



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:02 PM BST

PDB ID : 4UQ6
EMDB ID: : EMD-2684
Title : Electron density map of GluA2em in complex with LY451646 and glutamate
Authors : Meyerson, J.R.; Kumar, J.; Chittori, S.; Rao, P.; Pierson, J.; Bartesaghi, A.; Mayer, M.L.; Subramaniam, S.
Deposited on : 2014-06-20
Resolution : 12.80 Å(reported)
Based on PDB ID : 3KG2, 1FTJ

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

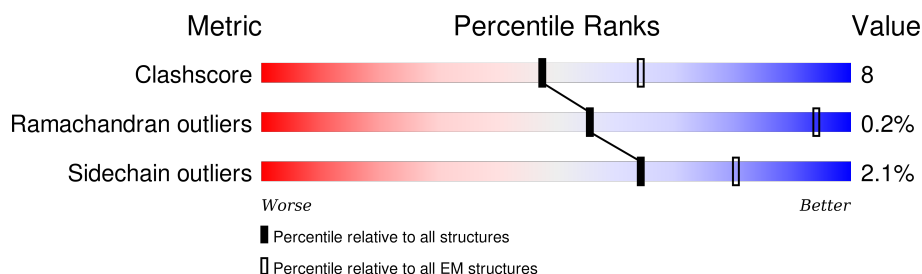
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 12.80 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	826	
1	B	826	
1	C	826	
1	D	826	

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
2	GLU	D	999	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18832 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	631	Total	C	N	O	S	0	0
			4685	2995	761	907	22		
1	B	632	Total	C	N	O	S	0	0
			4711	3011	765	912	23		
1	C	631	Total	C	N	O	S	0	0
			4685	2995	761	907	22		
1	D	632	Total	C	N	O	S	0	0
			4711	3011	765	912	23		

There are 28 discrepancies between the modelled and reference sequences:

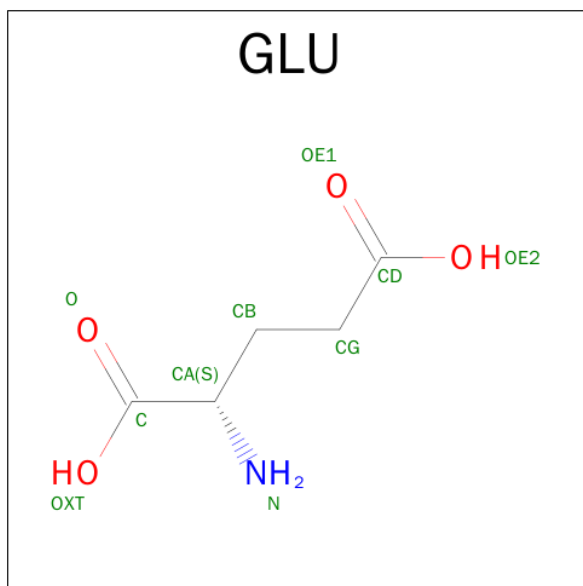
Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	CONFLICT	UNP P19491
A	382	LEU	VAL	CONFLICT	UNP P19491
A	384	GLU	LEU	CONFLICT	UNP P19491
A	385	ASP	THR	CONFLICT	UNP P19491
A	744	ASN	THR	VARIANT	UNP P19491
A	754	ASN	SER	VARIANT	UNP P19491
A	758	LEU	VAL	VARIANT	UNP P19491
B	241	GLU	ASN	CONFLICT	UNP P19491
B	382	LEU	VAL	CONFLICT	UNP P19491
B	384	GLU	LEU	CONFLICT	UNP P19491
B	385	ASP	THR	CONFLICT	UNP P19491
B	744	ASN	THR	VARIANT	UNP P19491
B	754	ASN	SER	VARIANT	UNP P19491
B	758	LEU	VAL	VARIANT	UNP P19491
C	241	GLU	ASN	CONFLICT	UNP P19491
C	382	LEU	VAL	CONFLICT	UNP P19491
C	384	GLU	LEU	CONFLICT	UNP P19491
C	385	ASP	THR	CONFLICT	UNP P19491
C	744	ASN	THR	VARIANT	UNP P19491
C	754	ASN	SER	VARIANT	UNP P19491
C	758	LEU	VAL	VARIANT	UNP P19491
D	241	GLU	ASN	CONFLICT	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
D	382	LEU	VAL	CONFLICT	UNP P19491
D	384	GLU	LEU	CONFLICT	UNP P19491
D	385	ASP	THR	CONFLICT	UNP P19491
D	744	ASN	THR	VARIANT	UNP P19491
D	754	ASN	SER	VARIANT	UNP P19491
D	758	LEU	VAL	VARIANT	UNP P19491

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).

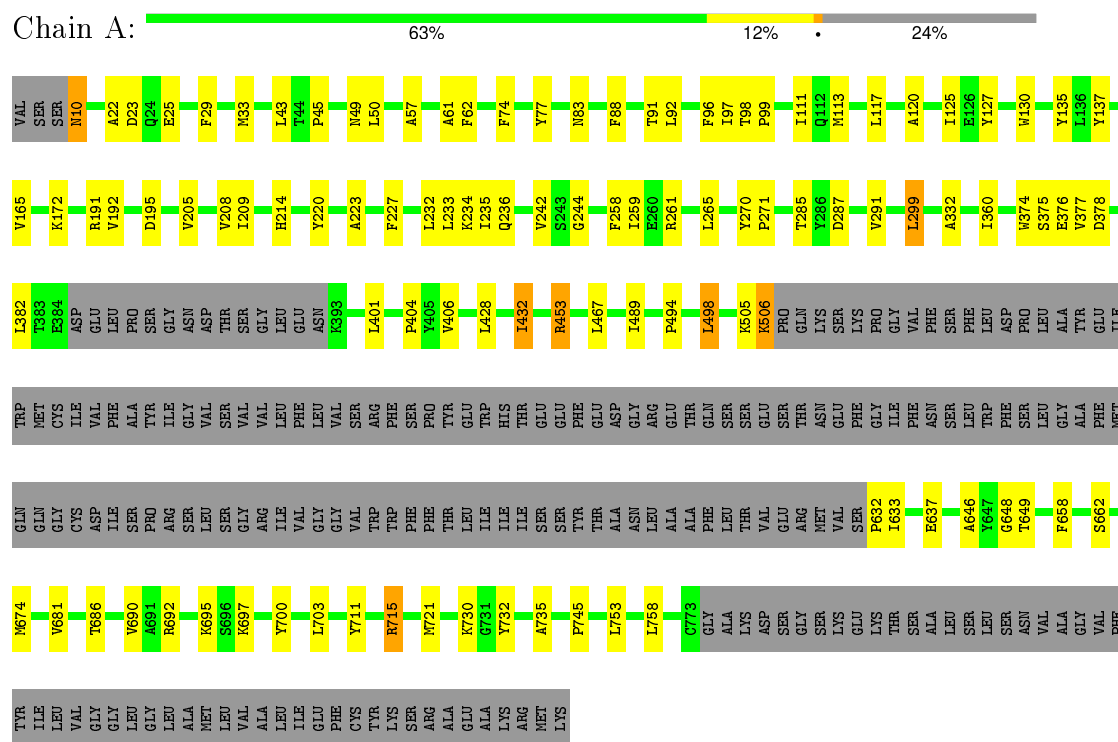


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			10	5	1	4	
2	B	1	Total	C	N	O	0
			10	5	1	4	
2	C	1	Total	C	N	O	0
			10	5	1	4	
2	D	1	Total	C	N	O	0
			10	5	1	4	

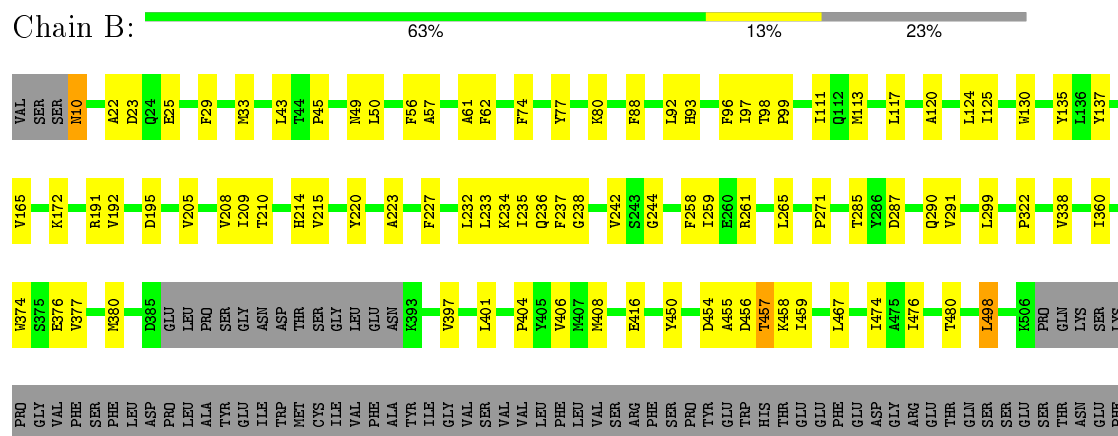
3 Residue-property plots

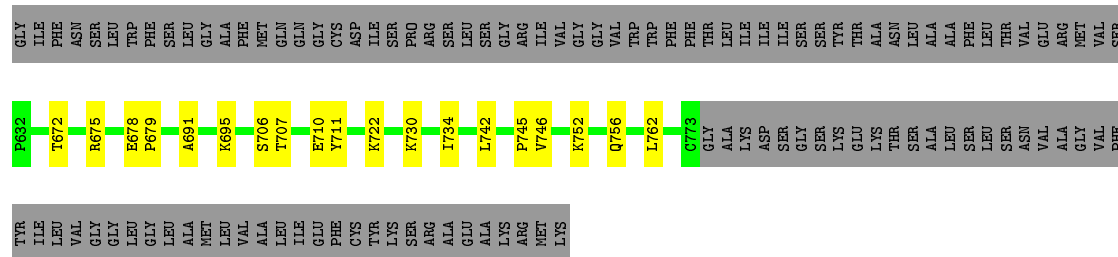
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. 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 2



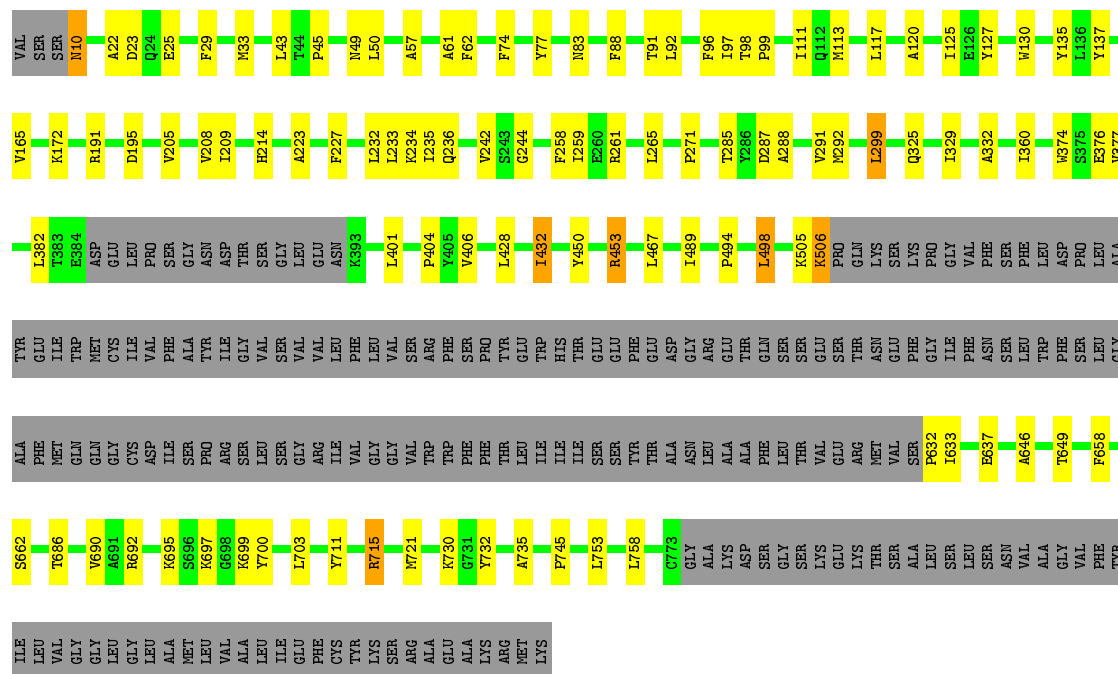
• Molecule 1: GLUTAMATE RECEPTOR 2





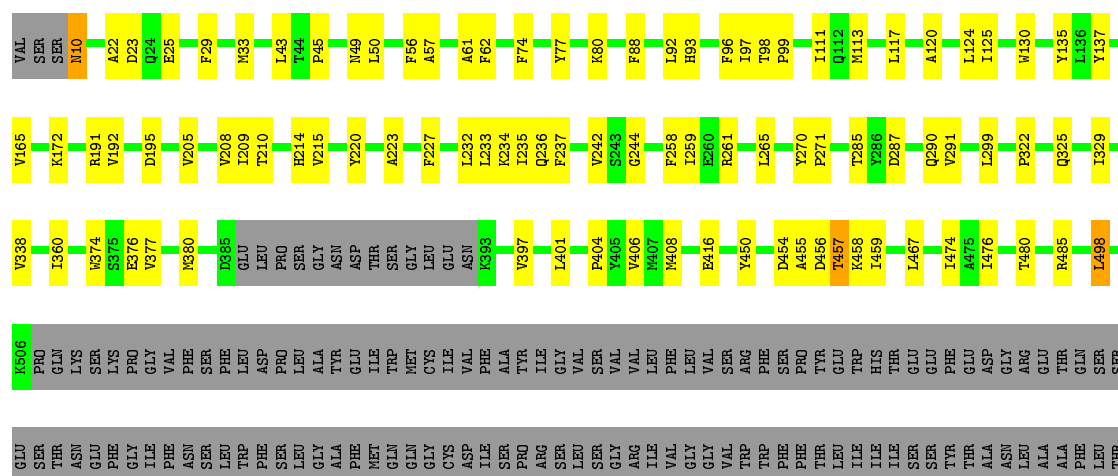
• Molecule 1: GLUTAMATE RECEPTOR 2

Chain C: 64% 12% 24%



• Molecule 1: GLUTAMATE RECEPTOR 2

Chain D: 62% 14% 23%



VAL	GLU	ARG	MET	VAL	SER	P632	6648	7649	1650	6653	7672	6675	6678	6679	6680	6681	A691	6695	S706	T707	E710	Y711	K722	K730	I734	L742	P745	V746	K752	Q756	L762	C773	GLY	ALA	LYS	ASP	SER	GLY	SER	LYS	GLU				
LYS	THR	SER	ALA	LEU	SER	LEU	SER	ASN	VAL	ALA	GLY	VAL	PHE	TYR	ILE	LEU	VAL	GLY	GLY	GLY	LEU	GLY	LEU	ALA	MET	LEU	VAL	ALA	LEU	ILE	GLU	PHE	CYS	TYR	LYS	SER	SER	ARG	ALA	GLU	ALA	LYS	ARG	MET	LYS

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE, Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	47000	Depositor
Image detector	FEI FALCON II (4K X 4K)	Depositor

5 Model quality

5.1 Standard geometry

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.36	0/4781	0.52	1/6501 (0.0%)
1	B	0.38	0/4807	0.53	1/6537 (0.0%)
1	C	0.36	0/4781	0.52	1/6501 (0.0%)
1	D	0.38	0/4807	0.53	1/6537 (0.0%)
All	All	0.37	0/19176	0.52	4/26076 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	745	PRO	N-CA-CB	5.87	110.35	103.30
1	D	745	PRO	N-CA-CB	5.84	110.31	103.30
1	C	745	PRO	N-CA-CB	5.47	109.87	103.30
1	A	745	PRO	N-CA-CB	5.45	109.83	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4685	0	4386	67	0
1	B	4711	0	4415	72	0
1	C	4685	0	4386	65	0
1	D	4711	0	4415	83	0
2	A	10	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	5	1	0
2	C	10	0	5	1	0
2	D	10	0	5	12	0
All	All	18832	0	17622	280	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 8.

The worst 5 of 280 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:215:VAL:HG11	1:D:215:VAL:HG11	1.42	1.00
1:B:454:ASP:HB3	1:B:457:THR:HG22	1.54	0.89
1:D:454:ASP:HB3	1:D:457:THR:HG22	1.54	0.88
1:D:650:LEU:HD23	2:D:999:GLU:HG3	1.58	0.85
1:D:691:ALA:O	1:D:695:LYS:HD3	1.81	0.81

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 PDB entries followed by that with respect to all EM entries.

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	625/826 (76%)	593 (95%)	31 (5%)	1 (0%)	52	86
1	B	626/826 (76%)	597 (95%)	28 (4%)	1 (0%)	52	86
1	C	625/826 (76%)	593 (95%)	31 (5%)	1 (0%)	52	86
1	D	626/826 (76%)	597 (95%)	28 (4%)	1 (0%)	52	86
All	All	2502/3304 (76%)	2380 (95%)	118 (5%)	4 (0%)	56	86

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	LYS
1	B	172	LYS
1	C	172	LYS
1	D	172	LYS

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 PDB entries followed by that with respect to all EM entries.

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	472/706 (67%)	461 (98%)	11 (2%)	58	83
1	B	475/706 (67%)	466 (98%)	9 (2%)	65	86
1	C	472/706 (67%)	461 (98%)	11 (2%)	58	83
1	D	475/706 (67%)	466 (98%)	9 (2%)	65	86
All	All	1894/2824 (67%)	1854 (98%)	40 (2%)	64	84

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	722	LYS
1	C	432	ILE
1	D	467	LEU
1	C	10	ASN
1	C	453	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	C	83	ASN

5.3.3 RNA ⓘ

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](#)

4 ligands are modelled in this entry.

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	$\# Z > 2$
2	GLU	A	999	-	3,9,9	0.13	0	3,11,11	0.13	0
2	GLU	B	999	-	3,9,9	0.14	0	3,11,11	0.15	0
2	GLU	C	999	-	3,9,9	0.14	0	3,11,11	0.13	0
2	GLU	D	999	-	3,9,9	0.13	0	3,11,11	0.15	0

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
2	GLU	A	999	-	-	0/3/9/9	0/0/0/0
2	GLU	B	999	-	-	0/3/9/9	0/0/0/0
2	GLU	C	999	-	-	0/3/9/9	0/0/0/0
2	GLU	D	999	-	-	0/3/9/9	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	999	GLU	1	0
2	C	999	GLU	1	0
2	D	999	GLU	12	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.