Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 08:27 AM EDT

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PDB ID	:	2QS1
Title	:	Crystal structure of the GluR5 ligand binding core dimer in complex with UBP315 at 1.80 Angstroms resolution
Authors	:	Alushin, G.M.; Jane, D.E.; Mayer, M.L.
Deposited on	:	2007-07-30
Resolution	:	1.80 Å(reported)

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
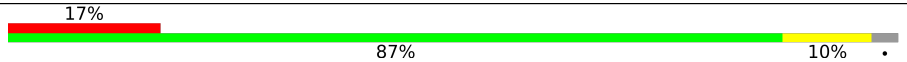
The reported resolution of this entry is 1.80 Å.

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.
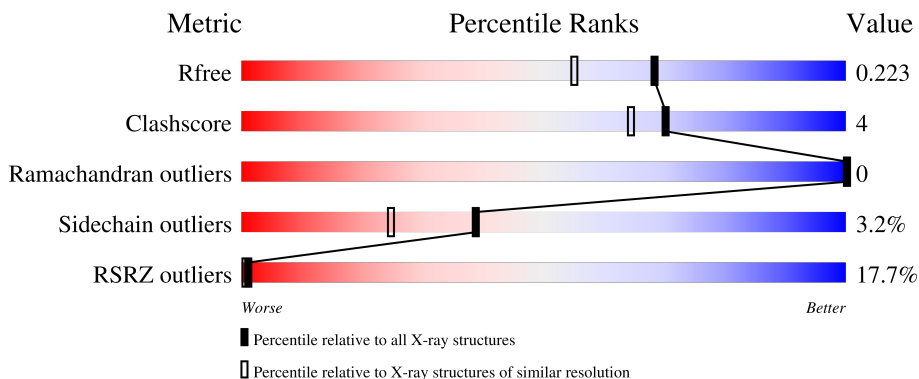
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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% / 88% / 9% · ·
1	B	258	17% / 87% / 10% ·

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 4620 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	10	0
			2089	1333	347	396	13			
1	B	251	Total	C	N	O	S	0	9	0
			2079	1327	345	393	14			

There are 10 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	117	GLY	-	linker	UNP P22756
A	118	THR	-	linker	UNP P22756
A	258	SER	GLU	engineered mutation	UNP P22756
B	1	GLY	-	expression tag	UNP P22756
B	2	SER	-	expression tag	UNP P22756
B	117	GLY	-	linker	UNP P22756
B	118	THR	-	linker	UNP P22756
B	258	SER	GLU	engineered mutation	UNP P22756

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	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 16	C 10	O 6	0	0
3	B	1	Total 16	C 10	O 6	0	0

- Molecule 4 is 3-({3-[(2S)-2-amino-2-carboxyethyl]-5-methyl-2,6-dioxo-3,6-dihydropyrim idin-1(2H)-yl}methyl)-4,5-dibromothiophene-2-carboxylic acid (three-letter code: UB1) (formula: $C_{14}H_{13}Br_2N_3O_6S$).
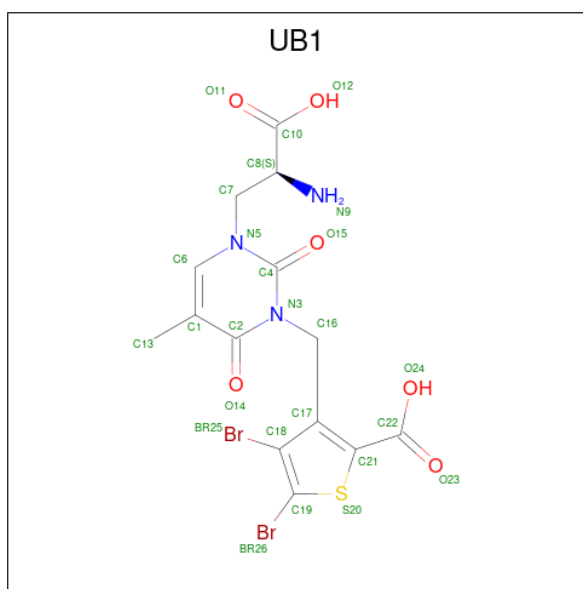
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 26	Br 2	C 14	N 3	O 6	S 1	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	N	O	S		
4	B	1	26	2	14	3	6	1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	190	Total 190	O 190	0	0
5	B	176	Total 176	O 176	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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

Chain A:

• Molecule 1: Glutamate receptor, ionotropic kainate 1

Chain B:
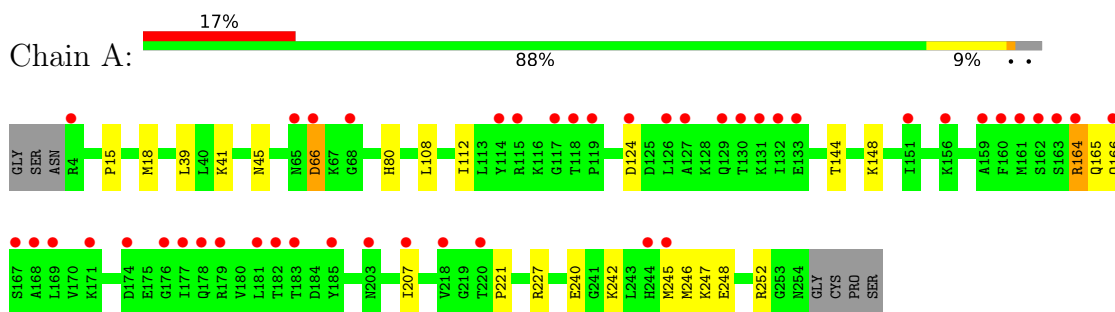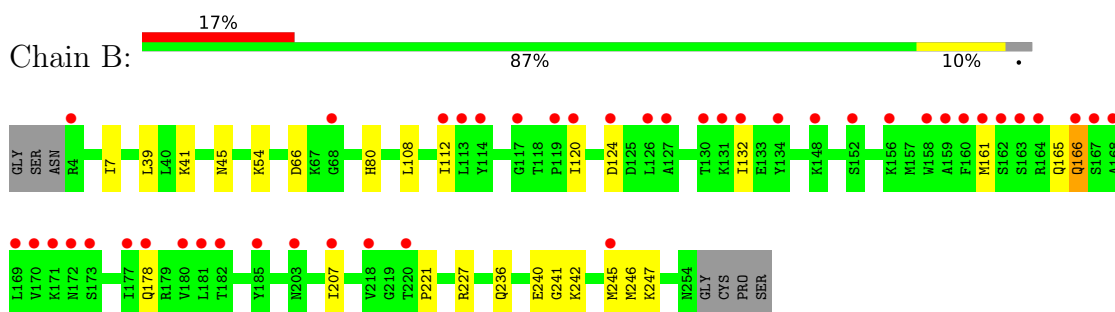
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	97.82Å 97.82Å 129.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.57 – 1.80 21.57 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (21.57-1.80) 99.9 (21.57-1.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.16 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.219 0.206 , 0.223	Depositor DCC
R_{free} test set	2884 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.3	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.486 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4620	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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: UB1, 1PE, CL

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	0.42	0/2128	0.55	0/2865
1	B	0.42	0/2118	0.55	0/2852
All	All	0.42	0/4246	0.55	0/5717

There are no bond length outliers.

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	2089	0	2108	14	0
1	B	2079	0	2100	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	16	0	22	0	0
3	B	16	0	22	1	0
4	A	26	0	11	0	0
4	B	26	0	11	0	0
5	A	190	0	0	3	0
5	B	176	0	0	6	0
All	All	4620	0	4274	31	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 4.

All (31) 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:221[A]:PRO:HG3	5:A:671:HOH:O	1.74	0.87
1:B:221[A]:PRO:HG3	5:B:705:HOH:O	1.76	0.86
1:A:248:GLU:O	1:A:252:ARG:HG3	1.93	0.68
1:B:240[A]:GLU:HG3	1:B:242:LYS:HG3	1.76	0.67
1:B:120:ILE:HD11	1:B:132:ILE:HD13	1.78	0.66
1:B:80:HIS:HA	5:B:705:HOH:O	1.95	0.65
1:A:80:HIS:HA	5:A:671:HOH:O	1.96	0.65
3:B:601:1PE:OH7	5:B:761:HOH:O	2.16	0.63
1:B:245[B]:MET:HG3	5:B:764:HOH:O	2.01	0.60
1:B:166:GLN:H	1:B:166:GLN:CD	2.05	0.59
1:A:242:LYS:HA	1:A:245[B]:MET:HG2	1.84	0.58
1:A:112:ILE:HB	1:A:207:ILE:HB	1.87	0.57
1:A:240[A]:GLU:HG3	1:A:242:LYS:HG3	1.91	0.53
1:A:66:ASP:OD2	1:A:66:ASP:N	2.43	0.51
1:B:112:ILE:HB	1:B:207:ILE:HB	1.92	0.51
1:A:144:THR:O	1:A:148:LYS:HG2	2.11	0.51
1:A:41:LYS:HE2	1:A:45:ASN:HD21	1.75	0.50
1:B:39:LEU:N	1:B:246[B]:MET:HE1	2.26	0.49
1:B:161:MET:O	1:B:165:GLN:HA	2.13	0.48
1:B:41:LYS:HE2	1:B:45:ASN:HD21	1.77	0.48
1:B:242:LYS:HA	1:B:245[B]:MET:HG2	1.97	0.46
1:A:248:GLU:O	1:A:252:ARG:CG	2.63	0.45
1:A:164:ARG:HH21	1:A:166:GLN:HB3	1.82	0.45
1:A:80:HIS:CE1	5:A:769:HOH:O	2.70	0.45
1:B:236:GLN:OE1	5:B:774:HOH:O	2.21	0.44
1:A:15:PRO:HA	1:A:18[A]:MET:SD	2.57	0.44
1:B:7[B]:ILE:CG2	1:B:54[B]:LYS:HD2	2.48	0.43
1:A:39:LEU:HB2	1:A:246:MET:HE1	2.01	0.42
1:B:7[B]:ILE:HG23	1:B:54[B]:LYS:HD2	2.01	0.42
1:B:80:HIS:CE1	5:B:775:HOH:O	2.72	0.41
1:B:241:GLY:O	1:B:245[B]:MET:HG2	2.21	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	259/258 (100%)	249 (96%)	10 (4%)	0	100	100
1	B	258/258 (100%)	253 (98%)	5 (2%)	0	100	100
All	All	517/516 (100%)	502 (97%)	15 (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	230/225 (102%)	223 (97%)	7 (3%)	41	27
1	B	229/225 (102%)	222 (97%)	7 (3%)	40	25
All	All	459/450 (102%)	445 (97%)	14 (3%)	39	25

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ASP
1	A	108	LEU
1	A	124	ASP
1	A	164	ARG
1	A	165	GLN
1	A	227	ARG
1	A	247	LYS
1	B	66	ASP

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Mol	Chain	Res	Type
1	B	108	LEU
1	B	124	ASP
1	B	166	GLN
1	B	178	GLN
1	B	227	ARG
1	B	247	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	B	45	ASN
1	B	178	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides 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
4	UB1	B	602	-	21,27,27	1.93	5 (23%)	25,40,40	2.17	6 (24%)
3	1PE	A	602	-	15,15,15	0.47	0	14,14,14	0.34	0
3	1PE	B	601	-	15,15,15	0.48	0	14,14,14	0.36	0
4	UB1	A	603	-	21,27,27	1.93	5 (23%)	25,40,40	2.16	5 (20%)

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
4	UB1	B	602	-	-	2/11/16/16	0/2/2/2
3	1PE	A	602	-	-	3/13/13/13	-
3	1PE	B	601	-	-	2/13/13/13	-
4	UB1	A	603	-	-	2/11/16/16	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	UB1	C18-C19	4.38	1.47	1.38
4	B	602	UB1	C18-C19	4.38	1.47	1.38
4	B	602	UB1	BR25-C18	4.12	1.98	1.89
4	A	603	UB1	BR25-C18	4.08	1.97	1.89
4	B	602	UB1	C6-C1	3.11	1.39	1.34
4	A	603	UB1	C6-C1	2.99	1.39	1.34
4	A	603	UB1	C4-N5	2.68	1.42	1.38
4	B	602	UB1	C4-N5	2.48	1.42	1.38
4	B	602	UB1	C4-N3	2.18	1.42	1.38
4	A	603	UB1	C4-N3	2.11	1.42	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	UB1	BR25-C18-C19	-6.16	121.13	127.67
4	B	602	UB1	BR25-C18-C19	-6.00	121.30	127.67
4	A	603	UB1	C2-N3-C4	-4.57	119.68	125.46
4	B	602	UB1	C2-N3-C4	-4.50	119.77	125.46
4	B	602	UB1	C16-N3-C4	4.39	123.29	116.97
4	A	603	UB1	C16-N3-C4	4.32	123.20	116.97
4	B	602	UB1	N5-C4-N3	3.51	119.92	115.57
4	A	603	UB1	N5-C4-N3	3.40	119.78	115.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	602	UB1	O15-C4-N5	-3.08	118.02	122.42
4	A	603	UB1	O15-C4-N5	-2.91	118.26	122.42
4	B	602	UB1	C17-C16-N3	-2.05	109.53	113.43

There are no chirality outliers.
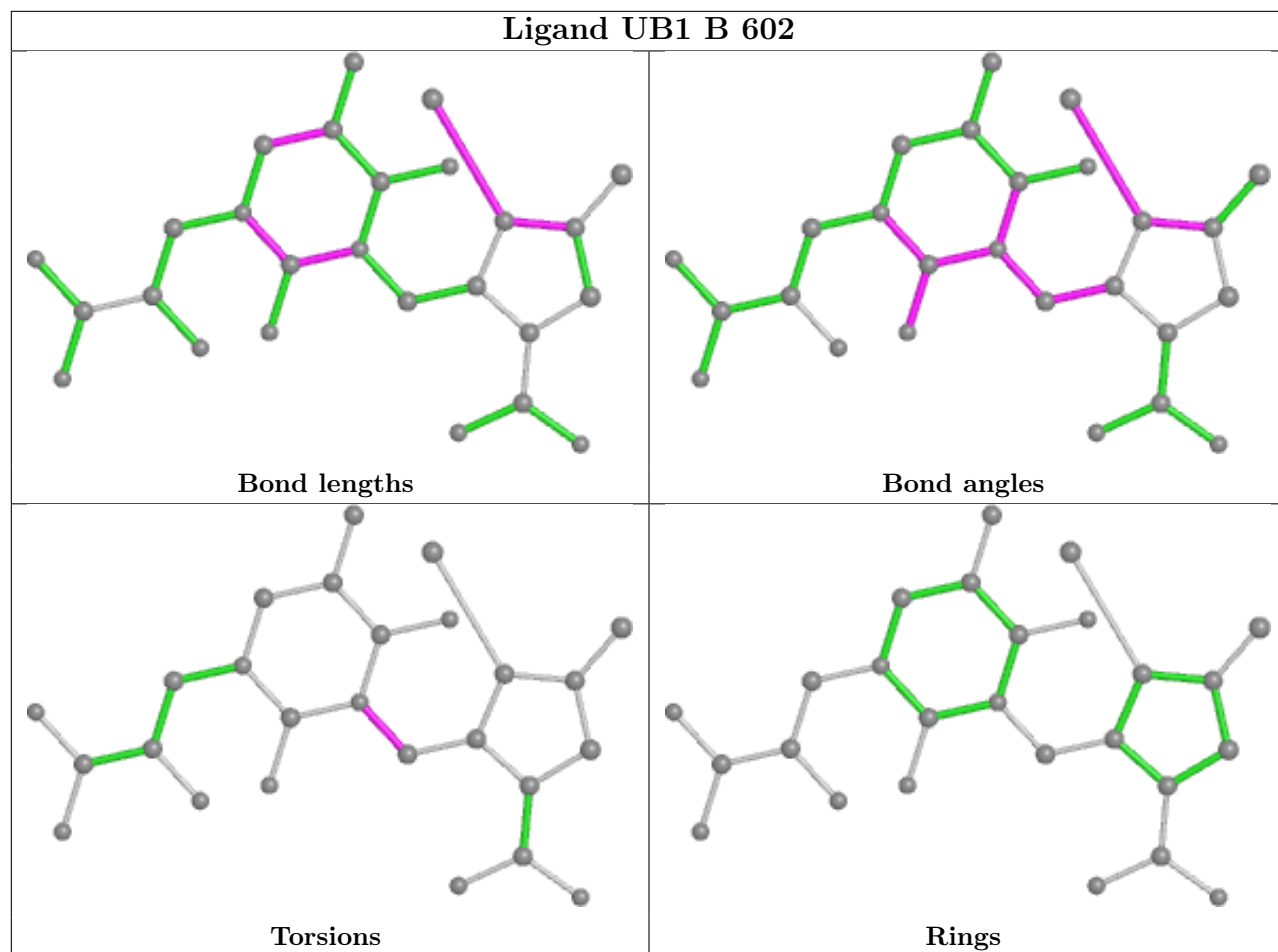
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	UB1	C17-C16-N3-C4
4	B	602	UB1	C17-C16-N3-C4
4	B	602	UB1	C17-C16-N3-C2
4	A	603	UB1	C17-C16-N3-C2
3	B	601	1PE	C16-C26-OH6-C15
3	A	602	1PE	OH6-C15-C25-OH5
3	B	601	1PE	OH4-C13-C23-OH3
3	A	602	1PE	C12-C22-OH3-C23
3	A	602	1PE	OH4-C13-C23-OH3

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand UB1 B 602

Bond lengths

Bond angles

Torsions

Rings

Ligand UB1 A 603

Bond lengths

Bond angles

Torsions

Rings
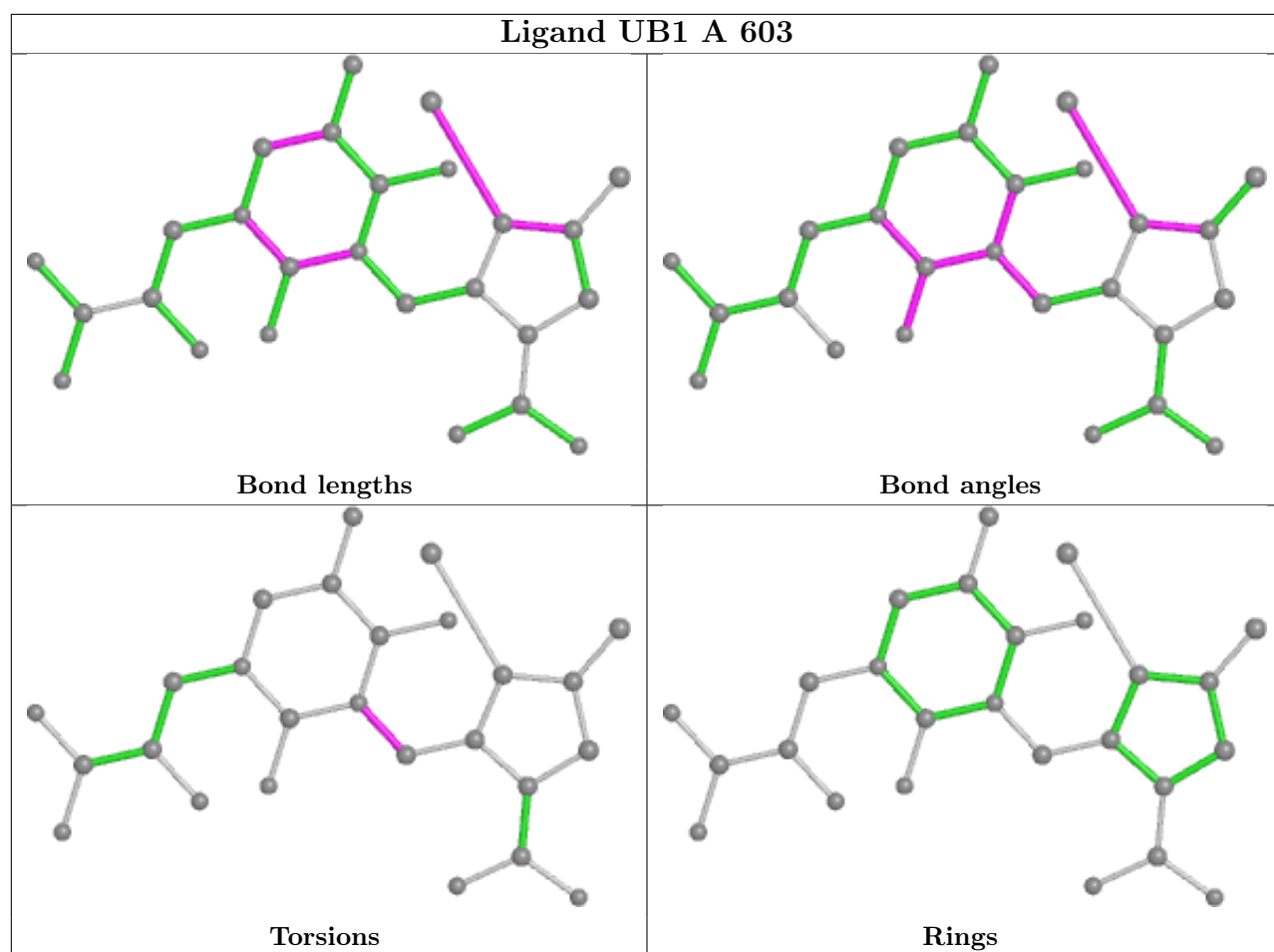
5.7 Other polymers ⓘ

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%)	0.82	45 (17%)	1	0	14, 35, 56, 60	0
1	B	251/258 (97%)	0.84	44 (17%)	1	1	14, 34, 55, 60	0
All	All	502/516 (97%)	0.83	89 (17%)	1	1	14, 35, 56, 60	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	166	GLN	8.3
1	B	163	SER	7.2
1	A	127	ALA	6.9
1	B	160	PHE	6.8
1	A	163	SER	6.4
1	B	161	MET	6.2
1	A	160	PHE	6.1
1	A	119	PRO	5.9
1	B	114	TYR	5.7
1	A	161	MET	5.7
1	B	131	LYS	5.7
1	B	124	ASP	5.3
1	B	127	ALA	5.2
1	B	171	LYS	4.8
1	B	119	PRO	4.8
1	B	178	GLN	4.6
1	B	167	SER	4.5
1	A	131	LYS	4.5
1	B	117	GLY	4.4
1	A	114	TYR	4.3
1	A	124	ASP	4.3
1	B	148	LYS	4.2
1	A	167	SER	4.2
1	A	178	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	173	SER	4.0
1	A	159	ALA	4.0
1	A	126	LEU	3.8
1	B	168	ALA	3.8
1	B	159	ALA	3.7
1	B	166	GLN	3.7
1	B	162	SER	3.7
1	A	183	THR	3.7
1	B	164	ARG	3.5
1	B	207	ILE	3.4
1	B	130	THR	3.4
1	B	68	GLY	3.4
1	A	171	LYS	3.4
1	B	181	LEU	3.4
1	A	130	THR	3.3
1	A	162	SER	3.3
1	A	133	GLU	3.2
1	B	177	ILE	3.2
1	B	182	THR	3.1
1	A	132	ILE	3.0
1	A	68	GLY	3.0
1	A	66	ASP	3.0
1	B	203	ASN	2.9
1	A	245[A]	MET	2.9
1	B	126	LEU	2.9
1	B	112	ILE	2.9
1	A	207	ILE	2.9
1	A	168	ALA	2.9
1	A	181	LEU	2.8
1	B	132	ILE	2.8
1	B	134	TYR	2.8
1	A	129	GLN	2.8
1	A	117	GLY	2.8
1	B	169	LEU	2.7
1	B	156	LYS	2.7
1	A	185	TYR	2.7
1	A	182	THR	2.6
1	A	203	ASN	2.6
1	A	156	LYS	2.6
1	A	218	VAL	2.6
1	B	180	VAL	2.6
1	A	169	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	170	VAL	2.5
1	A	177	ILE	2.5
1	B	245[A]	MET	2.4
1	B	220	THR	2.4
1	B	185	TYR	2.3
1	B	120	ILE	2.3
1	B	113	LEU	2.3
1	A	220	THR	2.2
1	B	158	TRP	2.2
1	A	179	ARG	2.2
1	B	218	VAL	2.2
1	A	4	ARG	2.2
1	A	164	ARG	2.1
1	B	4	ARG	2.1
1	A	151	ILE	2.1
1	A	115	ARG	2.1
1	A	174	ASP	2.1
1	A	65	ASN	2.1
1	A	176	GLY	2.1
1	B	172	ASN	2.0
1	A	118	THR	2.0
1	A	244	HIS	2.0
1	B	152	SER	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 ⓘ

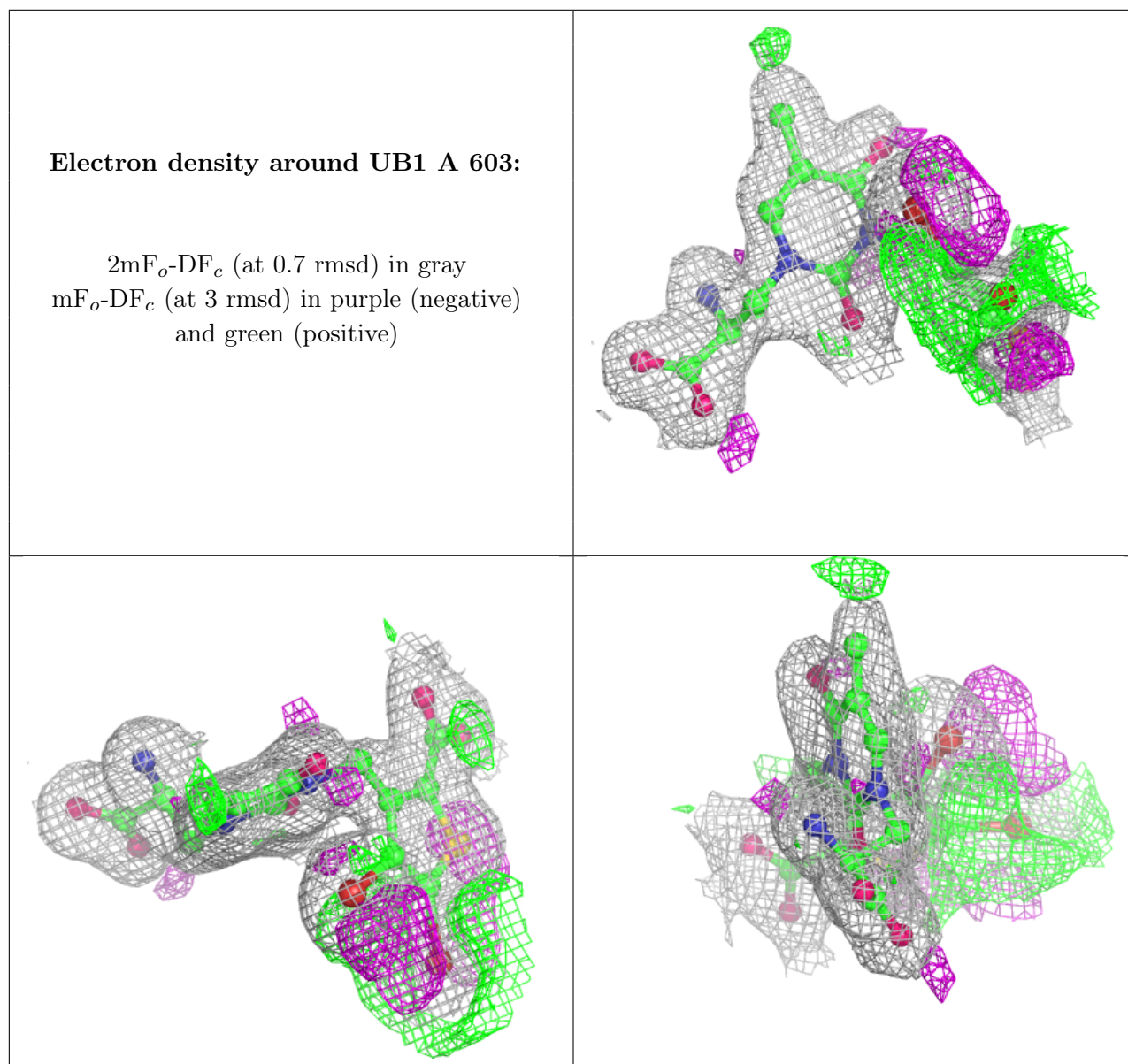There are no monosaccharides in this entry.

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. 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.

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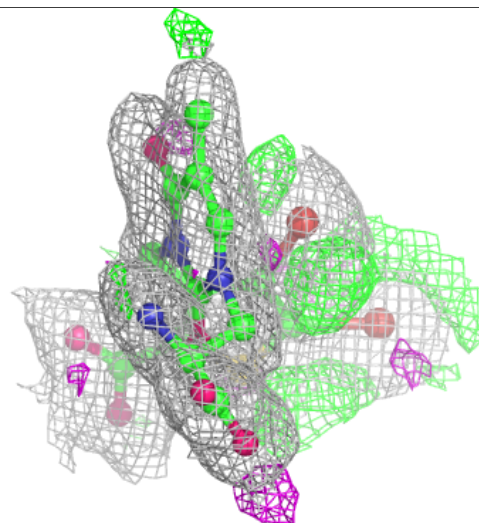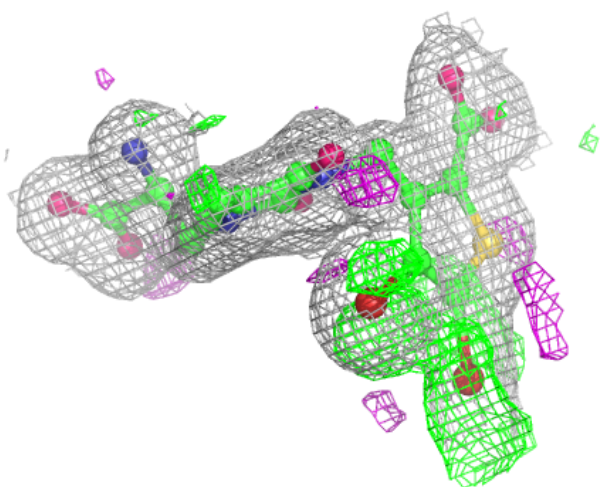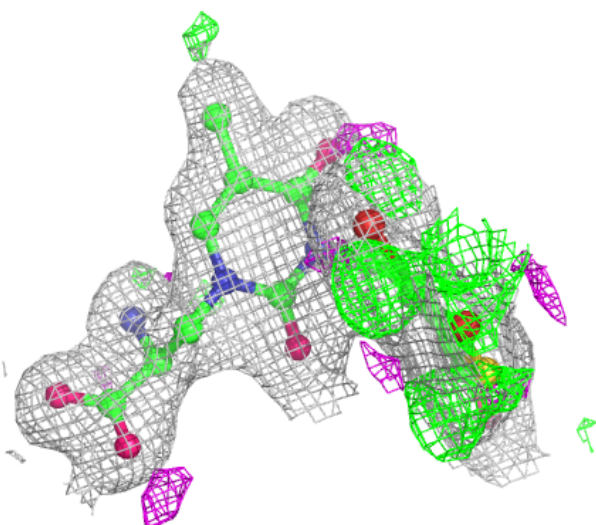
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	1PE	A	602	16/16	0.93	0.13	20,24,29,31	16
4	UB1	A	603	26/26	0.93	0.10	30,37,43,45	2
4	UB1	B	602	26/26	0.94	0.10	30,38,43,45	2
3	1PE	B	601	16/16	0.95	0.11	18,24,31,31	16
2	CL	A	501	1/1	0.99	0.06	24,24,24,24	1
2	CL	B	502	1/1	0.99	0.06	24,24,24,24	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UB1 A 603:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around UB1 B 602:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5　Other polymers ⓘ

There are no such residues in this entry.