



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 08:15 PM GMT

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 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 <http://wwpdb.org/ValidationPDFNotes.html>

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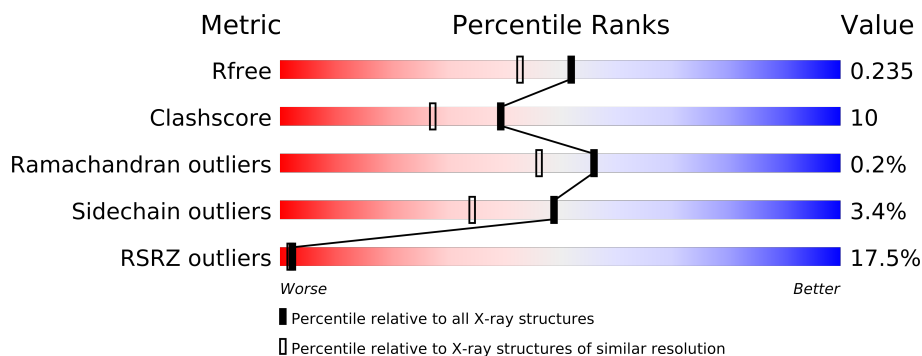
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	258	
1	B	258	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	1PE	B	401	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4706 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

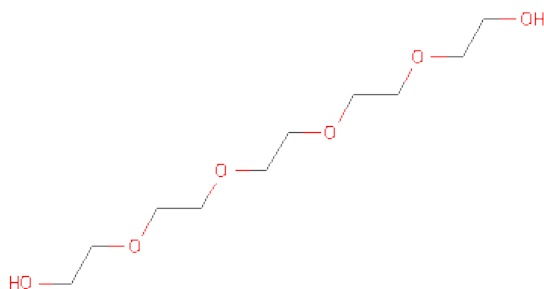
There are 12 discrepancies between the modelled and reference sequences:

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	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	UNP P22756

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

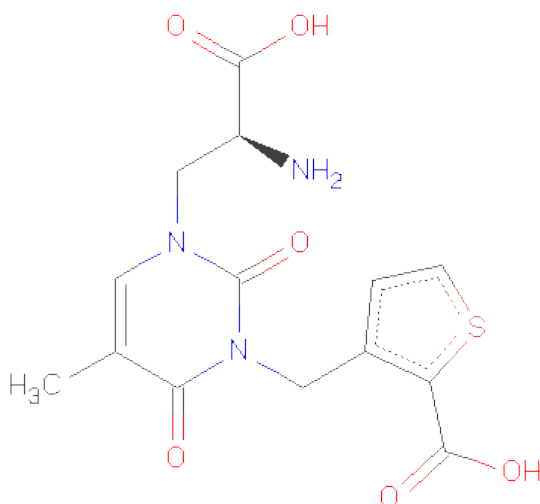
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Br	0	0
			1	1		
2	A	1	Total	Br	0	0
			1	1		

- 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-Y L-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		

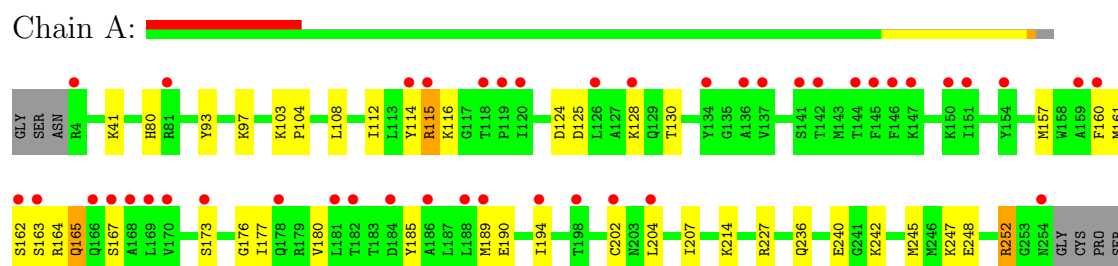
- Molecule 5 is water.

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

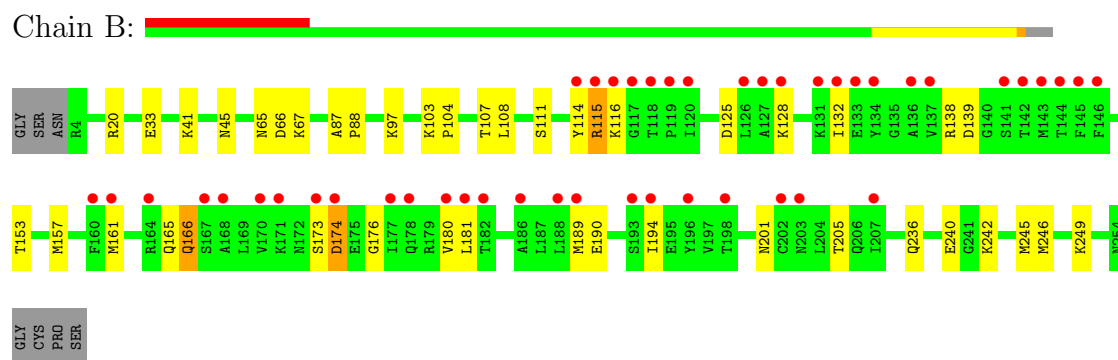
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 , 0.235	Depositor DCC
$R_{free}$ test set	2184 reflections (5.29%)	DCC
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> )	0.33 , 43.4	EDS
Estimated twinning fraction	0.476 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 43450 reflections	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.

## 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: UBA, BR, 1PE

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	22	1	0
4	A	24	0	13	0	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (86) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:CD	1:A:252:ARG:O	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	Distance(Å)	Clash(Å)
1:B:20[A]:ARG:HD3	1:B:33:GLU:HB3	1.87	0.56
1:A:236[A]:GLN:O	1:A:240[A]:GLU:HG2	2.05	0.56
1:A:163:SER:C	1:A:165:GLN:H	2.08	0.56
1:A:252:ARG:HD3	1:A:252:ARG:O	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:N	1:B:174:ASP:OD2	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:252:ARG:HD2	1:A:252:ARG:O	2.10	0.52
1:A:115:ARG:H	1:A:115:ARG:NH1	2.08	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:115:ARG:H	1:B:115:ARG:NH1	2.09	0.50
1:B:97[B]:LYS:N	1:B:97[B]:LYS:HE3	2.27	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:B:115:ARG:NH1	1:B:180:VAL:HG13	2.28	0.49
1:A:157:MET:O	1:A:161:MET:HG3	2.12	0.49
1:B:115:ARG:N	1:B:115:ARG:HH11	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:HE21	1:B:166:GLN:H	1.61	0.47
1:B:97[B]:LYS:CD	5:B:606:HOH:O	2.63	0.46
1:A:130:THR:HG23	1:A:160:PHE:CE1	2.51	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
1:A:116:LYS:NZ	1:A:202:CYS:O	2.43	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:HD2	1:A:41:LYS:HA	1.96	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	266/258 (103%)	258 (97%)	8 (3%)	0	100	100
1	B	270/258 (105%)	260 (96%)	9 (3%)	1 (0%)	43	30
All	All	536/516 (104%)	518 (97%)	17 (3%)	1 (0%)	56	46

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%)	44	29
1	B	241/225 (107%)	235 (98%)	6 (2%)	60	48
All	All	478/450 (106%)	463 (97%)	15 (3%)	49	38

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

Some 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 chains 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 ⓘ

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	$\# Z  > 2$
3	1PE	A	401	-	15,15,15	0.51	0	14,14,14	0.31	0
4	UBA	A	501	-	25,25,25	1.47	5 (20%)	30,36,36	2.60	10 (33%)
3	1PE	B	401	-	15,15,15	0.51	0	14,14,14	0.38	0
4	UBA	B	501	-	25,25,25	1.30	5 (20%)	30,36,36	2.35	11 (36%)

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	1PE	A	401	-	-	0/13/13/13	0/0/0/0
4	UBA	A	501	-	-	0/13/16/16	0/2/2/2
3	1PE	B	401	-	-	0/13/13/13	0/0/0/0
4	UBA	B	501	-	-	0/13/16/16	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	UBA	C5-N4	3.71	1.42	1.38
4	A	501	UBA	C19-C18	2.93	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	UBA	C19-C18	2.85	1.47	1.38
4	A	501	UBA	C1-C2	2.27	1.47	1.42
4	B	501	UBA	C5-N4	2.18	1.40	1.38
4	B	501	UBA	CB-N4	-2.18	1.46	1.48
4	A	501	UBA	CB-N4	-2.17	1.46	1.48
4	B	501	UBA	C1-C2	2.12	1.47	1.42
4	B	501	UBA	C5-N6	2.11	1.40	1.38
4	A	501	UBA	C5-N6	2.04	1.40	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	UBA	C3-N4-C5	9.28	122.19	118.59
4	B	501	UBA	C3-N4-C5	6.42	121.08	118.59
4	A	501	UBA	C1-N6-C5	-4.64	119.77	123.42
4	B	501	UBA	C1-N6-C5	-4.49	119.90	123.42
4	B	501	UBA	CA-CB-N4	-4.34	106.28	112.44
4	A	501	UBA	CA-CB-N4	-3.89	106.92	112.44
4	B	501	UBA	O1-C10-C19	-3.45	116.78	123.11
4	B	501	UBA	C17-C18-C19	-3.44	119.34	127.43
4	A	501	UBA	O1-C10-C19	-3.36	116.95	123.11
4	A	501	UBA	C17-C18-C19	-3.14	120.03	127.43
4	A	501	UBA	C22-S20-C19	3.10	96.00	91.47
4	A	501	UBA	C17-N6-C5	2.87	124.78	119.50
4	B	501	UBA	C6-C2-C3	2.80	124.54	118.59
4	B	501	UBA	C17-N6-C5	2.80	124.66	119.50
4	B	501	UBA	C22-S20-C19	2.79	95.55	91.47
4	B	501	UBA	C6-C2-C1	-2.65	117.60	122.88
4	A	501	UBA	C6-C2-C3	2.61	124.14	118.59
4	A	501	UBA	C6-C2-C1	-2.51	117.88	122.88
4	B	501	UBA	CB-N4-C5	-2.35	116.61	119.37
4	A	501	UBA	C18-C19-S20	-2.30	108.24	111.00
4	B	501	UBA	C18-C19-S20	-2.04	108.55	111.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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%)	0.94	43 (17%) 2 2	17, 30, 62, 71	0
1	B	251/258 (97%)	1.08	46 (18%) 2 1	17, 30, 64, 71	0
All	All	502/516 (97%)	1.01	89 (17%) 2 2	17, 31, 63, 71	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	117	GLY	9.0
1	A	168	ALA	8.9
1	B	114	TYR	5.9
1	B	115	ARG	5.4
1	B	131	LYS	5.3
1	B	180	VAL	4.9
1	B	126	LEU	4.9
1	B	160	PHE	4.8
1	A	159	ALA	4.6
1	B	181	LEU	4.4
1	A	160	PHE	4.2
1	A	181	LEU	4.1
1	B	132	ILE	4.1
1	B	120	ILE	3.9
1	B	168	ALA	3.8
1	A	184	ASP	3.7
1	A	154	TYR	3.7
1	A	162	SER	3.7
1	A	163	SER	3.6
1	B	178	GLN	3.6
1	B	137	VAL	3.6
1	B	167	SER	3.5
1	A	118	THR	3.5
1	B	174	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	186	ALA	3.2
1	B	182	THR	3.1
1	A	188	LEU	3.1
1	B	189[A]	MET	3.1
1	B	134	TYR	3.0
1	A	178	GLN	3.0
1	B	202	CYS	3.0
1	B	164	ARG	3.0
1	A	167	SER	3.0
1	B	128	LYS	3.0
1	B	177	ILE	2.9
1	B	141	SER	2.9
1	A	136	ALA	2.8
1	B	145	PHE	2.8
1	A	115	ARG	2.7
1	A	189[A]	MET	2.7
1	A	144	THR	2.7
1	B	188	LEU	2.7
1	A	137	VAL	2.6
1	B	170	VAL	2.6
1	B	203	ASN	2.6
1	A	151	ILE	2.6
1	A	150	LYS	2.5
1	B	144	THR	2.5
1	B	173	SER	2.5
1	A	194	ILE	2.5
1	B	119	PRO	2.5
1	A	126	LEU	2.5
1	A	202	CYS	2.5
1	B	143	MET	2.5
1	B	171	LYS	2.5
1	A	173	SER	2.5
1	A	134	TYR	2.4
1	A	142	THR	2.4
1	A	169	LEU	2.4
1	B	207	ILE	2.4
1	B	136	ALA	2.3
1	B	146	PHE	2.3
1	A	170	VAL	2.3
1	A	145	PHE	2.3
1	A	119	PRO	2.3
1	A	4	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	198	THR	2.3
1	B	118	THR	2.2
1	A	146	PHE	2.2
1	A	120	ILE	2.2
1	B	193	SER	2.2
1	A	182	THR	2.2
1	B	133	GLU	2.2
1	A	128	LYS	2.2
1	B	161	MET	2.2
1	B	116	LYS	2.2
1	A	254	ASN	2.2
1	A	204	LEU	2.2
1	A	147	LYS	2.2
1	B	142	THR	2.2
1	A	114	TYR	2.1
1	A	186	ALA	2.1
1	A	81[A]	ARG	2.1
1	A	141[A]	SER	2.1
1	A	166	GLN	2.1
1	B	194	ILE	2.1
1	B	198	THR	2.0
1	B	196	TYR	2.0
1	B	127	ALA	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	1PE	B	401	16/16	0.14	6.61	23,26,33,34	16
3	1PE	A	401	16/16	0.12	-0.04	24,25,31,32	16
4	UBA	A	501	24/24	0.15	-0.62	32,36,43,45	0
4	UBA	B	501	24/24	0.14	-0.67	31,36,43,45	0
2	BR	A	301	1/1	0.08	-2.90	39,39,39,39	1
2	BR	B	301	1/1	0.03	-5.32	38,38,38,38	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.