



Full wwPDB X-ray Structure Validation Report i

May 23, 2023 – 01:55 am BST

PDB ID : 8OJF
Title : Arabidopsis thaliana Phosphoenolpyruvate carboxylase PPC1 with bound phosphate
Authors : Haesaerts, S.; Loris, R.; Larsen, P.B.
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 i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.33
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) : 2.33

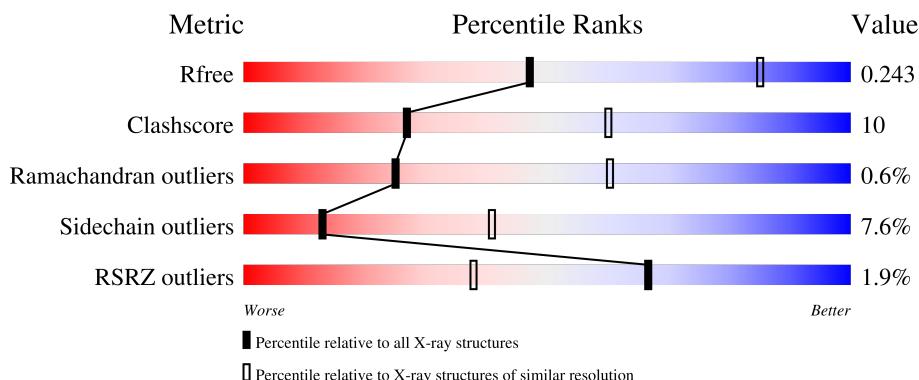
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

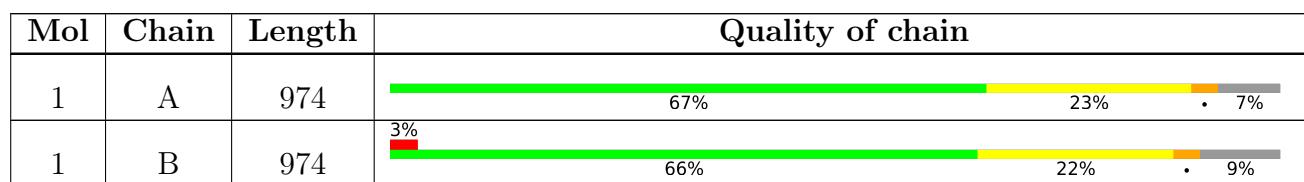
The reported resolution of this entry is 3.04 Å.

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}	130704	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (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.



2 Entry composition (i)

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.

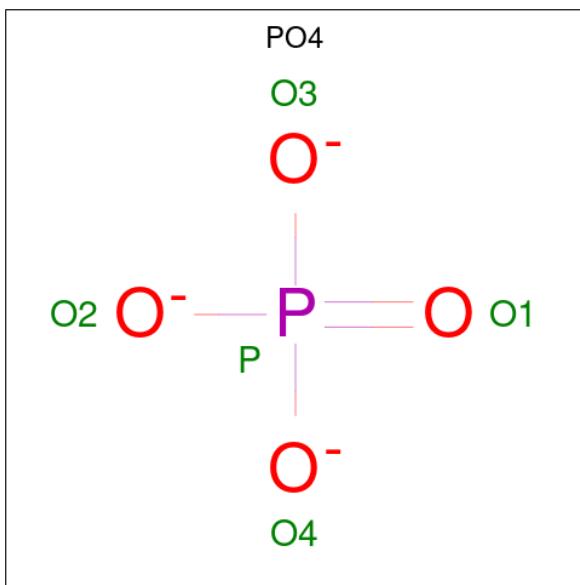
- Molecule 1 is a protein called Phosphoenolpyruvate carboxylase 1.

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

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 (three-letter code: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

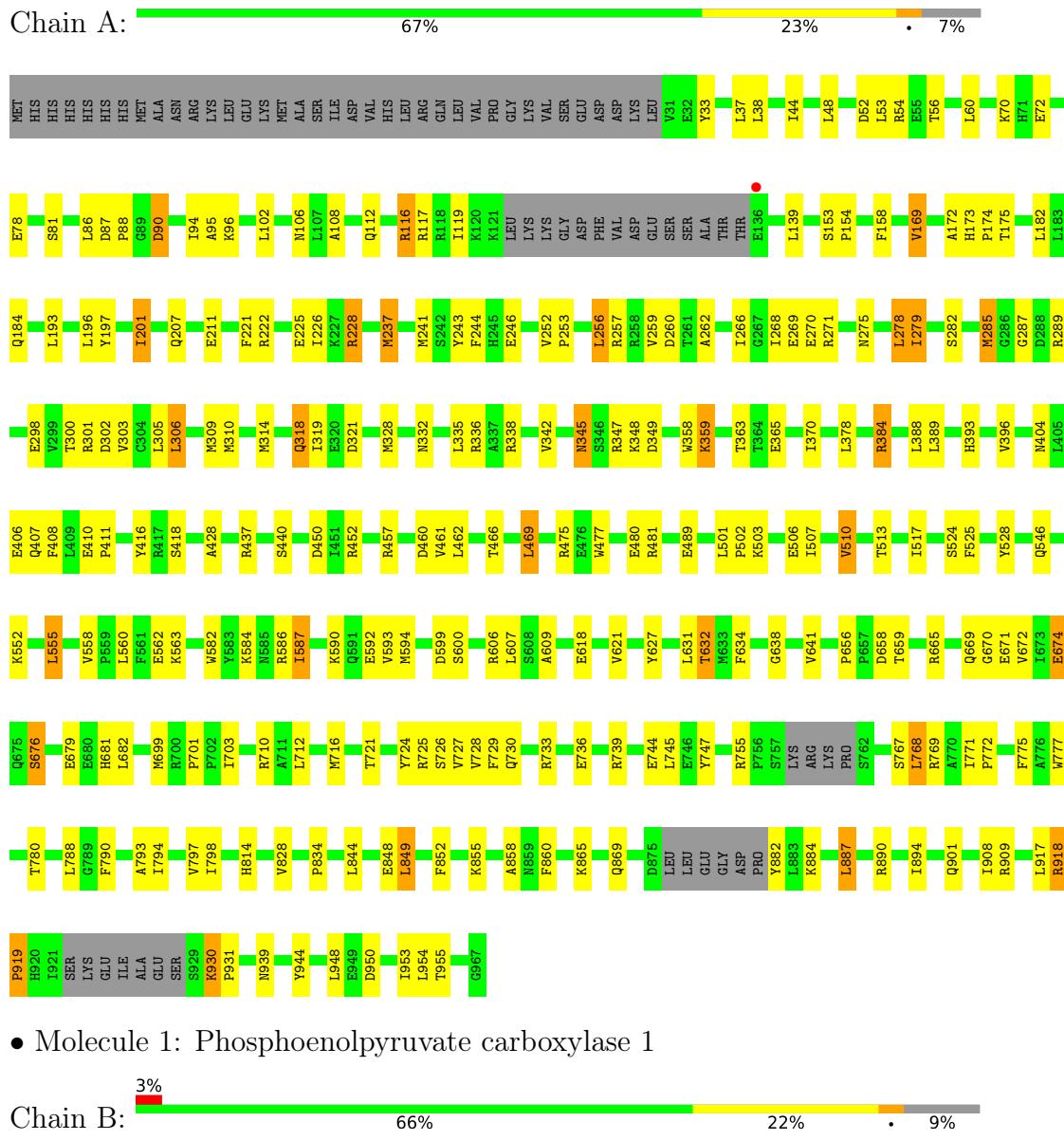
- Molecule 4 is water.

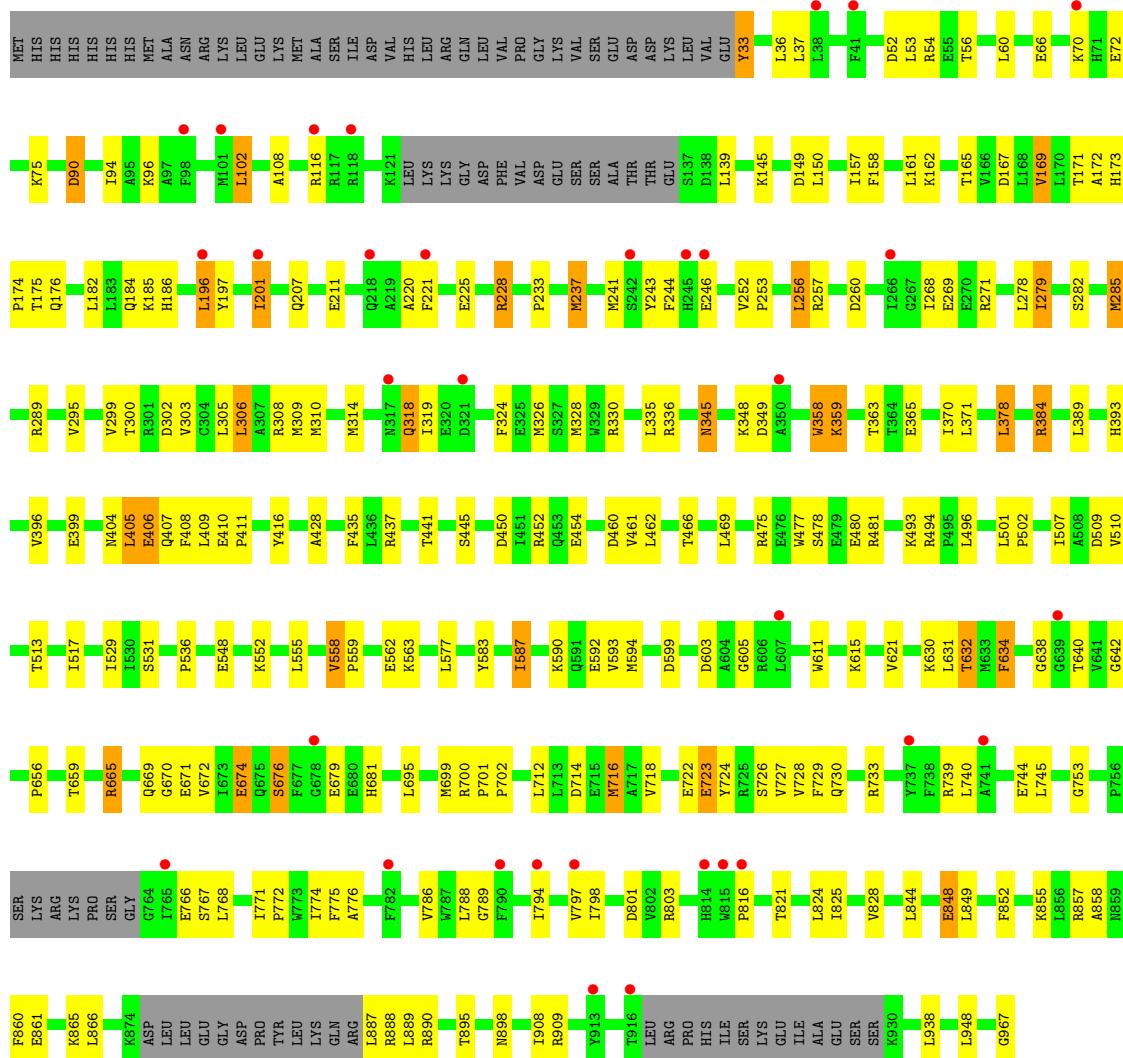
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	13	Total O 13 13	0	0
4	B	5	Total O 5 5	0	0

3 Residue-property plots [\(i\)](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Phosphoenolpyruvate carboxylase 1





4 Data and refinement statistics (i)

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 – 3.03	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.71-3.04) 90.3 (48.71-3.03)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	0.15 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R , R_{free}	0.203 , 0.243 0.203 , 0.243	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)	0.28 , 77.5	EDS
L-test for twinning ²	$< L > = 0.49$, $< L^2 > = 0.32$	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 $< |L| >$, $< L^2 >$ 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: CL, 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	0.39	0/7418	0.59	2/10048 (0.0%)
1	B	0.30	0/7259	0.47	0/9833
All	All	0.35	0/14677	0.54	2/19881 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	768	LEU	CA-CB-CG	5.92	128.93	115.30
1	A	849	LEU	CA-CB-CG	5.76	128.56	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7252	0	7166	149	0
1	B	7106	0	7025	142	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14393	0	14191	290	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (290) 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: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:A:237:MET:HA	1:A:285:MET:HE3	1.71	0.71
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:A:739:ARG:NH1	1:A:744:GLU:OE1	2.26	0.68
1:A:345:ASN:OD1	1:A:345:ASN:N	2.26	0.67
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: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:A:726:SER:HA	1:A:730:GLN:CG	2.29	0.62
1:B:739:ARG:NH1	1:B:744:GLU:OE1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:712:LEU:HG	1:A:716:MET:HE2	1.86	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:244:PHE:C	1:B:246:GLU:H	2.13	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:A:712:LEU:HG	1:A:716:MET:CE	2.39	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:B:260:ASP:CG	1:B:271:ARG:HG2	2.32	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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:244:PHE:C	1:A:246:GLU:H	2.20	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:260:ASP:CG	1:A:271:ARG:HG2	2.37	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
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:B:237:MET:HE3	1:B:303:VAL:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:285:MET:HE2	1:A:285:MET:HB2	1.87	0.43
1:A:618:GLU:CD	1:A:710:ARG:HH22	2.12	0.43
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:314:MET:HE2	1:A:314:MET:HB3	1.94	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:560:LEU:HD13	1:A:594:MET:HG2	2.03	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:285:MET:HE2	1:B:285:MET:HB2	1.99	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: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
1:A:582:TRP:O	1:A:586:ARG:HD3	2.21	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:196:LEU:HD12	1:B:196:LEU:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:201:ILE:HG12	1:B:201:ILE:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	899/974 (92%)	855 (95%)	38 (4%)	6 (1%)	22 57
1	B	878/974 (90%)	837 (95%)	37 (4%)	4 (0%)	29 65
All	All	1777/1948 (91%)	1692 (95%)	75 (4%)	10 (1%)	25 60

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

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Mol	Chain	Res	Type
1	A	918	ARG
1	A	848	GLU
1	A	119	ILE

5.3.2 Protein sidechains [\(i\)](#)

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%)	716 (92%)	59 (8%)	13 41
1	B	763/849 (90%)	705 (92%)	58 (8%)	13 41
All	All	1538/1698 (91%)	1421 (92%)	117 (8%)	13 41

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	TYR
1	A	54	ARG
1	A	60	LEU
1	A	90	ASP
1	A	102	LEU
1	A	116	ARG
1	A	117	ARG
1	A	153	SER
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
1	A	278	LEU
1	A	279	ILE

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Mol	Chain	Res	Type
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	321	ASP
1	A	328	MET
1	A	345	ASN
1	A	358	TRP
1	A	359	LYS
1	A	365	GLU
1	A	378	LEU
1	A	384	ARG
1	A	393	HIS
1	A	406	GLU
1	A	469	LEU
1	A	480	GLU
1	A	510	VAL
1	A	524	SER
1	A	555	LEU
1	A	558	VAL
1	A	587	ILE
1	A	606[A]	ARG
1	A	606[B]	ARG
1	A	632	THR
1	A	634	PHE
1	A	665	ARG
1	A	674	GLU
1	A	676	SER
1	A	727	VAL
1	A	767	SER
1	A	768	LEU
1	A	771	ILE
1	A	849	LEU
1	A	882	TYR
1	A	887	LEU
1	A	917	LEU
1	A	930	LYS
1	B	33	TYR
1	B	54	ARG
1	B	60	LEU

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Mol	Chain	Res	Type
1	B	90	ASP
1	B	102	LEU
1	B	116	ARG
1	B	139	LEU
1	B	165	THR
1	B	169	VAL
1	B	182	LEU
1	B	184	GLN
1	B	186	HIS
1	B	196	LEU
1	B	197	TYR
1	B	201	ILE
1	B	228	ARG
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	306	LEU
1	B	309	MET
1	B	318	GLN
1	B	319	ILE
1	B	324	PHE
1	B	328	MET
1	B	345	ASN
1	B	349	ASP
1	B	358	TRP
1	B	359	LYS
1	B	365	GLU
1	B	378	LEU
1	B	384	ARG
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	510	VAL
1	B	555	LEU
1	B	558	VAL

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Mol	Chain	Res	Type
1	B	587	ILE
1	B	632	THR
1	B	634	PHE
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	767	SER
1	B	768	LEU
1	B	771	ILE
1	B	887	LEU

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

Mol	Chain	Res	Type
1	A	914	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)

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	B	1001	-	4,4,4	0.78	0	6,6,6	0.74	0
2	PO4	A	1002	-	4,4,4	0.90	0	6,6,6	0.54	0
2	PO4	A	1001	-	4,4,4	1.02	0	6,6,6	0.67	0

There are no bond length outliers.

There are no bond angle outliers.

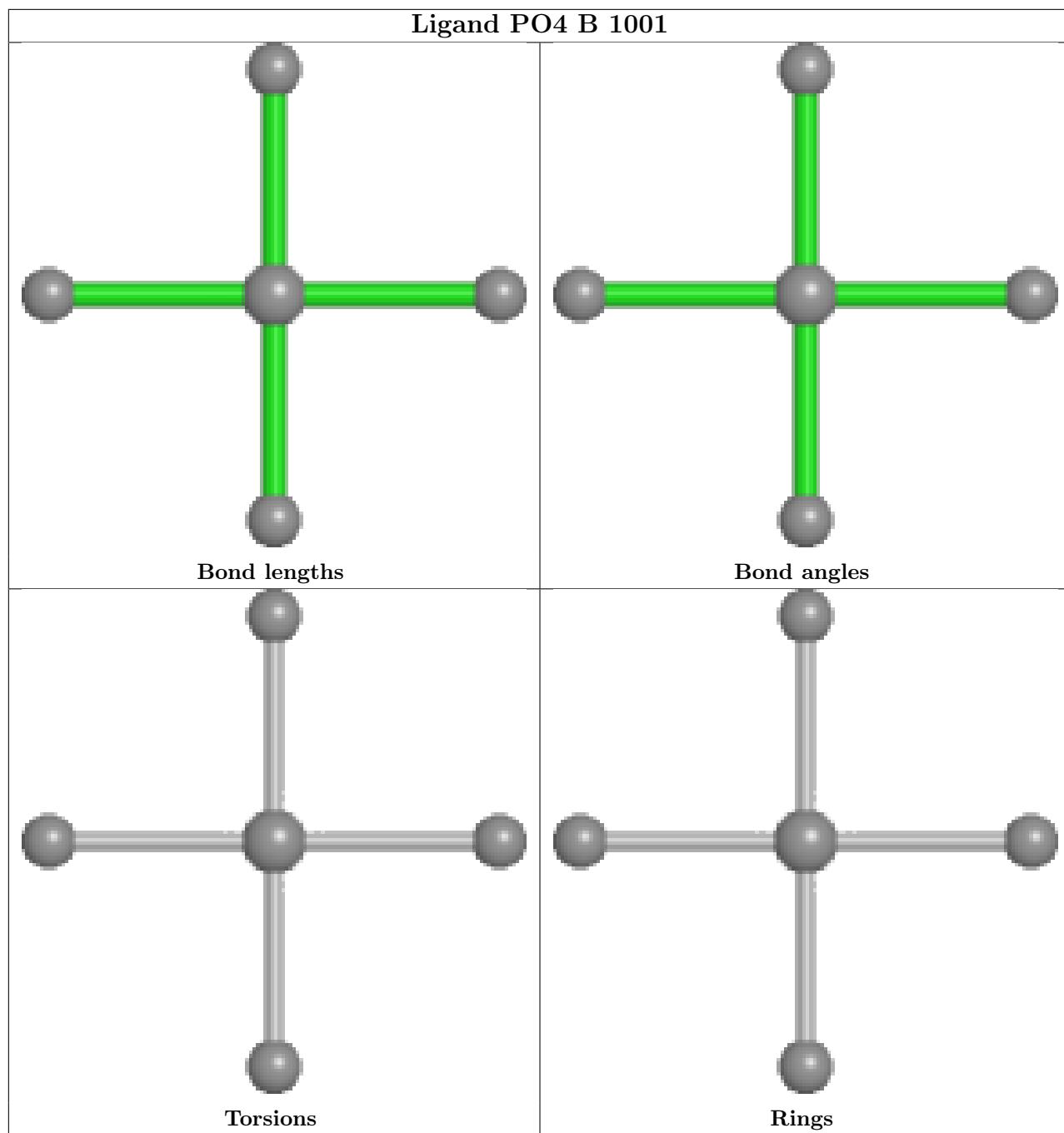
There are no chirality outliers.

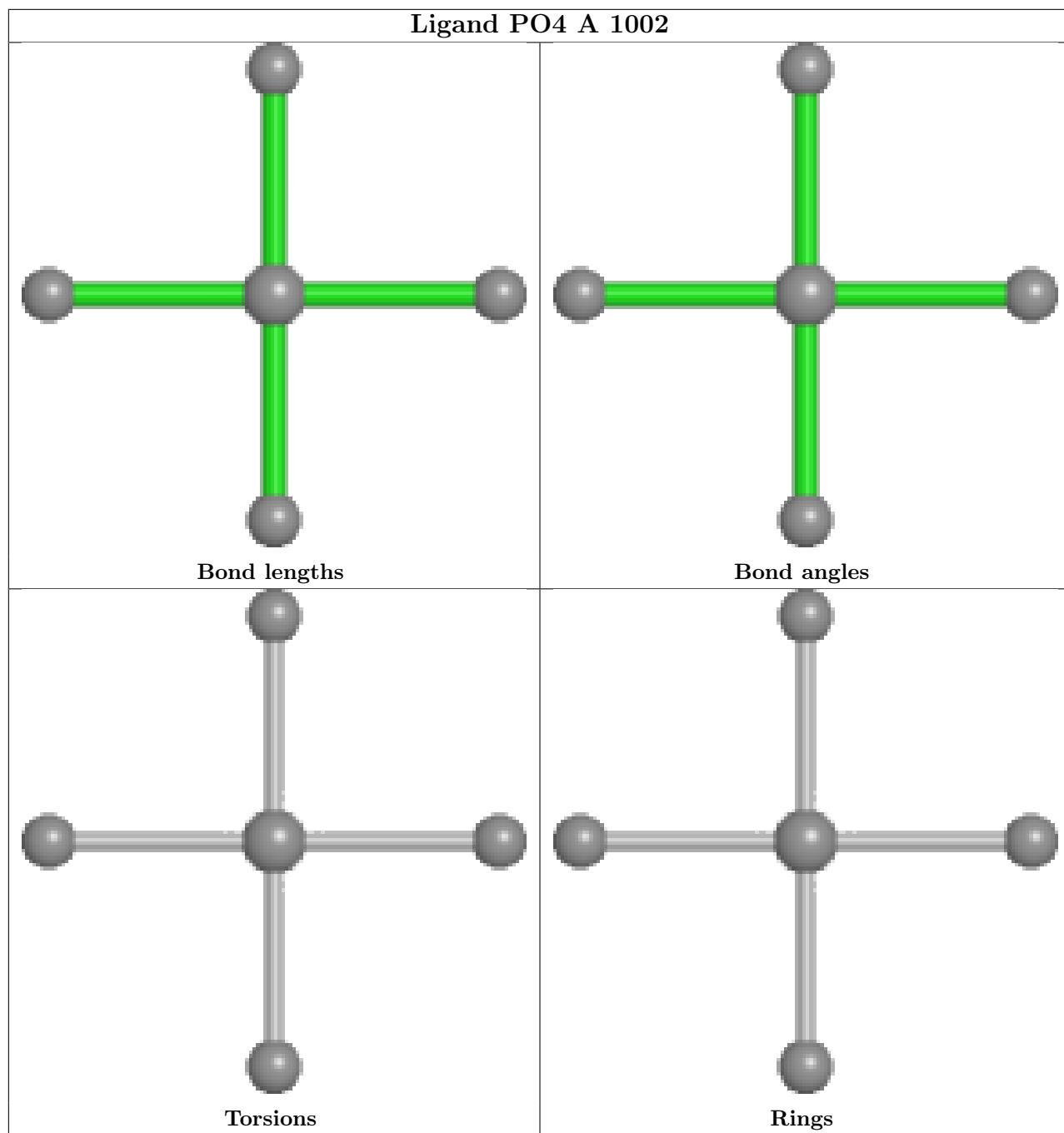
There are no torsion outliers.

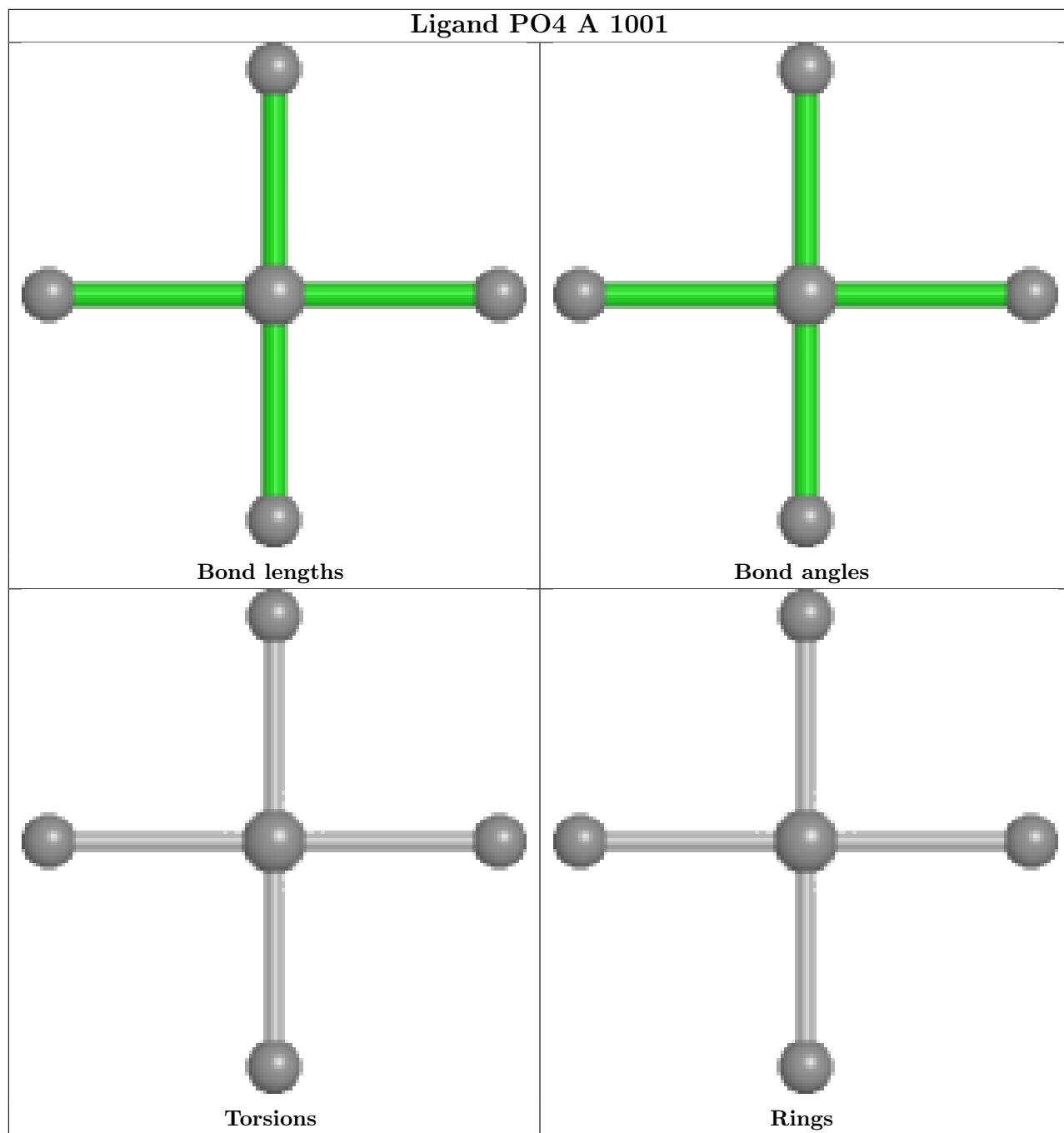
There are no ring outliers.

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%)	-0.39	1 (0%) 95 89	68, 98, 153, 223	0
1	B	888/974 (91%)	0.03	33 (3%) 41 17	103, 165, 244, 285	0
All	All	1794/1948 (92%)	-0.18	34 (1%) 66 38	68, 126, 228, 285	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	790	PHE	5.3
1	B	201	ILE	4.0
1	B	815	TRP	3.9
1	B	794	ILE	3.8
1	B	782	PHE	3.8
1	B	245	HIS	3.7
1	B	116	ARG	3.4
1	B	916	THR	3.4
1	B	246	GLU	3.2
1	B	196	LEU	3.1
1	B	913	TYR	3.0
1	B	70	LYS	3.0
1	B	797	VAL	3.0
1	B	765	ILE	2.8
1	B	816	PRO	2.8
1	B	98	PHE	2.8
1	B	221	PHE	2.7
1	B	266	ILE	2.6
1	B	741	ALA	2.5
1	B	321	ASP	2.5
1	B	639	GLY	2.5
1	B	317	ASN	2.5
1	B	814	HIS	2.5
1	B	101	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	118	ARG	2.3
1	B	38	LEU	2.3
1	A	136	GLU	2.2
1	B	678	GLY	2.2
1	B	218	GLN	2.1
1	B	737	TYR	2.1
1	B	350	ALA	2.1
1	B	242	SER	2.0
1	B	607	LEU	2.0
1	B	41	PHE	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 [\(i\)](#)

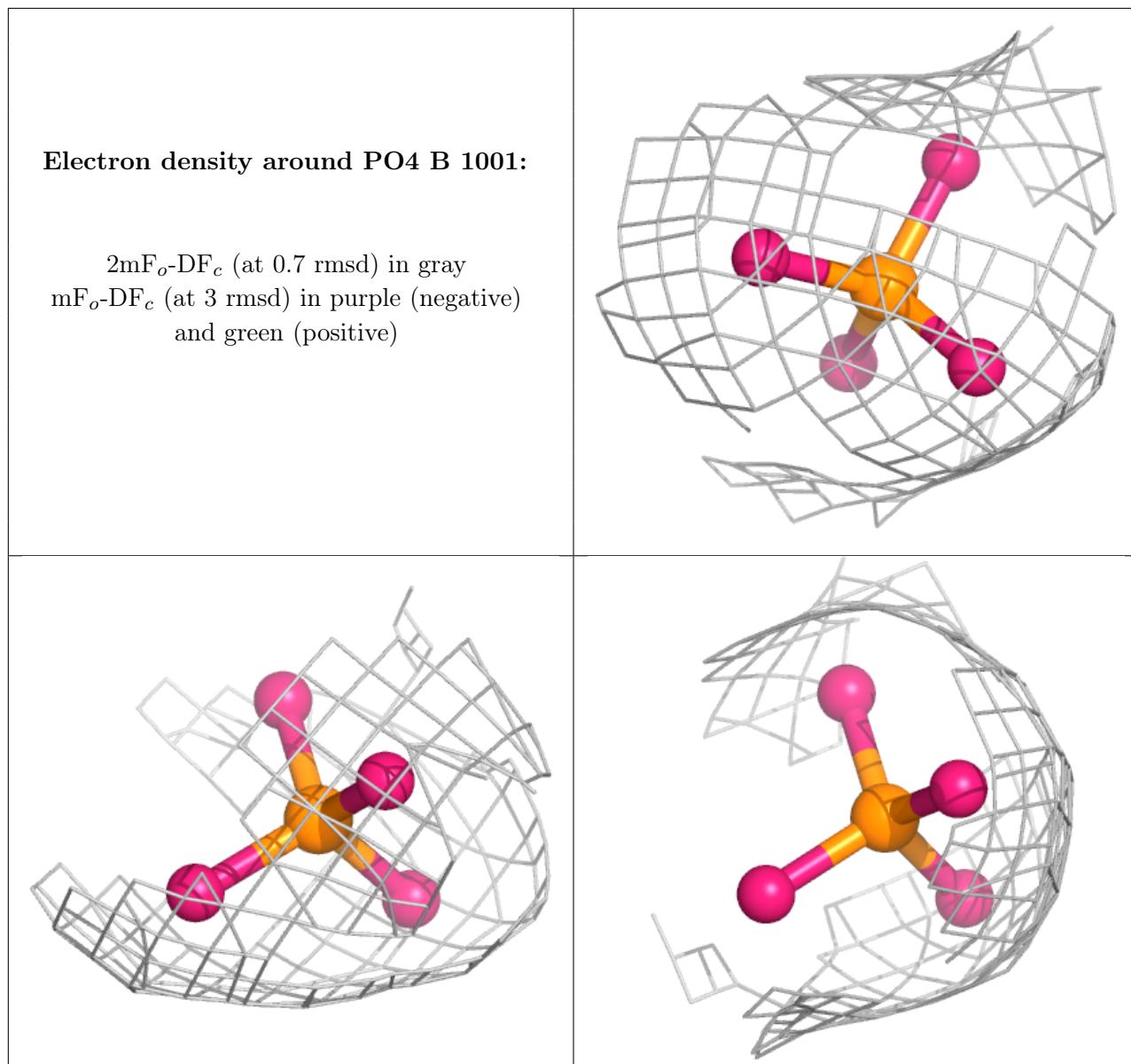
There are no monosaccharides in this entry.

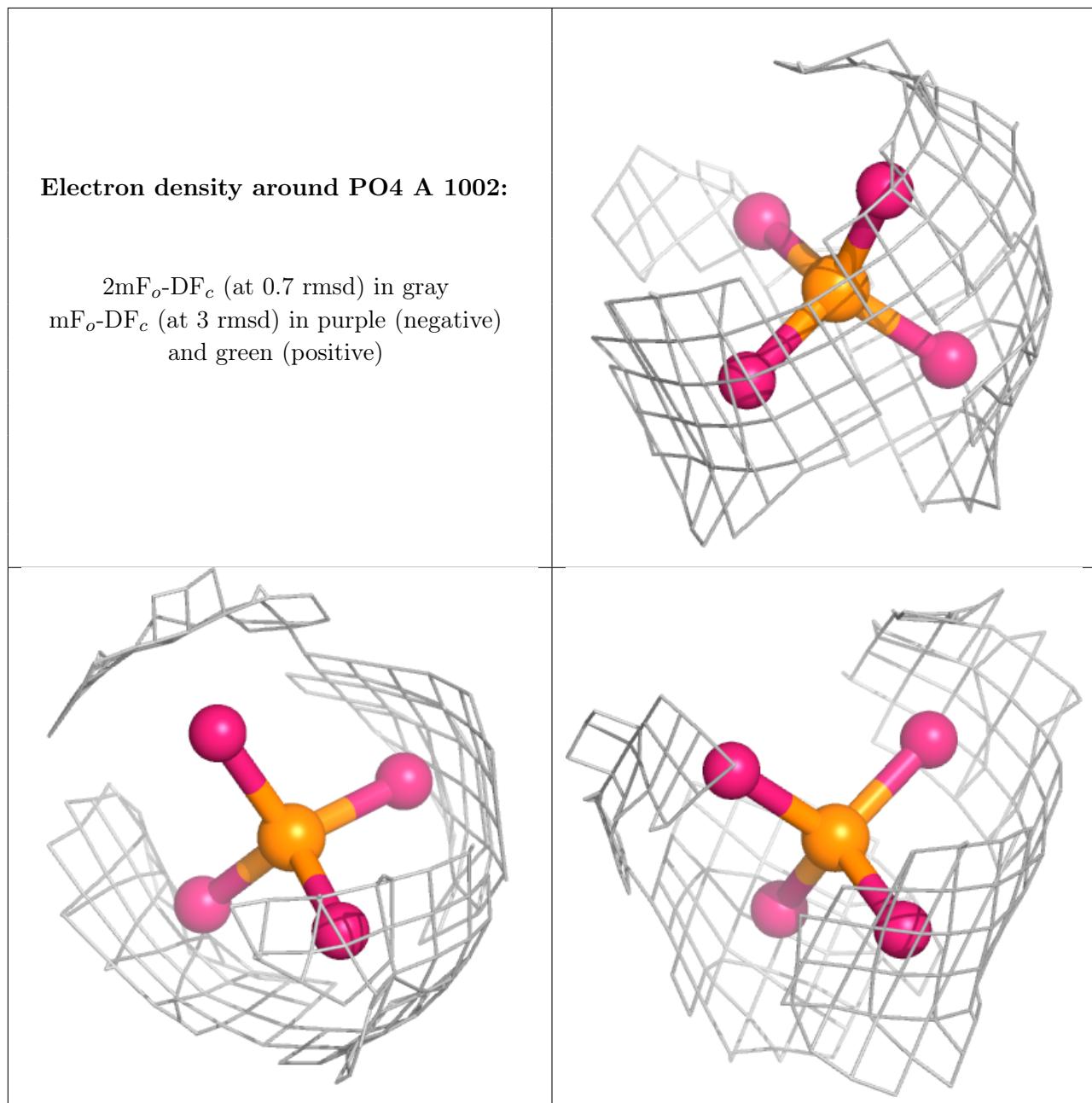
6.4 Ligands [\(i\)](#)

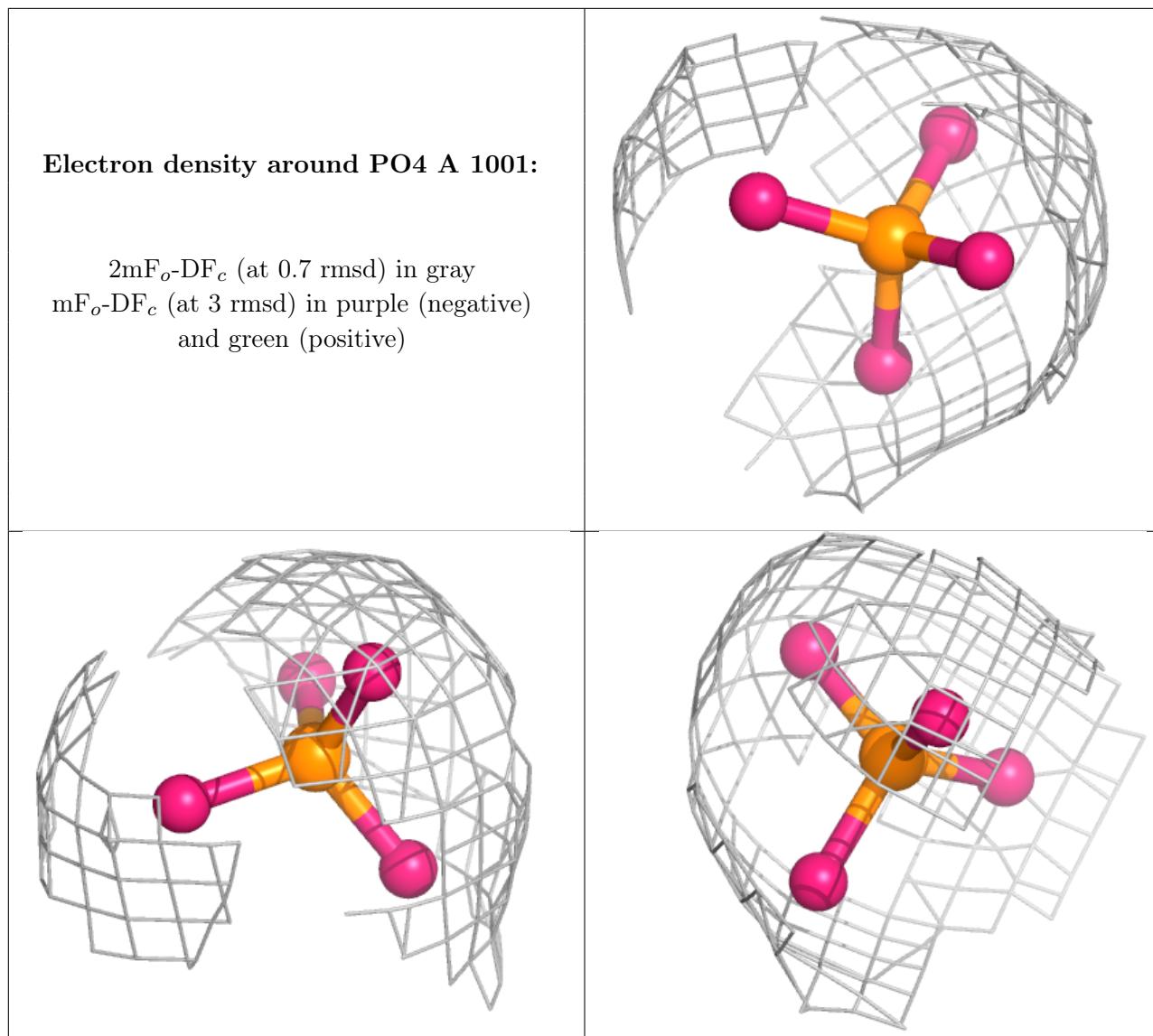
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CL	A	1004	1/1	0.82	0.33	119,119,119,119	0
3	CL	A	1003	1/1	0.87	0.28	108,108,108,108	0
2	PO4	B	1001	5/5	0.94	0.34	126,145,146,152	0
2	PO4	A	1002	5/5	0.96	0.11	148,149,152,154	0
2	PO4	A	1001	5/5	0.98	0.23	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.







6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.