Full wwPDB X-ray Structure Validation Report (i)

Jul 25, 2017 – 07:04 PM EDT

PDB ID	:	2OJT
Title	:	Structure and mechanism of kainate receptor modulation by anions
Authors	:	Mayer, M.L.
Deposited on	:	unknown
Resolution	:	1.95 Å(reported)

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

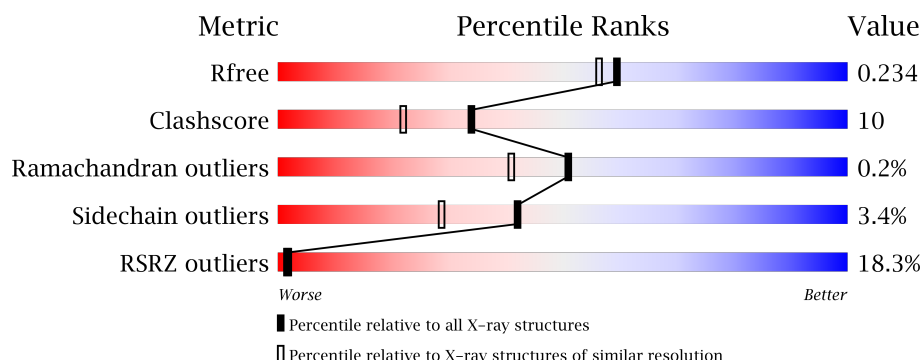|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

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	Percentile Ranks	Value
Rfree		0.234
Clashscore		10
Ramachandran outliers		0.2%
Sidechain outliers		3.4%
RSRZ outliers		18.3%

Worse ————————————————————— Better

▉ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (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 >=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 <=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	17% / 81% / 16% / ••
1	B	258	19% / 80% / 16% / ••

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	401	-	-	-	X

2 Entry composition (i)

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.

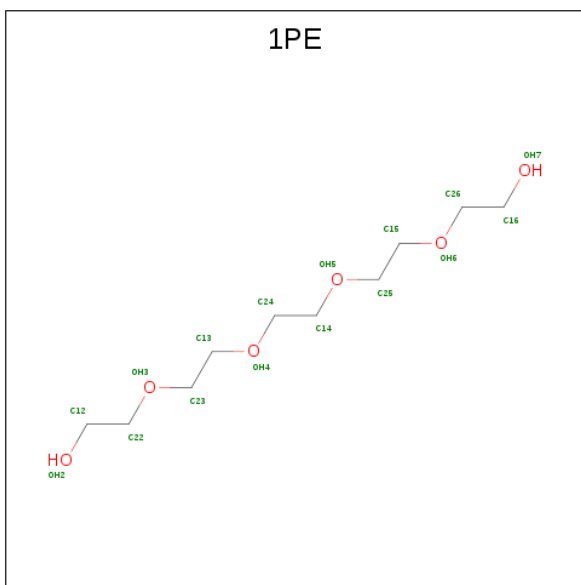| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	17	0
			2148	1367	359	408	14			
1	B	251	Total	C	N	O	S	0	21	0
			2188	1392	369	411	16			

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	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

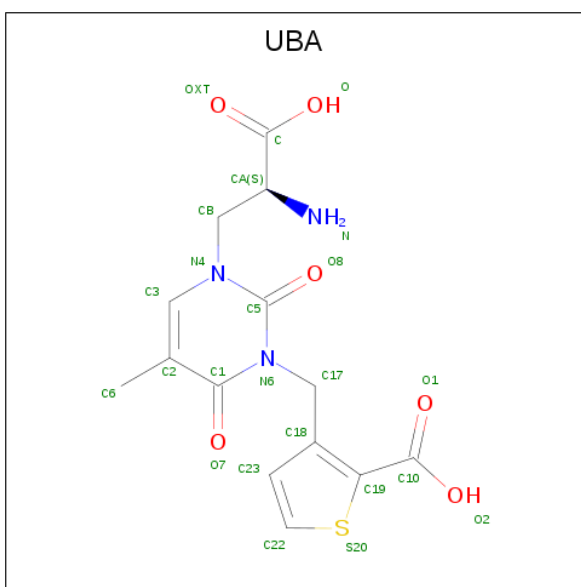- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

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: $C_{10}H_{22}O_6$).

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: $C_{14}H_{15}N_3O_6S$).

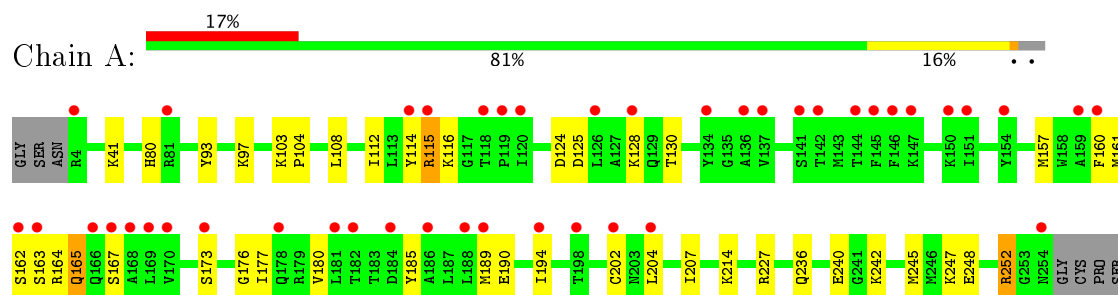| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			24	14	3	6	1		

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

- Molecule 5 is water.

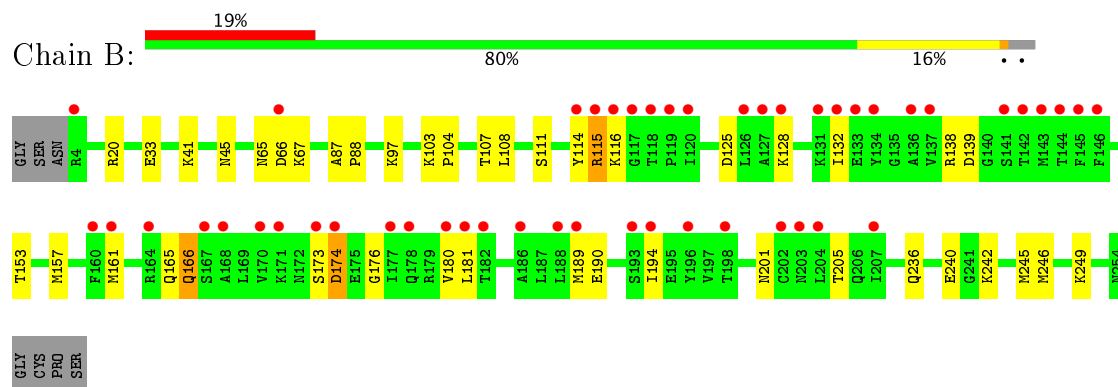| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	141	Total 141	O 141	0	2
5	B	147	Total 147	O 147	0	2

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 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

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4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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 (5.29%)	DCC
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.8	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	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^2)	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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 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: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	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: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:115:ARG:H	1:A:115:ARG:NH1	2.08	0.52
1:A:252:ARG:HD2	1:A:252:ARG:O	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: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: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: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: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:HD2	1:A:41:LYS:HA	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%)	38	25
All	All	536/516 (104%)	518 (97%)	17 (3%)	1 (0%)	51	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	ASP

5.3.2   Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	237/225 (105%)	228 (96%)	9 (4%)	38	24
1	B	241/225 (107%)	235 (98%)	6 (2%)	53	42
All	All	478/450 (106%)	463 (97%)	15 (3%)	42	32

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 (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	401	-	15,15,15	0.51	0	14,14,14	0.30	0
4	UBA	A	501	-	11,25,25	1.12	1 (9%)	10,36,36	2.87	5 (50%)
3	1PE	B	401	-	15,15,15	0.51	0	14,14,14	0.38	0
4	UBA	B	501	-	11,25,25	1.11	1 (9%)	10,36,36	2.95	6 (60%)

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	-	-	0/6/16/16	0/2/2/2
3	1PE	B	401	-	-	0/13/13/13	0/0/0/0
4	UBA	B	501	-	-	0/6/16/16	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	UBA	CB-N4	-2.38	1.46	1.48
4	A	501	UBA	CB-N4	-2.37	1.46	1.48

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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-C1	-2.37	117.60	122.56
4	A	501	UBA	C6-C2-C1	-2.24	117.88	122.56
4	B	501	UBA	CB-N4-C3	2.09	122.31	118.59
4	B	501	UBA	C2-C1-N6	2.41	119.40	116.60
4	A	501	UBA	C6-C2-C3	2.74	124.14	118.67
4	A	501	UBA	C2-C1-N6	2.82	119.88	116.60
4	B	501	UBA	C6-C2-C3	2.94	124.54	118.67
4	B	501	UBA	C17-N6-C5	5.76	124.66	117.92
4	A	501	UBA	C17-N6-C5	5.86	124.78	117.92

There are no chirality outliers.

There are no torsion outliers.

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

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.95	43 (17%)	2	2	17, 30, 62, 71	0
1	B	251/258 (97%)	1.11	49 (19%)	1	1	17, 30, 64, 71	0
All	All	502/516 (97%)	1.03	92 (18%)	1	2	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	9.2
1	B	114	TYR	6.4
1	B	126	LEU	5.9
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	B	164	ARG	3.1
1	A	126	LEU	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	136	ALA	2.9
1	A	137	VAL	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	A	4	ARG	2.5
1	B	136	ALA	2.5
1	A	146	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	142	THR	2.5
1	A	147	LYS	2.4
1	B	133	GLU	2.4
1	A	119	PRO	2.4
1	B	161	MET	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	116	LYS	2.3
1	B	118	THR	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 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, 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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	1PE	B	401	16/16	0.94	0.14	6.26	23,26,33,34	16
4	UBA	A	501	24/24	0.87	0.14	-0.63	32,36,43,45	0
4	UBA	B	501	24/24	0.90	0.14	-0.71	31,36,43,45	0
3	1PE	A	401	16/16	0.94	0.12	-	24,25,31,32	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

6.5 Other polymers (i)

There are no such residues in this entry.