



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:53 PM 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

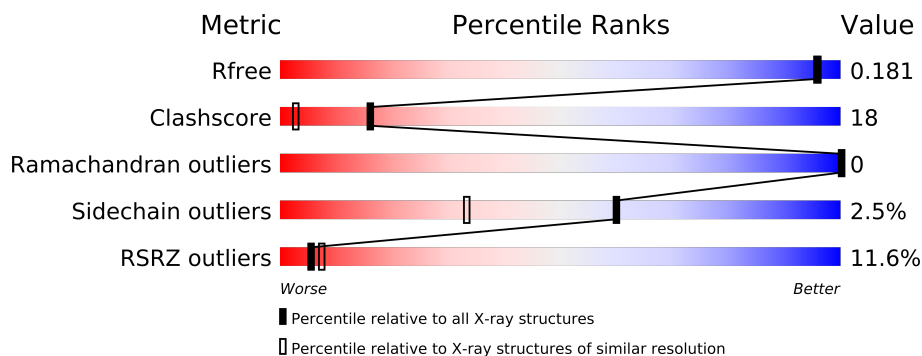
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.74 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}	66092	1657 (1.76-1.72)
Clashscore	79885	1881 (1.76-1.72)
Ramachandran outliers	78287	1859 (1.76-1.72)
Sidechain outliers	78261	1859 (1.76-1.72)
RSRZ outliers	66119	1658 (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 ≥ 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	A	602	-	X
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 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	19	0
			2165	1379	362	410	14			
1	B	251	Total	C	N	O	S	0	21	0
			2188	1392	369	411	16			

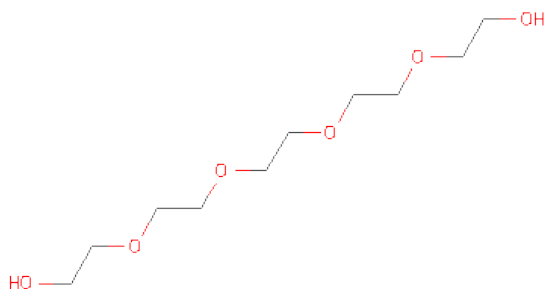
There are 10 discrepancies between the modelled and reference sequences:

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).

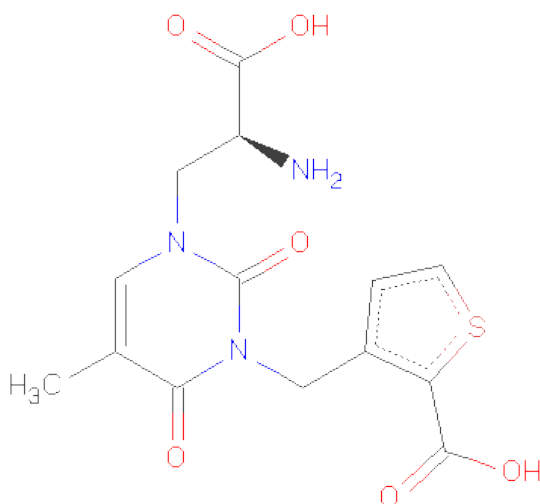
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



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: C₁₄H₁₅N₃O₆S).



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.

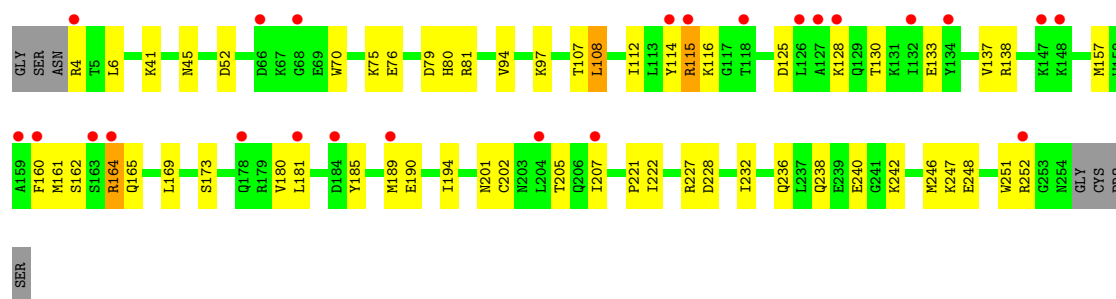
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	239	Total	O	0	8
			239	239		
5	B	243	Total	O	0	9
			243	243		

3 Residue-property plots

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.

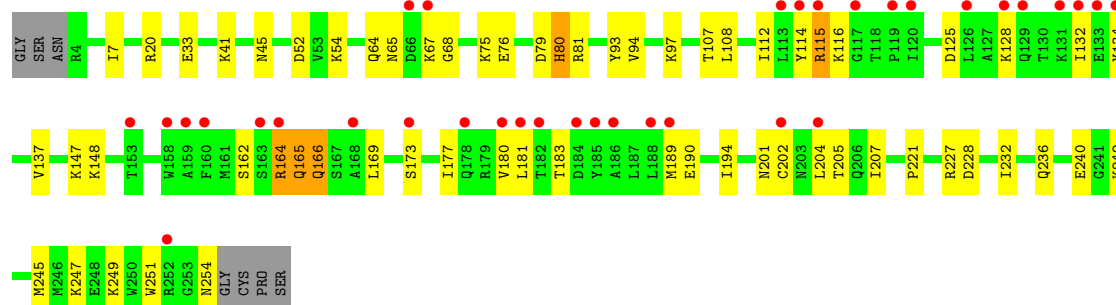
- Molecule 1: GLUTAMATE RECEPTOR, IONOTROPIC KAINATE 1

Chain A: 



- Molecule 1: GLUTAMATE RECEPTOR, IONOTROPIC KAINATE 1

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	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) 98.7 (33.41-1.73)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.181 , 0.211 0.178 , 0.181	Depositor DCC
R_{free} test set	3211 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.5	EDS
Estimated twinning fraction	0.460 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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 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 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	2165	0	2187	85	0
1	B	2188	0	2214	82	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	16	0	22	0	2
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	2
5	B	243	0	0	18	4
All	All	4917	0	4471	164	6

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 18.

All (164) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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 (6) 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	Distance(Å)	Clash(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
3:A:602:1PE:OH6	5:A:950:HOH:O[3_555]	2.06	0.14
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
1:B:107[A]:THR:CG2	5:B:972:HOH:O[3_455]	2.15	0.05

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
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%)	73	53
1	B	241/225 (107%)	234 (97%)	7 (3%)	55	27
All	All	480/450 (107%)	469 (98%)	11 (2%)	60	37

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
1	A	254	ASN
1	B	45	ASN
1	B	64	GLN
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	602	-	15,15,15	0.50	0	14,14,14	0.39	0
4	UBA	A	801	-	25,25,25	1.51	4 (16%)	30,36,36	2.23	8 (26%)
3	1PE	B	601	-	15,15,15	0.48	0	14,14,14	0.48	0
4	UBA	B	802	-	25,25,25	1.37	4 (16%)	30,36,36	2.48	12 (40%)

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	-	-	0/13/16/16	0/2/2/2
3	1PE	B	601	-	-	0/13/13/13	0/0/0/0
4	UBA	B	802	-	-	0/13/16/16	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	UBA	C5-N4	3.91	1.42	1.38
4	B	802	UBA	C5-N4	2.81	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	UBA	C1-C2	2.74	1.48	1.42
4	A	801	UBA	C19-C18	2.72	1.47	1.38
4	B	802	UBA	C19-C18	2.68	1.46	1.38
4	B	802	UBA	CB-N4	-2.42	1.45	1.48
4	B	802	UBA	C1-C2	2.34	1.48	1.42
4	A	801	UBA	CB-N4	-2.01	1.46	1.48

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	802	UBA	C3-N4-C5	6.61	121.15	118.59
4	A	801	UBA	O1-C10-C19	-4.80	114.30	123.11
4	A	801	UBA	C3-N4-C5	4.79	120.45	118.59
4	B	802	UBA	O1-C10-C19	-4.78	114.34	123.11
4	B	802	UBA	CA-CB-N4	-4.52	106.03	112.44
4	A	801	UBA	CA-CB-N4	-4.33	106.30	112.44
4	B	802	UBA	C17-C18-C19	-4.13	117.70	127.43
4	A	801	UBA	C17-C18-C19	-3.83	118.40	127.43
4	A	801	UBA	C1-N6-C5	-3.30	120.83	123.42
4	B	802	UBA	CB-N4-C5	-3.19	115.63	119.37
4	B	802	UBA	C1-N6-C5	-3.11	120.97	123.42
4	B	802	UBA	C22-S20-C19	2.97	95.81	91.47
4	A	801	UBA	C22-S20-C19	2.95	95.78	91.47
4	B	802	UBA	C6-C2-C3	2.63	124.17	118.59
4	B	802	UBA	C18-C19-S20	-2.51	107.99	111.00
4	A	801	UBA	CB-N4-C5	-2.42	116.53	119.37
4	B	802	UBA	O2-C10-C19	2.28	121.35	115.69
4	A	801	UBA	C6-C2-C3	2.11	123.08	118.59
4	B	802	UBA	CB-N4-C3	2.06	123.21	118.11
4	B	802	UBA	O-C-CA	2.03	121.44	116.88

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, 95th 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 ²)	Q<0.9
1	A	251/258 (97%)	0.54	24 (9%) 8 10	2, 14, 32, 45	0
1	B	251/258 (97%)	0.74	35 (13%) 4 4	9, 17, 32, 43	0
All	All	502/516 (97%)	0.64	59 (11%) 5 7	2, 16, 32, 45	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	114	TYR	8.0
1	A	66	ASP	7.9
1	B	131	LYS	7.7
1	B	160	PHE	5.9
1	A	115	ARG	5.5
1	B	132	ILE	5.4
1	B	181	LEU	5.3
1	A	163	SER	4.9
1	B	120	ILE	4.9
1	B	164	ARG	4.7
1	B	185	TYR	4.6
1	B	134	TYR	4.2
1	B	126	LEU	4.1
1	B	66	ASP	4.0
1	B	178	GLN	3.8
1	B	115	ARG	3.6
1	B	133	GLU	3.6
1	B	186	ALA	3.3
1	A	181	LEU	3.1
1	A	4	ARG	3.1
1	B	117	GLY	3.0
1	A	159	ALA	3.0
1	B	119	PRO	2.9
1	A	114	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	134	TYR	2.7
1	B	168	ALA	2.7
1	B	204	LEU	2.7
1	A	160	PHE	2.7
1	B	189[A]	MET	2.7
1	A	204	LEU	2.6
1	A	184	ASP	2.6
1	A	178	GLN	2.6
1	A	252	ARG	2.6
1	B	67	LYS	2.5
1	A	189[A]	MET	2.5
1	A	148	LYS	2.5
1	B	180	VAL	2.4
1	B	202	CYS	2.4
1	A	164	ARG	2.4
1	B	182	THR	2.4
1	A	126	LEU	2.3
1	A	127	ALA	2.3
1	A	132	ILE	2.3
1	B	173	SER	2.3
1	B	159	ALA	2.2
1	A	207	ILE	2.2
1	A	147	LYS	2.2
1	B	129	GLN	2.2
1	A	68	GLY	2.2
1	B	128	LYS	2.1
1	B	163	SER	2.1
1	B	188	LEU	2.1
1	B	252	ARG	2.1
1	B	184	ASP	2.1
1	A	118	THR	2.1
1	B	153	THR	2.0
1	A	128	LYS	2.0
1	B	158	TRP	2.0
1	B	113	LEU	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, 95th 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(Å ²)	Q<0.9
3	1PE	B	601	16/16	0.14	18.93	17,21,28,30	16
3	1PE	A	602	16/16	0.11	4.96	18,20,26,27	16
2	CL	B	502	1/1	0.07	0.25	23,23,23,23	1
4	UBA	B	802	24/24	0.11	-0.59	25,29,35,37	0
4	UBA	A	801	24/24	0.11	-0.60	25,30,34,37	0
2	CL	A	501	1/1	0.06	-2.16	23,23,23,23	1

6.5 Other polymers ⓘ

There are no such residues in this entry.