



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:22 pm BST

PDB ID : 2R5E  
Title : Aedes kynurenine aminotransferase in complex with glutamine  
Authors : Han, Q.; Gao, Y.G.; Robinson, H.; Li, J.  
Deposited on : 2007-09-03  
Resolution : 1.84 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.

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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 : 2.11  
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) : 2.11

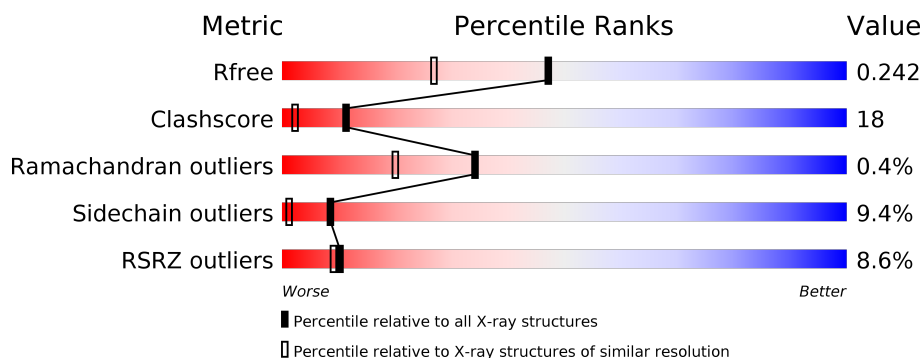
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.84 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 on 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	<div> <div>14%</div> <div> <div></div> <div>66%</div> <div>25%</div> <div>6% ..</div> </div> </div>
1	B	429	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>..</div> </div> </div>

## 2 Entry composition [i](#)

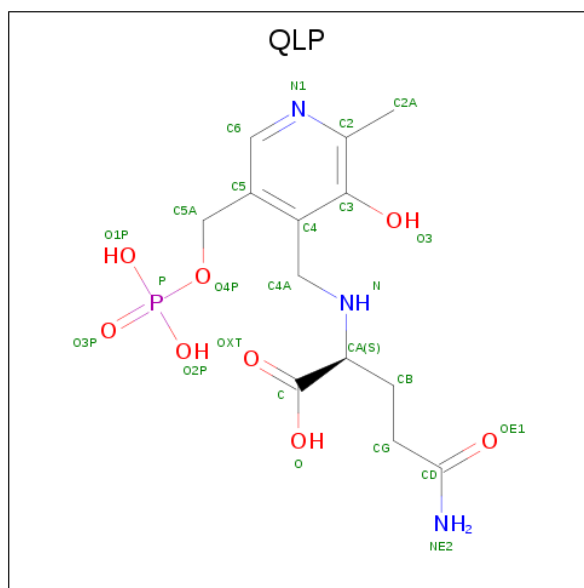
There are 3 unique types of molecules in this entry. The entry contains 7280 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	419	Total	C	N	O	S	0	0	0
			3323	2137	551	615	20			
1	B	419	Total	C	N	O	S	0	0	0
			3323	2137	551	615	20			

- Molecule 2 is N 2 -({3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4-YL}METHYL)-L-GLUTAMINE (three-letter code: QLP) (formula: C<sub>13</sub>H<sub>20</sub>N<sub>3</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	13	3	8	1		
2	B	1	Total	C	N	O	P	0	0
			25	13	3	8	1		

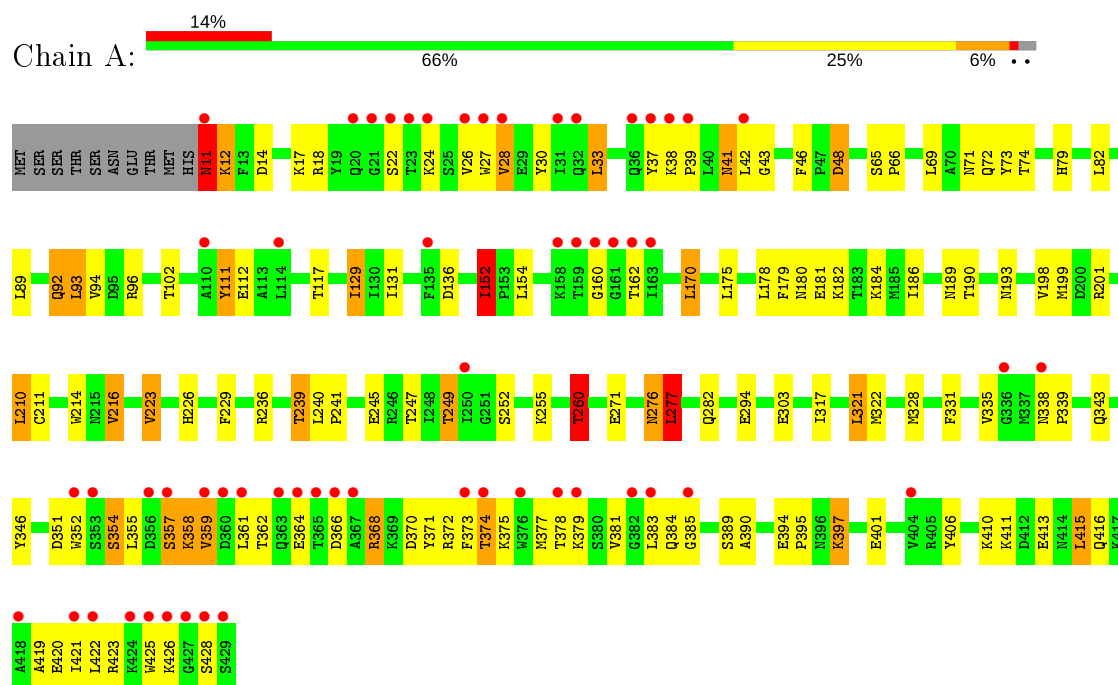
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	291	Total 291	O 291	0	0
3	B	293	Total 293	O 293	0	0

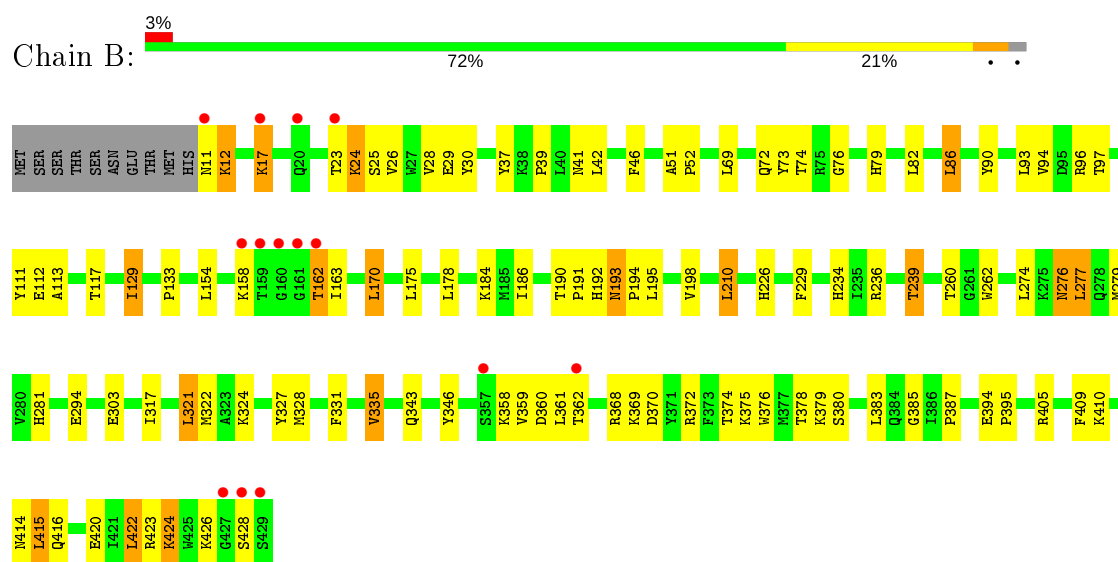
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 1: Kynurenine aminotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.37Å 95.59Å 165.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 1.84 29.74 – 1.84	Depositor EDS
% Data completeness (in resolution range)	90.2 (29.75-1.84) 90.2 (29.74-1.84)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.201 , 0.243 0.200 , 0.242	Depositor DCC
$R_{free}$ test set	3546 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7280	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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

### 5.1 Standard geometry

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

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	0.77	1/3411 (0.0%)	0.82	4/4629 (0.1%)
1	B	0.80	0/3411	0.81	3/4629 (0.1%)
All	All	0.79	1/6822 (0.0%)	0.82	7/9258 (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	1
1	B	1	0
All	All	1	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	TYR	CD2-CE2	-5.00	1.31	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	LEU	CA-CB-CG	5.81	128.67	115.30
1	A	48	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	B	277	LEU	CB-CG-CD2	5.36	120.11	111.00
1	B	86	LEU	CA-CB-CG	5.35	127.61	115.30
1	B	210	LEU	CA-CB-CG	5.33	127.55	115.30
1	A	260	THR	CA-CB-CG2	5.25	119.76	112.40
1	A	152	ILE	CB-CA-C	-5.22	101.16	111.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	260	THR	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ASN	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	3323	0	3278	158	0
1	B	3323	0	3278	96	0
2	A	25	0	16	1	0
2	B	25	0	16	1	0
3	A	291	0	0	51	0
3	B	293	0	0	19	0
All	All	7280	0	6588	237	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 18.

All (237) 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:41:ASN:HA	3:A:705:HOH:O	1.48	1.09
1:A:423:ARG:HG2	1:A:428:SER:HB2	1.37	1.05
1:A:72:GLN:OE1	1:B:260:THR:HG22	1.59	1.02
1:A:373:PHE:HA	3:A:696:HOH:O	1.58	1.00
1:A:92:GLN:HG2	3:A:647:HOH:O	1.61	0.99
1:B:322:MET:HE3	3:B:917:HOH:O	1.64	0.97
1:A:379:LYS:HG3	3:A:698:HOH:O	1.64	0.96
1:A:421:ILE:HG21	3:A:710:HOH:O	1.66	0.95
1:A:385:GLY:HA3	3:A:708:HOH:O	1.66	0.94
1:A:364:GLU:HG2	3:A:660:HOH:O	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:THR:OG1	1:A:384:GLN:HB2	1.71	0.89
1:A:201:ARG:HD2	3:A:715:HOH:O	1.72	0.89
1:A:39:PRO:HA	3:A:668:HOH:O	1.72	0.86
1:A:129:ILE:CD1	1:A:152:ILE:HD11	2.05	0.85
1:B:229:PHE:HB3	1:B:322:MET:HE1	1.57	0.85
1:A:420:GLU:HA	3:A:716:HOH:O	1.76	0.83
1:B:112:GLU:OE2	1:B:281:HIS:HD2	1.62	0.83
1:A:359:VAL:HA	3:A:648:HOH:O	1.78	0.83
1:A:22:SER:HB3	3:A:649:HOH:O	1.78	0.82
1:A:71:ASN:HD22	1:B:262:TRP:HE1	1.24	0.82
1:A:371:TYR:O	1:A:375:LYS:HG3	1.81	0.81
3:A:649:HOH:O	1:B:279:MET:SD	2.37	0.80
1:A:73:TYR:H	1:B:260:THR:HG23	1.45	0.79
1:B:322:MET:CE	3:B:917:HOH:O	2.25	0.79
1:A:223:VAL:HG13	1:A:255:LYS:HG3	1.66	0.78
1:A:249:THR:HG23	3:A:494:HOH:O	1.83	0.78
1:A:423:ARG:CG	1:A:428:SER:HB2	2.14	0.78
1:B:113:ALA:O	1:B:117:THR:HG23	1.85	0.77
1:A:362:THR:HB	3:A:699:HOH:O	1.84	0.77
1:A:152:ILE:HG12	1:A:178:LEU:CD2	2.15	0.76
1:A:152:ILE:HG12	1:A:178:LEU:HD22	1.67	0.75
1:A:383:LEU:HB2	3:A:710:HOH:O	1.85	0.75
1:A:357:SER:HB2	1:A:358:LYS:HD3	1.66	0.75
1:A:260:THR:CG2	1:B:73:TYR:H	2.00	0.75
1:A:73:TYR:N	1:B:260:THR:HG23	2.02	0.75
1:B:424:LYS:O	1:B:428:SER:HB2	1.88	0.73
1:A:79:HIS:HE1	1:A:294:GLU:OE1	1.72	0.73
1:A:129:ILE:HD13	1:A:152:ILE:HD11	1.69	0.73
1:A:236:ARG:O	1:A:239:THR:HG22	1.89	0.72
1:A:11:ASN:HD22	1:A:11:ASN:N	1.86	0.72
1:A:385:GLY:CA	3:A:708:HOH:O	2.30	0.72
1:B:79:HIS:HE1	1:B:294:GLU:OE2	1.73	0.71
1:B:226:HIS:HD2	3:B:856:HOH:O	1.73	0.71
1:A:30:TYR:HE1	1:A:374:THR:HG1	1.36	0.71
1:A:42:LEU:HD22	1:A:383:LEU:HD11	1.72	0.70
1:A:370:ASP:O	1:A:374:THR:HG22	1.92	0.70
1:A:30:TYR:HE1	1:A:374:THR:OG1	1.74	0.70
1:B:158:LYS:HE3	1:B:163:ILE:HG22	1.74	0.70
1:A:30:TYR:OH	1:A:374:THR:CG2	2.39	0.69
3:A:649:HOH:O	1:B:279:MET:HB3	1.91	0.69
1:A:30:TYR:OH	1:A:374:THR:HG21	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:GLU:OE2	1:B:423:ARG:NH2	2.25	0.68
1:B:335:VAL:HG21	1:B:422:LEU:HB3	1.73	0.68
1:A:423:ARG:HB2	3:A:716:HOH:O	1.94	0.68
1:A:102:THR:HB	1:A:271:GLU:HG3	1.76	0.67
1:A:385:GLY:N	3:A:721:HOH:O	2.28	0.67
1:A:18:ARG:HG3	3:B:881:HOH:O	1.93	0.67
1:B:117:THR:HA	1:B:277:LEU:HD22	1.76	0.67
1:A:71:ASN:ND2	1:B:262:TRP:HE1	1.94	0.66
1:A:368:ARG:HD3	1:A:397:LYS:HD3	1.78	0.66
1:B:193:ASN:HD21	1:B:405:ARG:HH11	1.43	0.65
1:B:360:ASP:OD1	1:B:362:THR:HB	1.96	0.65
1:B:229:PHE:HB3	1:B:322:MET:CE	2.24	0.65
1:A:249:THR:CG2	3:A:494:HOH:O	2.44	0.65
1:A:410:LYS:HB2	1:A:415:LEU:HD13	1.78	0.65
1:A:239:THR:HG23	3:A:589:HOH:O	1.95	0.65
1:A:361:LEU:HA	3:A:660:HOH:O	1.96	0.65
1:B:193:ASN:HD22	1:B:194:PRO:HA	1.61	0.64
1:A:162:THR:HG22	1:A:339:PRO:HG2	1.79	0.64
1:B:359:VAL:HG12	1:B:376:TRP:CZ3	2.33	0.64
1:B:117:THR:HG22	1:B:277:LEU:HD11	1.80	0.64
1:B:239:THR:HG23	3:B:882:HOH:O	1.98	0.63
1:A:413:GLU:HG2	3:A:624:HOH:O	1.98	0.63
1:A:190:THR:HG22	3:A:546:HOH:O	1.97	0.63
1:B:117:THR:HG22	1:B:277:LEU:CD1	2.30	0.62
1:A:260:THR:HG22	1:B:72:GLN:HA	1.81	0.61
1:A:423:ARG:HG2	1:A:428:SER:CB	2.21	0.61
1:B:112:GLU:OE2	1:B:281:HIS:CD2	2.50	0.61
1:B:226:HIS:HE1	3:B:715:HOH:O	1.85	0.60
1:A:162:THR:HG22	1:A:339:PRO:HD2	1.84	0.60
1:B:236:ARG:O	1:B:239:THR:HB	2.00	0.60
1:A:229:PHE:HB3	1:A:322:MET:CE	2.32	0.60
1:A:260:THR:HG23	1:B:73:TYR:H	1.65	0.60
1:A:240:LEU:HB3	1:A:241:PRO:HD2	1.82	0.59
1:A:198:VAL:HG13	1:A:343:GLN:CB	2.32	0.59
1:A:117:THR:HA	1:A:277:LEU:HD22	1.83	0.59
1:B:17:LYS:HB3	1:B:17:LYS:NZ	2.17	0.59
1:B:374:THR:HG21	1:B:387:PRO:HD3	1.84	0.59
1:A:38:LYS:HB3	1:A:38:LYS:NZ	2.18	0.59
1:A:190:THR:CG2	1:A:199:MET:H	2.16	0.59
1:A:184:LYS:HA	1:B:11:ASN:HD21	1.68	0.59
1:A:42:LEU:N	3:A:705:HOH:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:HIS:HD2	3:A:631:HOH:O	1.85	0.58
1:A:411:LYS:HE3	3:A:673:HOH:O	2.04	0.58
1:B:74:THR:OG1	1:B:79:HIS:HD2	1.87	0.57
1:A:377:MET:HA	1:A:381:VAL:HG12	1.86	0.57
1:A:190:THR:HG21	1:A:199:MET:H	1.70	0.56
1:A:229:PHE:HB3	1:A:322:MET:HE2	1.86	0.56
1:A:384:GLN:C	3:A:721:HOH:O	2.43	0.56
1:B:12:LYS:HD3	3:B:791:HOH:O	2.05	0.56
1:A:198:VAL:HG13	1:A:343:GLN:HB3	1.87	0.56
1:A:381:VAL:HG22	3:A:682:HOH:O	2.05	0.56
1:A:184:LYS:HA	1:B:11:ASN:ND2	2.21	0.56
1:B:193:ASN:HD22	1:B:194:PRO:CA	2.19	0.56
1:A:260:THR:HB	1:B:72:GLN:OE1	2.06	0.55
1:A:12:LYS:HA	1:A:12:LYS:HE3	1.88	0.55
1:B:370:ASP:O	1:B:374:THR:HG22	2.07	0.55
1:B:12:LYS:HG2	3:B:791:HOH:O	2.06	0.55
1:A:383:LEU:CB	3:A:710:HOH:O	2.50	0.54
1:A:226:HIS:HE1	3:A:510:HOH:O	1.89	0.54
1:B:162:THR:HG21	3:B:775:HOH:O	2.05	0.54
1:A:30:TYR:OH	1:A:374:THR:HG23	2.08	0.54
1:B:420:GLU:OE2	1:B:423:ARG:NE	2.41	0.54
1:B:192:HIS:HD2	1:B:195:LEU:H	1.56	0.53
1:B:30:TYR:OH	1:B:374:THR:HG23	2.09	0.53
1:B:129:ILE:HG13	1:B:186:ILE:HG13	1.91	0.52
1:A:94:VAL:HG23	1:A:96:ARG:HG2	1.92	0.52
1:A:48:ASP:HB2	1:A:410:LYS:HA	1.92	0.52
1:A:366:ASP:OD2	1:A:372:ARG:HG2	2.10	0.52
1:A:379:LYS:CG	3:A:698:HOH:O	2.35	0.52
1:B:414:ASN:ND2	3:B:894:HOH:O	2.43	0.52
1:A:26:VAL:HG21	1:A:390:ALA:HB1	1.92	0.52
1:B:234:HIS:HD2	3:B:853:HOH:O	1.93	0.51
1:B:303:GLU:OE1	1:B:303:GLU:HA	2.11	0.51
1:A:373:PHE:HD2	3:A:679:HOH:O	1.93	0.51
1:A:28:VAL:HB	3:B:874:HOH:O	2.10	0.51
1:A:378:THR:CG2	3:A:629:HOH:O	2.58	0.51
1:A:73:TYR:H	1:B:260:THR:CG2	2.17	0.51
3:A:649:HOH:O	1:B:279:MET:CB	2.55	0.51
1:A:260:THR:HG23	1:B:73:TYR:CG	2.45	0.51
1:B:29:GLU:OE2	1:B:375:LYS:NZ	2.42	0.51
1:A:328:MET:HA	1:A:331:PHE:CE2	2.45	0.51
1:A:27:TRP:NE1	1:A:136:ASP:OD2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:LYS:CE	2:A:430:QLP:H4A1	2.40	0.50
1:B:276:ASN:HD22	1:B:276:ASN:N	2.09	0.50
1:A:361:LEU:HD23	1:A:372:ARG:HB2	1.94	0.50
1:A:74:THR:OG1	1:A:79:HIS:HD2	1.94	0.50
1:B:424:LYS:HB2	3:B:876:HOH:O	2.10	0.50
1:A:423:ARG:HB3	1:A:428:SER:O	2.12	0.50
1:A:41:ASN:CA	3:A:705:HOH:O	2.28	0.49
1:A:247:THR:HG22	1:A:249:THR:HG22	1.94	0.49
1:A:378:THR:OG1	1:A:384:GLN:CB	2.52	0.49
1:A:180:ASN:OD1	1:A:182:LYS:HB2	2.13	0.49
1:A:162:THR:HG22	1:A:339:PRO:CG	2.41	0.49
1:B:369:LYS:HG3	1:B:372:ARG:HH12	1.78	0.49
1:A:131:ILE:HG12	1:A:152:ILE:HD12	1.93	0.49
1:A:41:ASN:HD22	1:A:43:GLY:H	1.59	0.49
1:B:424:LYS:O	1:B:428:SER:CB	2.57	0.49
2:B:430:QLP:HA	3:B:855:HOH:O	2.12	0.49
1:A:361:LEU:HG	3:A:696:HOH:O	2.12	0.49
1:B:198:VAL:HG13	1:B:343:GLN:CB	2.43	0.48
1:A:317:ILE:HG12	1:A:321:LEU:HD22	1.94	0.48
1:A:129:ILE:HG13	1:A:186:ILE:HG13	1.95	0.48
1:A:46:PHE:HB3	1:A:260:THR:HG21	1.96	0.48
1:A:198:VAL:HG13	1:A:343:GLN:HB2	1.95	0.48
1:A:282:GLN:HE22	1:B:25:SER:H	1.61	0.48
1:B:133:PRO:O	1:B:192:HIS:CE1	2.66	0.48
1:A:372:ARG:HD3	3:A:565:HOH:O	2.13	0.48
1:B:374:THR:OG1	1:B:385:GLY:O	2.27	0.48
1:A:223:VAL:HG22	1:A:252:SER:CB	2.44	0.47
1:A:189:ASN:ND2	1:A:193:ASN:H	2.12	0.47
1:A:245:GLU:HG3	3:A:643:HOH:O	2.14	0.47
1:A:162:THR:HG22	1:A:339:PRO:CD	2.45	0.47
1:A:11:ASN:HD21	1:B:184:LYS:HA	1.80	0.47
1:A:423:ARG:CB	1:A:428:SER:HB2	2.45	0.47
1:B:154:LEU:HD23	1:B:170:LEU:HD13	1.96	0.47
1:A:11:ASN:ND2	1:A:11:ASN:N	2.58	0.47
1:B:76:GLY:O	1:B:281:HIS:HE1	1.98	0.47
1:B:90:TYR:O	1:B:94:VAL:HG22	2.15	0.46
1:A:154:LEU:HD23	1:A:170:LEU:HD13	1.97	0.46
1:A:358:LYS:N	1:A:358:LYS:HD3	2.30	0.46
1:A:370:ASP:OD2	1:A:389:SER:OG	2.31	0.46
1:A:12:LYS:HG3	1:A:14:ASP:H	1.79	0.46
1:A:41:ASN:ND2	1:A:43:GLY:H	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LYS:HB3	3:B:909:HOH:O	2.15	0.46
1:A:260:THR:HG22	1:B:72:GLN:CA	2.46	0.45
1:A:37:TYR:HB2	3:A:629:HOH:O	2.15	0.45
1:A:406:TYR:HE1	3:A:721:HOH:O	1.98	0.45
1:B:42:LEU:HD22	1:B:383:LEU:HD11	1.98	0.45
1:A:368:ARG:HD3	1:A:397:LYS:CD	2.45	0.45
1:A:419:ALA:HB3	1:A:423:ARG:NH2	2.32	0.45
1:A:354:SER:O	1:A:355:LEU:HD23	2.16	0.45
1:B:23:THR:HG22	3:B:793:HOH:O	2.16	0.45
1:A:179:PHE:HB3	1:A:214:TRP:CD1	2.51	0.44
1:A:236:ARG:O	1:A:239:THR:CG2	2.63	0.44
1:A:352:TRP:O	1:A:352:TRP:CE3	2.70	0.44
1:A:37:TYR:HD1	3:A:652:HOH:O	2.00	0.44
1:B:317:ILE:HG12	1:B:321:LEU:HD22	1.99	0.44
1:A:383:LEU:CD2	1:A:422:LEU:CD1	2.96	0.44
1:B:394:GLU:HB3	1:B:395:PRO:HD3	1.98	0.44
1:A:33:LEU:HD11	1:A:375:LYS:HE2	2.00	0.44
1:A:384:GLN:HA	3:A:697:HOH:O	2.16	0.44
1:B:192:HIS:CD2	1:B:195:LEU:H	2.34	0.44
1:B:51:ALA:HB1	1:B:52:PRO:HD2	1.99	0.44
1:A:416:GLN:O	1:A:420:GLU:HG2	2.17	0.44
1:B:24:LYS:NZ	1:B:24:LYS:H	2.16	0.43
1:A:411:LYS:HE2	3:A:592:HOH:O	2.17	0.43
1:B:198:VAL:HG13	1:B:343:GLN:HB2	2.00	0.43
1:A:355:LEU:HD22	1:A:426:LYS:HD3	2.00	0.43
1:A:89:LEU:HG	1:A:93:LEU:HD22	1.99	0.43
1:B:327:TYR:OH	1:B:416:GLN:HA	2.18	0.43
1:B:190:THR:HA	1:B:191:PRO:C	2.38	0.43
1:A:276:ASN:N	1:A:276:ASN:HD22	2.17	0.43
1:A:368:ARG:HG3	3:A:675:HOH:O	2.18	0.43
1:B:46:PHE:HB3	1:B:260:THR:HG21	2.00	0.43
1:B:30:TYR:OH	1:B:374:THR:CG2	2.66	0.43
1:B:24:LYS:HE3	1:B:24:LYS:HB3	1.76	0.43
1:A:419:ALA:CB	1:A:423:ARG:NH2	2.83	0.42
1:B:162:THR:HG23	3:B:920:HOH:O	2.19	0.42
1:B:376:TRP:O	1:B:380:SER:HB3	2.18	0.42
1:B:420:GLU:OE2	1:B:423:ARG:CZ	2.68	0.42
1:B:193:ASN:HD21	1:B:405:ARG:NH1	2.13	0.42
1:B:94:VAL:HG23	1:B:96:ARG:HG2	2.01	0.42
1:A:239:THR:CG2	3:A:589:HOH:O	2.60	0.42
1:A:394:GLU:HB3	1:A:395:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:LYS:HB3	1:B:415:LEU:HD21	2.01	0.42
1:A:260:THR:HG22	1:B:73:TYR:H	1.81	0.42
1:A:411:LYS:CE	3:A:673:HOH:O	2.65	0.41
1:B:234:HIS:CD2	3:B:853:HOH:O	2.70	0.41
1:A:303:GLU:HA	1:A:303:GLU:OE1	2.20	0.41
1:A:181:GLU:HA	3:B:843:HOH:O	2.21	0.41
1:A:154:LEU:CD2	1:A:170:LEU:HD13	2.50	0.41
1:B:410:LYS:HB2	1:B:415:LEU:HD13	2.03	0.41
1:A:211:CYS:HA	1:A:216:VAL:HG22	2.01	0.41
1:B:129:ILE:HD12	1:B:129:ILE:C	2.41	0.41
1:A:338:ASN:HB2	1:A:351:ASP:HB3	2.03	0.41
1:A:229:PHE:HB3	1:A:322:MET:HE3	2.02	0.41
1:A:37:TYR:HD2	3:A:676:HOH:O	2.04	0.41
1:B:37:TYR:CE1	1:B:379:LYS:HG2	2.56	0.40
1:A:381:VAL:HG21	1:A:425:TRP:HB2	2.03	0.40
1:B:39:PRO:HG3	1:B:378:THR:HG23	2.02	0.40
1:A:65:SER:HA	1:A:66:PRO:HD2	1.87	0.40
1:A:282:GLN:NE2	1:B:25:SER:H	2.18	0.40
1:A:210:LEU:HD13	3:A:661:HOH:O	2.21	0.40
1:A:223:VAL:HG22	1:A:252:SER:HB2	2.03	0.40
1:A:401:GLU:HB3	3:A:641:HOH:O	2.22	0.40
1:B:328:MET:HA	1:B:331:PHE:CE2	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	417/429 (97%)	402 (96%)	12 (3%)	3 (1%)	22	9
1	B	417/429 (97%)	407 (98%)	10 (2%)	0	100	100
All	All	834/858 (97%)	809 (97%)	22 (3%)	3 (0%)	34	20

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	SER
1	A	397	LYS
1	A	160	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	357/367 (97%)	323 (90%)	34 (10%)	8	1
1	B	357/367 (97%)	324 (91%)	33 (9%)	9	1
All	All	714/734 (97%)	647 (91%)	67 (9%)	8	1

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	12	LYS
1	A	17	LYS
1	A	24	LYS
1	A	28	VAL
1	A	33	LEU
1	A	41	ASN
1	A	69	LEU
1	A	82	LEU
1	A	92	GLN
1	A	93	LEU
1	A	111	TYR
1	A	112	GLU
1	A	129	ILE
1	A	152	ILE
1	A	170	LEU
1	A	175	LEU
1	A	210	LEU
1	A	216	VAL
1	A	223	VAL

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Mol	Chain	Res	Type
1	A	239	THR
1	A	249	THR
1	A	260	THR
1	A	276	ASN
1	A	277	LEU
1	A	321	LEU
1	A	335	VAL
1	A	346	TYR
1	A	357	SER
1	A	358	LYS
1	A	359	VAL
1	A	368	ARG
1	A	374	THR
1	A	415	LEU
1	B	12	LYS
1	B	17	LYS
1	B	24	LYS
1	B	26	VAL
1	B	28	VAL
1	B	41	ASN
1	B	69	LEU
1	B	82	LEU
1	B	86	LEU
1	B	93	LEU
1	B	97	THR
1	B	111	TYR
1	B	129	ILE
1	B	162	THR
1	B	170	LEU
1	B	175	LEU
1	B	178	LEU
1	B	193	ASN
1	B	210	LEU
1	B	239	THR
1	B	274	LEU
1	B	276	ASN
1	B	321	LEU
1	B	335	VAL
1	B	346	TYR
1	B	358	LYS
1	B	361	LEU
1	B	368	ARG

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Mol	Chain	Res	Type
1	B	409	PHE
1	B	415	LEU
1	B	422	LEU
1	B	424	LYS
1	B	426	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	36	GLN
1	A	41	ASN
1	A	71	ASN
1	A	79	HIS
1	A	84	GLN
1	A	119	GLN
1	A	121	HIS
1	A	189	ASN
1	A	226	HIS
1	A	276	ASN
1	A	278	GLN
1	A	282	GLN
1	B	11	ASN
1	B	36	GLN
1	B	41	ASN
1	B	79	HIS
1	B	84	GLN
1	B	192	HIS
1	B	193	ASN
1	B	226	HIS
1	B	234	HIS
1	B	276	ASN
1	B	278	GLN
1	B	281	HIS
1	B	282	GLN
1	B	414	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	QLP	A	430	-	22,25,25	1.03	1 (4%)	27,35,35	1.57	3 (11%)
2	QLP	B	430	-	22,25,25	1.47	3 (13%)	27,35,35	1.96	5 (18%)

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
2	QLP	A	430	-	-	8/16/20/20	0/1/1/1
2	QLP	B	430	-	-	6/16/20/20	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	430	QLP	O3-C3	-4.59	1.26	1.37
2	A	430	QLP	O3-C3	-3.21	1.29	1.37
2	B	430	QLP	C4A-C4	2.44	1.55	1.51
2	B	430	QLP	C2A-C2	2.13	1.54	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	430	QLP	C4A-N-CA	6.72	126.73	113.83
2	A	430	QLP	C4A-N-CA	5.24	123.89	113.83
2	B	430	QLP	C6-C5-C4	4.45	121.27	118.12
2	A	430	QLP	O2P-P-O4P	-3.35	97.81	106.73
2	B	430	QLP	C5-C6-N1	-2.97	118.87	123.82
2	B	430	QLP	CG-CB-CA	-2.87	106.29	113.41
2	B	430	QLP	C4A-C4-C5	2.43	122.41	119.71
2	A	430	QLP	C4A-C4-C5	2.24	122.20	119.71

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	430	QLP	C5-C4-C4A-N
2	B	430	QLP	C5-C4-C4A-N
2	A	430	QLP	CA-CB-CG-CD
2	B	430	QLP	CB-CA-N-C4A
2	B	430	QLP	C-CA-N-C4A
2	A	430	QLP	C3-C4-C4A-N
2	A	430	QLP	C4-C5-C5A-O4P
2	B	430	QLP	C4-C5-C5A-O4P
2	A	430	QLP	C-CA-N-C4A
2	B	430	QLP	CA-CB-CG-CD
2	A	430	QLP	C5A-O4P-P-O2P
2	B	430	QLP	C5A-O4P-P-O1P
2	A	430	QLP	NE2-CD-CG-CB
2	A	430	QLP	OE1-CD-CG-CB

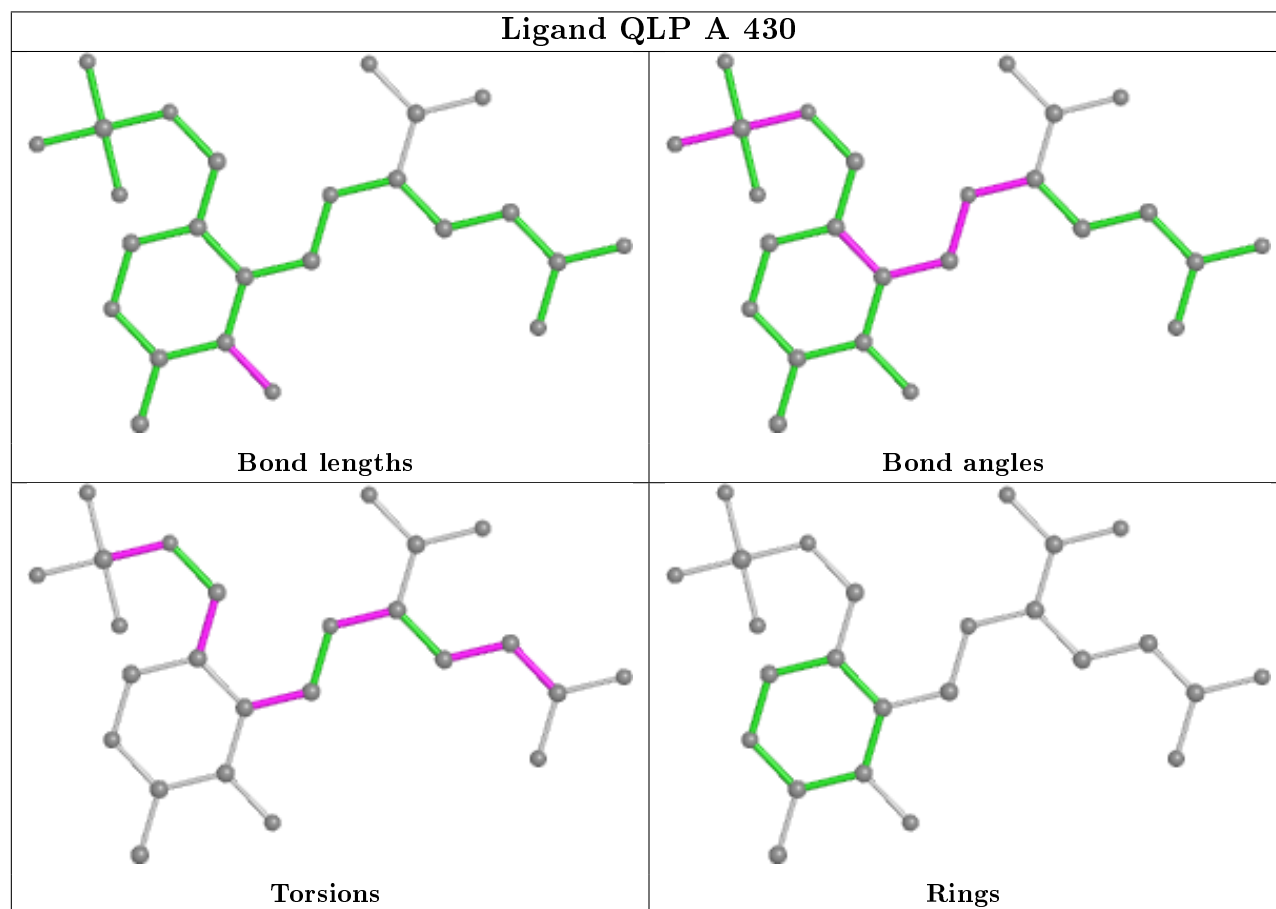
There are no ring outliers.

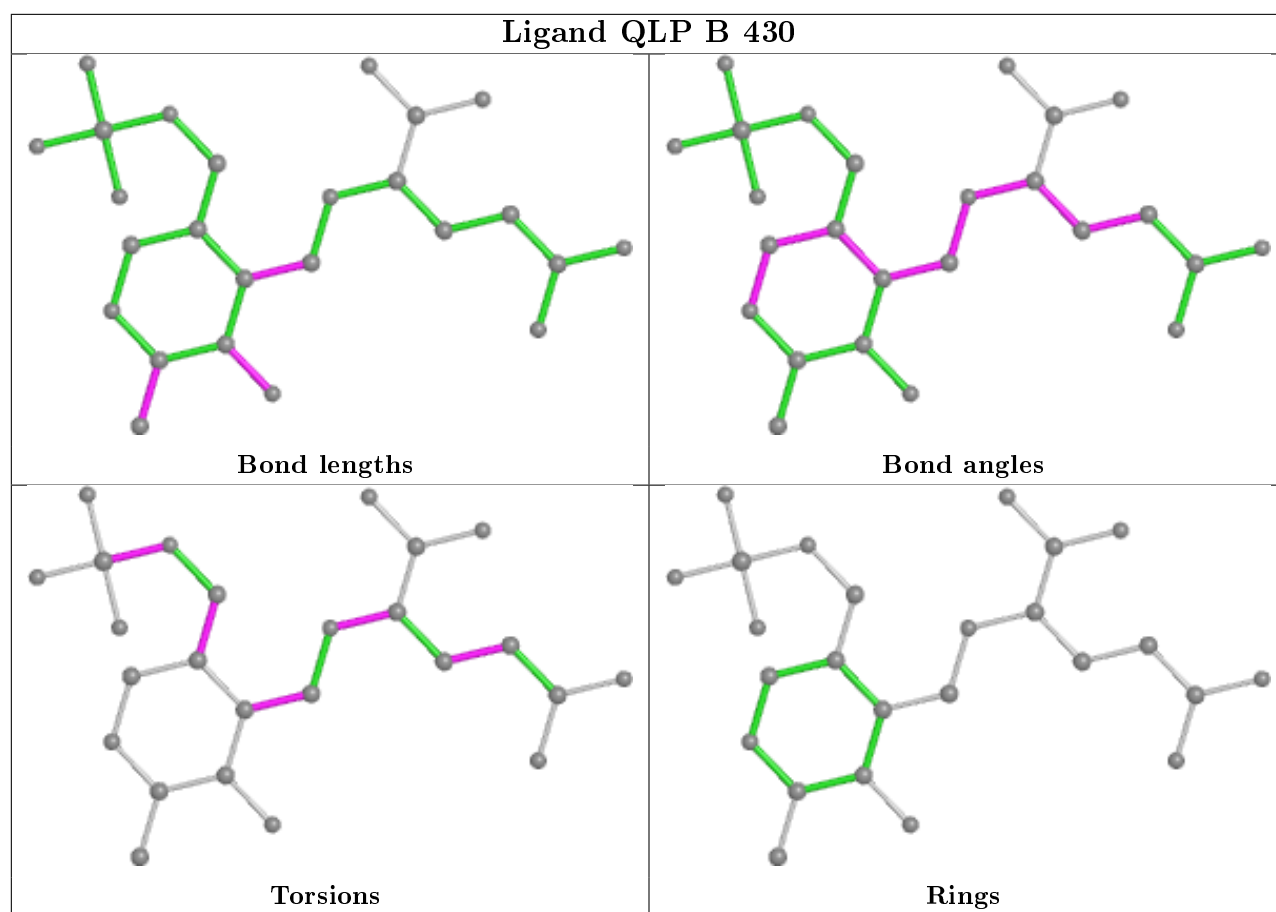
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	430	QLP	1	0
2	B	430	QLP	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 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	419/429 (97%)	0.59	58 (13%) 2 2	19, 32, 56, 73	0
1	B	419/429 (97%)	0.13	14 (3%) 46 43	18, 28, 45, 67	0
All	All	838/858 (97%)	0.36	72 (8%) 10 9	18, 29, 52, 73	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	429	SER	9.9
1	A	363	GLN	9.7
1	B	429	SER	7.5
1	A	428	SER	6.8
1	A	422	LEU	6.6
1	B	161	GLY	5.9
1	A	425	TRP	5.7
1	A	356	ASP	5.3
1	B	159	THR	5.1
1	B	428	SER	4.8
1	B	427	GLY	4.8
1	A	365	THR	4.7
1	A	374	THR	4.6
1	A	359	VAL	4.5
1	A	39	PRO	4.4
1	A	11	ASN	4.4
1	A	162	THR	4.3
1	A	159	THR	4.2
1	A	36	GLN	4.1
1	B	160	GLY	4.1
1	A	353	SER	4.0
1	A	364	GLU	4.0
1	A	23	THR	4.0
1	A	427	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	418	ALA	3.8
1	A	352	TRP	3.7
1	A	32	GLN	3.5
1	A	421	ILE	3.4
1	A	424	LYS	3.4
1	A	38	LYS	3.2
1	A	161	GLY	3.2
1	A	21	GLY	3.2
1	A	360	ASP	3.2
1	B	357	SER	3.0
1	A	367	ALA	3.0
1	B	158	LYS	3.0
1	A	163	ILE	3.0
1	A	426	LYS	3.0
1	A	383	LEU	3.0
1	A	22	SER	2.9
1	A	385	GLY	2.9
1	B	23	THR	2.9
1	A	338	ASN	2.9
1	B	11	ASN	2.8
1	A	31	ILE	2.8
1	A	366	ASP	2.7
1	A	160	GLY	2.7
1	A	361	LEU	2.7
1	A	24	LYS	2.6
1	A	376	TRP	2.6
1	A	110	ALA	2.5
1	A	404	VAL	2.4
1	A	250	ILE	2.4
1	A	20	GLN	2.4
1	A	378	THR	2.4
1	A	27	TRP	2.3
1	A	336	GLY	2.3
1	A	28	VAL	2.3
1	A	42	LEU	2.3
1	A	158	LYS	2.3
1	B	20	GLN	2.3
1	A	357	SER	2.3
1	B	362	THR	2.2
1	A	26	VAL	2.2
1	A	382	GLY	2.2
1	B	162	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	373	PHE	2.1
1	A	135	PHE	2.1
1	A	379	LYS	2.0
1	A	114	LEU	2.0
1	B	17	LYS	2.0
1	A	37	TYR	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 carbohydrates 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.

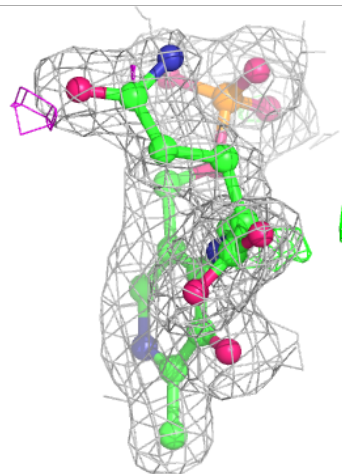
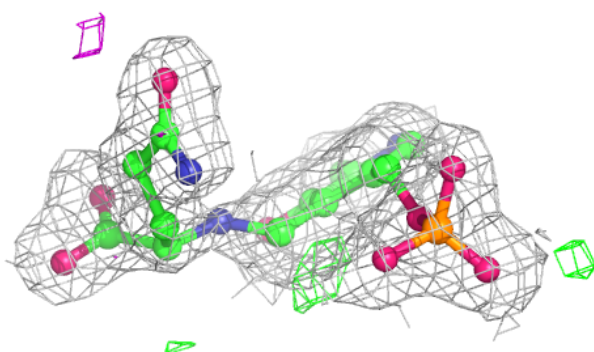
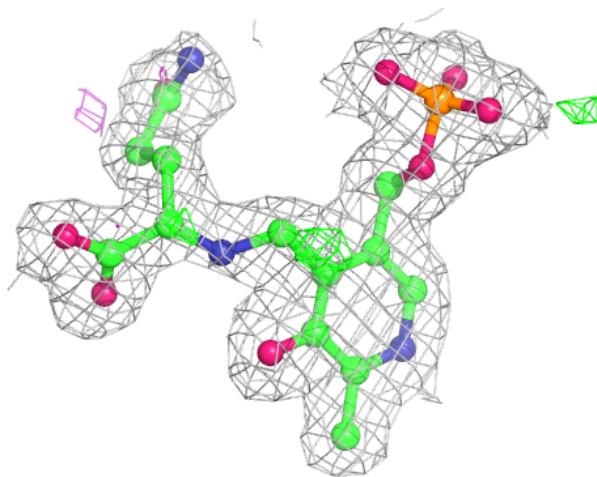
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	QLP	A	430	25/25	0.96	0.18	18,26,38,42	1
2	QLP	B	430	25/25	0.97	0.14	18,23,30,34	0

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.



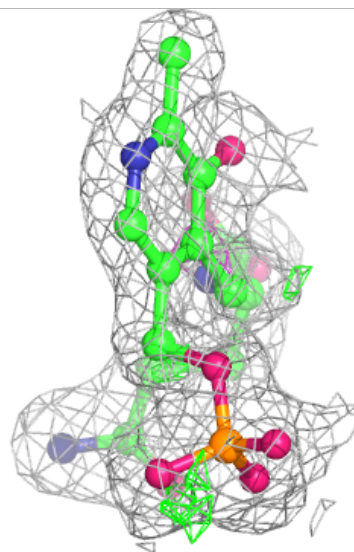
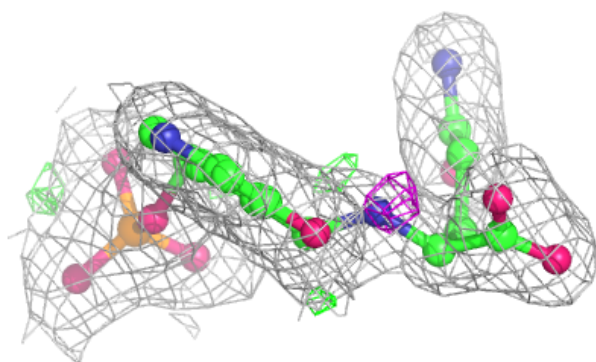
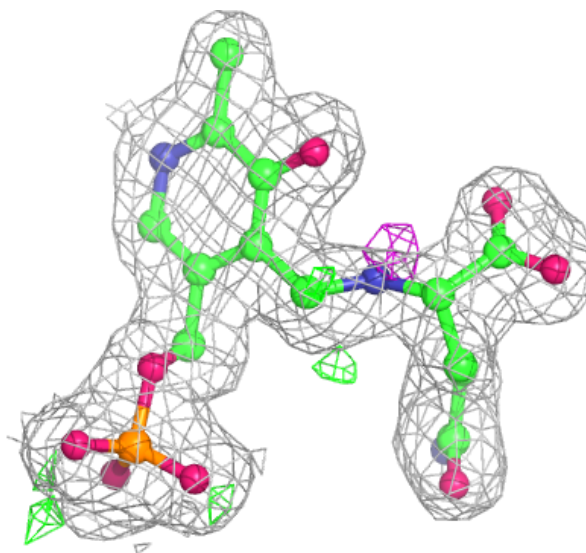
**Electron density around QLP A 430:**

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



**Electron density around QLP B 430:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.