



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 02:14 PM EDT

PDB ID : 2OJT  
Title : Structure and mechanism of kainate receptor modulation by anions  
Authors : Mayer, M.L.  
Deposited on : 2007-01-14  
Resolution : 1.95 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 : 2.23.2  
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) : 2.23.2

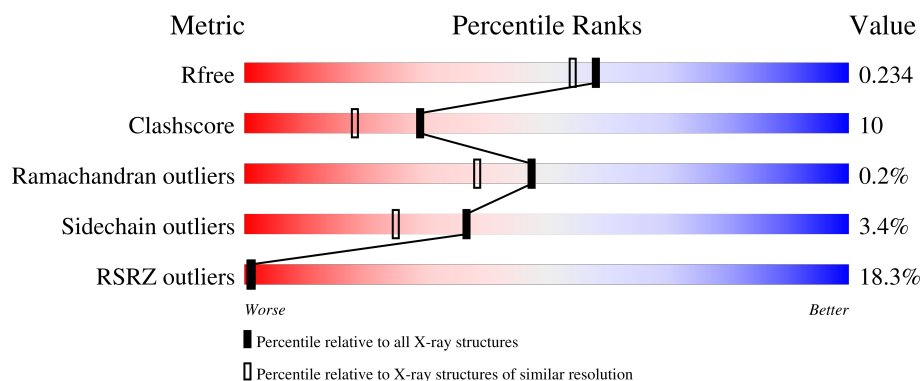
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	258	<div> <div>17%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>
1	B	258	<div> <div>19%</div> <div>80%</div> <div>16%</div> <div>..</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4706 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 Glutamate receptor, ionotropic kainate 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	17	0
			2148	1367	359	408	14			
1	B	251	Total	C	N	O	S	0	21	0
			2188	1392	369	411	16			

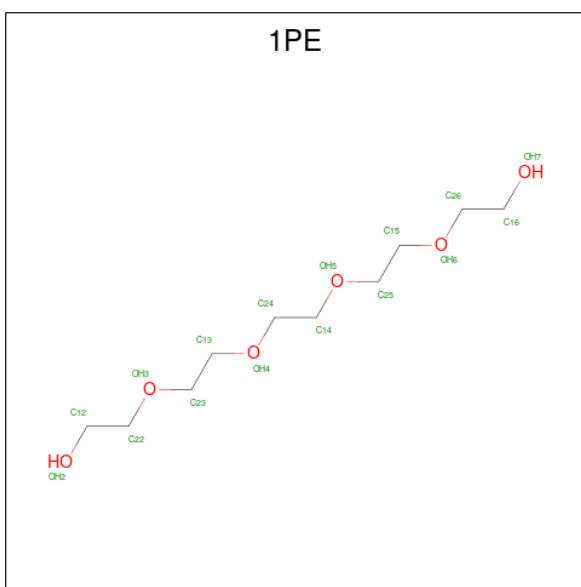
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P22756
A	2	SER	-	expression tag	UNP P22756
A	34	GLY	ALA	conflict	UNP P22756
A	117	GLY	-	SEE REMARK 999	UNP P22756
A	118	THR	-	SEE REMARK 999	UNP P22756
A	258	SER	GLU	engineered mutation	UNP P22756
B	1	GLY	-	expression tag	UNP P22756
B	2	SER	-	expression tag	UNP P22756
B	34	GLY	ALA	conflict	UNP P22756
B	117	GLY	-	SEE REMARK 999	UNP P22756
B	118	THR	-	SEE REMARK 999	UNP P22756
B	258	SER	GLU	engineered mutation	UNP P22756

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

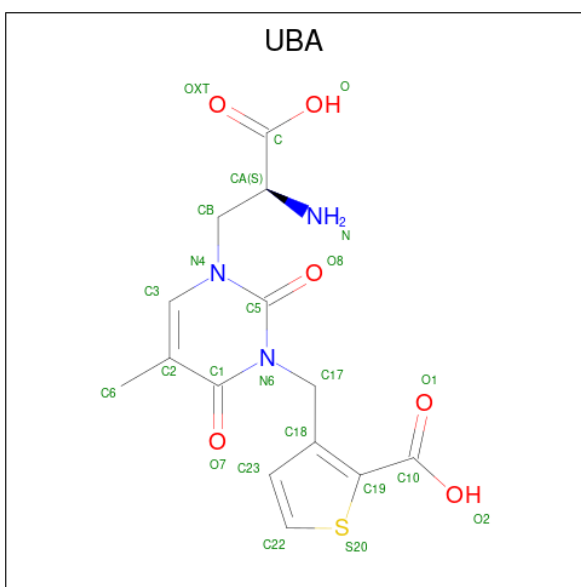
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Br	0	0
			1	1		
2	B	1	Total	Br	0	0
			1	1		

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is (S)-1-(2-AMINO-2-CARBOXYETHYL)-3(2-CARBOXYTHIOPHENE-3-YL-METHYL)-5-METHYLPYRIMIDINE-2,4-DIONE (three-letter code: UBA) (formula: C<sub>14</sub>H<sub>15</sub>N<sub>3</sub>O<sub>6</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			24	14	3	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			24	14	3	6	1		

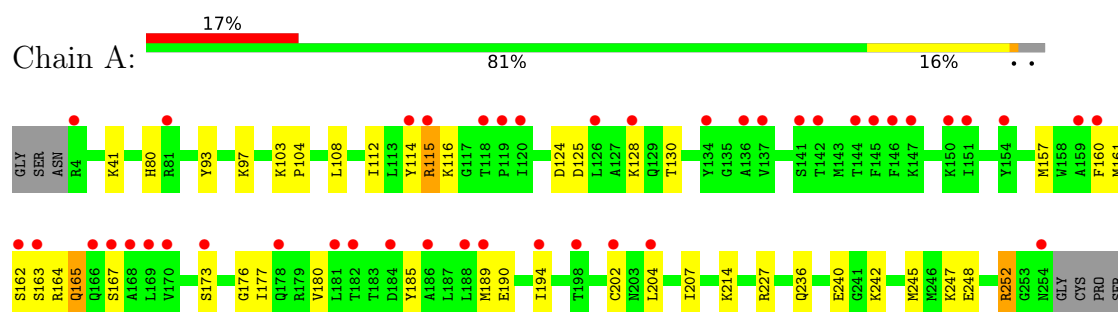
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	141	Total	O	0	2
			141	141		
5	B	147	Total	O	0	2
			147	147		

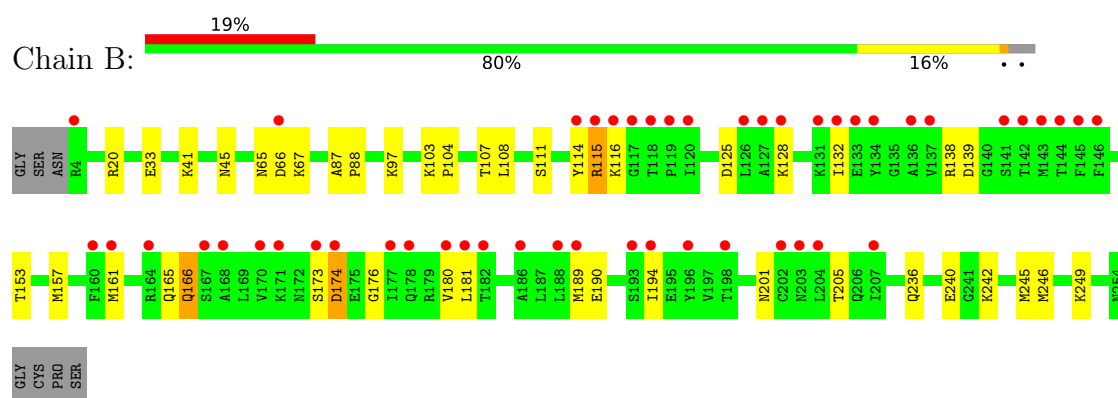
### 3 Residue-property plots

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: Glutamate receptor, ionotropic kainate 1



- Molecule 1: Glutamate receptor, ionotropic kainate 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.60Å 97.73Å 128.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.83 – 1.95 27.83 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.5 (27.83-1.95) 96.1 (27.83-1.95)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.190 , 0.233 0.208 , 0.234	Depositor DCC
$R_{free}$ test set	2184 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.0	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.476 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4706	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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: BR, 1PE, UBA

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	0.48	0/2186	0.60	0/2941
1	B	0.53	2/2226 (0.1%)	0.61	0/2991
All	All	0.50	2/4412 (0.0%)	0.60	0/5932

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	132	ILE	C-O	7.57	1.37	1.23
1	B	132	ILE	C-N	6.57	1.49	1.34

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	A	2148	0	2165	45	0
1	B	2188	0	2214	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	16	0	22	1	0
3	B	16	0	22	1	0
4	A	24	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	0	13	0	0
5	A	141	0	0	6	0
5	B	147	0	0	14	0
All	All	4706	0	4449	86	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (86) 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:97[B]:LYS:HD2	5:B:630:HOH:O	1.58	1.01
1:A:248[A]:GLU:O	1:A:252:ARG:HG3	1.73	0.89
1:B:107[A]:THR:HG21	5:B:521:HOH:O	1.73	0.86
3:B:401:1PE:OH2	5:B:608:HOH:O	1.94	0.86
1:A:248[B]:GLU:O	1:A:252:ARG:HG3	1.78	0.81
1:A:97[B]:LYS:CD	5:B:630:HOH:O	2.20	0.81
1:A:97[B]:LYS:CE	5:B:630:HOH:O	2.30	0.80
1:A:240[A]:GLU:HG3	1:A:242:LYS:HG3	1.66	0.77
1:B:240[A]:GLU:HG3	1:B:242:LYS:HG3	1.72	0.71
1:A:245:MET:HE3	5:A:571:HOH:O	1.91	0.71
1:A:173:SER:OG	1:A:189[B]:MET:SD	2.48	0.70
1:B:166:GLN:NE2	1:B:166:GLN:H	1.92	0.68
1:A:173:SER:O	1:A:177:ILE:HG13	1.96	0.66
1:A:189[A]:MET:CG	1:A:194:ILE:HG13	2.26	0.65
1:A:97[A]:LYS:HD2	5:A:613:HOH:O	1.97	0.65
1:A:173:SER:OG	1:A:189[B]:MET:CE	2.45	0.64
1:B:189[A]:MET:HG3	1:B:194:ILE:HG13	1.79	0.64
1:A:93:TYR:CZ	1:A:97[B]:LYS:NZ	2.66	0.64
1:A:164:ARG:HG3	1:A:167:SER:OG	1.99	0.62
1:A:252:ARG:O	1:A:252:ARG:CD	2.48	0.61
1:A:176:GLY:O	1:A:180:VAL:HG23	2.00	0.61
1:B:176:GLY:O	1:B:180:VAL:HG23	2.02	0.60
1:B:236[B]:GLN:NE2	5:B:548:HOH:O	2.32	0.60
1:A:189[A]:MET:HG3	1:A:194:ILE:HG13	1.84	0.59
3:A:401:1PE:C12	5:A:634:HOH:O	2.45	0.59
1:B:97[B]:LYS:HE2	5:B:606:HOH:O	2.01	0.59
1:A:97[B]:LYS:HD3	5:A:548:HOH:O	2.02	0.58
1:B:189[A]:MET:CG	1:B:194:ILE:HG13	2.34	0.58
1:B:236[A]:GLN:O	1:B:240[A]:GLU:HG2	2.04	0.58
1:A:97[B]:LYS:NZ	5:A:548:HOH:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20[A]:ARG:HD3	1:B:33:GLU:HB3	1.87	0.56
1:A:163:SER:C	1:A:165:GLN:H	2.08	0.56
1:A:236[A]:GLN:O	1:A:240[A]:GLU:HG2	2.05	0.56
1:A:252:ARG:O	1:A:252:ARG:HD3	2.05	0.56
1:A:130:THR:HG22	1:A:130:THR:O	2.06	0.55
1:A:162:SER:O	1:A:165:GLN:HB2	2.07	0.55
1:A:130:THR:HG23	1:A:160:PHE:HE1	1.71	0.55
1:B:97[B]:LYS:CE	5:B:606:HOH:O	2.55	0.54
1:B:174:ASP:OD2	1:B:174:ASP:N	2.41	0.54
1:A:97[B]:LYS:CD	5:A:548:HOH:O	2.57	0.52
1:B:245[A]:MET:HE3	5:B:579:HOH:O	2.08	0.52
1:A:114:TYR:CD1	1:A:115:ARG:NH1	2.74	0.52
1:A:115:ARG:NH1	1:A:115:ARG:H	2.08	0.52
1:A:252:ARG:O	1:A:252:ARG:HD2	2.10	0.52
1:B:190[A]:GLU:HA	1:B:190[A]:GLU:OE1	2.11	0.50
1:A:112:ILE:HB	1:A:207:ILE:HB	1.92	0.50
1:B:97[B]:LYS:N	1:B:97[B]:LYS:HE3	2.27	0.50
1:B:115:ARG:H	1:B:115:ARG:NH1	2.09	0.50
1:B:173:SER:OG	1:B:189[B]:MET:SD	2.63	0.50
1:B:236[B]:GLN:O	1:B:240[B]:GLU:HG3	2.12	0.50
1:A:125:ASP:HA	1:A:128:LYS:NZ	2.27	0.49
1:A:93:TYR:CE1	1:A:97[B]:LYS:NZ	2.80	0.49
1:A:157:MET:O	1:A:161:MET:HG3	2.12	0.49
1:B:115:ARG:NH1	1:B:180:VAL:HG13	2.28	0.49
1:B:115:ARG:HH11	1:B:115:ARG:N	2.11	0.48
1:B:107[A]:THR:CG2	5:B:521:HOH:O	2.45	0.48
1:A:80:HIS:HD2	5:B:648:HOH:O	1.97	0.48
1:B:242:LYS:O	1:B:246[A]:MET:HG3	2.15	0.47
1:B:65:ASN:C	1:B:67:LYS:H	2.18	0.47
1:B:166:GLN:H	1:B:166:GLN:HE21	1.61	0.47
1:A:130:THR:HG23	1:A:160:PHE:CE1	2.51	0.46
1:B:97[B]:LYS:CD	5:B:606:HOH:O	2.63	0.46
1:B:181:LEU:HD21	1:B:201[A]:ASN:ND2	2.30	0.46
1:B:115:ARG:NH1	1:B:115:ARG:N	2.64	0.45
1:B:125:ASP:HA	1:B:128:LYS:NZ	2.31	0.45
1:B:20[B]:ARG:HG2	1:B:33:GLU:HB3	1.98	0.45
1:A:97[B]:LYS:HE3	5:B:630:HOH:O	2.07	0.45
1:A:115:ARG:N	1:A:115:ARG:HH11	2.14	0.45
1:B:242:LYS:HA	1:B:245[B]:MET:HG2	1.99	0.45
1:A:115:ARG:NH1	1:A:180:VAL:HG13	2.32	0.45
1:A:115:ARG:NH2	1:A:185:TYR:H	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LYS:NZ	1:A:202:CYS:O	2.43	0.44
1:B:103:LYS:HB3	1:B:104:PRO:HD2	2.00	0.43
1:A:103:LYS:HB3	1:A:104:PRO:HD2	2.01	0.43
1:A:80:HIS:HB2	1:B:249:LYS:HG3	2.00	0.42
1:A:115:ARG:H	1:A:115:ARG:HH11	1.68	0.42
1:B:41[B]:LYS:HE3	1:B:45:ASN:HD21	1.85	0.42
1:B:87:ALA:HB1	1:B:88:PRO:HD2	2.01	0.42
1:B:111:SER:HB3	1:B:194:ILE:HD12	2.00	0.42
1:B:41[B]:LYS:NZ	5:B:586:HOH:O	2.53	0.41
1:B:116:LYS:HG2	1:B:205:THR:HB	2.02	0.41
1:A:190[A]:GLU:OE2	1:A:190[A]:GLU:HA	2.21	0.41
1:B:114:TYR:CD1	1:B:115:ARG:NH1	2.88	0.40
1:B:138:ARG:HG2	1:B:139:ASP:CG	2.42	0.40
1:B:157:MET:O	1:B:161:MET:HG3	2.21	0.40
1:A:41:LYS:HA	1:A:41:LYS:HD2	1.96	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	266/258 (103%)	258 (97%)	8 (3%)	0	100	100
1	B	270/258 (105%)	260 (96%)	9 (3%)	1 (0%)	34	22
All	All	536/516 (104%)	518 (97%)	17 (3%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	ASP

### 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	237/225 (105%)	228 (96%)	9 (4%)	33	21
1	B	241/225 (107%)	235 (98%)	6 (2%)	47	38
All	All	478/450 (106%)	463 (97%)	15 (3%)	37	28

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LEU
1	A	115	ARG
1	A	124	ASP
1	A	165	GLN
1	A	204	LEU
1	A	214	LYS
1	A	227	ARG
1	A	247	LYS
1	A	252	ARG
1	B	108	LEU
1	B	115	ARG
1	B	153	THR
1	B	165	GLN
1	B	166	GLN
1	B	174	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	166	GLN
1	A	201	ASN
1	A	254	ASN
1	B	166	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z  > 2$
4	UBA	B	501	-	12,25,25	1.26	2 (16%)	10,36,36	2.88	5 (50%)
3	1PE	A	401	-	15,15,15	0.50	0	14,14,14	0.30	0
4	UBA	A	501	-	12,25,25	1.31	2 (16%)	10,36,36	2.76	3 (30%)
3	1PE	B	401	-	15,15,15	0.50	0	14,14,14	0.38	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
4	UBA	B	501	-	-	1/7/16/16	0/2/2/2
3	1PE	A	401	-	-	4/13/13/13	-
4	UBA	A	501	-	-	0/7/16/16	0/2/2/2
3	1PE	B	401	-	-	6/13/13/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	UBA	C1-C2	2.96	1.47	1.41
4	B	501	UBA	C1-C2	2.80	1.47	1.41
4	B	501	UBA	CB-N4	-2.20	1.46	1.48
4	A	501	UBA	CB-N4	-2.19	1.46	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	UBA	C17-N6-C5	5.86	124.78	117.92
4	B	501	UBA	C17-N6-C5	5.76	124.66	117.92
4	B	501	UBA	C17-C18-C19	-5.04	119.34	127.43
4	A	501	UBA	C17-C18-C19	-4.61	120.03	127.43
4	B	501	UBA	C6-C2-C3	2.78	124.54	118.68
4	A	501	UBA	C6-C2-C3	2.59	124.14	118.68
4	B	501	UBA	CB-N4-C3	2.36	122.31	118.22
4	B	501	UBA	C6-C2-C1	-2.10	117.60	121.37

There are no chirality outliers.

All (11) torsion outliers are listed below:

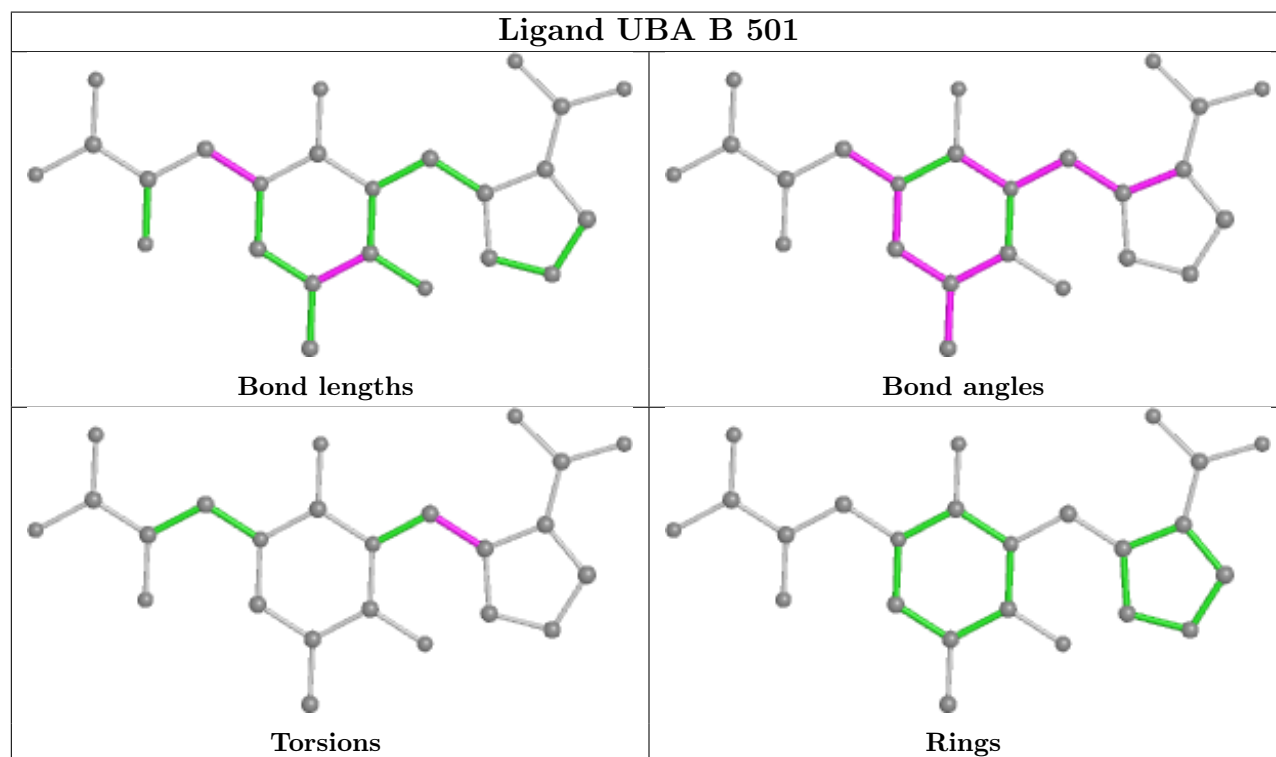
Mol	Chain	Res	Type	Atoms
3	B	401	1PE	OH6-C15-C25-OH5
3	A	401	1PE	OH6-C15-C25-OH5
3	B	401	1PE	OH4-C13-C23-OH3
3	B	401	1PE	OH7-C16-C26-OH6
4	B	501	UBA	N6-C17-C18-C23
3	A	401	1PE	C16-C26-OH6-C15
3	A	401	1PE	C25-C15-OH6-C26
3	B	401	1PE	C25-C15-OH6-C26
3	A	401	1PE	C15-C25-OH5-C14
3	B	401	1PE	OH2-C12-C22-OH3
3	B	401	1PE	C16-C26-OH6-C15

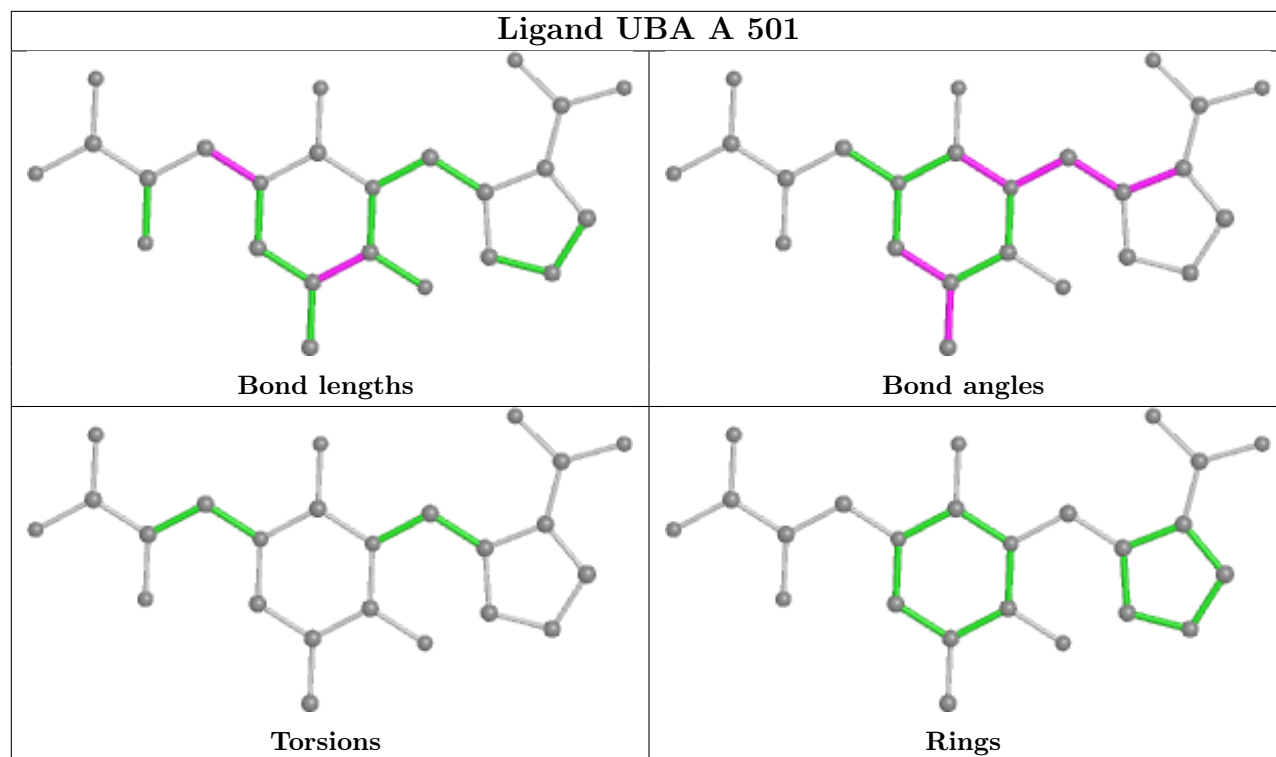
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	1PE	1	0
3	B	401	1PE	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	251/258 (97%)	0.95	43 (17%)  	17, 30, 62, 71	0
1	B	251/258 (97%)	1.10	49 (19%)  	17, 30, 64, 71	0
All	All	502/516 (97%)	1.02	92 (18%)  	17, 31, 63, 71	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	ALA	9.8
1	B	117	GLY	9.3
1	B	114	TYR	6.4
1	B	126	LEU	6.0
1	B	115	ARG	5.6
1	B	131	LYS	5.5
1	B	160	PHE	5.2
1	B	180	VAL	5.2
1	B	181	LEU	4.8
1	A	159	ALA	4.6
1	A	160	PHE	4.5
1	B	132	ILE	4.4
1	A	181	LEU	4.3
1	B	120	ILE	4.2
1	A	154	TYR	4.0
1	B	168	ALA	4.0
1	B	137	VAL	4.0
1	B	178	GLN	3.9
1	A	162	SER	3.9
1	B	202	CYS	3.9
1	A	184	ASP	3.8
1	B	167	SER	3.8
1	A	163	SER	3.8
1	B	186	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	189[A]	MET	3.5
1	A	118	THR	3.4
1	B	182	THR	3.4
1	B	174	ASP	3.4
1	A	188	LEU	3.3
1	A	189[A]	MET	3.3
1	B	134	TYR	3.2
1	A	167	SER	3.2
1	A	178	GLN	3.2
1	B	141	SER	3.2
1	A	126	LEU	3.1
1	B	164	ARG	3.1
1	B	145	PHE	3.1
1	B	177	ILE	3.0
1	B	128	LYS	3.0
1	A	144	THR	3.0
1	B	188	LEU	3.0
1	A	137	VAL	2.9
1	A	136	ALA	2.9
1	B	144	THR	2.9
1	A	202	CYS	2.9
1	B	203	ASN	2.9
1	A	150	LYS	2.9
1	A	151	ILE	2.8
1	A	115	ARG	2.8
1	A	142	THR	2.8
1	B	171	LYS	2.7
1	B	143	MET	2.7
1	B	173	SER	2.7
1	A	169	LEU	2.7
1	B	170	VAL	2.7
1	B	119	PRO	2.6
1	A	173	SER	2.6
1	B	146	PHE	2.6
1	A	145	PHE	2.6
1	A	194	ILE	2.5
1	B	207	ILE	2.5
1	A	170	VAL	2.5
1	A	134	TYR	2.5
1	B	142	THR	2.5
1	A	4	ARG	2.5
1	B	136	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	146	PHE	2.5
1	A	147	LYS	2.4
1	B	161	MET	2.4
1	B	133	GLU	2.4
1	A	119	PRO	2.4
1	A	141[A]	SER	2.4
1	A	204	LEU	2.4
1	A	254	ASN	2.4
1	A	198	THR	2.4
1	B	127	ALA	2.4
1	A	81[A]	ARG	2.4
1	A	128	LYS	2.3
1	B	118	THR	2.3
1	B	116	LYS	2.3
1	B	193	SER	2.3
1	A	114	TYR	2.2
1	A	120	ILE	2.2
1	A	182	THR	2.2
1	A	186	ALA	2.2
1	A	166	GLN	2.2
1	B	194	ILE	2.1
1	B	198	THR	2.1
1	B	196	TYR	2.1
1	B	204	LEU	2.0
1	B	66	ASP	2.0
1	B	4	ARG	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

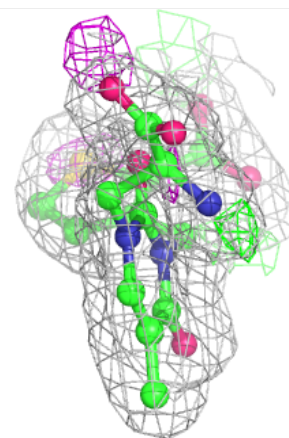
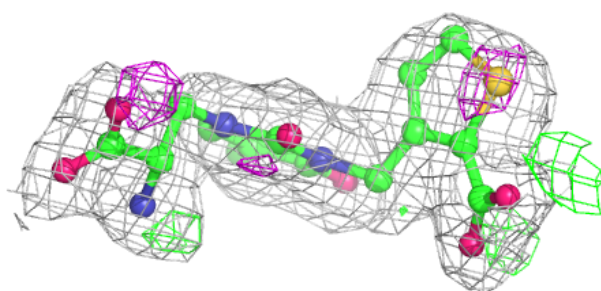
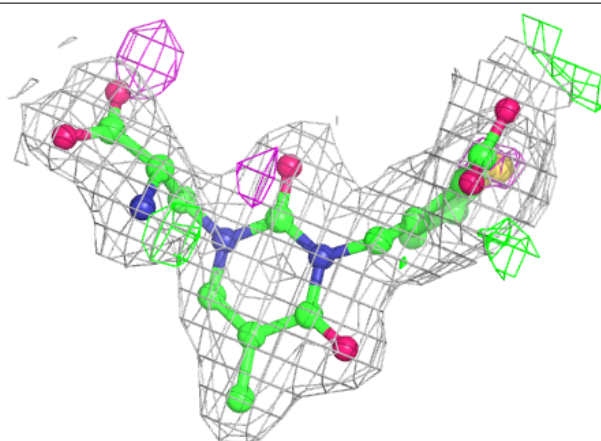
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	UBA	A	501	24/24	0.87	0.14	32,36,43,45	0
4	UBA	B	501	24/24	0.90	0.14	31,36,43,45	0
3	1PE	A	401	16/16	0.94	0.12	24,25,31,32	16
3	1PE	B	401	16/16	0.94	0.14	23,26,33,34	16
2	BR	A	301	1/1	0.99	0.10	39,39,39,39	1
2	BR	B	301	1/1	0.99	0.03	38,38,38,38	1

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.

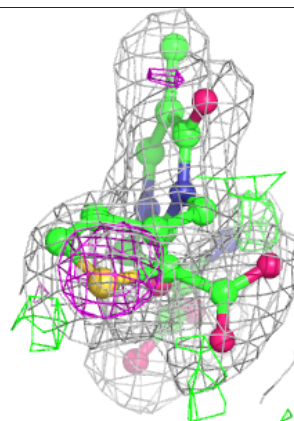
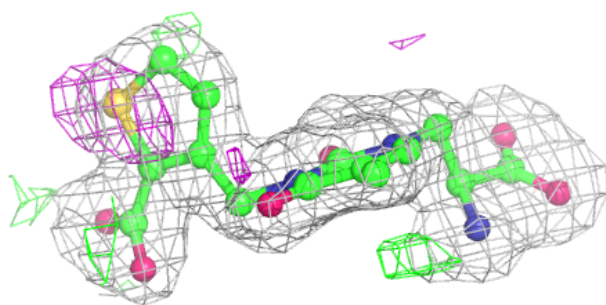
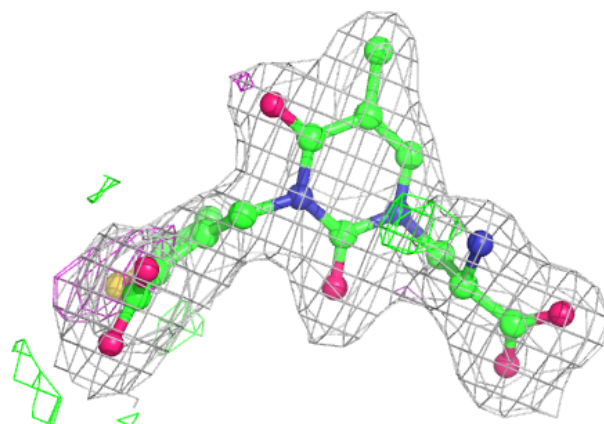
**Electron density around UBA A 501:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around UBA B 501:**

$2mF_o-DF_c$  (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.