



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 10:05 AM EDT

PDB ID : 2R5C  
Title : Aedes Kynurenine Aminotransferase in Complex with Cysteine  
Authors : Han, Q.; Gao, Y.G.; Robinson, H.; Li, J.  
Deposited on : 2007-09-03  
Resolution : 1.96 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

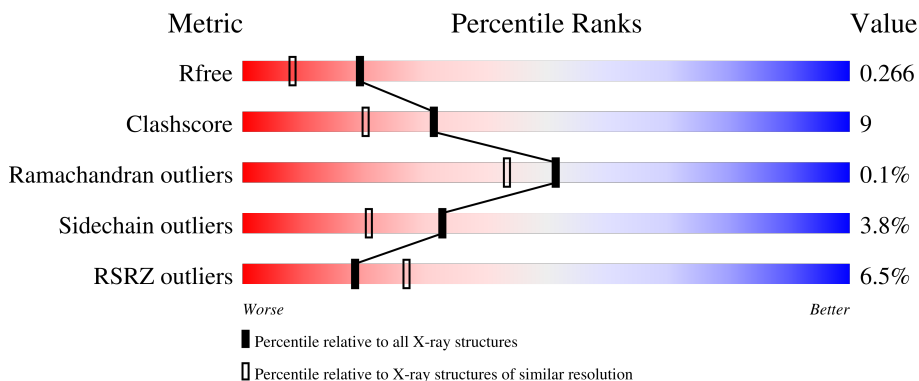
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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  $\geq 3$ , 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	429	
2	B	429	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7151 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.

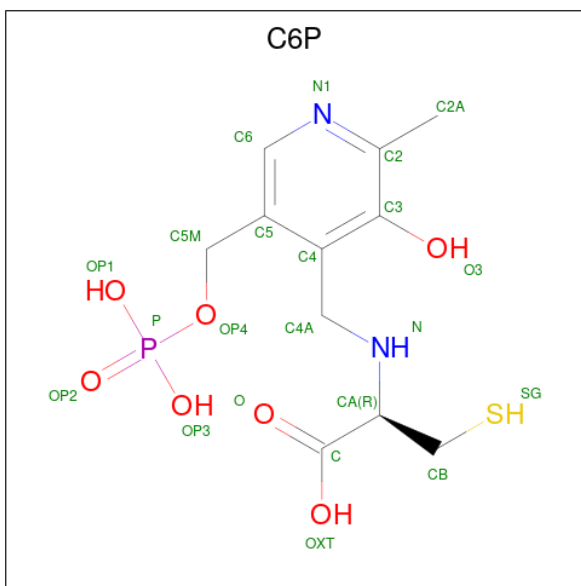
- Molecule 1 is a protein called Kynurenine aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	419	3338	2145	552	620	1	20	0	0	0

- Molecule 2 is a protein called Kynurenine aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	419	3323	2137	551	615	20	0	0	0

- Molecule 3 is N-({3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4-YL}METHYL)-L-CYSTEINE (three-letter code: C6P) (formula: C<sub>11</sub>H<sub>17</sub>N<sub>2</sub>O<sub>7</sub>PS).

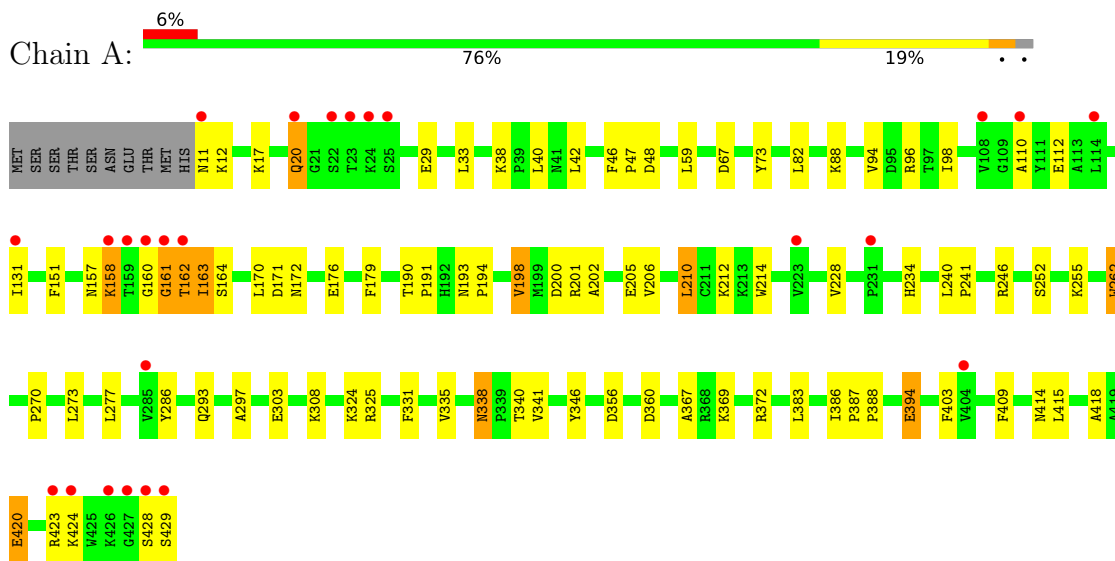


<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	252	Total 252	O 252	0	0
4	B	216	Total 216	O 216	0	0

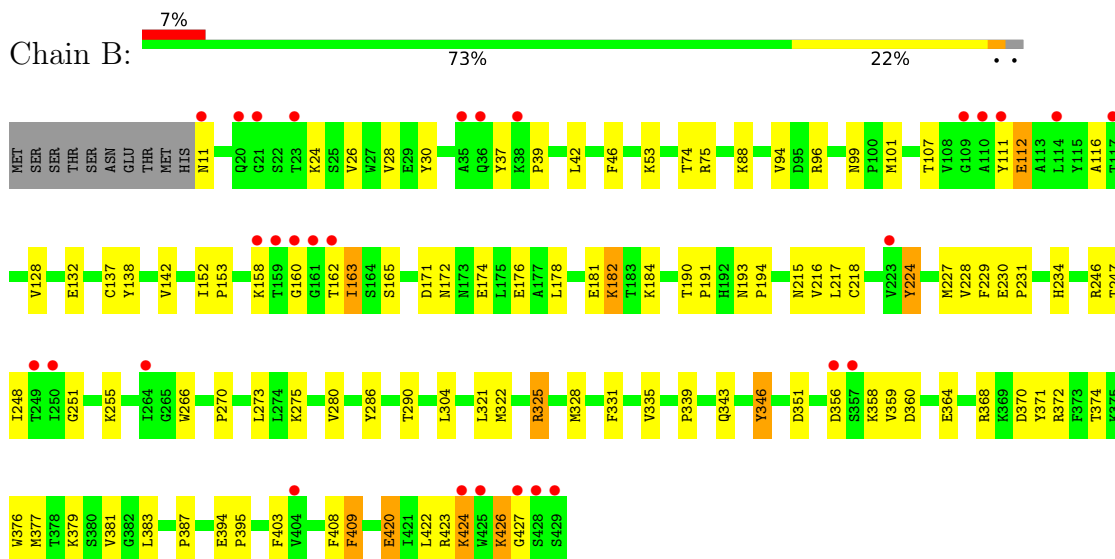
### 3 Residue-property plots i

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: Kynurenine aminotransferase



- Molecule 2: Kynurenine aminotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.05Å 95.68Å 166.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.67 – 1.96 28.66 – 1.96	Depositor EDS
% Data completeness (in resolution range)	91.5 (28.67-1.96) 91.4 (28.66-1.96)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.37 (at 1.96Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.220 , 0.267 0.219 , 0.266	Depositor DCC
$R_{free}$ test set	3057 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.6	Xtrriage
Anisotropy	0.040	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7151	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, LLP

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	1.16	9/3401 (0.3%)	0.92	7/4615 (0.2%)
2	B	1.23	8/3411 (0.2%)	0.93	4/4629 (0.1%)
All	All	1.20	17/6812 (0.2%)	0.93	11/9244 (0.1%)

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	3
2	B	0	1
All	All	0	4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	TYR	CD2-CE2	5.99	1.48	1.39
1	A	367	ALA	CA-CB	5.82	1.64	1.52
2	B	224	TYR	CE2-CZ	5.82	1.46	1.38
1	A	403	PHE	CD1-CE1	5.82	1.50	1.39
1	A	262	TRP	CE3-CZ3	5.77	1.48	1.38
1	A	151	PHE	CE2-CZ	5.54	1.47	1.37
1	A	420	GLU	CD-OE2	5.52	1.31	1.25
2	B	46	PHE	CE2-CZ	5.47	1.47	1.37
2	B	53	LYS	CE-NZ	5.46	1.62	1.49
2	B	248	ILE	C-O	5.45	1.33	1.23
1	A	394	GLU	CG-CD	5.44	1.60	1.51
1	A	308	LYS	CE-NZ	5.40	1.62	1.49
1	A	38	LYS	CE-NZ	5.34	1.62	1.49
2	B	286	TYR	CD1-CE1	5.33	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	128	VAL	CB-CG2	5.05	1.63	1.52
2	B	137	CYS	CB-SG	-5.03	1.73	1.81
2	B	424	LYS	CD-CE	5.00	1.63	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	255	LYS	CD-CE-NZ	-5.75	98.46	111.70
1	A	171	ASP	CB-CG-OD1	5.67	123.41	118.30
2	B	75	ARG	NE-CZ-NH1	-5.39	117.61	120.30
1	A	67	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	33	LEU	CB-CG-CD1	-5.23	102.11	111.00
1	A	48	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	356	ASP	CB-CG-OD2	5.20	122.98	118.30
2	B	370	ASP	CB-CG-OD2	-5.18	113.64	118.30
2	B	325	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	A	200	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	360	ASP	CB-CG-OD2	5.05	122.85	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	GLY	Peptide
1	A	161	GLY	Peptide
1	A	162	THR	Peptide
2	B	160	GLY	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	3338	0	3282	57	0
2	B	3323	0	3278	63	0
3	B	22	0	14	0	0
4	A	252	0	0	5	0
4	B	216	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7151	0	6574	119	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 9.

All (119) 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:157:ASN:OD1	1:A:158:LYS:HE3	1.40	1.18
1:A:162:THR:O	1:A:162:THR:HG22	1.54	1.03
1:A:162:THR:H	1:A:163:ILE:HG22	1.35	0.89
2:B:374:THR:HG21	2:B:387:PRO:HD3	1.57	0.86
2:B:88:LYS:HD3	2:B:304:LEU:HD13	1.60	0.84
1:A:161:GLY:O	1:A:338:ASN:HB3	1.78	0.82
1:A:157:ASN:OD1	1:A:158:LYS:CE	2.28	0.81
1:A:201:ARG:NH2	1:A:240:LEU:HD21	1.97	0.80
1:A:172:ASN:O	1:A:176:GLU:HG3	1.88	0.73
1:A:428:SER:O	1:A:429:SER:HB2	1.89	0.73
2:B:358:LYS:HE2	2:B:426:LYS:HG2	1.69	0.73
1:A:162:THR:O	1:A:162:THR:CG2	2.30	0.72
1:A:163:ILE:HG12	1:A:164:SER:N	2.03	0.72
2:B:215:ASN:HA	2:B:246:ARG:NH2	2.05	0.71
2:B:94:VAL:HG23	2:B:96:ARG:HG2	1.74	0.69
2:B:359:VAL:HG23	2:B:376:TRP:CZ3	2.26	0.69
1:A:201:ARG:HH21	1:A:240:LEU:HD21	1.57	0.69
1:A:162:THR:N	1:A:163:ILE:HG22	2.07	0.69
1:A:12:LYS:O	2:B:184:LYS:HE3	1.94	0.68
2:B:165:SER:OG	2:B:343:GLN:HG3	1.95	0.66
2:B:24:LYS:HB2	2:B:28:VAL:CG1	2.27	0.65
2:B:11:ASN:N	4:B:581:HOH:O	2.31	0.63
1:A:94:VAL:HG23	1:A:96:ARG:HG2	1.82	0.62
1:A:162:THR:HG21	4:A:489:HOH:O	2.00	0.61
1:A:228:VAL:HG21	1:A:234:HIS:HB2	1.83	0.61
2:B:152:ILE:HD12	2:B:174:GLU:HG2	1.84	0.58
2:B:377:MET:HG3	4:B:554:HOH:O	2.02	0.58
2:B:420:GLU:HB2	2:B:423:ARG:HH12	1.68	0.57
2:B:359:VAL:HG23	2:B:376:TRP:CE3	2.40	0.57
2:B:24:LYS:HB2	2:B:28:VAL:HG11	1.85	0.57
2:B:42:LEU:HD22	2:B:383:LEU:HD11	1.87	0.57
2:B:325:ARG:HB2	2:B:408:PHE:CE1	2.40	0.56
2:B:162:THR:CG2	2:B:163:ILE:N	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:GLU:HB3	2:B:395:PRO:HD3	1.88	0.56
2:B:107:THR:HB	2:B:112:GLU:HB3	1.88	0.55
1:A:29:GLU:HB3	4:A:555:HOH:O	2.06	0.55
1:A:212:LYS:HE2	1:A:241:PRO:O	2.07	0.55
2:B:162:THR:HG22	2:B:163:ILE:N	2.21	0.55
1:A:210:LEU:HD22	4:A:476:HOH:O	2.07	0.55
1:A:420:GLU:HA	1:A:423:ARG:HB2	1.88	0.55
2:B:162:THR:HG23	2:B:339:PRO:O	2.06	0.55
1:A:161:GLY:O	1:A:338:ASN:CB	2.53	0.55
2:B:216:VAL:HG12	2:B:217:LEU:N	2.22	0.54
1:A:82:LEU:HD22	1:A:293:GLN:HB3	1.90	0.53
1:A:46:PHE:HB2	1:A:47:PRO:HD2	1.90	0.53
2:B:420:GLU:HA	2:B:423:ARG:NH1	2.24	0.53
2:B:346:TYR:HA	2:B:408:PHE:CZ	2.44	0.52
1:A:335:VAL:O	1:A:335:VAL:HG22	2.10	0.51
2:B:24:LYS:HB2	2:B:28:VAL:HG13	1.93	0.51
2:B:356:ASP:HA	2:B:359:VAL:HG12	1.91	0.51
1:A:324:LYS:HB3	1:A:415:LEU:HD11	1.92	0.51
2:B:224:TYR:HD1	2:B:227:MET:CE	2.23	0.50
2:B:216:VAL:CG1	2:B:217:LEU:N	2.75	0.50
2:B:172:ASN:O	2:B:176:GLU:HG3	2.12	0.50
1:A:42:LEU:HD22	1:A:383:LEU:HD11	1.94	0.49
2:B:181:GLU:CD	2:B:181:GLU:H	2.16	0.49
2:B:224:TYR:HD1	2:B:227:MET:HE3	1.76	0.49
2:B:364:GLU:HB2	2:B:372:ARG:HG2	1.95	0.49
1:A:20:GLN:HB3	4:A:630:HOH:O	2.13	0.48
1:A:325:ARG:HD3	1:A:341:VAL:HG13	1.93	0.48
1:A:40:LEU:HD21	1:A:414:ASN:O	2.13	0.48
2:B:218:CYS:O	2:B:247:THR:HA	2.13	0.48
1:A:303:GLU:HA	1:A:303:GLU:OE1	2.14	0.48
1:A:82:LEU:HA	1:A:297:ALA:HB2	1.94	0.47
2:B:321:LEU:HD11	2:B:409:PHE:CE1	2.49	0.47
1:A:190:THR:HA	1:A:191:PRO:C	2.34	0.47
2:B:328:MET:HA	2:B:331:PHE:CE2	2.50	0.46
1:A:161:GLY:C	1:A:338:ASN:HB3	2.34	0.46
1:A:40:LEU:CD2	1:A:418:ALA:HB2	2.46	0.46
1:A:163:ILE:HD11	1:A:340:THR:OG1	2.15	0.46
2:B:424:LYS:O	2:B:427:GLY:N	2.47	0.46
2:B:230:GLU:OE2	2:B:231:PRO:HA	2.16	0.45
1:A:387:PRO:HA	1:A:388:PRO:HD3	1.75	0.45
2:B:358:LYS:HE2	2:B:426:LYS:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ILE:HG23	1:A:170:LEU:HD21	1.99	0.45
1:A:158:LYS:HB3	1:A:158:LYS:HE2	1.32	0.45
1:A:157:ASN:C	1:A:158:LYS:HE3	2.37	0.45
2:B:368:ARG:O	2:B:371:TYR:HB2	2.16	0.45
2:B:132:GLU:HB2	2:B:153:PRO:HA	1.99	0.45
2:B:182:LYS:HE2	2:B:182:LYS:HB2	1.70	0.45
2:B:26:VAL:HG22	2:B:30:TYR:CD2	2.52	0.44
1:A:193:ASN:HA	1:A:194:PRO:HA	1.61	0.44
2:B:99:ASN:OD1	2:B:101:MET:HB2	2.17	0.44
2:B:37:TYR:CE2	2:B:379:LYS:HG2	2.52	0.44
2:B:171:ASP:HB3	2:B:174:GLU:HB3	2.00	0.44
1:A:270:PRO:HG2	1:A:273:LEU:HD12	2.01	0.43
2:B:30:TYR:CE1	2:B:374:THR:HG23	2.54	0.43
1:A:110:ALA:HB2	1:A:252:SER:HB2	2.01	0.43
2:B:228:VAL:HG21	2:B:234:HIS:HB2	2.00	0.43
1:A:202:ALA:O	1:A:206:VAL:HG23	2.18	0.43
2:B:190:THR:HA	2:B:191:PRO:C	2.38	0.42
2:B:193:ASN:OD1	2:B:194:PRO:HA	2.19	0.42
1:A:198:VAL:O	1:A:198:VAL:CG2	2.68	0.42
1:A:201:ARG:HG2	1:A:205:GLU:OE1	2.19	0.42
2:B:215:ASN:OD1	2:B:246:ARG:NH2	2.49	0.42
1:A:179:PHE:HB3	1:A:214:TRP:CD1	2.55	0.42
1:A:386:ILE:HD13	1:A:386:ILE:HA	1.91	0.42
2:B:251:GLY:HA3	2:B:266:TRP:NE1	2.35	0.42
1:A:94:VAL:HG21	1:A:98:ILE:HD11	2.02	0.41
2:B:138:TYR:O	2:B:142:VAL:HG23	2.20	0.41
2:B:335:VAL:HG21	2:B:422:LEU:HB3	2.02	0.41
2:B:351:ASP:HB2	2:B:403:PHE:CE2	2.55	0.41
2:B:270:PRO:HD2	2:B:273:LEU:HD12	2.01	0.41
2:B:321:LEU:HD11	2:B:409:PHE:CD1	2.56	0.41
2:B:229:PHE:HB3	2:B:322:MET:HE2	2.02	0.41
1:A:82:LEU:HD22	1:A:293:GLN:CB	2.50	0.41
1:A:201:ARG:NH2	1:A:240:LEU:CD2	2.75	0.41
1:A:369:LYS:HG2	1:A:372:ARG:NH1	2.36	0.41
2:B:74:THR:HB	2:B:290:THR:HG23	2.03	0.41
2:B:116:ALA:HA	2:B:280:VAL:HG11	2.03	0.41
1:A:157:ASN:O	1:A:158:LYS:HE2	2.21	0.40
1:A:82:LEU:CD2	1:A:293:GLN:HB3	2.50	0.40
2:B:37:TYR:CZ	2:B:379:LYS:HG2	2.56	0.40
1:A:59:LEU:HD22	1:A:262:TRP:CZ2	2.56	0.40
1:A:277:LEU:N	1:A:277:LEU:HD12	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LEU:HD23	1:A:293:GLN:OE1	2.22	0.40
2:B:174:GLU:O	2:B:178:LEU:HD13	2.21	0.40
2:B:359:VAL:HG22	2:B:360:ASP:N	2.36	0.40
1:A:394:GLU:HB2	4:A:671:HOH: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	416/429 (97%)	401 (96%)	14 (3%)	1 (0%)	47 38
2	B	417/429 (97%)	409 (98%)	8 (2%)	0	100 100
All	All	833/858 (97%)	810 (97%)	22 (3%)	1 (0%)	51 43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	TYR

### 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	356/366 (97%)	341 (96%)	15 (4%)	30 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	357/367 (97%)	345 (97%)	12 (3%)	37	25
All	All	713/733 (97%)	686 (96%)	27 (4%)	33	21

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	17	LYS
1	A	20	GLN
1	A	88	LYS
1	A	112	GLU
1	A	158	LYS
1	A	163	ILE
1	A	198	VAL
1	A	210	LEU
1	A	246	ARG
1	A	331	PHE
1	A	338	ASN
1	A	346	TYR
1	A	409	PHE
1	A	424	LYS
2	B	39	PRO
2	B	111	TYR
2	B	112	GLU
2	B	158	LYS
2	B	163	ILE
2	B	182	LYS
2	B	275	LYS
2	B	346	TYR
2	B	381	VAL
2	B	409	PHE
2	B	420	GLU
2	B	426	LYS

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

Mol	Chain	Res	Type
2	B	50	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](#)

1 non-standard protein/DNA/RNA residue is 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
1	LLP	A	255	1	23,24,25	2.17	9 (39%)	25,32,34	1.77	6 (24%)

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
1	LLP	A	255	1	-	6/16/17/19	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	LLP	O3-C3	-5.33	1.24	1.37
1	A	255	LLP	C2-N1	3.60	1.40	1.33
1	A	255	LLP	C4-C4'	3.40	1.53	1.46
1	A	255	LLP	CD-CE	2.99	1.61	1.51
1	A	255	LLP	C4'-NZ	2.79	1.36	1.27
1	A	255	LLP	CE-NZ	2.59	1.52	1.46
1	A	255	LLP	C4-C5	-2.55	1.38	1.42
1	A	255	LLP	P-OP3	-2.34	1.45	1.54
1	A	255	LLP	C6-C5	2.26	1.42	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	LLP	OP4-C5'-C5	3.81	116.61	109.35
1	A	255	LLP	C4-C4'-NZ	-3.59	107.84	124.31
1	A	255	LLP	OP2-P-OP4	-3.00	98.76	106.73
1	A	255	LLP	CE-NZ-C4'	-2.82	110.25	118.90
1	A	255	LLP	C5-C6-N1	-2.32	119.95	123.82
1	A	255	LLP	OP3-P-OP1	2.12	118.97	110.68

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	255	LLP	C4-C4'-NZ-CE
1	A	255	LLP	O-C-CA-CB
1	A	255	LLP	C3-C4-C4'-NZ
1	A	255	LLP	CG-CD-CE-NZ
1	A	255	LLP	CD-CE-NZ-C4'
1	A	255	LLP	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	B	430	-	22,22,22	3.97	9 (40%)	28,31,31	2.15	5 (17%)

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	B	430	-	-	13/17/17/17	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	430	C6P	C3-C2	9.72	1.50	1.40
3	B	430	C6P	C3-C4	7.96	1.52	1.40
3	B	430	C6P	C5-C4	7.92	1.51	1.40
3	B	430	C6P	C6-C5	6.67	1.51	1.37
3	B	430	C6P	C2-N1	4.96	1.43	1.33
3	B	430	C6P	C6-N1	4.42	1.43	1.34
3	B	430	C6P	OXT-C	-3.79	1.18	1.30
3	B	430	C6P	P-OP1	-2.49	1.45	1.54
3	B	430	C6P	P-OP3	-2.33	1.45	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	430	C6P	C4A-N-CA	7.25	127.65	113.92
3	B	430	C6P	C6-C5-C4	4.92	121.60	118.12
3	B	430	C6P	C5-C6-N1	-3.71	117.63	123.82
3	B	430	C6P	C4A-C4-C3	2.91	123.16	120.04
3	B	430	C6P	C6-N1-C2	2.74	124.25	119.17

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	430	C6P	C5M-OP4-P-OP1
3	B	430	C6P	C5M-OP4-P-OP2
3	B	430	C6P	N-CA-CB-SG
3	B	430	C6P	C-CA-CB-SG
3	B	430	C6P	C5-C4-C4A-N
3	B	430	C6P	C-CA-N-C4A
3	B	430	C6P	O-C-CA-N
3	B	430	C6P	C3-C4-C4A-N
3	B	430	C6P	CB-CA-N-C4A

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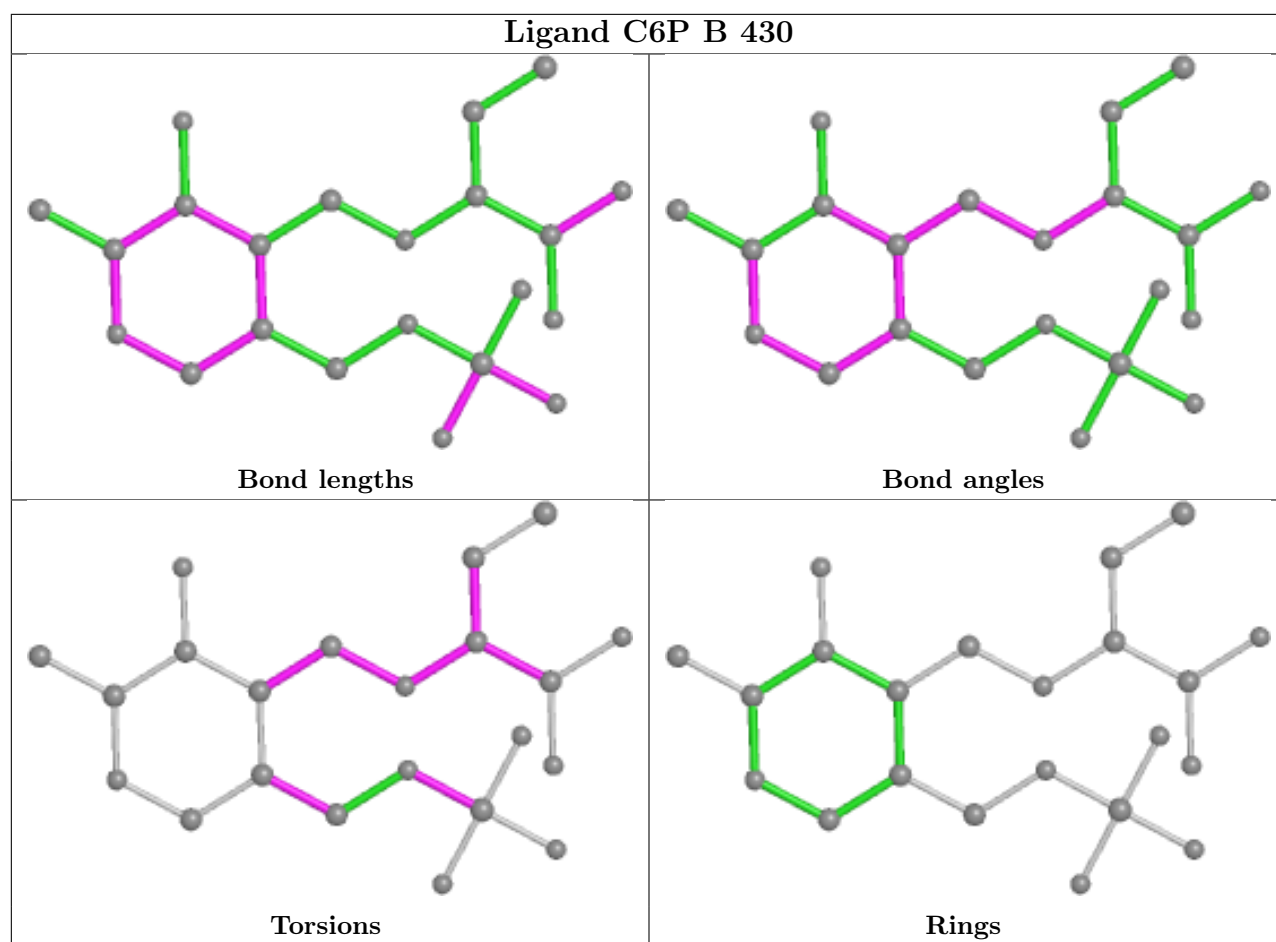
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Mol	Chain	Res	Type	Atoms
3	B	430	C6P	C4-C4A-N-CA
3	B	430	C6P	C5M-OP4-P-OP3
3	B	430	C6P	OXT-C-CA-N
3	B	430	C6P	C4-C5-C5M-OP4

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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	418/429 (97%)	0.21	25 (5%) 21 30	22, 37, 68, 126	0
2	B	419/429 (97%)	0.32	29 (6%) 16 25	23, 41, 74, 140	0
All	All	837/858 (97%)	0.26	54 (6%) 18 27	22, 39, 72, 140	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	428	SER	6.8
1	A	427	GLY	6.2
2	B	429	SER	6.0
2	B	162	THR	4.9
1	A	23	THR	4.7
2	B	159	THR	4.5
2	B	357	SER	4.5
1	A	429	SER	4.4
2	B	110	ALA	4.3
2	B	23	THR	4.1
1	A	161	GLY	4.0
2	B	11	ASN	4.0
1	A	158	LYS	3.9
1	A	159	THR	3.8
1	A	160	GLY	3.8
1	A	404	VAL	3.7
2	B	161	GLY	3.6
2	B	160	GLY	3.6
1	A	428	SER	3.5
1	A	11	ASN	3.5
2	B	20	GLN	3.4
2	B	264	ILE	3.4
1	A	223	VAL	3.2
2	B	158	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	22	SER	3.1
1	A	20	GLN	3.0
1	A	285	VAL	2.9
1	A	162	THR	2.8
1	A	110	ALA	2.8
2	B	356	ASP	2.8
2	B	427	GLY	2.7
1	A	24	LYS	2.7
1	A	25	SER	2.7
2	B	223	VAL	2.6
1	A	114	LEU	2.5
2	B	250	ILE	2.4
1	A	231	PRO	2.4
2	B	117	THR	2.2
1	A	423	ARG	2.2
2	B	425	TRP	2.2
2	B	21	GLY	2.2
2	B	249	THR	2.2
2	B	404	VAL	2.2
2	B	114	LEU	2.2
2	B	35	ALA	2.2
2	B	36	GLN	2.2
2	B	424	LYS	2.1
1	A	108	VAL	2.1
1	A	131	ILE	2.1
2	B	38	LYS	2.1
1	A	424	LYS	2.1
1	A	426	LYS	2.1
2	B	111	TYR	2.0
2	B	109	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	LLP	A	255	24/25	0.98	0.17	18,27,43,49	0

### 6.3 Carbohydrates [i](#)

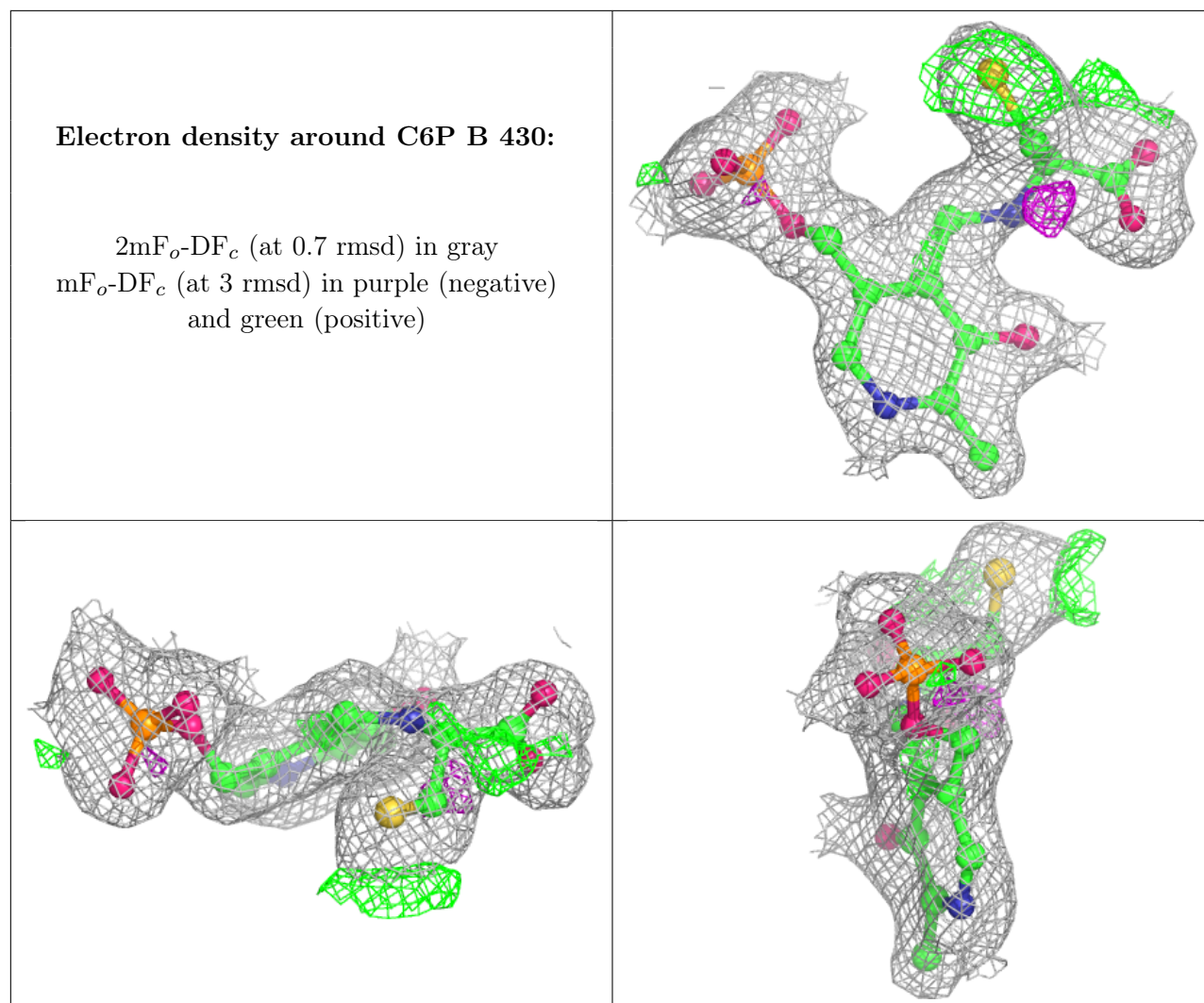
There are no monosaccharides in this entry.

### 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	C6P	B	430	22/22	0.95	0.17	19,30,51,60	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.