WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:59 AM GMT

PDB ID	:	2F35
Title	:	Crystal Structure of the GluR5 Ligand Binding Core with UBP302 At 1.87 Angstroms Resolution
Authors	:	Mayer, M.L.
Deposited on	:	2005-11-18
Resolution	:	1.87 Å(reported)

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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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		0.195
Clashscore		16
Ramachandran outliers		0
Sidechain outliers		3.0%
RSRZ outliers		30.1%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
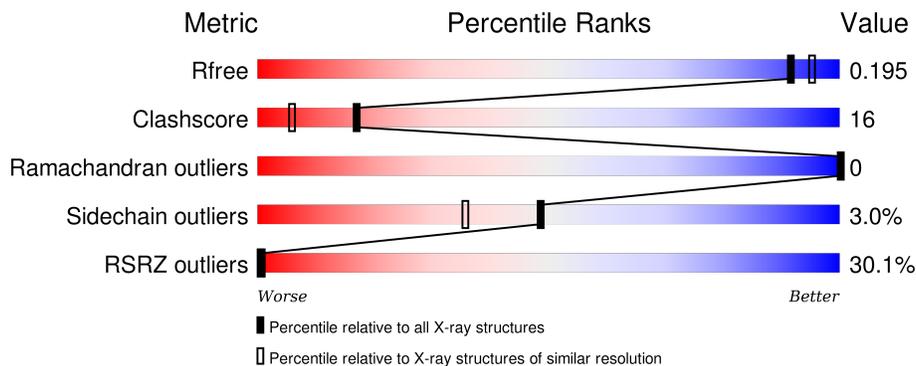
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (1.90-1.86)

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	29% / 73% / 23%
1	B	258	30% / 79% / 17%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4809 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 2143	C 1365	N 357	O 406	S 15	0	16	0
1	B	251	Total 2168	C 1377	N 363	O 413	S 15	0	19	0

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 1	Cl 1	0	0
2	A	1	Total 1	Cl 1	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).
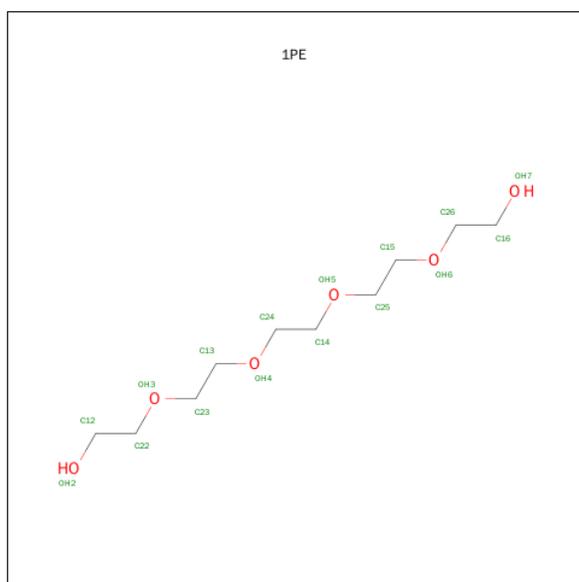
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 16	C 10	O 6	0	0
3	A	1	Total 16	C 10	O 6	0	0

- Molecule 4 is (S)-1-(2-AMINO-2-CARBOXYETHYL)-3-(2-CARBOXYBENZYL)PYRIMI
  DINE-2,4-DIONE (three-letter code: UBC) (formula: $C_{15}H_{15}N_3O_6$).
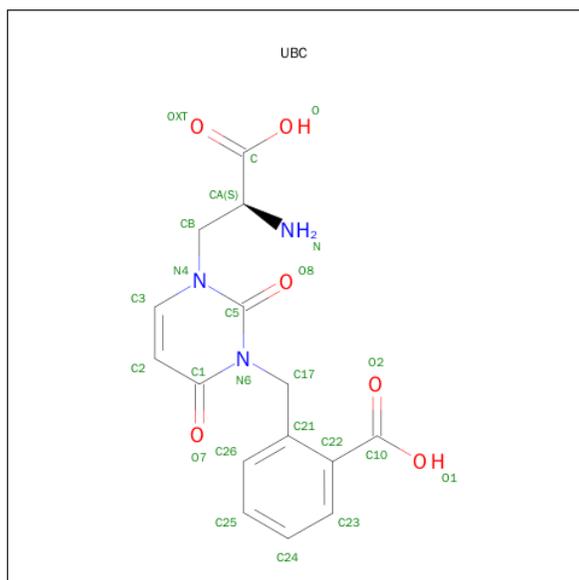
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 24	C 15	N 3	O 6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 24	C 15	N 3	O 6	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	205	Total 205	O 205	0	4
5	B	211	Total 211	O 211	0	5

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
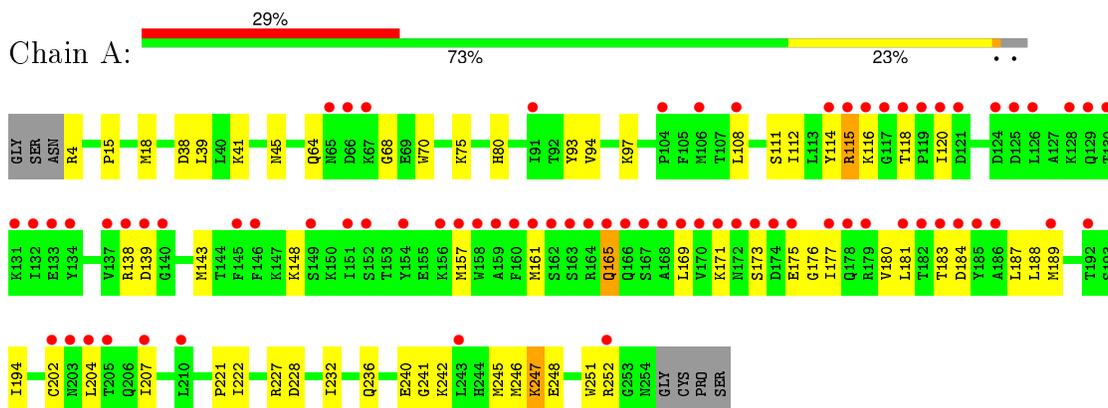
- Molecule 1: GLUTAMATE RECEPTOR, IONOTROPIC KAINATE 1
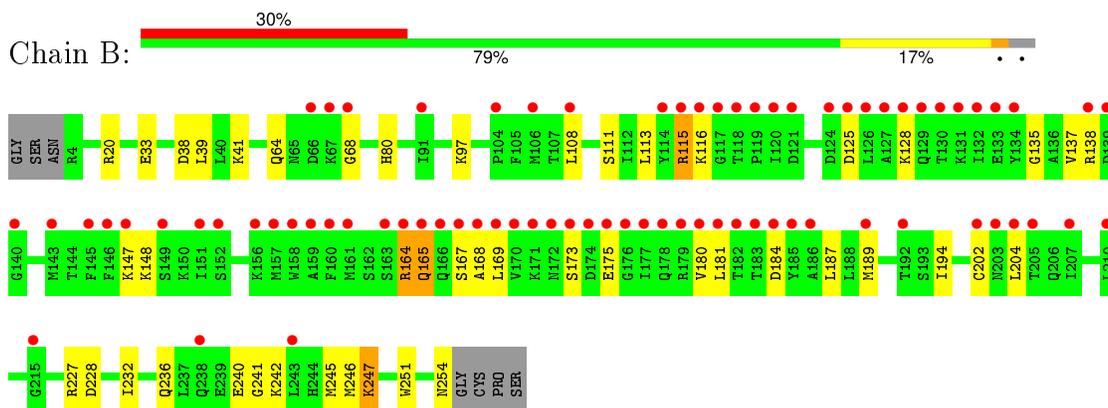
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	97.88Å 97.91Å 128.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.92 – 1.87 38.92 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.92-1.87) 99.8 (38.92-1.87)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.191 , 0.220 0.195 , 0.195	Depositor DCC
R_{free} test set	2589 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	26.6	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.3	EDS
Estimated twinning fraction	0.487 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Outliers	0 of 51373 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4809	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CL, UBC, 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	0.55	0/2181	0.71	0/2934
1	B	0.58	1/2206 (0.0%)	0.72	0/2966
All	All	0.56	1/4387 (0.0%)	0.72	0/5900

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	175	GLU	CD-OE1	6.85	1.33	1.25

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	2143	0	2161	75	0
1	B	2168	0	2176	71	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	0
4	A	24	0	13	0	0
4	B	24	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	205	0	0	13	1
5	B	211	0	0	10	0
All	All	4809	0	4407	144	1

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 16.

All (144) 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:B:115:ARG:HG2	1:B:115:ARG:HH11	1.11	1.12
1:A:115:ARG:HG2	1:A:115:ARG:HH11	1.15	1.11
1:B:64[A]:GLN:HE21	1:B:68[A]:GLY:HA2	1.13	1.07
1:A:221:PRO:HG3	5:A:973:HOH:O	1.58	1.04
1:B:181:LEU:HD23	1:B:204:LEU:HD11	1.45	0.99
1:B:164:ARG:HA	1:B:164:ARG:CZ	1.93	0.98
1:A:189[B]:MET:HE1	5:A:1004:HOH:O	1.66	0.93
1:B:64[A]:GLN:NE2	1:B:68[A]:GLY:HA2	1.87	0.90
1:B:115:ARG:CG	1:B:115:ARG:HH11	1.85	0.90
1:A:115:ARG:CG	1:A:115:ARG:HH11	1.86	0.87
1:B:137:VAL:HG21	1:B:189[B]:MET:HE3	1.55	0.86
1:B:64[A]:GLN:HE21	1:B:68[A]:GLY:CA	1.89	0.85
1:B:181:LEU:CD2	1:B:204:LEU:HD11	2.06	0.85
1:B:240[A]:GLU:OE2	1:B:242:LYS:HD2	1.76	0.84
1:B:137:VAL:CG2	1:B:189[B]:MET:HE3	2.10	0.82
1:A:165:GLN:HG2	1:A:169:LEU:HD12	1.61	0.82
1:A:181:LEU:HD23	1:A:204:LEU:HD11	1.65	0.78
1:A:97[A]:LYS:HD2	5:A:910:HOH:O	1.83	0.77
1:B:39:LEU:N	1:B:246[B]:MET:HE1	2.00	0.77
1:B:80:HIS:CE1	5:B:1010:HOH:O	2.39	0.75
1:A:4:ARG:HA	5:A:960:HOH:O	1.87	0.75
1:A:171:LYS:HB3	1:A:175:GLU:OE1	1.89	0.73
1:A:39:LEU:N	1:A:246[B]:MET:HE1	2.04	0.73
1:A:248[A]:GLU:O	1:A:252:ARG:HG2	1.88	0.72
1:A:240[A]:GLU:HG3	1:A:242:LYS:HG3	1.72	0.72
1:B:115:ARG:HD3	1:B:115:ARG:N	2.05	0.71
1:A:41:LYS:HD3	1:A:41:LYS:O	1.92	0.69
1:B:115:ARG:HD3	1:B:115:ARG:H	1.57	0.69
1:A:248[B]:GLU:O	1:A:252:ARG:HG2	1.92	0.68
1:B:115:ARG:NH1	1:B:115:ARG:HG2	1.92	0.68
1:B:241:GLY:O	1:B:245[B]:MET:HG3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97[A]:LYS:HD3	5:B:840:HOH:O	1.93	0.68
1:B:165:GLN:HG2	1:B:169:LEU:HD12	1.74	0.67
1:A:115:ARG:N	1:A:115:ARG:HD3	2.10	0.66
1:B:137:VAL:HG21	1:B:189[B]:MET:CE	2.23	0.65
1:B:173:SER:OG	1:B:189[B]:MET:CE	2.44	0.65
1:A:181:LEU:CD2	1:A:204:LEU:HD11	2.27	0.65
1:A:94[B]:VAL:O	1:A:97[B]:LYS:CG	2.43	0.65
1:B:236[A]:GLN:O	1:B:240[A]:GLU:HG2	1.96	0.65
1:A:115:ARG:HG2	1:A:115:ARG:NH1	1.95	0.63
1:A:115:ARG:H	1:A:115:ARG:HD3	1.64	0.62
1:B:164:ARG:HA	1:B:164:ARG:NH1	2.15	0.62
1:A:97[A]:LYS:HD3	5:A:845:HOH:O	1.98	0.61
1:A:189[A]:MET:HG2	1:A:194:ILE:HG13	1.82	0.61
1:A:241:GLY:O	1:A:245[B]:MET:HG3	2.01	0.60
1:B:236[B]:GLN:NE2	5:B:897:HOH:O	2.23	0.60
1:A:114:TYR:HE2	1:A:118:THR:HG1	1.50	0.59
1:B:189[A]:MET:HG2	1:B:194:ILE:HG13	1.84	0.59
1:B:147:LYS:CE	1:B:148:LYS:HG3	2.33	0.59
1:B:232[B]:ILE:HG22	1:B:236[B]:GLN:HE21	1.68	0.58
1:A:115:ARG:HD2	1:A:180:VAL:O	2.03	0.58
1:A:115:ARG:NH2	1:A:184:ASP:HA	2.19	0.58
1:A:70:TRP:O	1:A:75[B]:LYS:HD3	2.04	0.58
1:A:70:TRP:HH2	1:A:94[B]:VAL:HG12	1.69	0.57
1:B:137:VAL:CG2	1:B:189[B]:MET:CE	2.80	0.57
1:B:189[A]:MET:HG2	1:B:194:ILE:CG1	2.35	0.57
1:A:183:THR:HG22	1:A:184:ASP:N	2.19	0.57
1:B:115:ARG:HD2	1:B:180:VAL:O	2.05	0.57
1:B:232[B]:ILE:O	1:B:236[B]:GLN:HG3	2.05	0.57
1:A:138:ARG:NE	1:A:165:GLN:OE1	2.37	0.56
1:B:97[A]:LYS:HD2	5:B:906:HOH:O	2.05	0.56
1:A:189[A]:MET:HG2	1:A:194:ILE:CG1	2.35	0.56
1:B:111:SER:HB3	1:B:194:ILE:HD12	1.87	0.56
1:B:41:LYS:HD3	1:B:41:LYS:O	2.07	0.55
1:B:164:ARG:HA	1:B:164:ARG:NE	2.22	0.55
1:B:97[B]:LYS:HD2	5:B:934:HOH:O	2.07	0.55
1:A:236[A]:GLN:O	1:A:240[A]:GLU:HG2	2.06	0.55
1:B:115:ARG:NH2	1:B:184:ASP:OD1	2.40	0.54
1:B:147:LYS:HE3	1:B:148:LYS:CG	2.37	0.54
1:B:148:LYS:NZ	1:B:148:LYS:HB3	2.23	0.54
1:A:189[B]:MET:CE	5:A:968:HOH:O	2.55	0.54
1:A:70:TRP:CH2	1:A:94[B]:VAL:HG12	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LEU:HD23	1:A:204:LEU:CD1	2.37	0.54
1:A:176:GLY:O	1:A:180:VAL:HG23	2.08	0.53
1:B:116:LYS:NZ	1:B:202:CYS:O	2.36	0.53
1:B:147:LYS:HE2	1:B:148:LYS:HG3	1.90	0.53
1:A:116:LYS:NZ	1:A:202:CYS:O	2.41	0.53
1:A:94[B]:VAL:O	1:A:97[B]:LYS:HG3	2.09	0.52
1:B:164:ARG:HD3	1:B:167:SER:OG	2.09	0.52
1:B:115:ARG:CG	1:B:115:ARG:NH1	2.55	0.52
1:A:247:LYS:HD3	1:A:251:TRP:CE3	2.45	0.51
1:A:228:ASP:O	1:A:232[A]:ILE:HG12	2.11	0.51
1:B:20[A]:ARG:HD3	1:B:33:GLU:HB3	1.93	0.51
1:A:173:SER:OG	1:A:189[B]:MET:CE	2.59	0.51
1:B:97[A]:LYS:CE	5:B:840:HOH:O	2.59	0.51
1:B:173:SER:HG	1:B:189[B]:MET:CE	2.25	0.50
1:B:20[B]:ARG:HG2	1:B:33:GLU:HB3	1.93	0.50
1:A:232[B]:ILE:O	1:A:236[B]:GLN:HG3	2.11	0.50
1:A:189[B]:MET:HE2	5:A:968:HOH:O	2.11	0.50
1:B:80:HIS:HE1	5:B:1010:HOH:O	1.85	0.50
1:A:236[B]:GLN:NE2	5:A:901:HOH:O	2.43	0.50
1:B:38:ASP:HB2	1:B:246[B]:MET:HE3	1.94	0.50
1:A:111:SER:HB3	1:A:194:ILE:HD12	1.94	0.49
1:B:135:GLY:HA3	1:B:168:ALA:O	2.12	0.49
1:A:80:HIS:HA	5:A:973:HOH:O	2.11	0.49
1:B:137:VAL:HG23	1:B:189[B]:MET:HE3	1.91	0.49
1:B:147:LYS:C	1:B:147:LYS:HD2	2.33	0.48
1:B:97[A]:LYS:CD	5:B:840:HOH:O	2.55	0.48
1:B:164:ARG:HG3	1:B:164:ARG:O	2.13	0.48
1:B:125:ASP:HA	1:B:128:LYS:NZ	2.29	0.47
1:B:228:ASP:O	1:B:232[A]:ILE:HG12	2.15	0.47
1:A:112:ILE:HG12	1:A:188:LEU:HD13	1.94	0.47
1:A:252:ARG:HG3	1:A:252:ARG:O	2.14	0.47
1:B:147:LYS:HE3	1:B:148:LYS:HG3	1.96	0.47
1:B:245[B]:MET:HB2	5:B:997:HOH:O	2.13	0.47
1:A:148:LYS:NZ	1:A:148:LYS:HB3	2.30	0.47
1:A:181:LEU:CD2	1:A:204:LEU:CD1	2.92	0.47
1:A:41:LYS:C	1:A:41:LYS:HD3	2.32	0.47
1:A:222:ILE:HD12	1:B:20[B]:ARG:NH1	2.30	0.47
1:B:247:LYS:HD3	1:B:251:TRP:CE3	2.51	0.46
1:A:240[A]:GLU:OE2	1:A:242:LYS:HD2	2.15	0.46
1:A:112:ILE:HG12	1:A:188:LEU:CD1	2.45	0.46
1:A:139:ASP:HA	1:A:143:MET:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189[A]:MET:CG	1:A:194:ILE:HG13	2.44	0.46
1:A:38:ASP:HB2	1:A:246[B]:MET:HE3	1.98	0.46
1:A:112:ILE:HB	1:A:207:ILE:HB	1.97	0.45
1:A:173:SER:O	1:A:177:ILE:HG13	2.16	0.45
1:A:94[B]:VAL:O	1:A:97[B]:LYS:HG2	2.15	0.45
1:A:4:ARG:NH1	1:B:254:ASN:OD1	2.39	0.44
1:B:181:LEU:CD2	1:B:204:LEU:CD1	2.89	0.44
1:A:245[B]:MET:HE2	5:A:996:HOH:O	2.18	0.44
1:A:93:TYR:O	1:A:97[B]:LYS:HG2	2.18	0.44
1:A:183:THR:CG2	1:A:184:ASP:N	2.80	0.43
1:A:38:ASP:HB2	1:A:246[B]:MET:CE	2.48	0.43
1:B:113:LEU:HD11	1:B:204:LEU:HB3	2.00	0.43
1:A:245[B]:MET:HB2	5:A:996:HOH:O	2.18	0.43
1:B:115:ARG:NH2	1:B:184:ASP:HA	2.35	0.42
1:A:15:PRO:HA	1:A:18[A]:MET:SD	2.58	0.42
1:A:157:MET:O	1:A:161:MET:HG3	2.19	0.42
1:B:97[A]:LYS:HD3	5:B:935:HOH:O	2.19	0.42
1:A:38:ASP:C	1:A:246[B]:MET:HE1	2.39	0.41
1:A:115:ARG:NH1	1:A:115:ARG:CG	2.56	0.41
1:A:120:ILE:HG22	1:A:207:ILE:HG21	2.02	0.41
1:B:189[A]:MET:CG	1:B:194:ILE:HG13	2.50	0.41
1:A:97[A]:LYS:CE	5:A:845:HOH:O	2.68	0.41
1:B:138:ARG:NE	1:B:165:GLN:OE1	2.47	0.41
1:A:64[A]:GLN:OE1	1:A:68:GLY:HA2	2.20	0.41
1:B:164:ARG:CA	1:B:164:ARG:NE	2.84	0.41
1:A:41:LYS:HE2	1:A:45:ASN:OD1	2.21	0.41
1:B:247:LYS:HD2	1:B:251:TRP:CD2	2.56	0.41
1:B:148:LYS:HZ2	1:B:148:LYS:HB3	1.84	0.41
1:B:173:SER:OG	1:B:189[B]:MET:HE3	2.18	0.40
1:A:97[A]:LYS:CD	5:A:845:HOH:O	2.66	0.40
1:A:139:ASP:HA	1:A:143:MET:CE	2.52	0.40

All (1) 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:A:602:1PE:OH7	5:A:954:HOH:O[3_555]	2.06	0.14

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	265/258 (103%)	257 (97%)	8 (3%)	0	100	100
1	B	268/258 (104%)	261 (97%)	7 (3%)	0	100	100
All	All	533/516 (103%)	518 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	236/225 (105%)	230 (98%)	6 (2%)	55	44
1	B	238/225 (106%)	231 (97%)	7 (3%)	50	37
All	All	474/450 (105%)	461 (97%)	13 (3%)	48	40

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LEU
1	A	115	ARG
1	A	165	GLN
1	A	187	LEU
1	A	227	ARG
1	A	247	LYS
1	B	108	LEU
1	B	115	ARG

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Mol	Chain	Res	Type
1	B	164	ARG
1	B	165	GLN
1	B	187	LEU
1	B	227	ARG
1	B	247	LYS

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	166	GLN
1	A	201	ASN
1	A	254	ASN
1	B	166	GLN
1	B	201	ASN

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	0.53	0		14,14,14	0.44	0	
4	UBC	A	801	-	15,25,25	1.61	1 (6%)		15,35,35	1.45	1 (6%)	
3	1PE	B	601	-	15,15,15	0.48	0		14,14,14	0.43	0	
4	UBC	B	802	-	15,25,25	1.51	1 (6%)		15,35,35	1.26	1 (6%)	

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	UBC	A	801	-	-	0/8/16/16	0/2/2/2
3	1PE	B	601	-	-	0/13/13/13	0/0/0/0
4	UBC	B	802	-	-	0/8/16/16	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	802	UBC	C22-C21	5.15	1.48	1.40
4	A	801	UBC	C22-C21	5.62	1.48	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	802	UBC	C17-N6-C5	4.23	123.06	118.05
4	A	801	UBC	C17-N6-C5	5.04	124.01	118.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

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%)	1.54	74 (29%)	1	0	2, 15, 28, 37	0
1	B	251/258 (97%)	1.61	77 (30%)	1	0	8, 16, 28, 36	0
All	All	502/516 (97%)	1.58	151 (30%)	1	0	2, 16, 28, 37	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	ALA	11.5
1	B	168	ALA	10.1
1	B	159	ALA	9.7
1	B	160	PHE	9.0
1	B	132	ILE	9.0
1	A	132	ILE	8.8
1	B	163	SER	7.8
1	A	164	ARG	7.7
1	A	168	ALA	7.6
1	A	160	PHE	7.0
1	B	131	LYS	6.9
1	A	114	TYR	6.7
1	A	131	LYS	6.7
1	A	184	ASP	6.7
1	A	166	GLN	6.6
1	B	118	THR	6.6
1	B	184	ASP	6.5
1	A	183	THR	6.5
1	B	167	SER	6.5
1	A	118	THR	6.4
1	B	166	GLN	6.4
1	B	130	THR	6.3
1	B	129	GLN	6.3
1	B	114	TYR	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	181	LEU	6.0
1	B	119	PRO	5.9
1	A	134	TYR	5.8
1	A	182	THR	5.8
1	A	163	SER	5.8
1	A	185	TYR	5.7
1	A	130	THR	5.6
1	A	178	GLN	5.6
1	B	185	TYR	5.5
1	A	129	GLN	5.5
1	A	119	PRO	5.4
1	B	126	LEU	5.3
1	A	181	LEU	5.2
1	B	134	TYR	5.1
1	B	169	LEU	5.1
1	B	183	THR	5.1
1	A	120	ILE	5.1
1	B	128	LYS	5.1
1	B	120	ILE	5.0
1	B	117	GLY	4.9
1	B	178	GLN	4.8
1	A	117	GLY	4.8
1	A	124	ASP	4.7
1	A	167	SER	4.7
1	B	157	MET	4.5
1	B	124	ASP	4.5
1	A	157	MET	4.4
1	A	115	ARG	4.4
1	B	164	ARG	4.3
1	A	116	LYS	4.2
1	B	182	THR	4.2
1	B	115	ARG	4.2
1	A	156	LYS	4.2
1	B	116	LYS	4.2
1	B	177	ILE	4.1
1	B	146	PHE	4.1
1	A	121	ASP	4.0
1	B	170	VAL	3.8
1	A	126	LEU	3.8
1	B	133	GLU	3.7
1	A	145	PHE	3.7
1	A	170	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	133	GLU	3.7
1	B	121	ASP	3.6
1	A	169	LEU	3.6
1	B	203	ASN	3.5
1	B	171	LYS	3.5
1	B	156	LYS	3.4
1	B	165	GLN	3.4
1	B	125	ASP	3.4
1	B	108	LEU	3.4
1	A	173	SER	3.3
1	A	128	LYS	3.3
1	B	189[A]	MET	3.3
1	B	204	LEU	3.3
1	B	179	ARG	3.3
1	B	158	TRP	3.2
1	B	66	ASP	3.2
1	A	146	PHE	3.1
1	A	165	GLN	3.1
1	A	108	LEU	3.1
1	B	180	VAL	3.1
1	A	179	ARG	3.1
1	A	203	ASN	3.1
1	B	173	SER	3.1
1	A	161	MET	3.0
1	B	147	LYS	3.0
1	B	161	MET	3.0
1	B	175	GLU	2.9
1	A	152	SER	2.9
1	A	207	ILE	2.9
1	A	186	ALA	2.9
1	B	202	CYS	2.9
1	B	140	GLY	2.8
1	B	145	PHE	2.8
1	A	158	TRP	2.8
1	A	171	LYS	2.8
1	B	210	LEU	2.8
1	A	189[A]	MET	2.8
1	A	125	ASP	2.8
1	A	138	ARG	2.7
1	A	91	ILE	2.7
1	A	65[A]	ASN	2.7
1	B	172	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	139	ASP	2.6
1	B	205	THR	2.6
1	B	106	MET	2.6
1	B	149	SER	2.5
1	B	176	GLY	2.5
1	A	151	ILE	2.5
1	A	174	ASP	2.5
1	A	177	ILE	2.5
1	A	106	MET	2.5
1	A	67	LYS	2.5
1	B	186	ALA	2.5
1	A	202	CYS	2.4
1	B	91	ILE	2.4
1	B	127	ALA	2.4
1	A	149	SER	2.4
1	B	174	ASP	2.4
1	A	192	THR	2.4
1	A	139	ASP	2.4
1	B	138	ARG	2.3
1	A	204	LEU	2.3
1	A	243	LEU	2.3
1	B	151	ILE	2.3
1	B	143	MET	2.3
1	B	207	ILE	2.3
1	B	192	THR	2.2
1	B	243	LEU	2.2
1	B	238[A]	GLN	2.2
1	A	175	GLU	2.2
1	A	154	TYR	2.2
1	A	210	LEU	2.1
1	B	104	PRO	2.1
1	A	205	THR	2.1
1	A	104	PRO	2.1
1	A	140	GLY	2.1
1	B	67	LYS	2.1
1	A	162	SER	2.1
1	B	68[A]	GLY	2.1
1	A	66	ASP	2.1
1	A	172	ASN	2.0
1	B	152	SER	2.0
1	B	215	GLY	2.0
1	A	137	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	252	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	601	16/16	0.96	0.14	0.29	20,23,30,32	16
4	UBC	A	801	24/24	0.90	0.14	-0.67	28,34,39,40	0
4	UBC	B	802	24/24	0.90	0.13	-0.74	27,33,39,39	0
2	CL	A	501	1/1	0.99	0.19	-	24,24,24,24	1
3	1PE	A	602	16/16	0.95	0.15	-	20,22,24,25	16
2	CL	B	502	1/1	0.99	0.18	-	25,25,25,25	1

6.5 Other polymers (i)

There are no such residues in this entry.