:B:75:LYS:HE2	1.99	0.44
1:A:78:GLU:O	1:A:81:SER:OG	2.36	0.44
1:A:672:VAL:O	1:A:676:SER:OG	2.35	0.44
1:B:289:ARG:NH1	1:B:295:VAL:O	2.51	0.44
1:A:501:LEU:O	1:A:503:LYS:HG3	2.17	0.44
1:A:513:THR:O	1:A:517:ILE:HG13	2.18	0.43
1:B:157:ILE:HG23	1:B:695:LEU:HD21	1.99	0.43
1:A:139:LEU:HD11	1:A:259:VAL:HG22	1.99	0.43
1:A:416:TYR:CD2	1:A:428:ALA:HB1	2.53	0.43
1:B:330:ARG:HD2	1:B:330:ARG:HA	1.85	0.43
1:B:378:LEU:HD12	1:B:378:LEU:HA	1.79	0.43
1:B:895:THR:O	1:B:898:ASN:HB2	2.18	0.43
1:A:246:GLU:O	1:A:246:GLU:HG3	2.19	0.43
1:A:262:ALA:O	1:A:266:ILE:HG12	2.19	0.43
1:B:145:LYS:O	1:B:149:ASP:HB2	2.18	0.43
1:A:844:LEU:HD22	1:A:909:ARG:HH21	1.83	0.43
1:A:865:LYS:O	1:A:869:GLN:HB2	2.19	0.43
1:B:171:THR:OG1	1:B:669:GLN:HA	2.18	0.43
1:B:410:GLU:HB3	1:B:411:PRO:HD3	2.00	0.43
1:B:176:GLN:HA	1:B:671:GLU:HB2	2.00	0.43
1:B:335:LEU:HG	1:B:370:ILE:HD12	1.99	0.43
1:B:404:ASN:HB3	1:B:406:GLU:OE2	2.19	0.43
1:A:38:LEU:HD12	1:A:38:LEU:HA	1.82	0.43
1:A:777:TRP:HA	1:A:780:THR:HG22	2.00	0.43
1:A:890:ARG:O	1:A:894:ILE:HG13	2.18	0.43
1:B:285:MET:HE2	1:B:285:MET:HB2	1.85	0.43
1:B:496:LEU:HB3	1:B:548:GLU:HG2	1.99	0.43
1:A:699:MET:O	1:A:701:PRO:HD3	2.19	0.43
1:B:176:GLN:NE2	1:B:671:GLU:HA	2.34	0.43
1:B:603:ASP:OD1	1:B:603:ASP:N	2.51	0.43
1:B:611:TRP:CE2	1:B:615:LYS:HE3	2.54	0.43
1:A:600:SER:HB2	1:A:609:ALA:HB1	1.99	0.43
1:A:834:PRO:HG3	1:A:860:PHE:CE1	2.54	0.43
1:A:587:ILE:HD12	1:A:590:LYS:O	2.19	0.43
1:B:509:ASP:O	1:B:513:THR:HG23	2.19	0.43
1:B:452:ARG:HA	1:B:529:ILE:O	2.19	0.42
1:A:489:GLU:CD	1:B:494:ARG:HH22	2.26	0.42
1:B:699:MET:O	1:B:701:PRO:HD3	2.18	0.42
1:A:70:LYS:HB3	1:A:72:GLU:HG3	2.00	0.42
1:A:201:ILE:H	1:A:201:ILE:HD13	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLN:O	1:A:211:GLU:HG3	2.19	0.42
1:A:587:ILE:HD13	1:A:587:ILE:HA	1.77	0.42
1:A:703:ILE:HD12	1:A:814:HIS:O	2.18	0.42
1:B:801:ASP:OD2	1:B:803:ARG:NH2	2.52	0.42
1:A:53:LEU:HD12	1:A:53:LEU:HA	1.70	0.42
1:A:347:ARG:O	1:A:349:ASP:N	2.52	0.42
1:A:621:VAL:HG11	1:A:658:ASP:O	2.19	0.42
1:A:724:TYR:O	1:A:728:VAL:HG22	2.20	0.42
1:B:243:TYR:OH	1:B:674:GLU:HG2	2.20	0.42
1:B:501:LEU:HD12	1:B:502:PRO:HD2	2.01	0.42
1:A:275:ASN:HA	1:A:440:SER:OG	2.20	0.42
1:A:287:GLY:HA3	1:A:450:ASP:O	2.20	0.42
1:B:786:VAL:HG11	1:B:828:VAL:HG11	2.02	0.42
1:B:855:LYS:O	1:B:858:ALA:HB3	2.19	0.42
1:A:245:HIS:HA	1:A:314:MET:HE1	2.01	0.42
1:A:228:ARG:HH22	1:A:950:ASP:CG	2.27	0.42
1:B:772:PRO:HA	1:B:775:PHE:HB3	2.01	0.42
1:A:501:LEU:HD12	1:A:502:PRO:HD2	2.02	0.41
1:A:118:ARG:C	1:A:120:LYS:H	2.27	0.41
1:A:469:LEU:HD12	1:A:469:LEU:HA	1.86	0.41
1:A:844:LEU:HD13	1:A:909:ARG:HH21	1.85	0.41
1:B:233:PRO:HB2	1:B:299:VAL:HG11	2.02	0.41
1:A:463:ASP:CG	1:A:475:ARG:HG3	2.45	0.41
1:A:560:LEU:HD13	1:A:594:MET:HG2	2.03	0.41
1:B:716:MET:HB2	1:B:716:MET:HE2	1.85	0.41
1:B:326:MET:HG3	1:B:371:LEU:HD11	2.02	0.41
1:B:102:LEU:HD13	1:B:102:LEU:HA	1.90	0.41
1:B:605:GLY:HA2	1:B:724:TYR:CD1	2.55	0.41
1:A:384:ARG:O	1:A:388:LEU:HB2	2.21	0.41
1:A:852:PHE:O	1:A:855:LYS:HB2	2.20	0.41
1:B:70:LYS:HB3	1:B:72:GLU:HG3	2.02	0.41
1:B:496:LEU:CB	1:B:548:GLU:HG2	2.50	0.41
1:A:461:VAL:HG21	1:A:510:VAL:HG22	2.03	0.41
1:B:305:LEU:HD13	1:B:305:LEU:HA	1.84	0.41
1:A:228:ARG:NH2	1:A:939:ASN:HB2	2.36	0.41
1:B:744:GLU:HB2	1:B:776:ALA:HB2	2.02	0.41
1:A:201:ILE:HG12	1:A:201:ILE:O	2.21	0.41
1:A:253:PRO:O	1:A:257:ARG:HG3	2.21	0.41
1:A:323:MET:HE2	1:A:357:PHE:CD2	2.56	0.41
1:A:359:LYS:HE2	1:A:359:LYS:HB3	1.75	0.41
1:A:477:TRP:CD1	1:A:481:ARG:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:TRP:O	1:A:586:ARG:HD3	2.21	0.41
1:A:708:GLU:H	1:A:708:GLU:CD	2.28	0.41
1:B:558:VAL:HA	1:B:559:PRO:HD3	1.89	0.41
1:B:714:ASP:O	1:B:718:VAL:HG23	2.21	0.41
1:A:44:ILE:O	1:A:48:LEU:HG	2.20	0.41
1:A:278:LEU:HA	1:A:278:LEU:HD23	1.89	0.41
1:B:843:LEU:O	1:B:906:LYS:NZ	2.37	0.41
1:B:196:LEU:HD12	1:B:196:LEU:HA	1.87	0.40
1:B:326:MET:HE1	1:B:419:LEU:CD1	2.48	0.40
1:A:406:GLU:CD	1:A:406:GLU:C	2.88	0.40
1:B:590:LYS:HG2	1:B:630:LYS:HE2	2.03	0.40
1:B:726:SER:HA	1:B:730:GLN:CG	2.51	0.40
1:A:270:GLU:HG2	1:A:271:ARG:H	1.86	0.40
1:A:318:GLN:HE21	1:A:318:GLN:HB2	1.69	0.40
1:A:552:LYS:H	1:A:552:LYS:HG2	1.42	0.40
1:B:207:GLN:O	1:B:211:GLU:HG3	2.21	0.40
1:B:532:MET:HE2	1:B:532:MET:H	1.86	0.40
1:B:640:THR:OG1	1:B:967:GLY:OXT	2.38	0.40
1:A:172:ALA:HB2	1:A:285:MET:HG3	2.03	0.40
1:A:733:ARG:NH2	1:A:736:GLU:OE2	2.55	0.40
1:B:96:LYS:HE2	1:B:225:GLU:OE2	2.21	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	899/974 (92%)	855 (95%)	38 (4%)	6 (1%)	18	49
1	B	878/974 (90%)	837 (95%)	37 (4%)	4 (0%)	24	57
All	All	1777/1948 (91%)	1692 (95%)	75 (4%)	10 (1%)	21	53

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	919	PRO
1	B	889	LEU
1	A	348	LYS
1	A	670	GLY
1	B	348	LYS
1	B	670	GLY
1	B	848	GLU
1	A	918	ARG
1	A	848	GLU
1	A	119	ILE

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	775/849 (91%)	718 (93%)	57 (7%)	13	39
1	B	763/849 (90%)	711 (93%)	52 (7%)	14	42
All	All	1538/1698 (91%)	1429 (93%)	109 (7%)	13	40

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	102	LEU
1	A	117	ARG
1	A	169	VAL
1	A	182	LEU
1	A	184	GLN
1	A	196	LEU
1	A	197	TYR
1	A	201	ILE
1	A	228	ARG
1	A	237	MET
1	A	256	LEU
1	A	269	GLU

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Mol	Chain	Res	Type
1	A	278	LEU
1	A	279	ILE
1	A	285	MET
1	A	305	LEU
1	A	306	LEU
1	A	309	MET
1	A	318	GLN
1	A	319	ILE
1	A	320	GLU
1	A	321	ASP
1	A	345	ASN
1	A	359	LYS
1	A	365	GLU
1	A	378	LEU
1	A	388	LEU
1	A	393	HIS
1	A	398	VAL
1	A	399	GLU
1	A	406	GLU
1	A	441	THR
1	A	469	LEU
1	A	480	GLU
1	A	507	ILE
1	A	510	VAL
1	A	555	LEU
1	A	558	VAL
1	A	587	ILE
1	A	608	SER
1	A	632	THR
1	A	665	ARG
1	A	674	GLU
1	A	676	SER
1	A	713	LEU
1	A	727	VAL
1	A	767	SER
1	A	768	LEU
1	A	771	ILE
1	A	805	LEU
1	A	827	MET
1	A	849	LEU
1	A	869	GLN
1	A	887	LEU

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Mol	Chain	Res	Type
1	A	917	LEU
1	A	930	LYS
1	B	60	LEU
1	B	102	LEU
1	B	117	ARG
1	B	139	LEU
1	B	165	THR
1	B	169	VAL
1	B	182	LEU
1	B	184	GLN
1	B	196	LEU
1	B	201	ILE
1	B	237	MET
1	B	256	LEU
1	B	269	GLU
1	B	278	LEU
1	B	279	ILE
1	B	285	MET
1	B	305	LEU
1	B	306	LEU
1	B	309	MET
1	B	318	GLN
1	B	319	ILE
1	B	320	GLU
1	B	321	ASP
1	B	345	ASN
1	B	359	LYS
1	B	365	GLU
1	B	378	LEU
1	B	393	HIS
1	B	399	GLU
1	B	405	LEU
1	B	406	GLU
1	B	469	LEU
1	B	480	GLU
1	B	493	LYS
1	B	507	ILE
1	B	510	VAL
1	B	555	LEU
1	B	558	VAL
1	B	587	ILE
1	B	632	THR

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Mol	Chain	Res	Type
1	B	665	ARG
1	B	674	GLU
1	B	676	SER
1	B	716	MET
1	B	723	GLU
1	B	727	VAL
1	B	735	VAL
1	B	767	SER
1	B	771	ILE
1	B	805	LEU
1	B	849	LEU
1	B	887	LEU

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

Mol	Chain	Res	Type
1	A	184	GLN
1	A	380	HIS
1	A	591	GLN
1	A	914	HIS
1	B	163	ASN
1	B	186	HIS
1	B	655	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	1002	-	4,4,4	0.94	0	6,6,6	0.57	0
2	PO4	A	1001	-	4,4,4	1.06	0	6,6,6	0.71	0
2	PO4	B	1001	-	4,4,4	0.82	0	6,6,6	0.77	0

There are no bond length outliers.

There are no bond angle outliers.

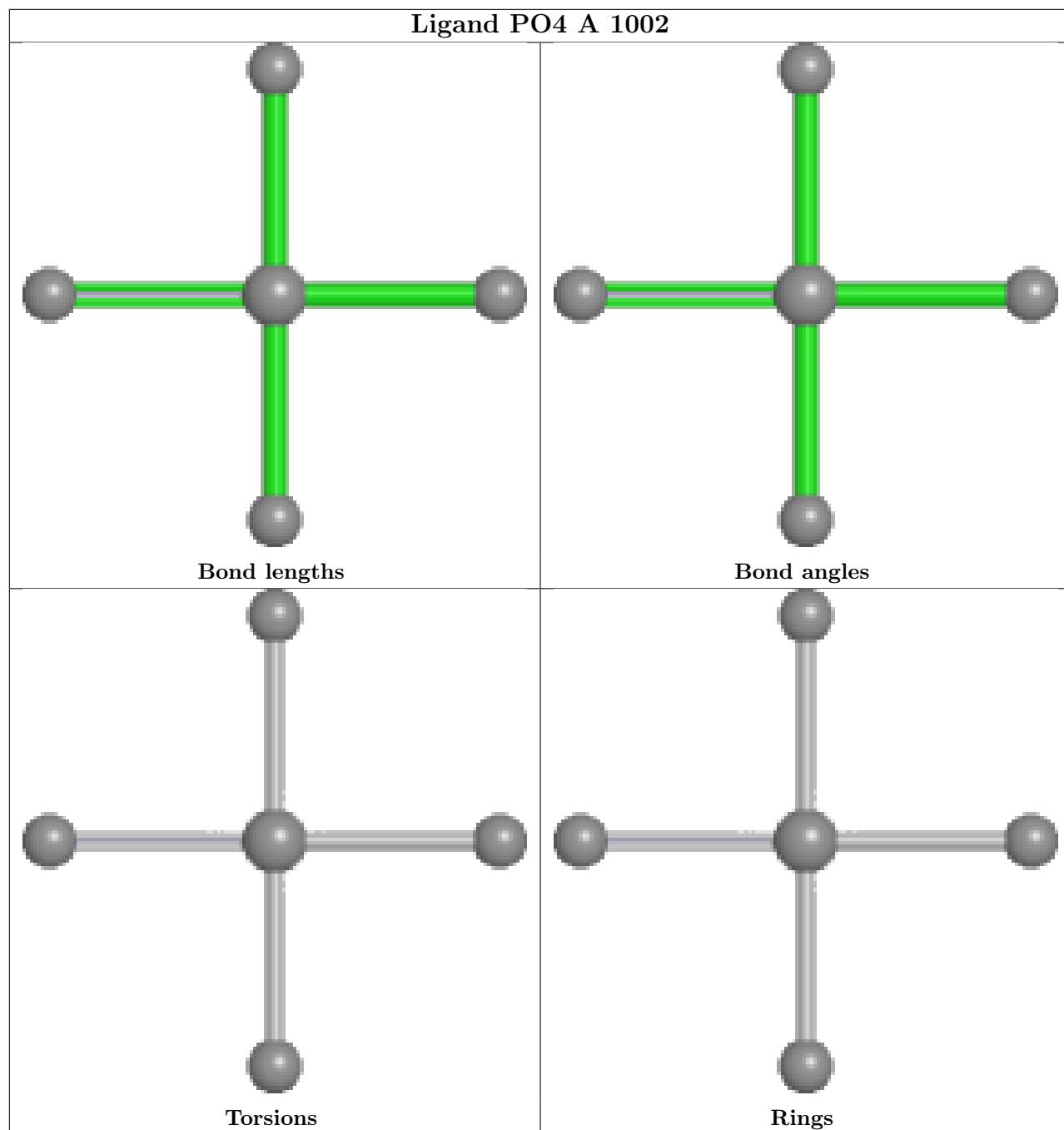
There are no chirality outliers.

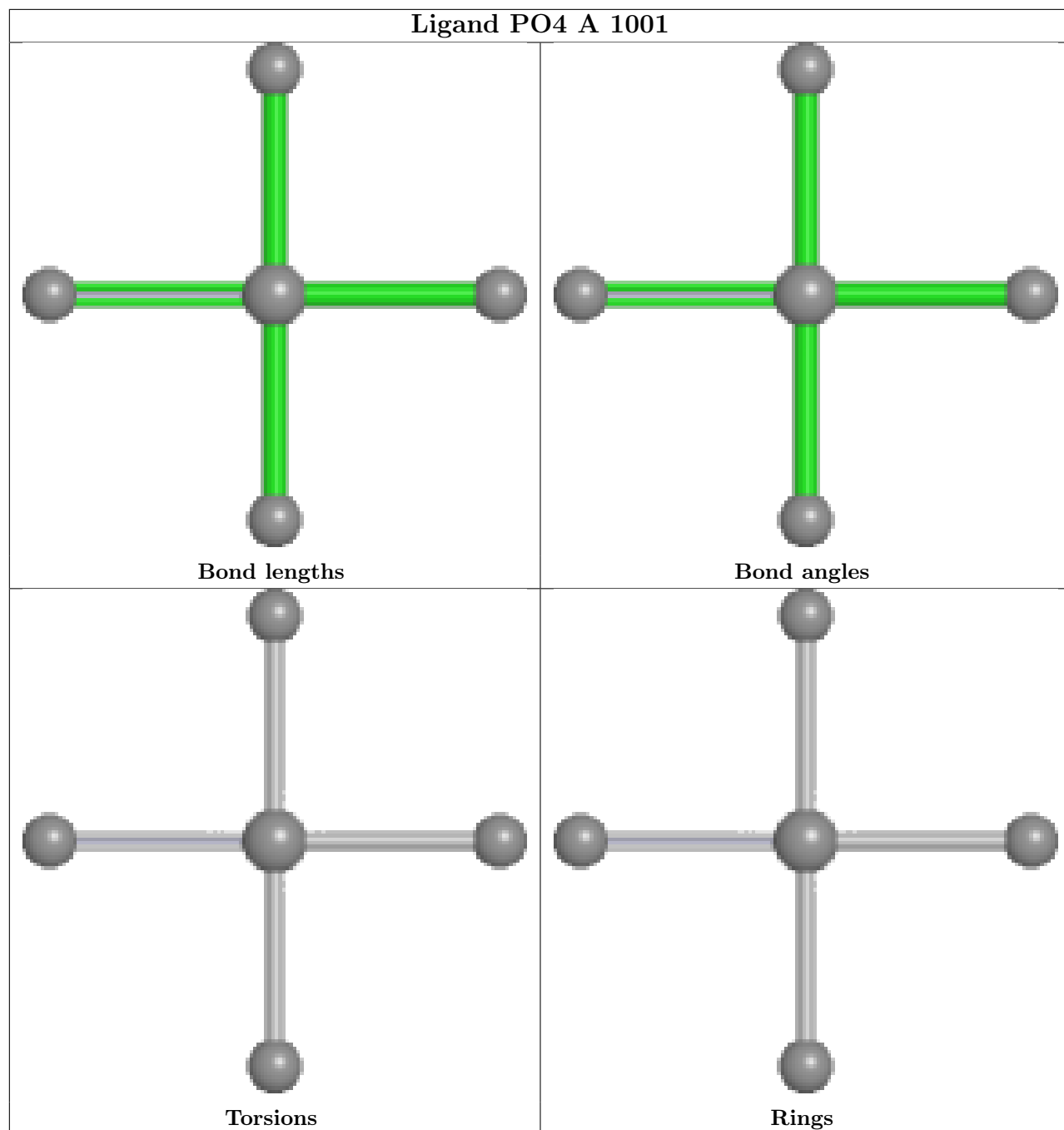
There are no torsion outliers.

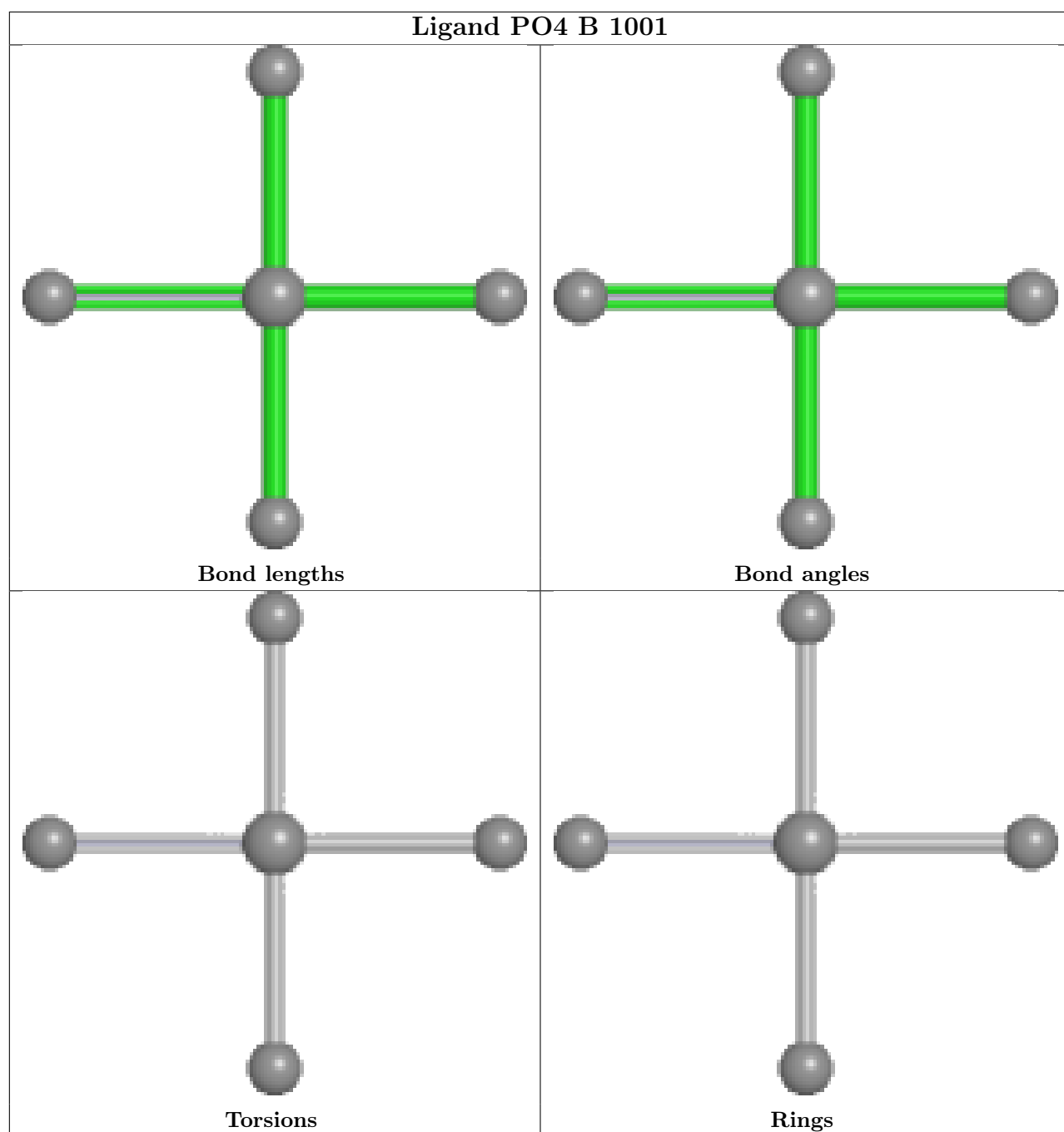
There are no ring outliers.

No monomer is involved in short contacts.

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	906/974 (93%)	-0.45	5 (0%)	85 69	54, 98, 153, 223	3 (0%)
1	B	888/974 (91%)	-0.31	4 (0%)	87 72	103, 165, 244, 285	0
All	All	1794/1948 (92%)	-0.38	9 (0%)	87 72	54, 126, 228, 285	3 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	875	ASP	3.0
1	B	601	GLY	2.8
1	B	771	ILE	2.8
1	B	196	LEU	2.8
1	A	88	PRO	2.6
1	B	245	HIS	2.6
1	A	136	GLU	2.5
1	A	245	HIS	2.4
1	A	601	GLY	2.1

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,

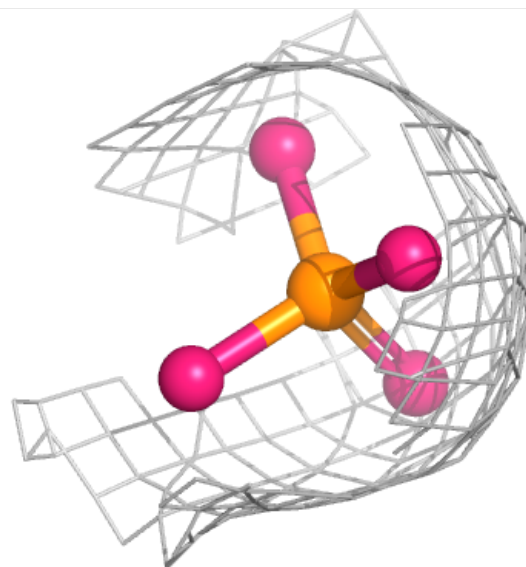
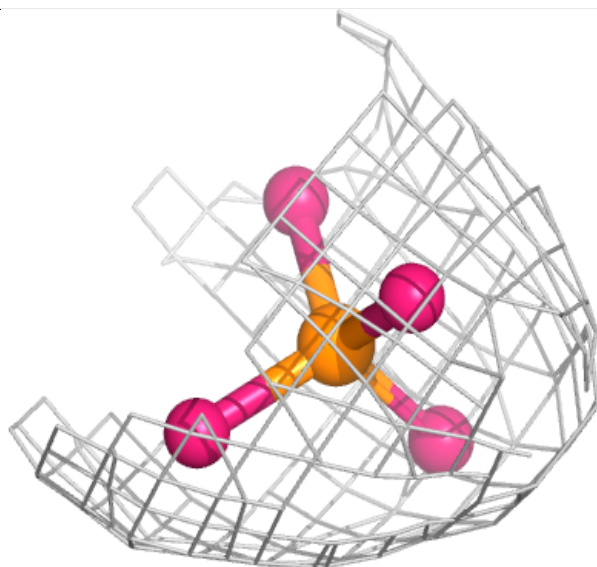
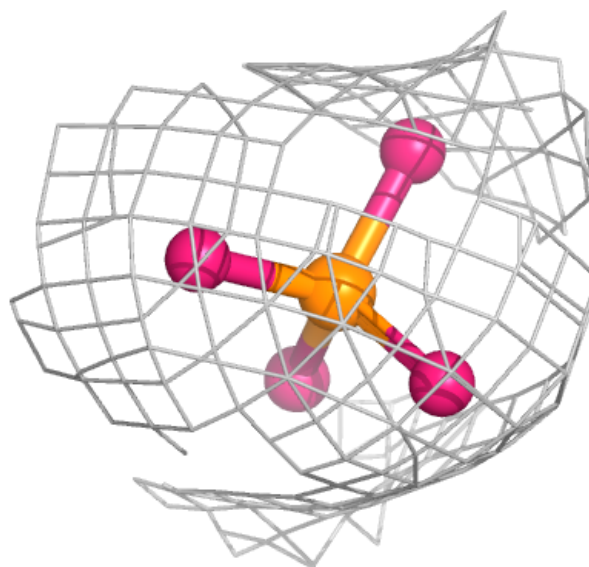
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CL	A	1004	1/1	0.92	0.16	119,119,119,119	0
2	PO4	B	1001	5/5	0.94	0.06	126,145,146,152	0
3	CL	A	1003	1/1	0.95	0.15	108,108,108,108	0
2	PO4	A	1002	5/5	0.95	0.05	148,149,152,154	0
2	PO4	A	1001	5/5	0.98	0.04	91,91,107,107	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

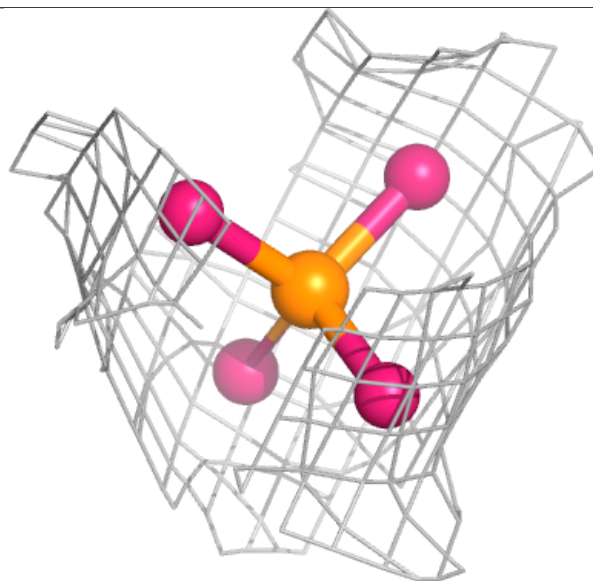
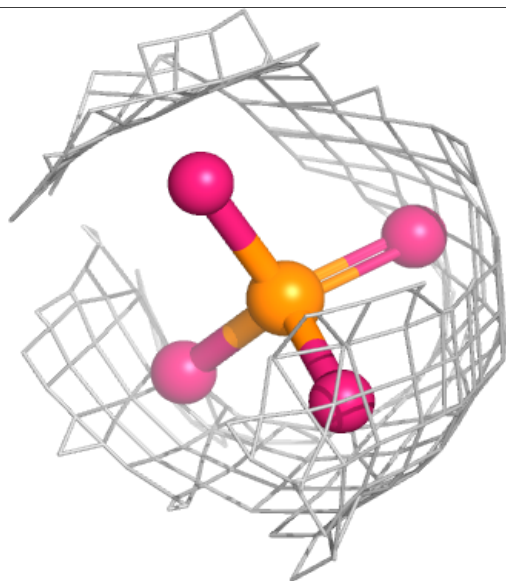
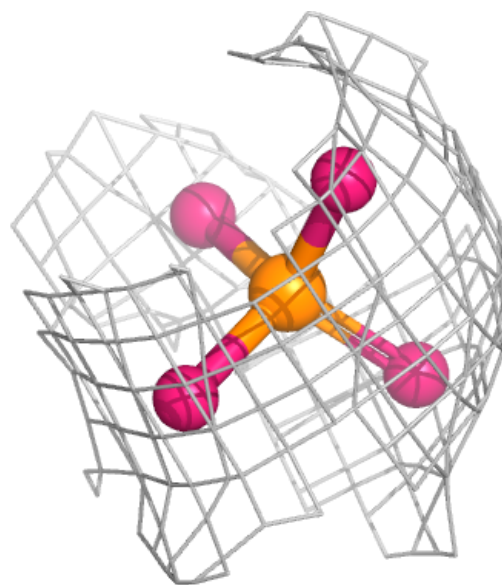
Electron density around PO4 B 1001:

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



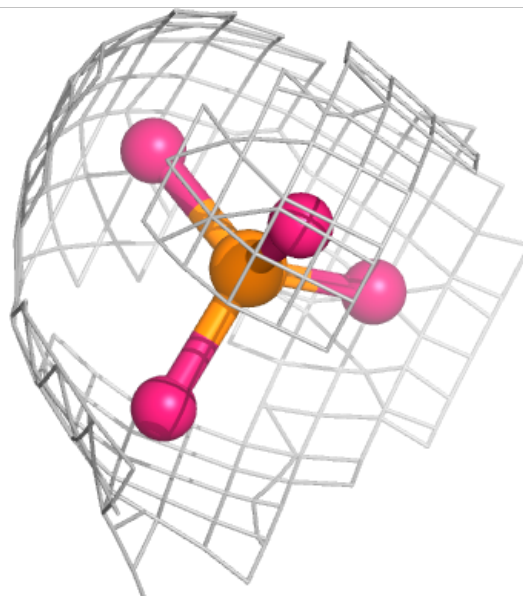
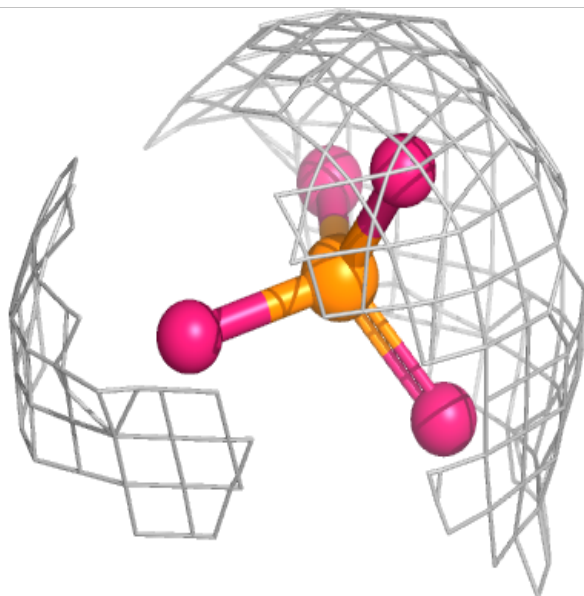
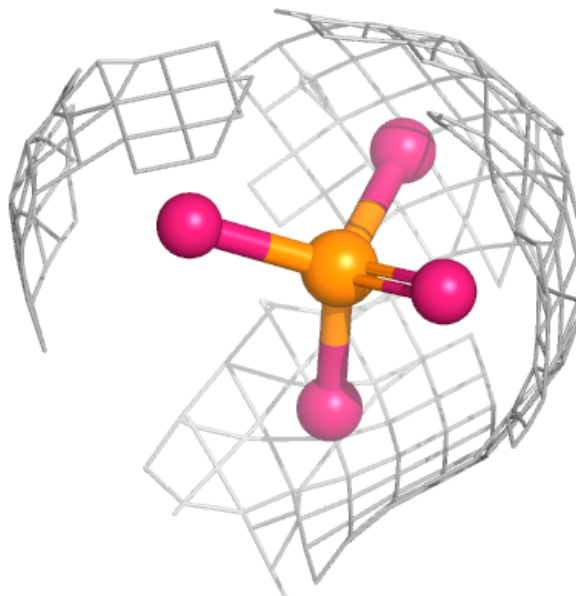
Electron density around PO4 A 1002:

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



Electron density around PO4 A 1001:

$2mF_o-DF_c$ (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.