



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:58 AM GMT

PDB ID : 2F34  
Title : Crystal Structure of the GluR5 Ligand Binding Core Dimer with UBP310 At  
1.74 Angstroms Resolution  
Authors : Mayer, M.L.  
Deposited on : 2005-11-18  
Resolution : 1.74 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

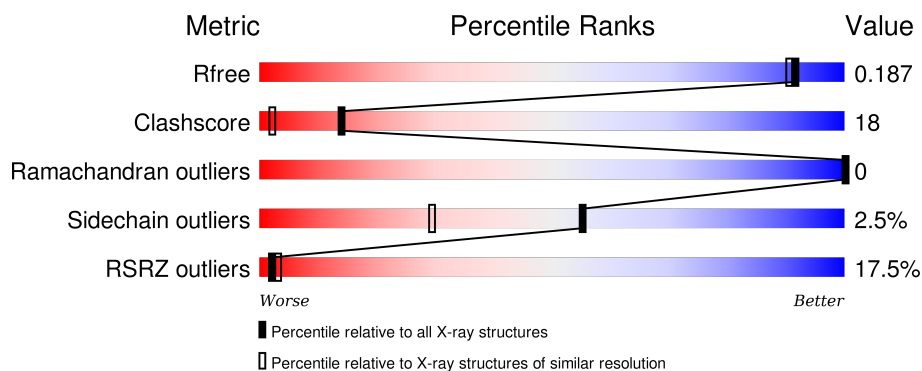
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.74 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))
$R_{free}$	91344	2417 (1.76-1.72)
Clashscore	102246	2570 (1.76-1.72)
Ramachandran outliers	100387	2544 (1.76-1.72)
Sidechain outliers	100360	2544 (1.76-1.72)
RSRZ outliers	91569	2420 (1.76-1.72)

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. 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	
1	B	258	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1PE	B	601	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4917 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	19	0
			2165	1379	362	410	14			
1	B	251	Total	C	N	O	S	0	21	0
			2188	1392	369	411	16			

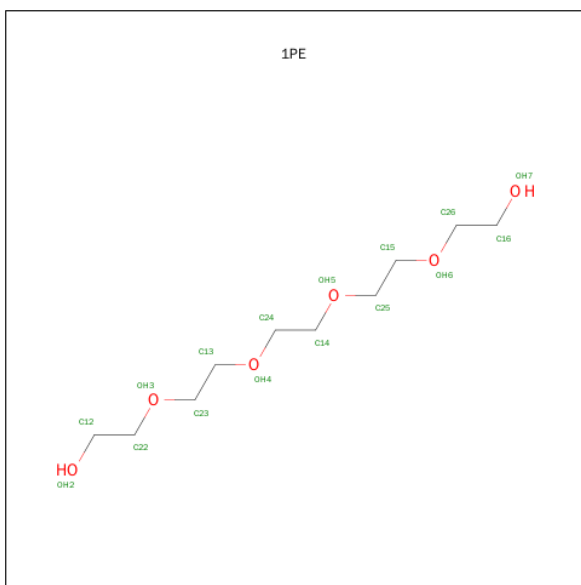
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP P22756
A	2	SER	-	CLONING ARTIFACT	UNP P22756
A	117	GLY	-	LINKER	UNP P22756
A	118	THR	-	LINKER	UNP P22756
A	258	SER	GLU	ENGINEERED	UNP P22756
B	1	GLY	-	CLONING ARTIFACT	UNP P22756
B	2	SER	-	CLONING ARTIFACT	UNP P22756
B	117	GLY	-	LINKER	UNP P22756
B	118	THR	-	LINKER	UNP P22756
B	258	SER	GLU	ENGINEERED	UNP P22756

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

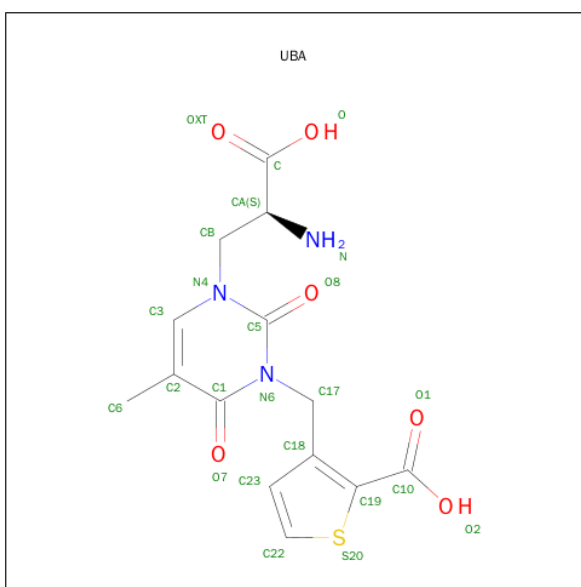
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- 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	B	1	Total	C	O	0	0
			16	10	6		
3	A	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		

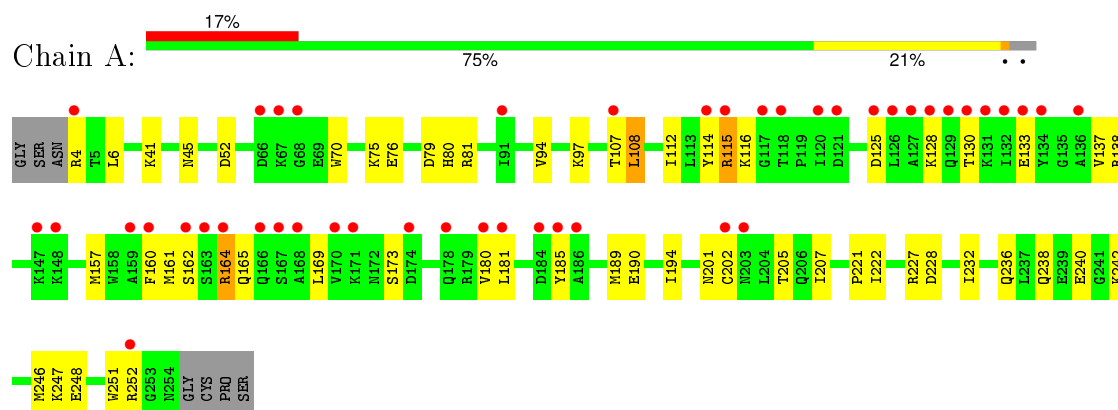
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	239	Total	O	0	8
			239	239		
5	B	243	Total	O	0	9
			243	243		

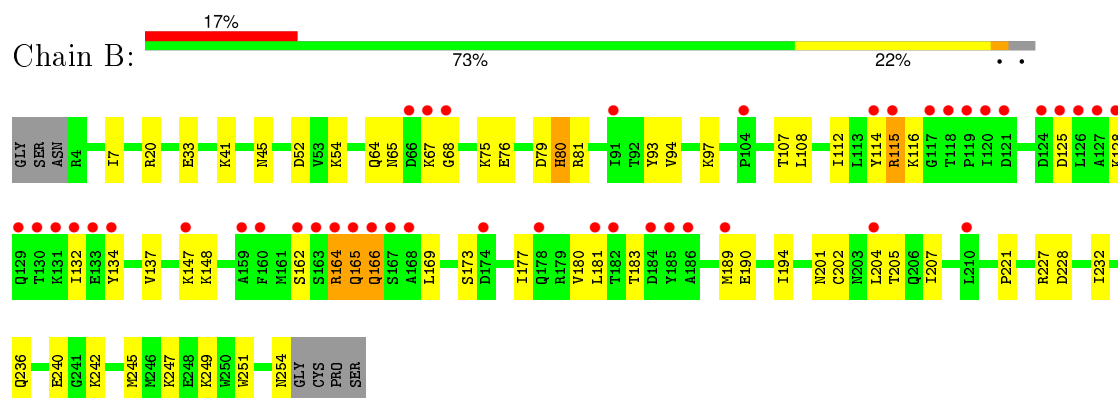
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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, $\alpha$ , $\beta$ , $\gamma$	97.70Å 97.95Å 129.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.41 – 1.74 33.41 – 1.73	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.41-1.74) 99.5 (33.41-1.73)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.11 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.181 , 0.211 0.183 , 0.187	Depositor DCC
$R_{free}$ test set	3189 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.8	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.5	EDS
Estimated twinning fraction	0.460 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 64048 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4917	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CL, UBA, 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	0.59	0/2203	0.77	1/2963 (0.0%)
1	B	0.78	4/2226 (0.2%)	0.80	1/2991 (0.0%)
All	All	0.69	4/4429 (0.1%)	0.79	2/5954 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	132	ILE	C-O	11.94	1.46	1.23
1	B	132	ILE	C-N	10.95	1.59	1.34
1	B	183	THR	C-O	5.71	1.34	1.23
1	B	134	TYR	CG-CD1	5.37	1.46	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	ILE	O-C-N	5.40	131.34	122.70
1	A	52	ASP	CB-CG-OD1	5.04	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2165	0	2187	85	0
1	B	2188	0	2214	82	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	16	0	22	0	1
3	B	16	0	22	0	2
4	A	24	0	13	0	0
4	B	24	0	13	0	0
5	A	239	0	0	15	1
5	B	243	0	0	18	3
All	All	4917	0	4471	164	4

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 (164) 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:238[B]:GLN:HG3	5:A:1039[B]:HOH:O	1.62	0.97
1:A:248[A]:GLU:O	1:A:252:ARG:HG3	1.65	0.96
1:B:164:ARG:HH11	1:B:164:ARG:HG2	1.27	0.94
1:A:248[B]:GLU:O	1:A:252:ARG:HG3	1.67	0.93
1:B:166:GLN:HE21	1:B:166:GLN:H	1.14	0.92
1:A:108:LEU:HD12	1:A:190[A]:GLU:HG3	1.49	0.92
1:B:166:GLN:NE2	1:B:166:GLN:H	1.68	0.91
1:A:164:ARG:HH11	1:A:164:ARG:HG2	1.34	0.90
1:A:162:SER:O	1:A:165:GLN:HB2	1.72	0.89
1:A:221:PRO:HG3	5:A:1008:HOH:O	1.72	0.88
1:B:221:PRO:HG3	5:B:1012:HOH:O	1.74	0.86
1:B:245[B]:MET:HG3	5:B:808:HOH:O	1.75	0.86
1:A:164:ARG:HH11	1:A:164:ARG:CG	1.91	0.83
1:B:164:ARG:HH11	1:B:164:ARG:CG	1.92	0.82
1:A:108:LEU:HD12	1:A:190[A]:GLU:CG	2.12	0.80
1:A:97[B]:LYS:HD2	5:A:954:HOH:O	1.82	0.79
1:B:189[A]:MET:HG3	1:B:194:ILE:HG13	1.64	0.79
1:B:245[B]:MET:CG	5:B:808:HOH:O	2.30	0.79
1:A:189[A]:MET:CG	1:A:194:ILE:HG13	2.12	0.79
1:B:115:ARG:H	1:B:115:ARG:NH1	1.81	0.78
1:B:173:SER:OG	1:B:189[B]:MET:CE	2.33	0.77
1:B:75[A]:LYS:HE3	1:B:79:ASP:OD2	1.84	0.77
1:B:181:LEU:CD2	1:B:204:LEU:HD11	2.16	0.75
1:A:189[A]:MET:HG2	1:A:194:ILE:HG13	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ARG:HD2	1:A:252:ARG:O	1.87	0.74
1:A:236[A]:GLN:O	1:A:240[A]:GLU:HG2	1.87	0.74
1:B:181:LEU:HD23	1:B:204:LEU:HD11	1.70	0.73
1:A:115:ARG:H	1:A:115:ARG:NH1	1.86	0.73
1:A:108:LEU:CD1	1:A:190[A]:GLU:HG3	2.19	0.72
1:B:116:LYS:NZ	1:B:202:CYS:O	2.17	0.72
1:A:189[A]:MET:HG2	1:A:194:ILE:CG1	2.20	0.71
1:B:189[A]:MET:HG3	1:B:194:ILE:CG1	2.20	0.71
1:A:115:ARG:N	1:A:115:ARG:HH11	1.90	0.70
1:B:93:TYR:CD1	1:B:97[B]:LYS:NZ	2.56	0.70
1:B:107[A]:THR:HG21	5:B:972:HOH:O	1.90	0.70
1:B:115:ARG:N	1:B:115:ARG:HH11	1.91	0.69
1:B:115:ARG:NH1	1:B:180:VAL:HG13	2.08	0.69
1:B:115:ARG:NH1	1:B:115:ARG:N	2.42	0.67
1:A:173:SER:OG	1:A:189[B]:MET:CE	2.43	0.66
1:B:240[A]:GLU:HG3	1:B:242:LYS:HG3	1.78	0.65
1:B:232[B]:ILE:HG22	1:B:236[B]:GLN:HE21	1.61	0.65
1:B:125:ASP:HA	1:B:128:LYS:NZ	2.11	0.65
1:A:232[B]:ILE:O	1:A:236[B]:GLN:HG3	1.97	0.64
1:A:107[A]:THR:HG21	5:A:1031:HOH:O	1.97	0.64
1:B:93:TYR:O	1:B:97[B]:LYS:HD3	1.97	0.64
1:A:130:THR:HG23	1:A:160:PHE:HE1	1.63	0.64
1:A:97[B]:LYS:CD	5:A:954:HOH:O	2.43	0.63
1:B:181:LEU:HD21	1:B:201[A]:ASN:ND2	2.14	0.63
1:A:115:ARG:N	1:A:115:ARG:NH1	2.47	0.63
1:B:80:HIS:HD2	5:B:998:HOH:O	1.82	0.62
1:B:173:SER:OG	1:B:189[B]:MET:HE3	2.00	0.62
1:B:80:HIS:HA	5:B:1012:HOH:O	2.00	0.61
1:A:115:ARG:NH1	1:A:180:VAL:HG13	2.15	0.61
1:B:97[A]:LYS:HD2	5:B:1022:HOH:O	2.01	0.60
1:B:166:GLN:HE21	1:B:166:GLN:N	1.93	0.60
1:B:20[A]:ARG:HD3	1:B:33:GLU:HB3	1.84	0.60
1:B:181:LEU:HD21	1:B:201[A]:ASN:HD21	1.66	0.60
1:A:116:LYS:NZ	1:A:202:CYS:O	2.32	0.60
1:B:80:HIS:CD2	5:B:998:HOH:O	2.55	0.59
1:B:173:SER:OG	1:B:189[B]:MET:HE1	2.02	0.59
1:A:125:ASP:HA	1:A:128:LYS:NZ	2.17	0.59
1:B:162:SER:O	1:B:165:GLN:HB2	2.02	0.59
1:A:107[A]:THR:CG2	5:A:1031:HOH:O	2.51	0.59
1:A:173:SER:OG	1:A:189[B]:MET:HE3	2.03	0.58
1:B:112:ILE:HB	1:B:207:ILE:HB	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:HIS:CE1	5:A:1030:HOH:O	2.57	0.57
1:B:80:HIS:CE1	5:B:1033:HOH:O	2.58	0.57
1:A:130:THR:HG22	1:A:130:THR:O	2.05	0.57
1:B:114:TYR:HA	1:B:115:ARG:NH1	2.20	0.56
1:B:236[B]:GLN:NE2	5:B:891:HOH:O	2.22	0.56
1:A:164:ARG:NH1	1:A:164:ARG:HB2	2.21	0.56
1:B:94[A]:VAL:HG13	5:B:1016:HOH:O	2.06	0.56
1:A:107[A]:THR:HG23	5:A:853:HOH:O	2.05	0.56
1:A:240[A]:GLU:HG3	1:A:242:LYS:HG3	1.88	0.55
1:A:97[A]:LYS:HD2	5:A:953:HOH:O	2.06	0.55
1:B:41[B]:LYS:HE3	1:B:45:ASN:HD21	1.70	0.55
1:B:181:LEU:HD21	1:B:204:LEU:HD11	1.89	0.54
1:A:164:ARG:NH1	1:A:164:ARG:HG2	2.14	0.54
1:B:114:TYR:HA	1:B:115:ARG:HH12	1.73	0.53
1:B:228:ASP:O	1:B:232[A]:ILE:HG12	2.09	0.53
1:B:7:ILE:HD13	1:B:52[A]:ASP:HB3	1.91	0.53
1:A:190[A]:GLU:OE2	1:A:190[A]:GLU:HA	2.09	0.53
1:A:222:ILE:HD12	1:B:20[A]:ARG:NH2	2.24	0.53
1:A:41:LYS:HE2	1:A:45:ASN:HD21	1.74	0.52
1:A:80:HIS:CD2	5:B:807:HOH:O	2.61	0.52
1:A:221:PRO:CG	5:A:1008:HOH:O	2.40	0.52
1:A:164:ARG:HH11	1:A:164:ARG:CB	2.23	0.52
1:A:125:ASP:HA	1:A:128:LYS:HZ1	1.75	0.52
1:B:181:LEU:HD21	1:B:204:LEU:CD1	2.39	0.51
1:A:112:ILE:HB	1:A:207:ILE:HB	1.92	0.51
1:A:75[A]:LYS:HE3	1:A:79:ASP:OD2	2.11	0.51
1:B:116:LYS:HG2	1:B:205:THR:HB	1.92	0.51
1:B:164:ARG:NH1	1:B:164:ARG:HG2	2.07	0.51
1:A:138:ARG:CZ	1:A:165:GLN:OE1	2.59	0.51
1:B:232[B]:ILE:O	1:B:236[B]:GLN:HG3	2.10	0.51
1:A:236[B]:GLN:NE2	5:A:883:HOH:O	2.37	0.51
1:B:125:ASP:HA	1:B:128:LYS:HZ3	1.74	0.50
1:A:114:TYR:HA	1:A:115:ARG:NH1	2.26	0.50
1:B:173:SER:O	1:B:177:ILE:HG13	2.12	0.50
1:B:221:PRO:CG	5:B:1012:HOH:O	2.47	0.50
1:A:80:HIS:HA	5:A:1008:HOH:O	2.11	0.49
1:A:80:HIS:HE1	5:A:1030:HOH:O	1.93	0.49
1:A:165:GLN:HG2	1:A:169:LEU:HD12	1.93	0.49
1:B:164:ARG:NH1	1:B:164:ARG:CG	2.62	0.49
1:A:80:HIS:HD2	5:B:807:HOH:O	1.96	0.49
1:A:252:ARG:HD2	1:A:252:ARG:C	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:HIS:HB2	1:B:249:LYS:HG3	1.95	0.48
1:A:240[A]:GLU:OE2	1:A:242:LYS:HD2	2.13	0.48
1:B:147:LYS:HD2	1:B:147:LYS:C	2.34	0.48
1:B:165:GLN:HG2	1:B:169:LEU:HD12	1.96	0.48
1:B:65:ASN:OD1	1:B:68:GLY:N	2.47	0.48
1:A:248[A]:GLU:O	1:A:252:ARG:CG	2.50	0.47
1:B:97[B]:LYS:N	1:B:97[B]:LYS:CD	2.76	0.47
1:A:41:LYS:HE2	1:A:45:ASN:ND2	2.29	0.47
1:A:181:LEU:HD21	1:A:201:ASN:ND2	2.30	0.47
1:B:236[A]:GLN:O	1:B:240[A]:GLU:HG2	2.14	0.47
1:A:242:LYS:O	1:A:246[A]:MET:HG3	2.14	0.47
1:B:81[A]:ARG:NH1	5:B:971:HOH:O	2.48	0.46
1:B:181:LEU:CD2	1:B:204:LEU:CD1	2.91	0.46
1:A:70:TRP:HH2	1:A:94[B]:VAL:HG12	1.80	0.46
1:A:189[A]:MET:HB2	5:A:947[A]:HOH:O	2.15	0.46
1:A:181:LEU:HD21	1:A:201:ASN:HD21	1.80	0.46
1:A:248[A]:GLU:HG2	5:A:1036:HOH:O	2.14	0.46
1:B:166:GLN:NE2	1:B:166:GLN:N	2.50	0.46
1:B:93:TYR:CE1	1:B:97[B]:LYS:NZ	2.77	0.45
1:A:108:LEU:CD1	1:A:190[A]:GLU:CG	2.87	0.45
1:A:116:LYS:HG2	1:A:205:THR:HB	1.99	0.45
1:A:164:ARG:NH1	1:A:164:ARG:CB	2.79	0.45
1:B:41[A]:LYS:HD2	5:B:944:HOH:O	2.17	0.45
1:A:247:LYS:HD2	1:A:251:TRP:CD2	2.51	0.45
1:B:148:LYS:NZ	1:B:148:LYS:HB3	2.33	0.44
1:B:181:LEU:CD2	1:B:201[A]:ASN:HD21	2.29	0.44
1:A:79:ASP:O	1:A:80:HIS:HB2	2.17	0.44
1:A:228:ASP:O	1:A:232[A]:ILE:HG12	2.17	0.44
1:B:20[A]:ARG:CD	1:B:33:GLU:HB3	2.47	0.44
1:B:242:LYS:HA	1:B:245[B]:MET:HG2	1.98	0.44
1:B:20[B]:ARG:HG2	1:B:33:GLU:HB3	2.00	0.44
1:A:189[A]:MET:HG3	1:A:194:ILE:HG13	1.94	0.44
1:B:137:VAL:HG21	1:B:189[B]:MET:CE	2.48	0.44
1:A:173:SER:OG	1:A:189[B]:MET:HE1	2.16	0.43
1:B:64:GLN:HG2	1:B:68:GLY:HA2	2.00	0.43
1:A:137:VAL:HG21	1:A:189[B]:MET:CE	2.48	0.43
1:B:125:ASP:HA	1:B:128:LYS:HZ2	1.80	0.43
1:B:189[A]:MET:HB2	5:B:953[A]:HOH:O	2.18	0.43
1:A:115:ARG:NH2	1:A:185:TYR:H	2.17	0.43
1:B:76:GLU:OE1	1:B:81[A]:ARG:CZ	2.66	0.43
1:A:138:ARG:NH2	1:A:165:GLN:OE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ARG:HG2	1:A:6:LEU:HD23	1.99	0.43
1:A:248[B]:GLU:O	1:A:252:ARG:CG	2.53	0.43
1:A:133:GLU:O	1:A:185:TYR:HA	2.19	0.43
1:A:70:TRP:CH2	1:A:94[B]:VAL:HG12	2.54	0.42
1:B:65:ASN:C	1:B:67:LYS:H	2.23	0.42
1:A:164:ARG:NH1	1:A:164:ARG:CG	2.61	0.41
1:A:108:LEU:HD12	1:A:190[A]:GLU:CD	2.41	0.41
1:A:4:ARG:HD2	1:B:254:ASN:OD1	2.19	0.41
1:A:137:VAL:HG21	1:A:189[B]:MET:HE3	2.02	0.41
1:B:80:HIS:HE1	5:B:1033:HOH:O	1.98	0.41
1:A:76:GLU:OE1	1:A:81[A]:ARG:CZ	2.69	0.41
1:B:190[A]:GLU:HA	1:B:190[A]:GLU:OE1	2.21	0.41
1:B:97[B]:LYS:N	1:B:97[B]:LYS:HD2	2.35	0.41
1:A:157:MET:O	1:A:161:MET:HG3	2.20	0.41
1:B:7:ILE:HD12	1:B:54[B]:LYS:HE3	2.02	0.41
1:A:75[B]:LYS:HE2	1:A:79:ASP:OD1	2.21	0.40
1:B:247:LYS:HD2	1:B:251:TRP:CD2	2.57	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:601:1PE:OH7	5:B:882:HOH:O[4_555]	1.92	0.28
3:A:602:1PE:OH7	5:A:874:HOH:O[3_555]	2.01	0.19
5:B:1024:HOH:O	5:B:1040:HOH:O[4_555]	2.13	0.07
3:B:601:1PE:OH2	5:B:906:HOH:O[4_555]	2.14	0.06

## 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	268/258 (104%)	260 (97%)	8 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	270/258 (105%)	262 (97%)	8 (3%)	0	100	100
All	All	538/516 (104%)	522 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	239/225 (106%)	235 (98%)	4 (2%)	68	48
1	B	241/225 (107%)	234 (97%)	7 (3%)	50	23
All	All	480/450 (107%)	469 (98%)	11 (2%)	55	33

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LEU
1	A	115	ARG
1	A	164	ARG
1	A	227	ARG
1	B	80	HIS
1	B	108	LEU
1	B	115	ARG
1	B	164	ARG
1	B	165	GLN
1	B	166	GLN
1	B	227	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	166	GLN

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Mol	Chain	Res	Type
1	A	254	ASN
1	B	45	ASN
1	B	64	GLN
1	B	166	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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	602	-	15,15,15	0.50	0	14,14,14	0.39	0
4	UBA	A	801	-	12,25,25	1.17	2 (16%)	7,36,36	3.10	4 (57%)
3	1PE	B	601	-	15,15,15	0.48	0	14,14,14	0.48	0
4	UBA	B	802	-	12,25,25	1.26	1 (8%)	7,36,36	3.20	4 (57%)

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	602	-	-	0/13/13/13	0/0/0/0
4	UBA	A	801	-	-	0/7/16/16	0/2/2/2
3	1PE	B	601	-	-	0/13/13/13	0/0/0/0
4	UBA	B	802	-	-	0/7/16/16	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	802	UBA	CB-N4	-2.59	1.45	1.48
4	A	801	UBA	CB-N4	-2.16	1.46	1.48
4	A	801	UBA	CB-CA	2.03	1.56	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	802	UBA	C17-C18-C19	-5.68	117.70	127.43
4	A	801	UBA	C17-C18-C19	-5.27	118.40	127.43
4	A	801	UBA	C6-C2-C3	2.22	123.08	118.62
4	B	802	UBA	C6-C2-C3	2.76	124.17	118.62
4	A	801	UBA	C22-S20-C19	3.57	95.78	91.50
4	B	802	UBA	C22-S20-C19	3.59	95.81	91.50
4	B	802	UBA	C17-N6-C5	3.75	122.49	118.05
4	A	801	UBA	C17-N6-C5	4.05	122.84	118.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	1PE	0	1
3	B	601	1PE	0	2

## 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%)	0.95	45 (17%) <b>2</b> <b>3</b>	2, 14, 32, 45	0
1	B	251/258 (97%)	1.01	43 (17%) <b>2</b> <b>3</b>	9, 17, 32, 43	0
All	All	502/516 (97%)	0.98	88 (17%) <b>2</b> <b>3</b>	2, 16, 32, 45	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	PHE	7.9
1	A	160	PHE	7.4
1	B	114	TYR	7.3
1	B	132	ILE	6.9
1	B	131	LYS	6.9
1	A	66	ASP	6.8
1	B	66	ASP	6.0
1	A	164	ARG	5.6
1	B	120	ILE	5.5
1	A	181	LEU	5.4
1	B	164	ARG	5.4
1	A	114	TYR	5.3
1	B	168	ALA	5.3
1	B	115	ARG	5.3
1	B	163	SER	5.2
1	A	159	ALA	5.1
1	A	163	SER	5.1
1	A	132	ILE	5.0
1	B	159	ALA	5.0
1	A	134	TYR	4.9
1	A	126	LEU	4.9
1	A	115	ARG	4.8
1	A	131	LYS	4.6
1	B	126	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	166	GLN	4.5
1	B	134	TYR	4.5
1	B	185	TYR	4.5
1	B	129	GLN	4.3
1	B	178	GLN	4.3
1	A	184	ASP	4.3
1	B	181	LEU	4.2
1	A	120	ILE	4.2
1	A	168	ALA	4.2
1	B	118	THR	4.1
1	B	130	THR	3.9
1	B	184	ASP	3.9
1	A	185	TYR	3.8
1	A	128	LYS	3.7
1	A	133	GLU	3.6
1	B	167	SER	3.6
1	A	167	SER	3.6
1	A	178	GLN	3.5
1	B	210	LEU	3.4
1	A	127	ALA	3.4
1	A	162	SER	3.2
1	B	124	ASP	3.2
1	A	174	ASP	3.1
1	A	129	GLN	3.1
1	A	121	ASP	3.1
1	A	118	THR	3.0
1	B	119	PRO	3.0
1	B	133	GLU	3.0
1	A	170	VAL	3.0
1	A	186	ALA	2.9
1	A	68	GLY	2.9
1	B	121	ASP	2.9
1	A	91	ILE	2.9
1	A	67	LYS	2.8
1	B	91	ILE	2.8
1	B	128	LYS	2.8
1	B	127	ALA	2.7
1	B	174	ASP	2.7
1	B	67	LYS	2.7
1	A	202	CYS	2.6
1	B	182	THR	2.6
1	B	166	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	180	VAL	2.5
1	A	130	THR	2.5
1	A	107[A]	THR	2.4
1	B	162	SER	2.4
1	A	4	ARG	2.4
1	B	189[A]	MET	2.4
1	B	186	ALA	2.4
1	B	125	ASP	2.4
1	B	204	LEU	2.3
1	A	252	ARG	2.3
1	B	68	GLY	2.2
1	A	125	ASP	2.2
1	A	203	ASN	2.2
1	A	171	LYS	2.2
1	B	117	GLY	2.1
1	A	147	LYS	2.1
1	A	117	GLY	2.1
1	A	148	LYS	2.1
1	B	165	GLN	2.0
1	B	104	PRO	2.0
1	A	136	ALA	2.0
1	B	147	LYS	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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	1PE	B	601	16/16	0.93	0.15	4.08	17,21,28,30	16
4	UBA	A	801	24/24	0.91	0.09	-0.83	25,30,34,37	0
4	UBA	B	802	24/24	0.90	0.09	-0.89	25,29,35,37	0
2	CL	B	502	1/1	0.98	0.13	-	23,23,23,23	1
2	CL	A	501	1/1	0.99	0.11	-	23,23,23,23	1
3	1PE	A	602	16/16	0.97	0.12	-	18,20,26,27	16

## 6.5 Other polymers [i](#)

There are no such residues in this entry.