Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2024 – 01:04 pm GMT

PDB ID	:	8CJ5
Title	:	Arabidopsis thaliana Phosphoenolpyruvate carboxylase PPC1 A651V mutant with bound phosphate
Authors	:	Haesaerts, S.; Loris, R.; Larsen, P.
Deposited on	:	2023-02-12
Resolution	:	3.00 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:

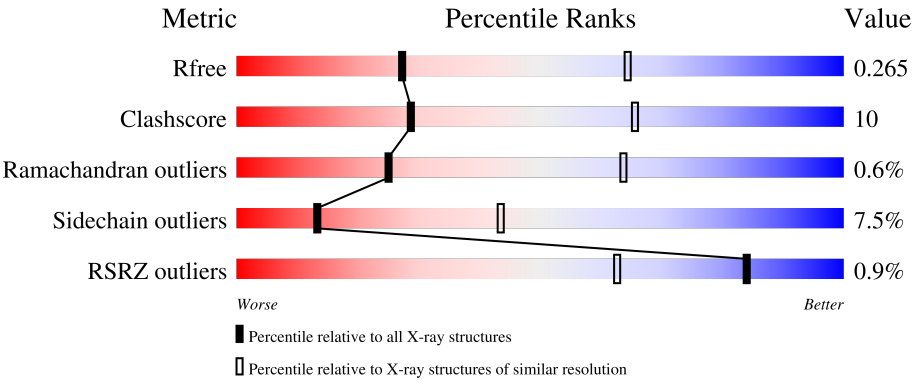
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	67% 23% · 7%
1	B	974	2% 67% 22% · 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14494 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.

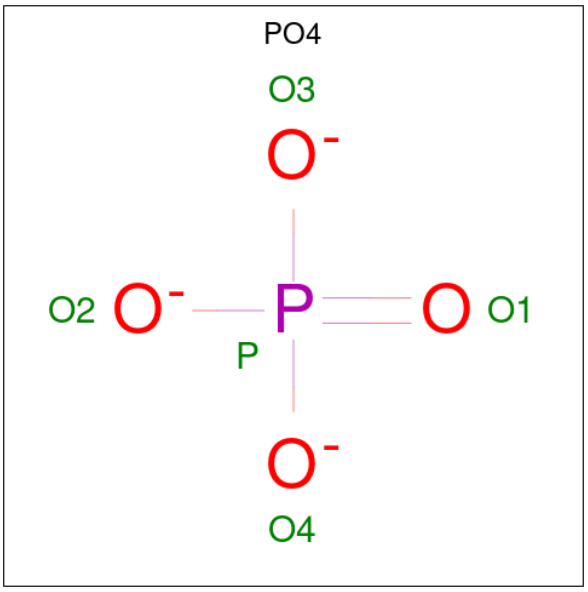
- Molecule 1 is a protein called Phosphoenolpyruvate carboxylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	908	Total	C	N	O	S	0	9	0
			7312	4644	1285	1354	29			
1	B	890	Total	C	N	O	S	0	1	0
			7145	4534	1248	1334	29			

There are 16 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
A	651	VAL	ALA	engineered mutation	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
B	651	VAL	ALA	engineered mutation	UNP Q9MAH0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (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	B	1	Total O P 5 4 1	0	0

- Molecule 3 is water.

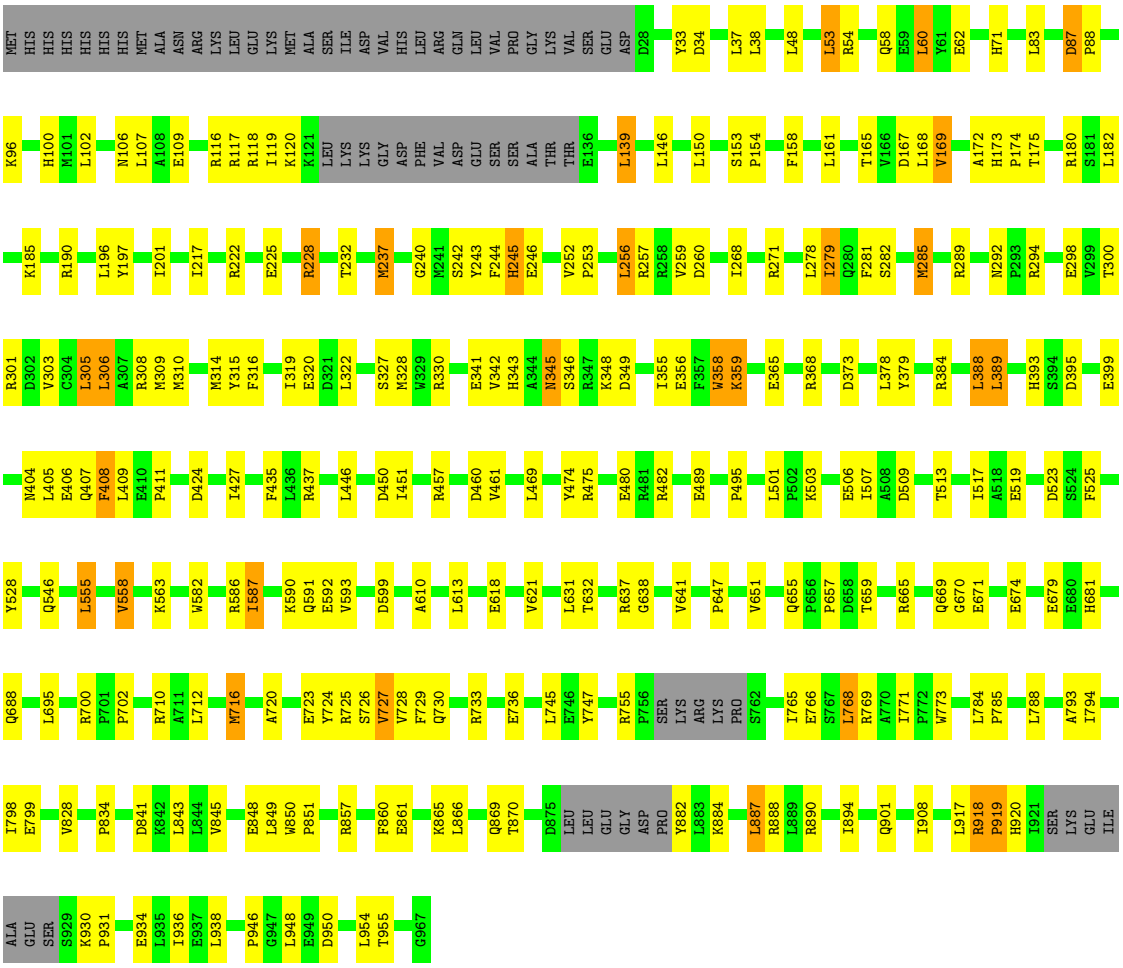
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	25	Total O 25 25	0	0
3	B	2	Total O 2 2	0	0

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.

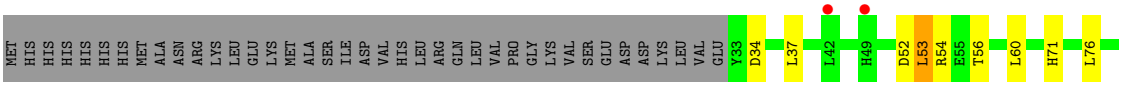
• Molecule 1: Phosphoenolpyruvate carboxylase 1

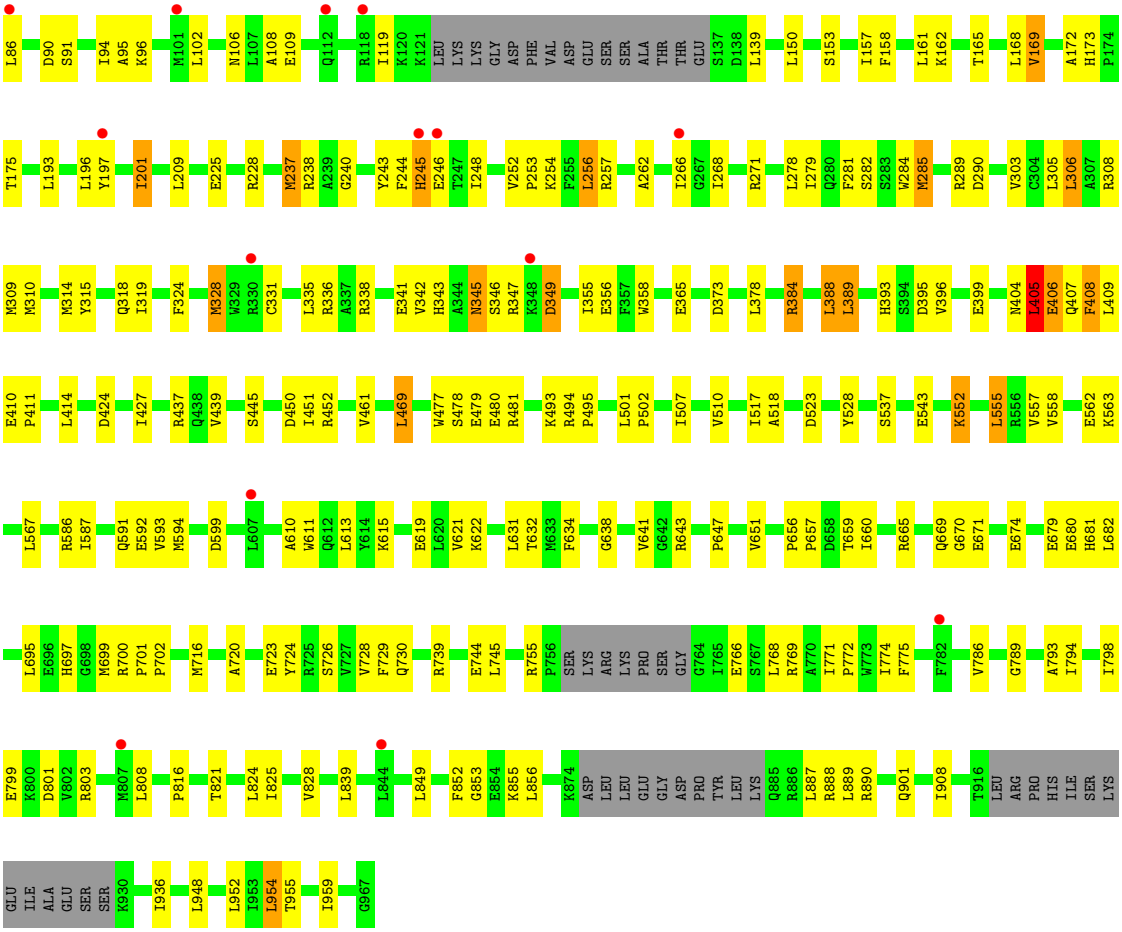
Chain A:



• Molecule 1: Phosphoenolpyruvate carboxylase 1

Chain B:




L86 D90 S91 I94 A95 K96 M101 L102 N106 L107 A108 E109 Q112 R118 I119 K120 K121 LEU LYS LYS GLY ASP PHE VAL ASP GLU SER SER ALA THR THR GLU S137 D138 L139 L150 S153 I157 F158 L161 K162 T165 L168 V169 A172 H173 P174
T175 L193 L196 Y197 I201 L209 E225 R228 M237 R238 A239 G240 Y243 F244 H245 E246 T247 I248 V252 P253 K254 F255 L256 R257 A262 I266 G267 I268 R271 L278 I279 Q280 F281 S282 S283 W284 M285 R289 D290 V303 C304 L305 L306 A307 R308
M309 M310 M314 Y315 Q318 I319 F324 M328 W329 R330 C331 L335 R336 A337 R338 E341 V342 H343 A344 N345 S346 R347 K348 D349 I355 E356 F357 W358 E365 D373 L378 R384 L388 L389 H393 S394 D395 V396 E399 N404 L405 E406 Q407 F408 L409
E410 P411 L414 D424 I427 R437 Q438 V439 S445 D450 I451 R452 V461 L469 W477 S478 E479 E480 R481 K493 R494 P495 L501 P502 I507 V510 I517 A518 D523 Y528 S537 E543 K552 L555 R556 V557 V558 E562 K563
L567 R586 I587 Q591 E592 V593 M594 D599 L607 A610 W611 G612 L613 Y614 K615 E619 L620 V621 K622 L631 T632 W633 F634 G638 V641 G642 R643 P647 V651 P656 P657 D658 T659 I660 R665 Q669 G670 E671 E674 E679 E680 H681 L682
L695 E696 H697 G698 M699 R700 P701 P702 M716 A720 E723 Y724 R725 S726 V727 V728 F729 Q730 R739 E744 L745 R755 P756 SER LYS ARG LYS PRO SER GLY G764 I765 E766 S767 L768 R769 A770 I771 P772 W773 I774 F775 F782 V786 G789 A793 T794 I798
E799 K800 D801 V802 R803 M807 L808 P816 T821 L824 I825 V828 L839 L844 L849 F852 G853 E854 K855 L856 K874 ASP LEU LEU GLU GLY ASP PRO TYR LEU LYS Q885 R886 L887 R888 L889 R890 Q901 I908 T916 LEU ARG PRO HIS ILE SER LYS
GLU ILE ALA GLU SER SER K930 I936 L948 L952 I953 L954 T955 I959 G967

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	128.83Å 156.62Å 142.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.04 – 3.00 49.04 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (49.04-3.00) 85.2 (49.04-3.00)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.24 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.215 , 0.266 0.214 , 0.265	Depositor DCC
R_{free} test set	2841 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	91.0	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 75.9	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	14494	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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

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	0.38	0/7497	0.56	1/10151 (0.0%)
1	B	0.31	0/7300	0.49	1/9882 (0.0%)
All	All	0.35	0/14797	0.52	2/20033 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	405	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	768	LEU	CA-CB-CG	5.43	127.79	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	918	ARG	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7312	0	7247	146	0
1	B	7145	0	7094	134	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	25	0	0	0	0
3	B	2	0	0	1	0
All	All	14494	0	14341	278	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 (278) 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	1.52	0.91
1:A:638:GLY:HA2	1:A:669:GLN:HG3	1.53	0.88
1:B:173:HIS:ND1	1:B:669:GLN:OE1	2.17	0.78
1:A:175:THR:HG23	1:A:671:GLU:H	1.47	0.77
1:A:169:VAL:HB	1:A:282:SER:HB2	1.66	0.77
1:A:298:GLU:OE1	1:A:301[A]:ARG:NH1	2.18	0.77
1:B:169:VAL:HB	1:B:282:SER:HB2	1.66	0.77
1:B:345:ASN:N	1:B:345:ASN:OD1	2.17	0.77
1:B:172:ALA:HB2	1:B:285:MET:HG3	1.66	0.76
1:A:884:LYS:HA	1:A:887:LEU:HB3	1.67	0.74
1:A:930:LYS:HG2	1:A:931:PRO:HD2	1.70	0.74
1:B:175:THR:HG23	1:B:671:GLU:H	1.51	0.74
1:A:355:ILE:HG22	1:A:356:GLU:HG2	1.69	0.73
1:B:888:ARG:O	1:B:890:ARG:N	2.21	0.73
1:A:618:GLU:OE1	1:A:710:ARG:NH2	2.21	0.73
1:B:355:ILE:HG22	1:B:356:GLU:HG2	1.70	0.73
1:A:315:TYR:HB3	1:A:378:LEU:HD21	1.71	0.72
1:A:173:HIS:ND1	1:A:669:GLN:OE1	2.22	0.72
1:A:716:MET:HG2	1:A:793:ALA:HB1	1.69	0.72
1:B:450:ASP:OD2	1:B:665:ARG:NH2	2.21	0.71
1:B:593:VAL:HG12	1:B:631:LEU:HD11	1.72	0.71
1:B:461:VAL:HG22	1:B:507:ILE:HG23	1.73	0.71
1:B:384:ARG:HD2	1:B:396:VAL:HB	1.72	0.70
1:B:723:GLU:HG2	1:B:789:GLY:HA2	1.71	0.69
1:A:139:LEU:HD11	1:A:259:VAL:HG22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:VAL:HG12	1:A:631:LEU:HD11	1.74	0.69
1:A:637:ARG:NH2	1:A:655:GLN:OE1	2.24	0.69
1:A:174:PRO:O	1:A:747:TYR:OH	2.12	0.68
1:B:591:GLN:NE2	1:B:592:GLU:O	2.26	0.68
1:A:100[A]:HIS:NE2	1:A:225:GLU:OE1	2.22	0.68
1:B:343:HIS:HA	1:B:346:SER:HB2	1.76	0.67
1:A:641:VAL:HG21	1:A:828:VAL:HG21	1.76	0.67
1:A:745:LEU:HD12	1:A:745:LEU:H	1.60	0.66
1:A:908:ILE:HD11	1:A:948:LEU:HB3	1.77	0.66
1:A:243:TYR:OH	1:A:674:GLU:HG2	1.94	0.66
1:B:305:LEU:HD11	1:B:388:LEU:HD23	1.79	0.65
1:B:106:ASN:OD1	1:B:890:ARG:NH2	2.30	0.64
1:A:919:PRO:O	1:A:920:HIS:ND1	2.29	0.64
1:A:679[B]:GLU:OE2	1:A:681:HIS:ND1	2.29	0.64
1:B:786:VAL:HG11	1:B:828:VAL:HG21	1.80	0.64
1:B:243:TYR:OH	1:B:674:GLU:HG2	1.99	0.63
1:A:495:PRO:HB2	1:B:495:PRO:HB2	1.81	0.63
1:A:106:ASN:OD1	1:A:890:ARG:NH2	2.32	0.63
1:A:345:ASN:OD1	1:A:345:ASN:N	2.30	0.62
1:A:343:HIS:HA	1:A:346:SER:HB2	1.82	0.61
1:B:315:TYR:HB3	1:B:378:LEU:HD21	1.83	0.61
1:A:610:ALA:HA	1:A:613:LEU:HD12	1.83	0.61
1:A:460:ASP:OD1	1:A:475:ARG:NH1	2.34	0.60
1:B:908:ILE:HD11	1:B:948:LEU:HB3	1.84	0.60
1:B:739:ARG:NH1	1:B:744:GLU:OE1	2.36	0.58
1:B:562:GLU:HG2	1:B:599:ASP:HB2	1.85	0.58
1:A:237:MET:HG2	1:A:303:VAL:HG12	1.85	0.58
1:B:306:LEU:HA	1:B:389:LEU:HD11	1.85	0.58
1:B:306:LEU:O	1:B:310:MET:HG3	2.03	0.58
1:B:328:MET:SD	1:B:328:MET:N	2.77	0.57
1:B:543:GLU:HG2	1:B:557:VAL:HG21	1.86	0.57
1:B:96:LYS:HE2	1:B:225:GLU:OE2	2.05	0.56
1:B:161:LEU:HD13	1:B:695:LEU:HD13	1.87	0.56
1:B:253:PRO:O	1:B:257:ARG:HG3	2.06	0.56
1:A:244:PHE:C	1:A:246:GLU:H	2.08	0.56
1:A:306:LEU:O	1:A:310:MET:HG3	2.05	0.55
1:A:232:THR:HA	1:A:294:ARG:HH21	1.71	0.55
1:A:563:LYS:NZ	1:A:766:GLU:OE2	2.39	0.55
1:B:745:LEU:HD12	1:B:745:LEU:H	1.71	0.55
1:A:48:LEU:HD22	1:A:222:ARG:NH1	2.21	0.55
1:B:237:MET:HG2	1:B:303:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ARG:NH2	1:A:950:ASP:OD1	2.39	0.55
1:B:238:ARG:HH22	1:B:306:LEU:HD21	1.70	0.55
1:A:289:ARG:NH2	1:A:300:THR:OG1	2.37	0.54
1:A:306:LEU:HD22	1:A:389:LEU:HD11	1.89	0.54
1:A:96:LYS:HE2	1:A:225:GLU:OE2	2.07	0.54
1:A:310:MET:O	1:A:314:MET:HG3	2.06	0.54
1:A:305:LEU:HB3	1:A:389:LEU:HG	1.90	0.54
1:B:702:PRO:HB3	1:B:816:PRO:HG2	1.90	0.54
1:B:592:GLU:OE2	1:B:665:ARG:NE	2.34	0.54
1:A:154:PRO:C	1:A:268:ILE:HD11	2.29	0.54
1:A:404:ASN:HB2	1:A:407:GLN:H	1.73	0.54
1:A:408:PHE:O	1:A:411:PRO:HD2	2.08	0.53
1:B:96:LYS:HG3	1:B:954:LEU:HD21	1.90	0.53
1:A:158:PHE:HB2	1:A:268:ILE:HD13	1.91	0.53
1:A:563:LYS:HE3	1:A:599:ASP:HB3	1.89	0.53
1:B:643:ARG:HG3	1:B:774:ILE:HG13	1.89	0.53
1:A:150:LEU:HD11	1:A:700:ARG:HD3	1.91	0.53
1:A:58:GLN:O	1:A:62:GLU:HG3	2.09	0.53
1:B:245:HIS:O	3:B:1101:HOH:O	2.18	0.53
1:B:501:LEU:HD12	1:B:502:PRO:HD2	1.89	0.53
1:B:801:ASP:OD2	1:B:803:ARG:NH2	2.43	0.52
1:B:244:PHE:HA	1:B:248:ILE:HB	1.91	0.52
1:B:256:LEU:HD23	1:B:437:ARG:HD3	1.91	0.52
1:B:610:ALA:HA	1:B:613:LEU:HD12	1.90	0.52
1:B:621:VAL:HG21	1:B:659:THR:HG22	1.91	0.52
1:B:656:PRO:HG2	1:B:659:THR:HG21	1.91	0.52
1:B:726:SER:HA	1:B:730:GLN:HG3	1.92	0.52
1:A:712:LEU:O	1:A:716:MET:HB2	2.10	0.52
1:A:726:SER:HA	1:A:730:GLN:HG3	1.90	0.52
1:B:244:PHE:C	1:B:246:GLU:H	2.12	0.52
1:A:342:VAL:HG11	1:A:373:ASP:HB2	1.92	0.51
1:A:841:ASP:HA	1:A:845:VAL:HG23	1.93	0.51
1:B:563:LYS:NZ	1:B:766:GLU:OE2	2.44	0.51
1:A:733:ARG:NH2	1:A:736:GLU:OE2	2.43	0.51
1:A:865:LYS:O	1:A:869:GLN:HB2	2.11	0.51
1:A:857:ARG:O	1:A:860:PHE:HB3	2.10	0.51
1:A:720:ALA:HB2	1:A:793:ALA:HB2	1.92	0.51
1:B:254:LYS:NZ	1:B:680:GLU:OE2	2.44	0.51
1:B:641:VAL:HG21	1:B:828:VAL:HG21	1.93	0.51
1:A:513:THR:O	1:A:517:ILE:HG13	2.11	0.51
1:B:679:GLU:HB3	1:B:682:LEU:HG	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:PRO:HG3	1:A:860:PHE:CE1	2.46	0.50
1:A:845:VAL:O	1:A:850:TRP:NE1	2.43	0.50
1:B:477:TRP:HA	1:B:481[A]:ARG:HH11	1.76	0.50
1:A:252:VAL:HB	1:A:253:PRO:HD3	1.94	0.50
1:B:641:VAL:HG21	1:B:828:VAL:CG2	2.42	0.50
1:B:657:PRO:HA	1:B:697:HIS:CE1	2.46	0.50
1:A:647:PRO:O	1:A:651:VAL:HG23	2.11	0.50
1:B:150:LEU:HD11	1:B:700:ARG:HB2	1.94	0.50
1:B:477:TRP:HA	1:B:481[A]:ARG:NH1	2.27	0.50
1:B:772:PRO:HA	1:B:775:PHE:HB3	1.91	0.50
1:A:107:LEU:HD22	1:A:190:ARG:HB3	1.92	0.50
1:A:724:TYR:CD1	1:A:788:LEU:HD23	2.47	0.50
1:A:794:ILE:O	1:A:798:ILE:HG12	2.12	0.49
1:B:821:THR:O	1:B:825:ILE:HG12	2.12	0.49
1:A:501:LEU:O	1:A:503:LYS:HG3	2.12	0.49
1:A:528:TYR:HB2	1:A:555:LEU:HD13	1.93	0.49
1:A:279:ILE:HD13	1:A:279:ILE:H	1.77	0.49
1:A:139:LEU:N	1:A:688:GLN:OE1	2.46	0.49
1:B:621:VAL:HG21	1:B:659:THR:HA	1.94	0.49
1:B:201:ILE:HD13	1:B:201:ILE:H	1.77	0.49
1:A:474:TYR:CZ	1:A:482:ARG:HD3	2.47	0.49
1:B:331:CYS:SG	1:B:336:ARG:HD2	2.53	0.49
1:B:404:ASN:HB2	1:B:407:GLN:H	1.78	0.49
1:B:405:LEU:HD12	1:B:405:LEU:H	1.77	0.49
1:A:316:PHE:HE1	1:A:379:TYR:HB2	1.78	0.49
1:A:657:PRO:HB3	1:A:702:PRO:HD2	1.95	0.49
1:B:406:GLU:HA	1:B:409:LEU:H	1.78	0.48
1:B:647:PRO:O	1:B:651:VAL:HG23	2.13	0.48
1:A:180:ARG:N	2:A:1001:PO4:O4	2.46	0.48
1:B:798:ILE:HD11	1:B:808:LEU:HD12	1.95	0.48
1:A:242:SER:HA	1:A:245:HIS:CE1	2.48	0.48
1:A:173:HIS:O	1:A:175:THR:N	2.45	0.48
1:B:720:ALA:HB2	1:B:793:ALA:HB2	1.96	0.48
1:B:769:ARG:HB2	1:B:772:PRO:HD2	1.96	0.48
1:A:168:LEU:O	1:A:281:PHE:HA	2.14	0.47
1:B:240:GLY:HA3	1:B:285:MET:HE1	1.95	0.47
1:A:461:VAL:HA	1:A:507:ILE:HD12	1.97	0.47
1:B:952:LEU:O	1:B:955:THR:OG1	2.25	0.47
1:A:901:GLN:HB2	1:A:955:THR:HB	1.96	0.47
1:A:172:ALA:HB2	1:A:285:MET:HG3	1.97	0.47
1:A:244:PHE:O	1:A:246:GLU:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:ARG:HD3	1:A:769:ARG:NH2	2.29	0.47
1:B:518:ALA:O	1:B:552:LYS:HE2	2.14	0.47
1:A:728:VAL:HG23	1:A:729:PHE:CD2	2.50	0.47
1:B:755:ARG:HD3	1:B:769:ARG:CZ	2.44	0.47
1:A:256:LEU:HB3	1:A:437:ARG:NH1	2.29	0.47
1:A:461:VAL:HG22	1:A:507:ILE:HG23	1.95	0.47
1:B:395:ASP:OD1	1:B:395:ASP:N	2.42	0.47
1:B:794:ILE:O	1:B:798:ILE:HG12	2.15	0.47
1:A:399:GLU:CD	1:A:399:GLU:H	2.17	0.47
1:B:158:PHE:HB2	1:B:268:ILE:HD13	1.97	0.47
1:B:853:GLY:HA2	1:B:856:LEU:HD12	1.97	0.47
1:B:37:LEU:HD11	1:B:108:ALA:HB2	1.97	0.47
1:B:308:ARG:HG3	1:B:445:SER:HB3	1.97	0.47
1:B:477:TRP:CG	1:B:481[A]:ARG:HD2	2.50	0.47
1:A:359:LYS:H	1:A:359:LYS:HG2	1.57	0.46
1:B:657:PRO:HB3	1:B:702:PRO:HD2	1.96	0.46
1:B:679:GLU:HG3	1:B:681:HIS:H	1.80	0.46
1:B:852:PHE:O	1:B:855:LYS:HB2	2.16	0.46
1:B:523:ASP:OD1	1:B:523:ASP:N	2.47	0.46
1:A:395:ASP:OD1	1:A:395:ASP:N	2.47	0.46
1:A:424:ASP:HB3	1:A:427:ILE:HD12	1.97	0.46
1:A:794:ILE:HD13	1:A:870:THR:HG21	1.97	0.46
1:B:289:ARG:HG2	1:B:452:ARG:O	2.16	0.46
1:A:87:ASP:OD1	1:A:87:ASP:N	2.49	0.46
1:A:582:TRP:O	1:A:586:ARG:HD3	2.15	0.46
1:B:404:ASN:HB3	1:B:406:GLU:OE2	2.16	0.46
1:B:157:ILE:O	1:B:161:LEU:HB2	2.15	0.45
1:A:358:TRP:CD1	1:A:359:LYS:N	2.84	0.45
1:A:406:GLU:HA	1:A:409:LEU:H	1.81	0.45
1:A:517:ILE:HA	1:A:525:PHE:CZ	2.52	0.45
1:B:37:LEU:HD21	1:B:193:LEU:HD11	1.99	0.45
1:A:587:ILE:HD12	1:A:590:LYS:O	2.17	0.45
1:A:849:LEU:HD23	1:A:849:LEU:H	1.82	0.45
1:A:161:LEU:HD13	1:A:695:LEU:HD13	1.98	0.45
1:A:330:ARG:HD2	1:A:330:ARG:HA	1.80	0.45
1:B:52:ASP:O	1:B:56:THR:HG23	2.15	0.45
1:B:168:LEU:O	1:B:281:PHE:HA	2.17	0.45
1:B:150:LEU:HD21	1:B:700:ARG:HD3	1.98	0.45
1:A:451:ILE:HG13	1:A:517:ILE:HD11	1.99	0.45
1:B:256:LEU:HB3	1:B:437:ARG:NH1	2.32	0.45
1:B:408:PHE:O	1:B:411:PRO:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:GLU:HG2	1:A:356:GLU:HB2	1.99	0.44
1:B:728:VAL:HG23	1:B:729:PHE:CD2	2.52	0.44
1:A:260:ASP:CG	1:A:271:ARG:HG2	2.38	0.44
1:A:489:GLU:OE2	1:B:494:ARG:NH2	2.38	0.44
1:A:841:ASP:HA	1:A:845:VAL:CG2	2.46	0.44
1:B:252:VAL:HB	1:B:253:PRO:HD3	1.99	0.44
1:B:173:HIS:O	1:B:175:THR:N	2.46	0.44
1:B:315:TYR:OH	1:B:439:VAL:HA	2.18	0.44
1:B:479:GLU:OE1	1:B:537:SER:HB3	2.17	0.44
1:B:849:LEU:H	1:B:849:LEU:HD23	1.83	0.44
1:A:558:VAL:HB	1:A:592:GLU:O	2.18	0.43
1:B:824:LEU:O	1:B:828:VAL:HG23	2.18	0.43
1:A:450:ASP:OD2	1:A:665:ARG:NH2	2.52	0.43
1:A:322:LEU:HD22	1:A:435:PHE:CD2	2.53	0.43
1:A:591:GLN:NE2	1:A:592:GLU:O	2.48	0.43
1:A:725:ARG:O	1:A:730:GLN:HG2	2.19	0.43
1:A:726:SER:HA	1:A:730:GLN:CG	2.48	0.43
1:A:621:VAL:HG21	1:A:659:THR:HA	1.99	0.43
1:B:611:TRP:CE2	1:B:615:LYS:HE3	2.54	0.43
1:A:173:HIS:O	1:A:175:THR:HG22	2.18	0.43
1:A:457:ARG:NE	1:A:506:GLU:HB3	2.34	0.43
1:A:936:ILE:HG22	1:A:946:PRO:HB2	2.00	0.43
1:A:316:PHE:CE1	1:A:379:TYR:HB2	2.53	0.43
1:A:523:ASP:OD1	1:A:523:ASP:N	2.52	0.43
1:B:53:LEU:HD12	1:B:53:LEU:HA	1.81	0.43
1:B:262:ALA:O	1:B:266:ILE:HG12	2.18	0.43
1:B:478:SER:H	1:B:481[A]:ARG:NH1	2.17	0.43
1:B:290:ASP:HB3	1:B:452:ARG:HH21	1.84	0.43
1:B:424:ASP:HB3	1:B:427:ILE:HD12	2.01	0.43
1:B:726:SER:HA	1:B:730:GLN:CG	2.49	0.43
1:B:594:MET:HA	1:B:634:PHE:HB3	2.00	0.42
1:A:388:LEU:HA	1:A:388:LEU:HD12	1.86	0.42
1:B:90:ASP:O	1:B:94:ILE:HG12	2.19	0.42
1:B:699:MET:O	1:B:701:PRO:HD3	2.19	0.42
1:A:890:ARG:O	1:A:894:ILE:HG13	2.18	0.42
1:B:95:ALA:HB3	1:B:954:LEU:HD23	2.00	0.42
1:B:256:LEU:HD12	1:B:256:LEU:HA	1.93	0.42
1:A:253:PRO:O	1:A:257:ARG:HG3	2.19	0.42
1:A:509:ASP:O	1:A:513:THR:HG23	2.20	0.42
1:B:347:ARG:O	1:B:349:ASP:N	2.53	0.42
1:A:301[A]:ARG:NH2	1:A:519:GLU:OE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:ILE:HG13	1:B:517:ILE:HD11	2.01	0.42
1:B:342:VAL:HG11	1:B:373:ASP:HB2	2.02	0.42
1:B:724:TYR:O	1:B:728:VAL:HG22	2.19	0.42
1:A:866:LEU:O	1:A:870:THR:HG23	2.20	0.42
1:A:723:GLU:O	1:A:727:VAL:HG12	2.19	0.42
1:A:37:LEU:HD23	1:A:37:LEU:HA	1.94	0.41
1:A:784:LEU:HB3	1:A:785:PRO:HD3	2.02	0.41
1:B:284:TRP:CD1	1:B:450:ASP:HB2	2.55	0.41
1:B:347:ARG:CG	1:B:349:ASP:HB2	2.50	0.41
1:A:60:LEU:HD21	1:A:83:LEU:HD21	2.03	0.41
1:A:546:GLN:OE1	1:A:555:LEU:HD12	2.19	0.41
1:B:528:TYR:HB2	1:B:555:LEU:CD1	2.51	0.41
1:A:53:LEU:HD12	1:A:53:LEU:HA	1.74	0.41
1:A:843:LEU:HD23	1:A:843:LEU:HA	1.89	0.41
1:B:338:ARG:O	1:B:341:GLU:HB2	2.20	0.41
1:A:292:ASN:OD1	1:A:294:ARG:HB2	2.21	0.41
1:B:86:LEU:HD13	1:B:91:SER:HA	2.02	0.41
1:B:158:PHE:CE2	1:B:162:LYS:HD2	2.54	0.41
1:B:410:GLU:HB3	1:B:411:PRO:HD3	2.03	0.41
1:A:48:LEU:HD22	1:A:222:ARG:HH12	1.85	0.41
1:A:118:ARG:C	1:A:120:LYS:H	2.23	0.41
1:B:755:ARG:HD3	1:B:769:ARG:NH2	2.35	0.41
1:B:469:LEU:HD12	1:B:469:LEU:HA	1.92	0.41
1:B:660:ILE:HD12	1:B:697:HIS:ND1	2.36	0.41
1:A:167:ASP:HB3	1:A:665:ARG:HG3	2.03	0.41
1:A:240:GLY:HA3	1:A:285:MET:CE	2.51	0.41
1:B:619:GLU:O	1:B:622:LYS:HB2	2.20	0.41
1:A:34:ASP:O	1:A:38:LEU:HB2	2.21	0.41
1:A:87:ASP:HB3	1:A:88:PRO:HD2	2.02	0.41
1:A:405:LEU:HG	1:A:406:GLU:HG3	2.03	0.41
1:A:591:GLN:O	1:A:631:LEU:HD12	2.21	0.41
1:B:209:LEU:HA	1:B:209:LEU:HD23	1.88	0.41
1:B:245:HIS:HA	1:B:314:MET:HE1	2.03	0.41
1:B:335:LEU:HD12	1:B:414:LEU:HG	2.03	0.41
1:A:169:VAL:HA	1:A:282:SER:O	2.21	0.40
1:A:765:ILE:HD13	1:A:773:TRP:CZ3	2.56	0.40
1:A:217:ILE:HD13	1:A:217:ILE:HG21	1.82	0.40
1:A:306:LEU:HA	1:A:389:LEU:HD11	2.04	0.40
1:B:936:ILE:H	1:B:936:ILE:HG13	1.67	0.40
1:A:146:LEU:HA	1:A:146:LEU:HD23	1.79	0.40
1:A:850:TRP:N	1:A:851:PRO:HD2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:HIS:CD2	1:A:245:HIS:H	2.39	0.40
1:A:327:SER:HB3	1:A:368:ARG:NH2	2.36	0.40
1:B:76:LEU:HB3	1:B:839:LEU:HD22	2.04	0.40
1:B:901:GLN:NE2	1:B:959:ILE:HD12	2.36	0.40
1:A:120:LYS:HB3	1:A:120:LYS:HE2	1.94	0.40
1:A:938:LEU:HD23	1:A:938:LEU:HA	1.75	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	907/974 (93%)	858 (95%)	42 (5%)	7 (1%)	19	57
1	B	881/974 (90%)	833 (95%)	44 (5%)	4 (0%)	29	68
All	All	1788/1948 (92%)	1691 (95%)	86 (5%)	11 (1%)	25	64

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	670	GLY
1	A	919	PRO
1	B	670	GLY
1	B	889	LEU
1	A	888	ARG
1	A	245	HIS
1	A	918	ARG
1	B	119	ILE
1	B	245	HIS
1	A	446	LEU
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	782/850 (92%)	721 (92%)	61 (8%)	12 42
1	B	769/850 (90%)	713 (93%)	56 (7%)	14 44
All	All	1551/1700 (91%)	1434 (92%)	117 (8%)	13 43

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

Mol	Chain	Res	Type
1	A	33	TYR
1	A	53	LEU
1	A	54	ARG
1	A	60	LEU
1	A	71	HIS
1	A	87	ASP
1	A	102	LEU
1	A	109	GLU
1	A	116	ARG
1	A	117	ARG
1	A	139	LEU
1	A	153	SER
1	A	165	THR
1	A	169	VAL
1	A	182	LEU
1	A	185	LYS
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	278	LEU
1	A	279	ILE
1	A	285	MET
1	A	305	LEU
1	A	306	LEU

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Mol	Chain	Res	Type
1	A	308	ARG
1	A	309	MET
1	A	319	ILE
1	A	328	MET
1	A	345	ASN
1	A	348	LYS
1	A	349	ASP
1	A	358	TRP
1	A	359	LYS
1	A	365	GLU
1	A	384	ARG
1	A	388	LEU
1	A	389	LEU
1	A	393	HIS
1	A	408	PHE
1	A	469	LEU
1	A	480	GLU
1	A	555	LEU
1	A	558	VAL
1	A	587	ILE
1	A	632	THR
1	A	716	MET
1	A	727	VAL
1	A	768	LEU
1	A	771	ILE
1	A	799	GLU
1	A	848	GLU
1	A	861	GLU
1	A	882	TYR
1	A	887	LEU
1	A	917	LEU
1	A	934[A]	GLU
1	A	934[B]	GLU
1	A	954	LEU
1	B	34	ASP
1	B	53	LEU
1	B	54	ARG
1	B	60	LEU
1	B	71	HIS
1	B	102	LEU
1	B	109	GLU
1	B	139	LEU

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Mol	Chain	Res	Type
1	B	153	SER
1	B	165	THR
1	B	169	VAL
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	271	ARG
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	365	GLU
1	B	384	ARG
1	B	388	LEU
1	B	389	LEU
1	B	393	HIS
1	B	399	GLU
1	B	405	LEU
1	B	406	GLU
1	B	408	PHE
1	B	469	LEU
1	B	480	GLU
1	B	493	LYS
1	B	510	VAL
1	B	552	LYS
1	B	555	LEU
1	B	558	VAL
1	B	567	LEU
1	B	586	ARG
1	B	587	ILE
1	B	632	THR

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Mol	Chain	Res	Type
1	B	716	MET
1	B	768	LEU
1	B	771	ILE
1	B	799	GLU
1	B	887	LEU
1	B	954	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	B	1001	-	4,4,4	0.85	0	6,6,6	0.37	0
2	PO4	A	1001	-	4,4,4	1.09	0	6,6,6	0.27	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

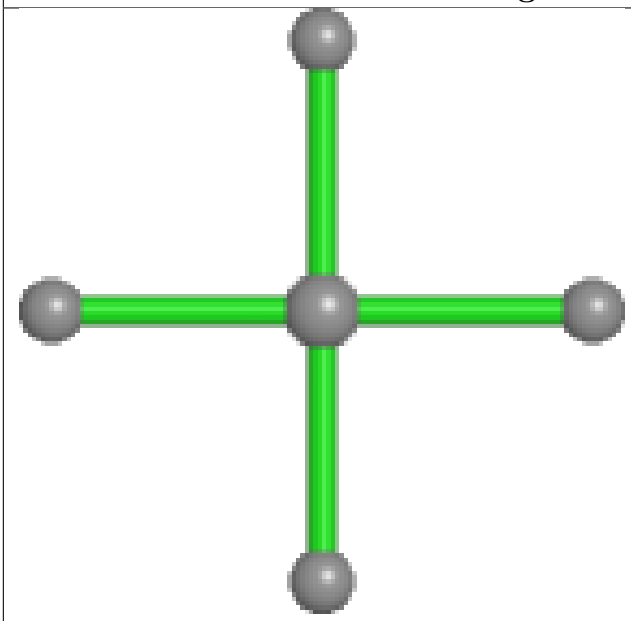
There are no ring outliers.

1 monomer is involved in 1 short contact:

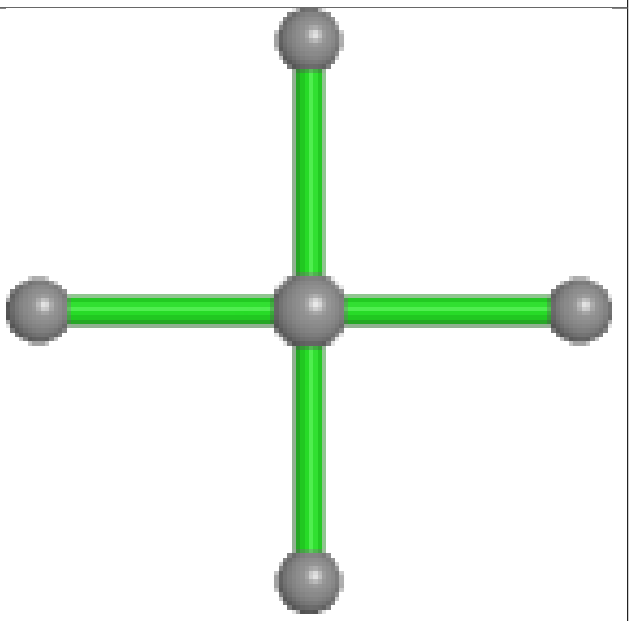
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	PO4	1	0

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 then 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.

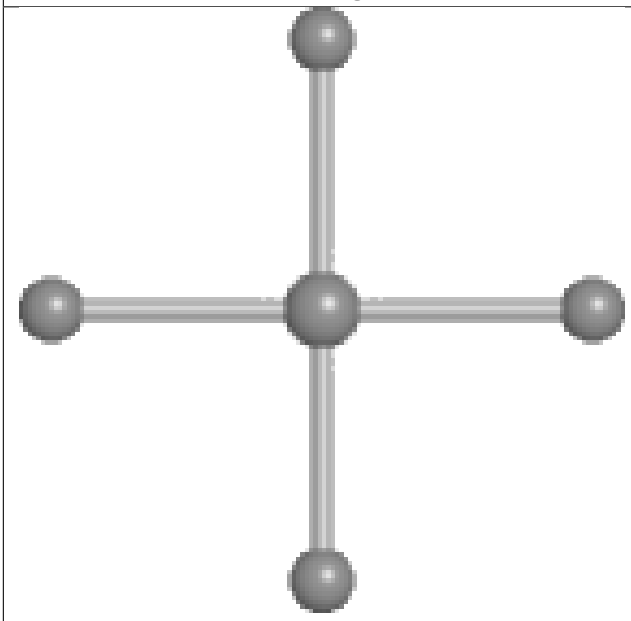
Ligand PO4 B 1001



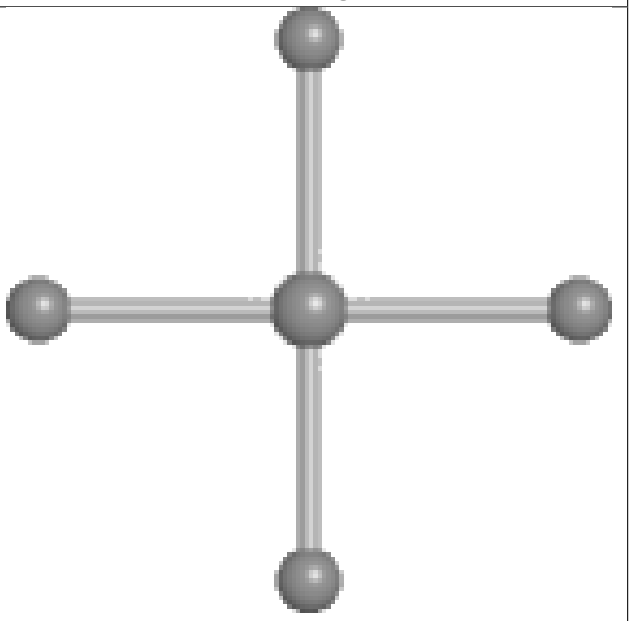
Bond lengths



Bond angles

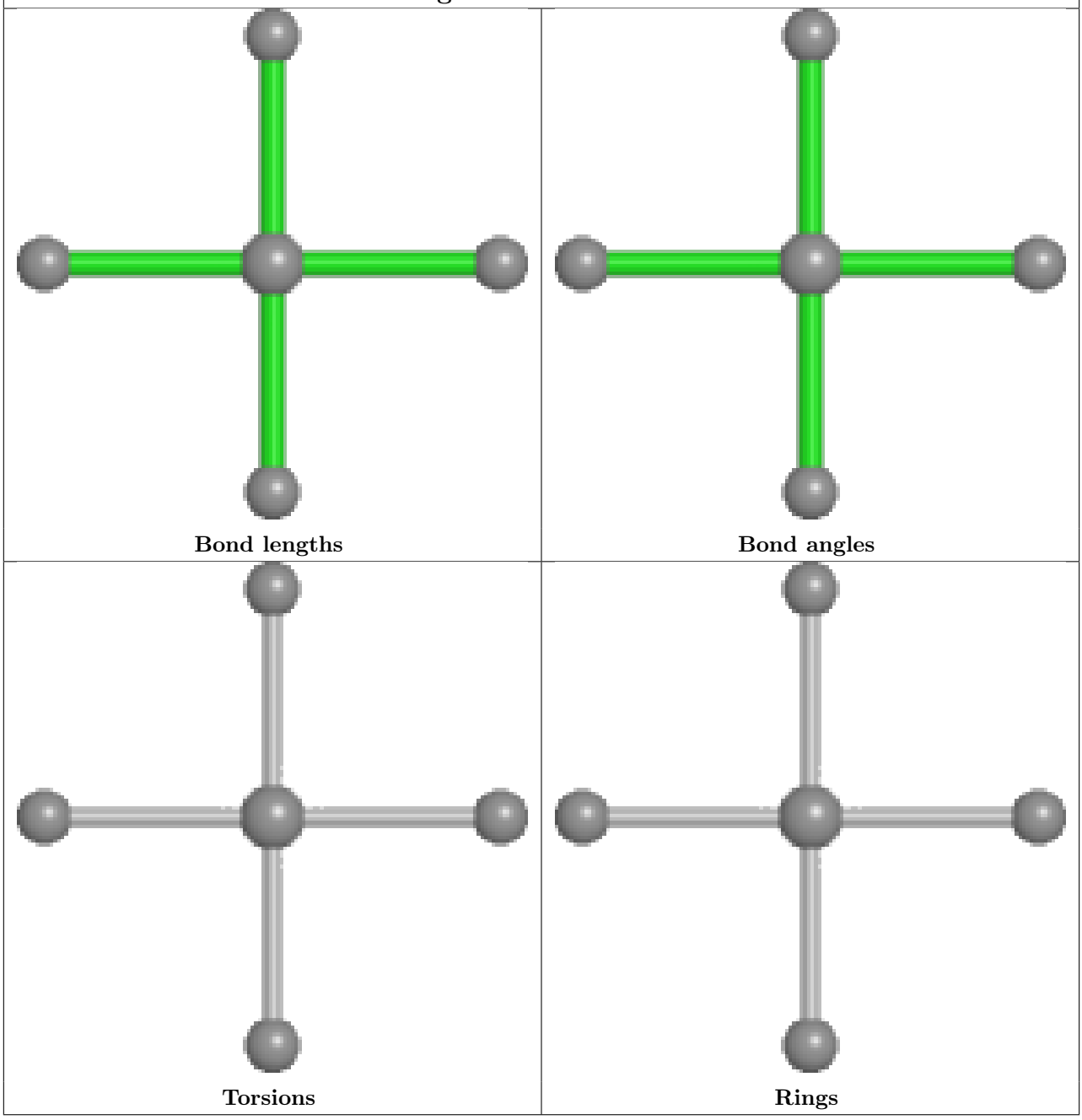


Torsions



Rings

Ligand PO4 A 1001



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, 95^{th} 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	908/974 (93%)	-0.46	0 100 100	63, 92, 141, 211	0
1	B	890/974 (91%)	-0.08	16 (1%) 68 40	87, 156, 223, 255	0
All	All	1798/1948 (92%)	-0.27	16 (0%) 84 63	63, 117, 212, 255	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	245	HIS	3.3
1	B	246	GLU	3.3
1	B	118	ARG	3.1
1	B	49	HIS	3.1
1	B	197	TYR	3.0
1	B	101	MET	2.8
1	B	348	LYS	2.8
1	B	782	PHE	2.6
1	B	86	LEU	2.5
1	B	330	ARG	2.4
1	B	844	LEU	2.2
1	B	266	ILE	2.2
1	B	112	GLN	2.2
1	B	807	MET	2.1
1	B	607	LEU	2.1
1	B	42	LEU	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)

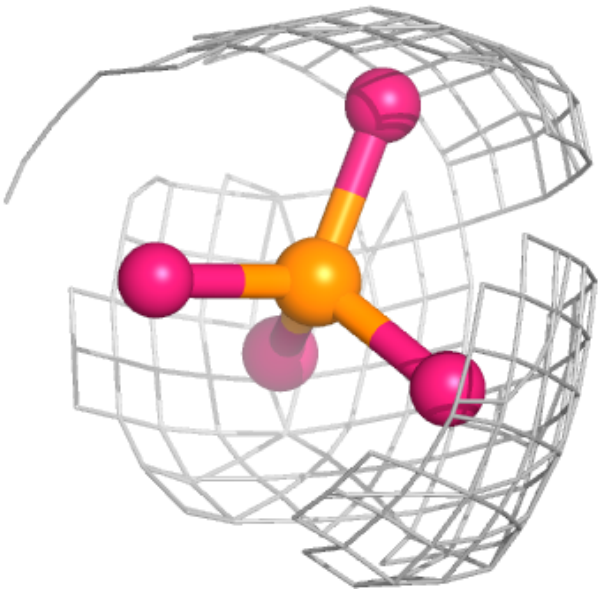
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

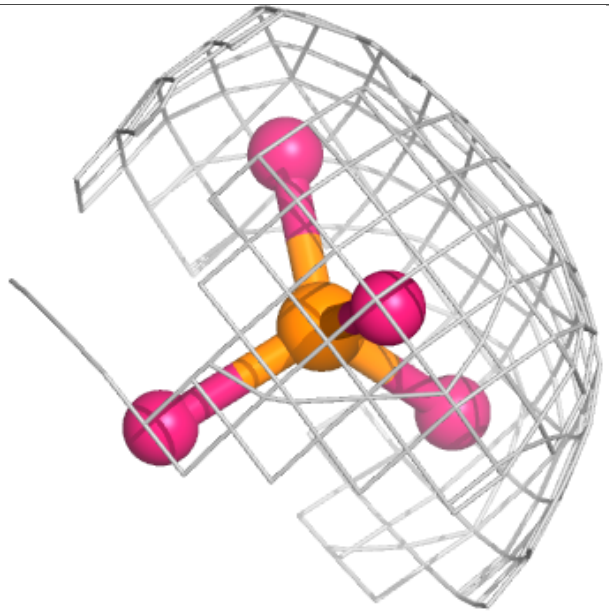
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	B	1001	5/5	0.95	0.38	140,143,145,150	0
2	PO4	A	1001	5/5	0.99	0.27	83,85,93,100	0

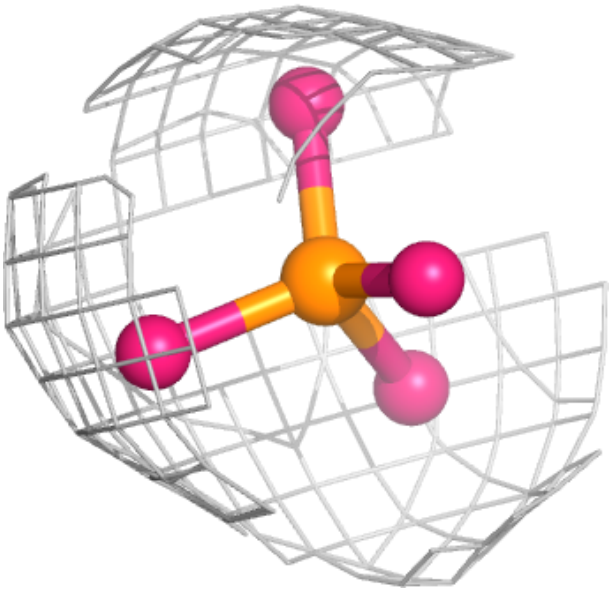
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

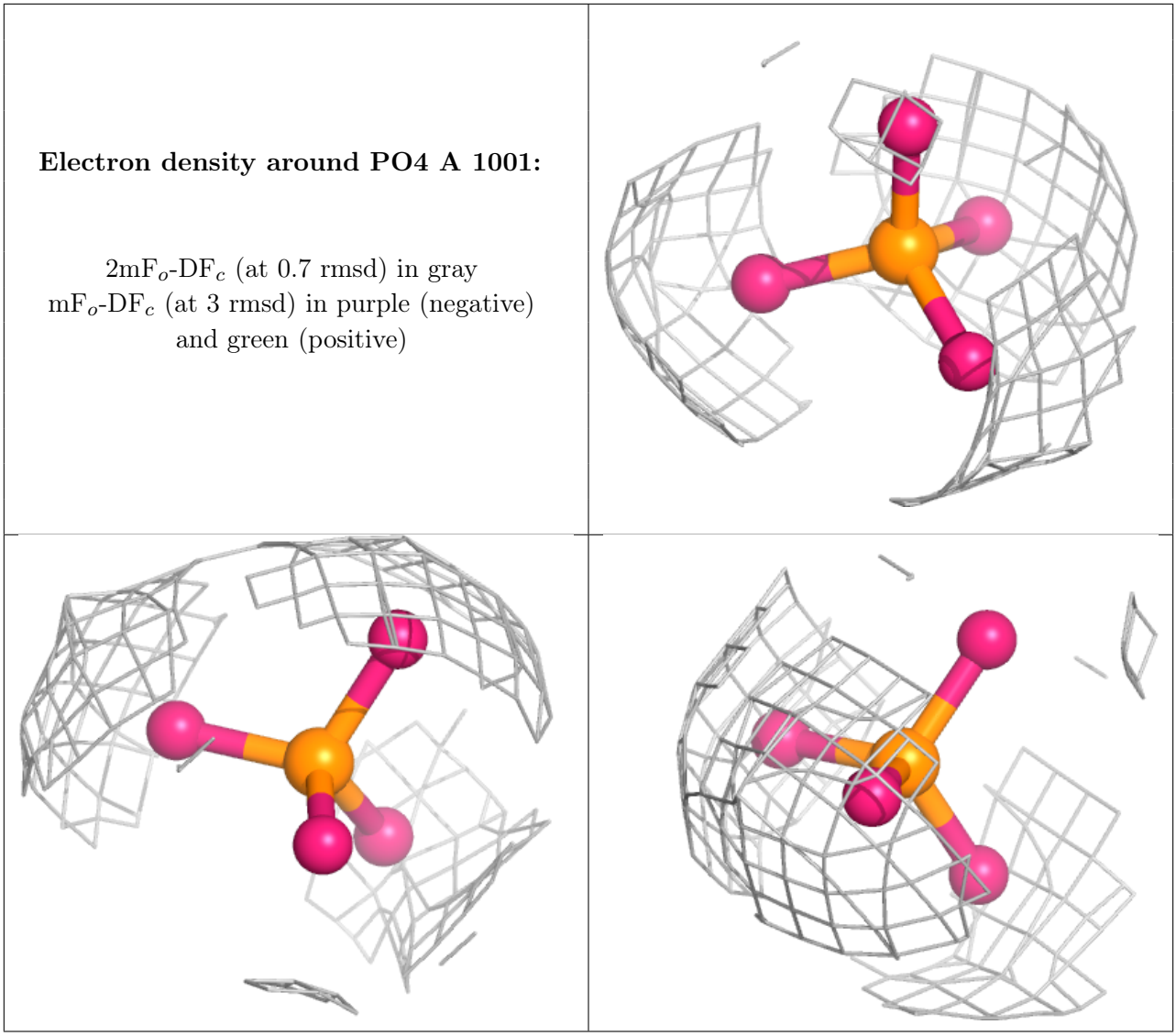






Electron density around PO4 A 1001:

$2mF_o$-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

There are no such residues in this entry.