

Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2023 – 07:17 AM EDT

PDB ID	:	4GE7
Title	:	Kynurenine Aminotransferase II Inhibitors
Authors	:	Pandit, J.
Deposited on		
Resolution	:	2.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

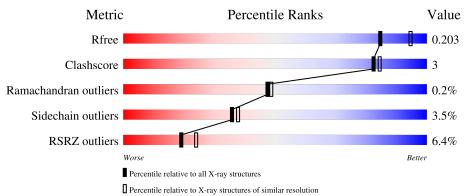
Xtriage (Phenix) EDS buster-report Percentile statistics Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA)	::	20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001) Parkinson et al. (1996)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		Parkinson et al. (1996) 2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.10 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	5197(2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	А	439	90%	7% •					
1	В	439	90%	7% ••					



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7390 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/alpha-aminoadipate aminotransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	428	Total 3345	C 2145		0 621	S 18	0	0	0
1	В	428	Total 3345	C 2145		O 621	S 18	0	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	240	SER	LYS	engineered mutation	UNP Q8N5Z0
А	241	GLY	PHE	engineered mutation	UNP Q8N5Z0
А	426	LEU	-	expression tag	UNP Q8N5Z0
А	427	VAL	-	expression tag	UNP Q8N5Z0
А	428	PRO	-	expression tag	UNP Q8N5Z0
А	429	ARG	-	expression tag	UNP Q8N5Z0
А	430	GLY	-	expression tag	UNP Q8N5Z0
А	431	SER	-	expression tag	UNP Q8N5Z0
А	432	LEU	-	expression tag	UNP Q8N5Z0
А	433	GLU	-	expression tag	UNP Q8N5Z0
А	434	HIS	-	expression tag	UNP Q8N5Z0
А	435	HIS	-	expression tag	UNP Q8N5Z0
А	436	HIS	-	expression tag	UNP Q8N5Z0
А	437	HIS	-	expression tag	UNP Q8N5Z0
А	438	HIS	-	expression tag	UNP Q8N5Z0
А	439	HIS	-	expression tag	UNP Q8N5Z0
В	240	SER	LYS	engineered mutation	UNP Q8N5Z0
В	241	GLY	PHE	engineered mutation	UNP Q8N5Z0
В	426	LEU	-	expression tag	UNP Q8N5Z0
В	427	VAL	-	expression tag	UNP Q8N5Z0
В	428	PRO	-	expression tag	UNP Q8N5Z0
В	429	ARG	-	expression tag	UNP Q8N5Z0
В	430	GLY	-	expression tag	UNP Q8N5Z0
В	431	SER	-	expression tag	UNP Q8N5Z0

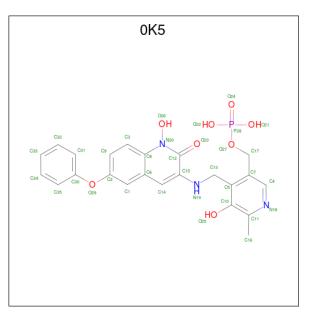
There are 32 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
В	432	LEU	-	expression tag	UNP Q8N5Z0
В	433	GLU	-	expression tag	UNP Q8N5Z0
В	434	HIS	-	expression tag	UNP Q8N5Z0
В	435	HIS	-	expression tag	UNP Q8N5Z0
В	436	HIS	-	expression tag	UNP Q8N5Z0
В	437	HIS	-	expression tag	UNP Q8N5Z0
В	438	HIS	-	expression tag	UNP Q8N5Z0
В	439	HIS	-	expression tag	UNP Q8N5Z0

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• Molecule 2 is (5-hydroxy-4-{[(1-hydroxy-2-oxo-6-phenoxy-1,2-dihydroquinolin-3-yl)am ino]methyl}-6-methylpyridin-3-yl)methyl dihydrogen phosphate (three-letter code: 0K5) (formula: $C_{23}H_{22}N_3O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
0	۸	1	Total	С	Ν	Ο	Р	0	0	
	Z A	1	35	23	3	8	1	0	0	
0	P	1	Total	С	Ν	Ο	Р	0	0	
	D		35	23	3	8	1	0		

• Molecule 3 is water.

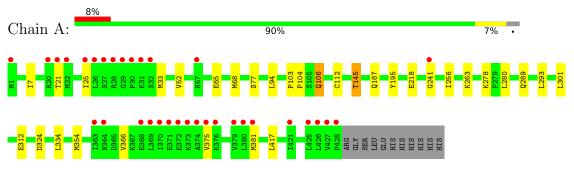
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	307	Total O 307 307	0	0
3	В	323	Total O 323 323	0	0



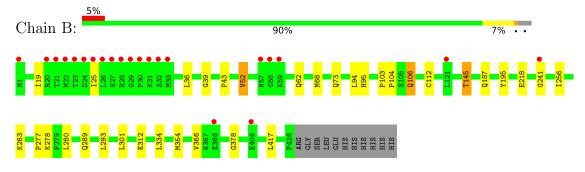
3 Residue-property plots (i)

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/alpha-aminoadipate aminotransferase, mitochondrial



• Molecule 1: Kynurenine/alpha-aminoadipate aminotransferase, mitochondrial





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	85.74Å 114.97Å 116.55Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.51 - 2.10	Depositor
Resolution (A)	33.51 - 2.10	EDS
% Data completeness	(Not available) $(33.51-2.10)$	Depositor
(in resolution range)	89.0 (33.51-2.10)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.16 (at 2.10 \text{\AA})$	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.9.2, BUSTER 2.9.2	Depositor
R, R_{free}	0.178 , 0.202	Depositor
It, It _{free}	0.180 , 0.203	DCC
R_{free} test set	3075 reflections $(5.10%)$	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34, 62.9	EDS
L-test for twinning ²	$< L > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7390	wwPDB-VP
Average B, all atoms $(Å^2)$	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: 0K5, CSO $\,$

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			lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.44	0/3419	0.65	0/4642	
1	В	0.44	0/3419	0.64	0/4642	
All	All	0.44	0/6838	0.64	0/9284	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3345	0	3366	19	0
1	В	3345	0	3366	19	0
2	А	35	0	20	2	0
2	В	35	0	20	1	0
3	А	307	0	0	6	0
3	В	323	0	0	4	0
All	All	7390	0	6772	34	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 3.

All (34) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:112:CYS:HB2	3:A:885:HOH:O	1.56	1.03
1:A:112:CYS:SG	3:A:885:HOH:O	2.40	0.80
2:A:501:0K5:O26	1:B:39:GLY:HA3	1.82	0.79
1:A:112:CYS:CB	3:A:885:HOH:O	2.23	0.75
1:B:145:THR:HG21	1:B:195:TYR:CZ	2.33	0.64
1:A:145:THR:HG21	1:A:195:TYR:CZ	2.34	0.62
1:A:263:LYS:HG2	3:A:886:HOH:O	2.03	0.58
1:A:104:PRO:HB3	1:A:278:LYS:HD3	1.88	0.56
1:B:145:THR:HG21	1:B:195:TYR:OH	2.08	0.54
1:A:289:GLN:O	1:A:293:LEU:HD23	2.07	0.53
1:B:289:GLN:O	1:B:293:LEU:HD23	2.08	0.53
1:B:95:HIS:HE1	3:B:607:HOH:O	1.91	0.53
1:B:104:PRO:HB3	1:B:278:LYS:HD3	1.89	0.53
1:A:324:ASP:HB2	3:A:624:HOH:O	2.09	0.51
1:A:145:THR:HG21	1:A:195:TYR:OH	2.10	0.50
1:A:21:THR:HG22	1:A:25:ILE:HD13	1.95	0.48
1:A:375:VAL:HG21	1:B:25:ILE:HD12	1.96	0.47
1:A:77:SER:OG	2:B:501:0K5:H2	2.14	0.47
1:B:263:LYS:HD2	1:B:354:MET:CE	2.45	0.46
1:A:381:MET:HG2	1:B:36:LEU:HB2	1.98	0.46
1:B:73:GLN:HB2	3:B:909:HOH:O	2.17	0.45
2:A:501:0K5:N20	1:B:39:GLY:HA3	2.32	0.45
1:A:65:GLU:HG2	3:A:684:HOH:O	2.17	0.44
1:A:375:VAL:HG11	1:B:25:ILE:HB	1.99	0.44
1:A:263:LYS:HD2	1:A:354:MET:CE	2.48	0.44
1:A:256:ILE:HD11	1:A:280:LEU:HD13	2.00	0.43
1:A:33:MET:HG2	1:B:378:GLY:HA2	2.02	0.42
1:B:277:PRO:HG2	1:B:280:LEU:HD12	2.02	0.41
1:B:43:PRO:HB3	3:B:909:HOH:O	2.20	0.41
1:B:52:VAL:HB	1:B:62:GLN:HG2	2.03	0.41
1:B:256:ILE:HD11	1:B:280:LEU:HD13	2.01	0.41
1:B:103:PRO:HD2	1:B:106:GLN:HB2	2.04	0.40
1:B:112:CYS:HB2	3:B:888:HOH:O	2.20	0.40
1:A:103:PRO:HD2	1:A:106:GLN:HB2	2.04	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	А	425/439~(97%)	417 (98%)	7 (2%)	1 (0%)	47 49
1	В	425/439~(97%)	418 (98%)	6 (1%)	1 (0%)	47 49
All	All	850/878~(97%)	835~(98%)	13~(2%)	2 (0%)	47 49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	241	GLY
1	В	241	GLY

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	А	371/381~(97%)	358~(96%)	13 (4%)	36 38		
1	В	371/381~(97%)	358~(96%)	13 (4%)	36 38		
All	All	742/762~(97%)	716 (96%)	26 (4%)	36 38		

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	7	ILE
1	А	52	VAL
1	А	68	MET
1	А	94	LEU



Mol	Chain	Res	Dus page Type
1	А	106	GLN
1	А	145	THR
1	А	187	GLN
1	А	218	GLU
1	А	301	LEU
1	А	312	GLU
1	А	334	LEU
1	А	366	VAL
1	А	417	LEU
1	В	19	ILE
1	В	52	VAL
1	В	68	MET
1	В	94	LEU
1	В	106	GLN
1	В	145	THR
1	В	187	GLN
1	В	218	GLU
1	В	301	LEU
1	В	312	GLU
1	В	334	LEU
1	В	366	VAL
1	В	417	LEU

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Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such side chains are listed below:

Mol	Chain	Res	Type
1	А	95	HIS
1	А	150	HIS
1	А	237	GLN
1	А	305	GLN
1	А	328	ASN
1	В	95	HIS
1	В	237	GLN
1	В	305	GLN
1	В	328	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

2 non-standard protein/DNA/RNA residues 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	Aol Type Chain Res Link		Link	B	ond leng	$_{ m gths}$	Bond angles			
WIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
1	CSO	А	122	1	3,6,7	0.65	0	$0,\!6,\!8$	-	-
1	CSO	В	122	1	3,6,7	0.67	0	0,6,8	-	-

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	CSO	А	122	1	-	0/1/5/7	-
1	CSO	В	122	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	Turne	Type Chain		Link	Bond lengths			Bond angles		
IVIOI	туре	Unam	\mathbf{Res}	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	0K5	А	501	-	38,38,38	1.23	3 (7%)	48,55,55	1.31	5 (10%)
2	0K5	В	501	-	38,38,38	0.91	3 (7%)	48,55,55	1.41	4 (8%)

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	0K5	А	501	-	-	6/15/15/15	0/4/4/4
2	0K5	В	501	-	-	5/15/15/15	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	А	501	0 K5	C15-N19	4.80	1.43	1.34
2	А	501	0 K5	C6-C8	-3.02	1.36	1.41
2	В	501	0K5	C15-N19	2.87	1.39	1.34
2	В	501	0 K5	C10-C11	-2.50	1.38	1.40
2	А	501	0K5	O26-N20	2.20	1.42	1.39
2	В	501	0K5	C6-C8	-2.13	1.37	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$\mathbf{Ideal}(^{o})$
2	В	501	0 K5	C6-C14-C15	5.75	123.42	120.27
2	А	501	0 K5	C12-C15-N19	3.73	118.56	113.20
2	В	501	0 K5	C14-C15-C12	-3.72	117.84	120.22
2	А	501	0 K5	C14-C15-N19	-2.62	120.65	124.91
2	А	501	0 K5	C16-C11-C10	-2.52	117.77	120.89
2	А	501	0 K5	C13-C5-C7	2.39	122.36	119.71
2	А	501	0 K5	C6-C14-C15	2.29	121.52	120.27
2	В	501	0 K5	C13-C5-C10	2.16	122.36	120.04



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	501	0K5	C2-O29-C30	-2.13	113.82	118.80

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	501	0 K5	C14-C15-N19-C13
2	А	501	0 K5	C12-C15-N19-C13
2	А	501	0 K5	C17-O27-P28-O22
2	А	501	0 K5	C17-O27-P28-O24
2	А	501	0 K5	C17-O27-P28-O21
2	В	501	0 K5	C17-O27-P28-O22
2	В	501	0 K5	C17-O27-P28-O24
2	В	501	0 K5	C17-O27-P28-O21
2	В	501	0 K5	N19-C13-C5-C7
2	В	501	0 K5	N19-C13-C5-C10
2	А	501	0 K5	N19-C13-C5-C7

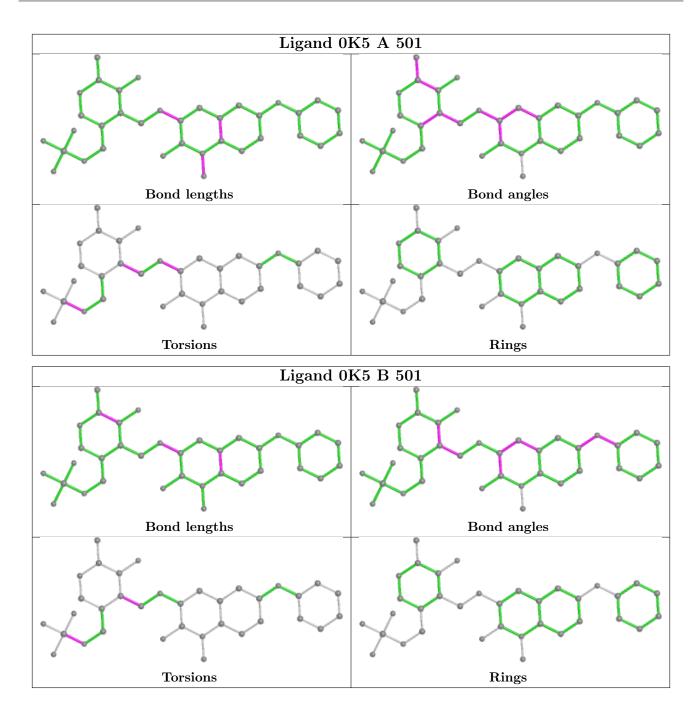
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	501	0K5	2	0
2	В	501	0K5	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 sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	$\langle RSRZ \rangle$	#RS	$\#RSRZ{>}2$		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	427/439~(97%)	0.05	33 (7%)	13	17	15, 29, 93, 122	0
1	В	427/439~(97%)	-0.07	22~(5%)	27	32	17, 27, 64, 125	0
All	All	854/878~(97%)	-0.01	55 (6%)	19	24	15, 28, 86, 125	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	26	LEU	11.5
1	А	25	ILE	9.0
1	В	25	ILE	9.0
1	А	428	PRO	8.9
1	А	427	VAL	8.6
1	В	23	THR	7.6
1	В	29	GLY	7.5
1	А	27	SER	7.1
1	А	426	LEU	7.0
1	А	380	LEU	6.9
1	В	27	SER	6.6
1	А	376	LYS	6.0
1	А	370	ILE	5.9
1	В	24	ASP	5.6
1	А	28	ARG	5.6
1	А	29	GLY	5.5
1	В	21	THR	5.5
1	В	28	ARG	5.4
1	В	59	LYS	5.4
1	В	20	ARG	5.4
1	А	21	THR	5.2
1	А	371	GLU	5.0
1	А	241	GLY	5.0
1	А	31	LYS	4.9



Mol	Chain	Res	Type	RSRZ
1	В	33	MET	4.7
1	А	26	LEU	4.6
1	А	372	GLU	4.6
1	В	32	SER	4.2
1	А	375	VAL	4.1
1	В	30	PRO	4.0
1	В	31	LYS	4.0
1	А	22	MET	4.0
1	А	425	LEU	3.9
1	А	374	ALA	3.8
1	А	381	MET	3.7
1	А	32	SER	3.4
1	А	1	MET	3.0
1	А	363	ILE	2.9
1	А	373	LYS	2.7
1	А	369	LEU	2.7
1	А	20	ARG	2.7
1	А	421	ILE	2.6
1	А	57	ASN	2.5
1	А	368	GLU	2.5
1	В	57	ASN	2.5
1	А	379	VAL	2.4
1	В	1	MET	2.4
1	В	408	GLU	2.3
1	В	58	GLY	2.3
1	В	22	MET	2.3
1	А	30	PRO	2.2
1	В	121	LEU	2.1
1	А	364	ASN	2.1
1	В	368	GLU	2.1
1	В	241	GLY	2.1

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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^{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	$\mathbf{B} extsf{-}\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{A}^2)$	Q<0.9
1	CSO	А	122	7/8	0.97	0.09	16,18,27,30	0
1	CSO	В	122	7/8	0.98	0.13	17,18,26,27	0



6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

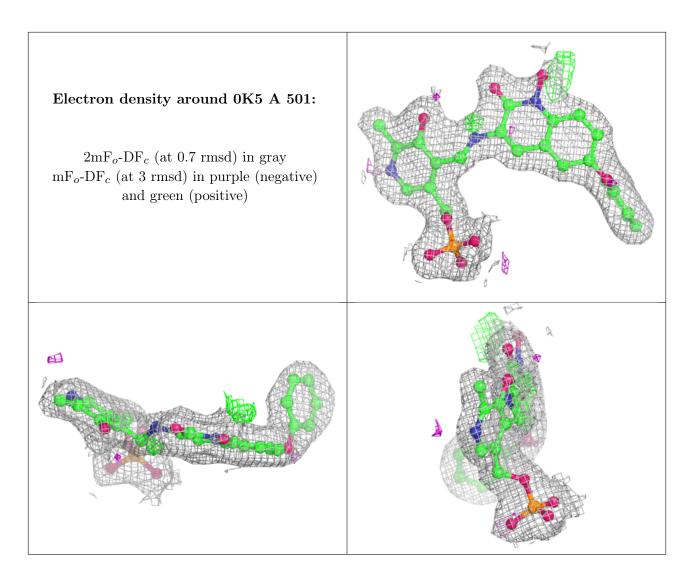
6.4 Ligands (i)

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^{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.

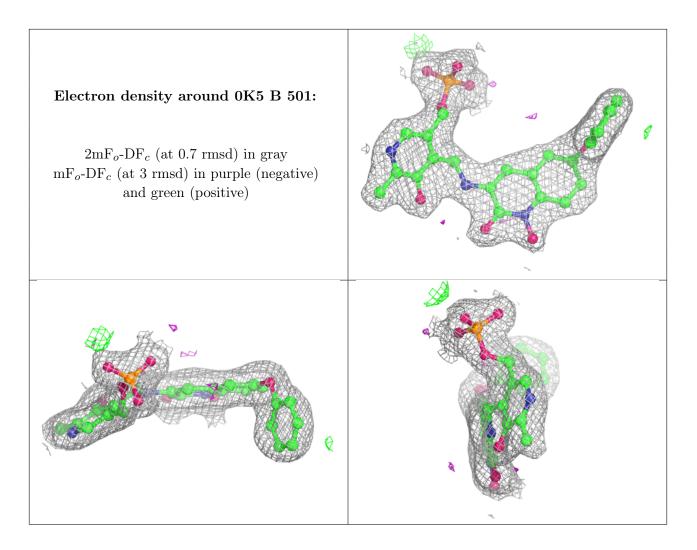
Mo	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
2	0K5	А	501	35/35	0.96	0.12	$15,\!26,\!38,\!56$	0
2	0K5	В	501	35/35	0.98	0.11	17,20,35,41	0

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.

