



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:17 AM UTC

PDB ID : 5WT4 / pdb_00005wt4
Title : L-Cysteine-PLP intermediate of NifS from Helicobacter pylori
Authors : Fujishiro, T.; Nakamura, R.; Takahashi, T.
Deposited on : 2016-12-09
Resolution : 2.92 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

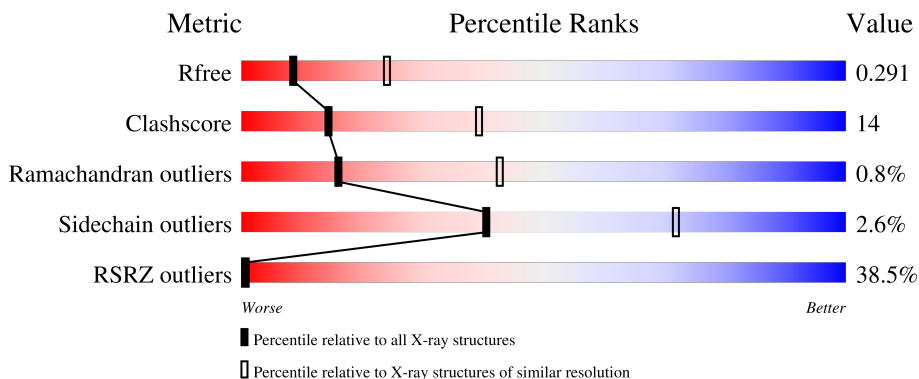
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	401	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2810 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 Cysteine desulfurase IscS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	358	2775	1754	486	524	11	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

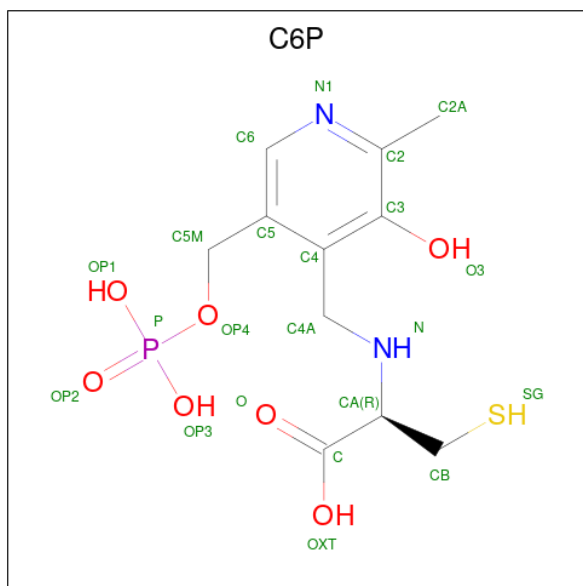
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	engineered mutation	UNP O25008
A	138	ARG	LYS	engineered mutation	UNP O25008
A	388	VAL	-	expression tag	UNP O25008
A	389	ASP	-	expression tag	UNP O25008
A	390	LEU	-	expression tag	UNP O25008
A	391	VAL	-	expression tag	UNP O25008
A	392	PRO	-	expression tag	UNP O25008
A	393	ARG	-	expression tag	UNP O25008
A	394	GLY	-	expression tag	UNP O25008
A	395	SER	-	expression tag	UNP O25008
A	396	HIS	-	expression tag	UNP O25008
A	397	HIS	-	expression tag	UNP O25008
A	398	HIS	-	expression tag	UNP O25008
A	399	HIS	-	expression tag	UNP O25008
A	400	HIS	-	expression tag	UNP O25008
A	401	HIS	-	expression tag	UNP O25008

- Molecule 2 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	3	1		

- Molecule 3 is N-({3-HYDROXY-2-METHYL-5-[(PHOSPHONOXY)METHYL]PYRIDIN-4-YL}METHYL)-L-CYSTEINE (CCD ID: C6P) (formula: $C_{11}H_{17}N_2O_7PS$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	N	O	P	S	0	0
			22	11	2	7	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.17Å 103.17Å 133.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.12 – 2.92 48.12 – 2.92	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.12-2.92) 98.6 (48.12-2.92)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 2.91Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.268 , 0.292 0.270 , 0.291	Depositor DCC
R_{free} test set	802 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	62.9	Xtrriage
Anisotropy	0.812	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	2810	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: C6P, IPA

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	0.47	0/2825	0.95	6/3826 (0.2%)

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	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	VAL	N-CA-C	-6.14	100.57	109.29
1	A	281	LYS	N-CA-C	-5.92	106.70	112.97
1	A	291	ARG	CA-C-N	-5.89	117.13	123.08
1	A	291	ARG	C-N-CA	-5.89	117.13	123.08
1	A	358	SER	CA-C-N	5.34	129.15	120.60
1	A	358	SER	C-N-CA	5.34	129.15	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	305	GLY	Mainchain
1	A	306	ILE	Mainchain

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	2775	0	2793	78	0
2	A	4	0	8	0	0
3	A	22	0	13	3	0
4	A	9	0	0	0	0
All	All	2810	0	2814	79	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 14.

All (79) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:HD1	1:A:145:THR:HG22	1.43	0.83
1:A:275:LEU:O	1:A:279:LEU:HD12	1.82	0.79
1:A:357:LEU:HD21	1:A:366:ILE:HD11	1.67	0.77
1:A:272:ARG:HH21	1:A:294:ARG:NH1	1.86	0.73
1:A:99:THR:HG22	1:A:100:THR:H	1.53	0.71
1:A:96:HIS:ND1	1:A:145:THR:HG22	2.06	0.69
1:A:320:ILE:HD12	1:A:372:VAL:HG21	1.74	0.69
1:A:134:ALA:O	1:A:137:VAL:HG22	1.93	0.69
1:A:179:THR:HG23	1:A:200:LEU:HD12	1.77	0.65
1:A:64:ILE:HG22	1:A:220:SER:HB2	1.79	0.65
1:A:206:LYS:NZ	3:A:502:C6P:H4A1	2.12	0.64
1:A:314:ASP:OD1	1:A:379:ARG:NH2	2.29	0.63
1:A:187:LYS:HA	1:A:264:GLU:HG2	1.81	0.63
1:A:81:LEU:HD11	1:A:107:VAL:HG13	1.79	0.62
1:A:88:GLU:OE1	1:A:92:LYS:HD3	1.99	0.62
1:A:272:ARG:HH21	1:A:294:ARG:HH11	1.48	0.62
1:A:148:VAL:HG11	1:A:170:CYS:SG	2.41	0.61
1:A:99:THR:HG23	1:A:149:SER:O	2.01	0.60
1:A:382:ASN:N	1:A:382:ASN:OD1	2.34	0.60
1:A:182:VAL:HG22	1:A:202:PHE:HA	1.84	0.60
1:A:275:LEU:HD12	1:A:370:ILE:HG13	1.83	0.60
1:A:381:ARG:O	1:A:383:ILE:N	2.35	0.59
1:A:290:ASP:OD1	1:A:292:ILE:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ILE:CD1	1:A:372:VAL:HG21	2.34	0.56
1:A:270:LYS:HG2	1:A:271:LEU:HD12	1.86	0.56
1:A:133:THR:OG1	1:A:136:GLN:HG3	2.07	0.55
1:A:159:LEU:HD21	1:A:290:ASP:HB3	1.89	0.54
1:A:369:THR:HA	1:A:372:VAL:HG22	1.90	0.54
1:A:99:THR:HG22	1:A:100:THR:N	2.23	0.53
1:A:292:ILE:HD12	1:A:293:HIS:CG	2.44	0.52
1:A:290:ASP:OD1	1:A:291:ARG:N	2.42	0.52
1:A:200:LEU:HB3	1:A:217:TYR:HB3	1.91	0.52
1:A:64:ILE:HG22	1:A:220:SER:CB	2.39	0.52
1:A:96:HIS:HD2	1:A:120:GLU:O	1.93	0.51
1:A:99:THR:CG2	1:A:103:GLU:HG3	2.41	0.51
1:A:206:LYS:HZ2	3:A:502:C6P:H4A1	1.75	0.50
1:A:133:THR:N	1:A:136:GLN:OE1	2.38	0.49
1:A:39:GLN:O	1:A:43:GLU:CB	2.60	0.49
1:A:182:VAL:HG11	1:A:206:LYS:HZ3	1.78	0.49
1:A:95:ASN:HB3	1:A:144:LYS:HE2	1.95	0.48
1:A:267:VAL:O	1:A:271:LEU:HD13	2.13	0.48
1:A:379:ARG:HD2	1:A:379:ARG:O	2.14	0.48
1:A:88:GLU:HA	1:A:92:LYS:HB2	1.96	0.47
1:A:283:PRO:O	1:A:285:VAL:HG13	2.14	0.47
1:A:100:THR:HG23	1:A:150:VAL:HG12	1.97	0.47
1:A:98:VAL:HG22	1:A:122:THR:OG1	2.15	0.46
1:A:182:VAL:CG1	1:A:206:LYS:HZ3	2.28	0.46
1:A:96:HIS:HD1	1:A:145:THR:CG2	2.22	0.46
1:A:169:ILE:O	1:A:173:LYS:HG2	2.15	0.46
1:A:103:GLU:OE1	1:A:151:MET:N	2.41	0.45
1:A:202:PHE:CZ	1:A:215:GLY:HA3	2.51	0.45
1:A:138:ARG:HA	1:A:141:ILE:HG22	1.98	0.45
1:A:309:GLU:OE1	1:A:309:GLU:N	2.50	0.45
1:A:281:LYS:C	1:A:282:ILE:HD12	2.43	0.44
1:A:152:TRP:HA	1:A:163:ILE:HD11	2.00	0.44
1:A:280:LEU:HD23	1:A:285:VAL:HG23	1.99	0.44
1:A:138:ARG:NH1	1:A:173:LYS:HE3	2.32	0.44
1:A:39:GLN:HG3	1:A:40:PHE:N	2.33	0.44
1:A:102:ALA:HB1	1:A:154:ASN:ND2	2.32	0.43
1:A:138:ARG:O	1:A:141:ILE:HG22	2.18	0.43
1:A:141:ILE:HA	1:A:145:THR:HG21	2.00	0.43
1:A:102:ALA:HB1	1:A:154:ASN:HD22	1.84	0.43
1:A:106:ALA:O	1:A:110:THR:HG23	2.17	0.43
1:A:178:HIS:HB2	1:A:199:PHE:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LEU:HG	1:A:279:LEU:CD1	2.48	0.43
1:A:134:ALA:HB1	1:A:169:ILE:HD12	2.02	0.42
1:A:181:ALA:O	1:A:185:ILE:HD12	2.20	0.42
1:A:306:ILE:HG21	1:A:380:LEU:HD13	2.01	0.42
1:A:7:LEU:HD11	1:A:369:THR:HG21	2.02	0.42
1:A:39:GLN:O	1:A:43:GLU:HB3	2.20	0.42
1:A:90:LEU:HA	1:A:90:LEU:HD23	1.88	0.41
3:A:502:C6P:H5M2	3:A:502:C6P:H4A2	1.64	0.41
1:A:94:LYS:HD3	1:A:145:THR:O	2.20	0.41
1:A:39:GLN:O	1:A:43:GLU:HB2	2.20	0.41
1:A:269:GLY:HA2	1:A:296:PRO:O	2.21	0.41
1:A:113:PHE:CE1	1:A:117:LEU:HD11	2.56	0.41
1:A:282:ILE:O	1:A:285:VAL:HG22	2.21	0.41
1:A:73:ALA:HB2	1:A:203:SER:HB2	2.03	0.41
1:A:38:HIS:CE1	1:A:40:PHE:HB2	2.57	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	354/401 (88%)	340 (96%)	11 (3%)	3 (1%)	16 43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	ASP
1	A	304	ARG
1	A	382	ASN

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	302/337 (90%)	294 (97%)	8 (3%)	40 72

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	203	SER
1	A	232	GLU
1	A	270	LYS
1	A	277	GLU
1	A	292	ILE
1	A	307	GLU
1	A	383	ILE

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 oligosaccharides 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	$\# Z > 2$
3	C6P	A	502	-	22,22,22	2.98	7 (31%)	28,31,31	1.51	5 (17%)
2	IPA	A	501	-	3,3,3	0.52	0	3,3,3	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C6P	A	502	-	-	6/17/17/17	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	C6P	C4A-C4	-7.97	1.40	1.52
3	A	502	C6P	C2A-C2	-6.84	1.39	1.50
3	A	502	C6P	C5M-C5	-4.76	1.38	1.50
3	A	502	C6P	C4A-N	-4.35	1.34	1.46
3	A	502	C6P	P-OP2	3.69	1.62	1.50
3	A	502	C6P	C6-N1	3.10	1.40	1.34
3	A	502	C6P	P-OP1	2.18	1.62	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	C6P	C4A-N-CA	3.68	120.74	113.84
3	A	502	C6P	C6-C5-C4	2.91	120.26	118.06
3	A	502	C6P	C4A-C4-C3	2.70	123.57	119.98
3	A	502	C6P	OP3-P-OP4	2.17	112.33	106.67
3	A	502	C6P	C5-C6-N1	-2.16	120.31	123.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

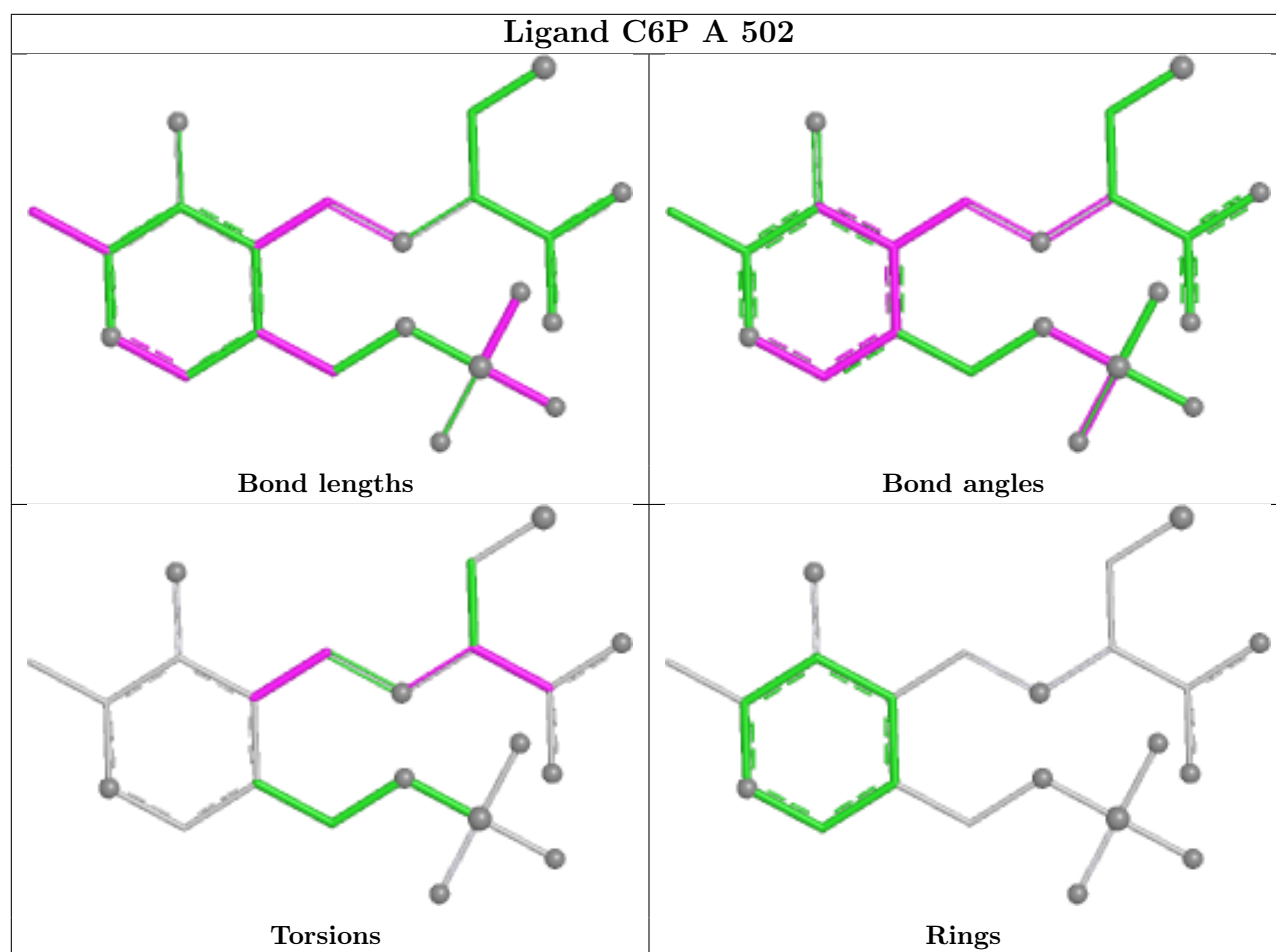
Mol	Chain	Res	Type	Atoms
3	A	502	C6P	C3-C4-C4A-N
3	A	502	C6P	C5-C4-C4A-N
3	A	502	C6P	CB-CA-N-C4A
3	A	502	C6P	C-CA-N-C4A
3	A	502	C6P	O-C-CA-CB
3	A	502	C6P	OXT-C-CA-CB

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	C6P	3	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	358/401 (89%)	1.74	138 (38%) 1 0	35, 81, 133, 207	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	LYS	5.2
1	A	286	MET	5.1
1	A	325	GLY	5.1
1	A	303	VAL	4.4
1	A	351	THR	4.0
1	A	99	THR	4.0
1	A	129	HIS	4.0
1	A	384	SER	4.0
1	A	2	VAL	4.0
1	A	301	VAL	3.9
1	A	225	THR	3.8
1	A	288	VAL	3.7
1	A	4	ARG	3.7
1	A	381	ARG	3.6
1	A	319	ASN	3.6
1	A	383	ILE	3.6
1	A	85	TYR	3.6
1	A	312	LEU	3.5
1	A	126	ILE	3.3
1	A	122	THR	3.3
1	A	304	ARG	3.3
1	A	90	LEU	3.2
1	A	172	GLU	3.2
1	A	182	VAL	3.2
1	A	300	LEU	3.2
1	A	118	GLY	3.2
1	A	130	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	302	SER	3.2
1	A	279	LEU	3.1
1	A	110	THR	3.1
1	A	289	GLY	3.1
1	A	378	VAL	3.0
1	A	39	GLN	3.0
1	A	306	ILE	3.0
1	A	284	ASP	3.0
1	A	285	VAL	3.0
1	A	88	GLU	3.0
1	A	232	GLU	3.0
1	A	278	ALA	3.0
1	A	313	TRP	2.9
1	A	377	ALA	2.9
1	A	354	ARG	2.9
1	A	380	LEU	2.9
1	A	270	LYS	2.8
1	A	291	ARG	2.8
1	A	160	ILE	2.8
1	A	91	LYS	2.8
1	A	323	SER	2.7
1	A	135	GLU	2.7
1	A	271	LEU	2.7
1	A	322	ALA	2.7
1	A	293	HIS	2.7
1	A	128	GLU	2.7
1	A	153	ALA	2.7
1	A	231	GLY	2.7
1	A	165	GLU	2.7
1	A	100	THR	2.7
1	A	139	GLU	2.7
1	A	287	VAL	2.7
1	A	282	ILE	2.6
1	A	117	LEU	2.6
1	A	106	ALA	2.6
1	A	186	GLY	2.6
1	A	169	ILE	2.6
1	A	112	ASN	2.6
1	A	320	ILE	2.6
1	A	280	LEU	2.5
1	A	357	LEU	2.5
1	A	143	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	360	PHE	2.5
1	A	171	LYS	2.5
1	A	221	GLY	2.5
1	A	161	PHE	2.5
1	A	144	LYS	2.5
1	A	175	VAL	2.5
1	A	277	GLU	2.5
1	A	145	THR	2.5
1	A	180	ASP	2.4
1	A	283	PRO	2.4
1	A	290	ASP	2.4
1	A	138	ARG	2.4
1	A	36	SER	2.4
1	A	113	PHE	2.4
1	A	92	LYS	2.3
1	A	125	PRO	2.3
1	A	5	ILE	2.3
1	A	292	ILE	2.3
1	A	14	ARG	2.3
1	A	98	VAL	2.3
1	A	227	LEU	2.3
1	A	199	PHE	2.3
1	A	324	THR	2.3
1	A	218	ILE	2.2
1	A	80	VAL	2.2
1	A	148	VAL	2.2
1	A	215	GLY	2.2
1	A	311	MET	2.2
1	A	223	GLY	2.2
1	A	355	LEU	2.2
1	A	375	GLN	2.2
1	A	119	VAL	2.2
1	A	374	SER	2.2
1	A	140	ALA	2.2
1	A	141	ILE	2.2
1	A	163	ILE	2.2
1	A	219	ARG	2.2
1	A	379	ARG	2.2
1	A	162	PRO	2.2
1	A	18	LYS	2.2
1	A	147	LEU	2.2
1	A	176	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	321	ALA	2.2
1	A	317	ARG	2.1
1	A	84	VAL	2.1
1	A	296	PRO	2.1
1	A	82	LYS	2.1
1	A	194	LYS	2.1
1	A	362	THR	2.1
1	A	6	TYR	2.1
1	A	89	CYS	2.1
1	A	28	ARG	2.1
1	A	307	GLU	2.1
1	A	376	ALA	2.1
1	A	203	SER	2.1
1	A	189	PRO	2.1
1	A	316	ASN	2.1
1	A	202	PHE	2.1
1	A	294	ARG	2.1
1	A	132	ILE	2.1
1	A	174	GLY	2.1
1	A	142	THR	2.1
1	A	64	ILE	2.1
1	A	116	SER	2.0
1	A	124	LEU	2.0
1	A	193	LEU	2.0
1	A	121	VAL	2.0
1	A	382	ASN	2.0
1	A	367	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

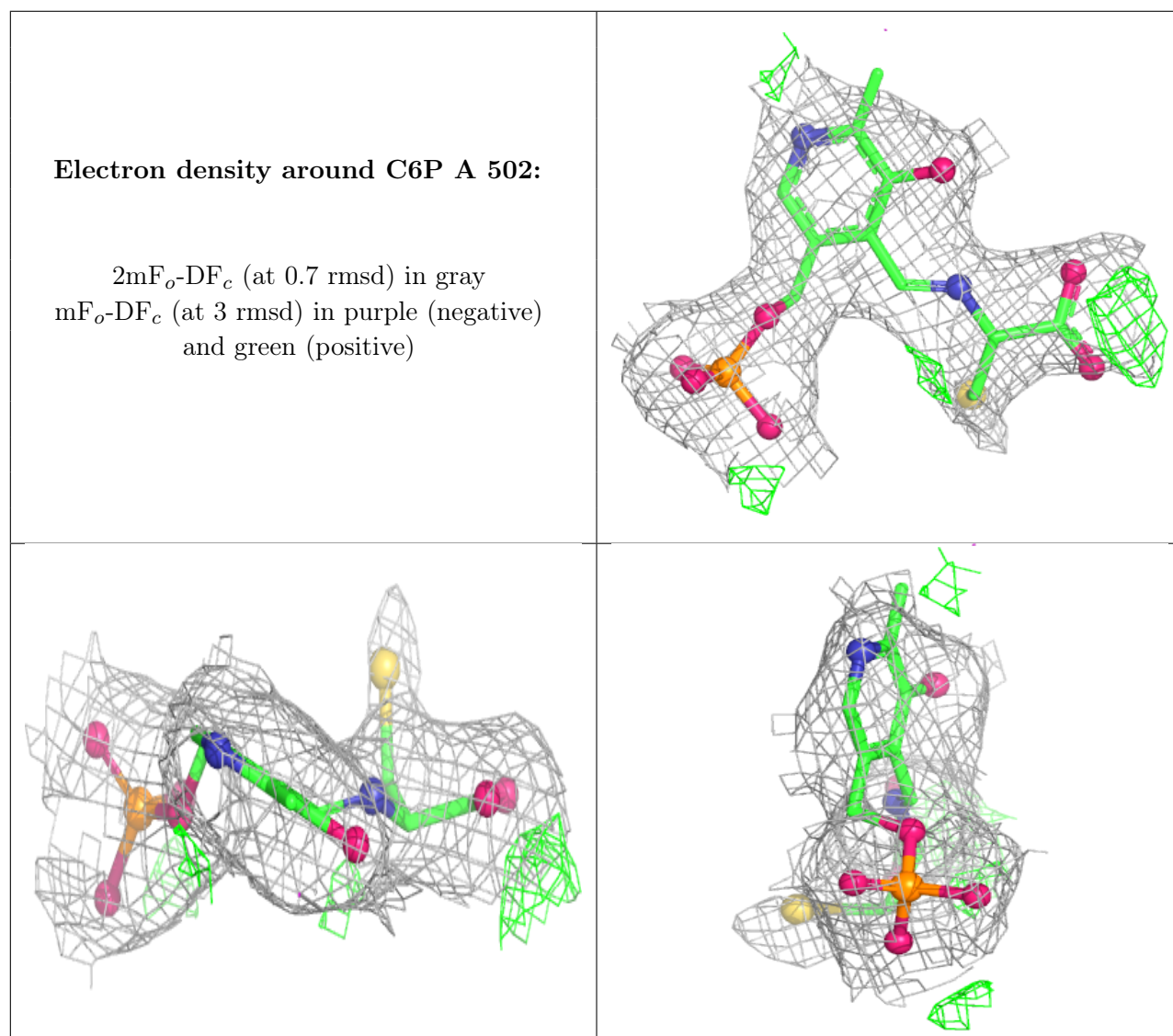
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	IPA	A	501	4/4	0.68	0.38	56,60,63,68	0
3	C6P	A	502	22/22	0.91	0.15	24,69,83,89	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.