



## wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Sep 3, 2017 – 06:30 PM EDT

PDB ID : 5KUF  
EMDB ID: : EMD-8289  
Title : GluK2EM with 2S,4R-4-methylglutamate  
Authors : Meyerson, J.R.; Chittori, S.; Merk, A.; Rao, P.; Han, T.H.; Serpe, M.; Mayer, M.L.; Subramaniam, S.  
Deposited on : unknown  
Resolution : 3.80 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

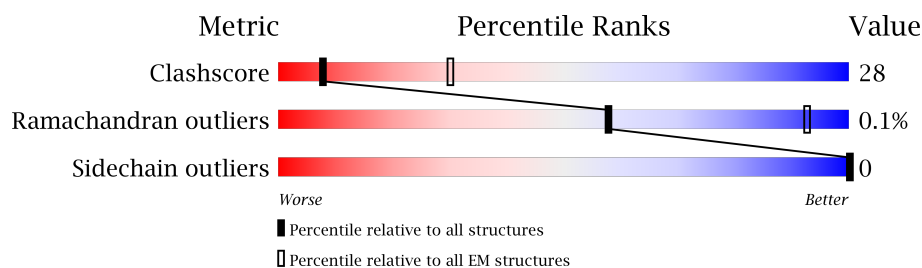
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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  $\geq 3$ , 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	877	<div> <div style="width: 44%; background-color: green;"></div> <div style="width: 42%; background-color: yellow;"></div> <div style="width: 14%; background-color: grey;"></div> </div> <div>44% 42% 14%</div>
1	B	877	<div> <div style="width: 41%; background-color: green;"></div> <div style="width: 44%; background-color: yellow;"></div> <div style="width: 14%; background-color: grey;"></div> </div> <div>41% 44% 14%</div>
1	C	877	<div> <div style="width: 43%; background-color: green;"></div> <div style="width: 42%; background-color: yellow;"></div> <div style="width: 14%; background-color: grey;"></div> </div> <div>43% 42% 14%</div>
1	D	877	<div> <div style="width: 41%; background-color: green;"></div> <div style="width: 44%; background-color: yellow;"></div> <div style="width: 14%; background-color: grey;"></div> </div> <div>41% 44% 14%</div>

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	SYM	B	901	-	-	X	-
2	SYM	D	901	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23728 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 ionotropic, kainate 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	750	Total	C	N	O	S	0	0
			5921	3802	985	1103	31		
1	B	750	Total	C	N	O	S	0	0
			5921	3802	985	1103	31		
1	C	750	Total	C	N	O	S	0	0
			5921	3802	985	1103	31		
1	D	750	Total	C	N	O	S	0	0
			5921	3802	985	1103	31		

There are 24 discrepancies between the modelled and reference sequences:

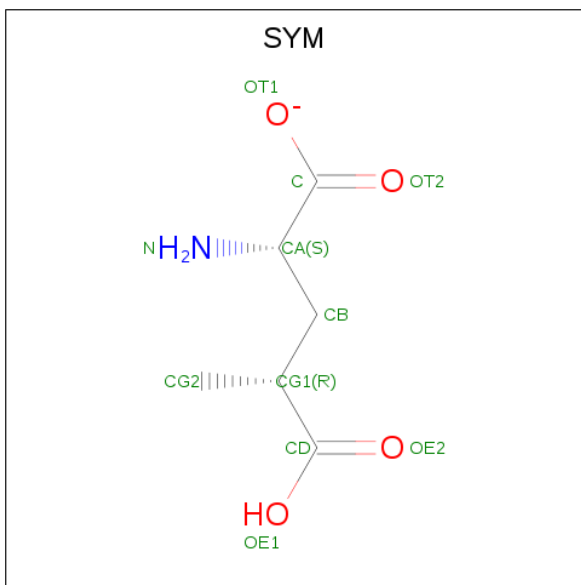
Chain	Residue	Modelled	Actual	Comment	Reference
A	487	THR	ALA	engineered mutation	UNP P42260
A	536	VAL	ILE	variant	UNP P42260
A	545	VAL	CYS	variant	UNP P42260
A	658	SER	ALA	engineered mutation	UNP P42260
A	690	SER	ASN	engineered mutation	UNP P42260
A	704	LEU	PHE	engineered mutation	UNP P42260
B	487	THR	ALA	engineered mutation	UNP P42260
B	536	VAL	ILE	variant	UNP P42260
B	545	VAL	CYS	variant	UNP P42260
B	658	SER	ALA	engineered mutation	UNP P42260
B	690	SER	ASN	engineered mutation	UNP P42260
B	704	LEU	PHE	engineered mutation	UNP P42260
C	487	THR	ALA	engineered mutation	UNP P42260
C	536	VAL	ILE	variant	UNP P42260
C	545	VAL	CYS	variant	UNP P42260
C	658	SER	ALA	engineered mutation	UNP P42260
C	690	SER	ASN	engineered mutation	UNP P42260
C	704	LEU	PHE	engineered mutation	UNP P42260
D	487	THR	ALA	engineered mutation	UNP P42260
D	536	VAL	ILE	variant	UNP P42260
D	545	VAL	CYS	variant	UNP P42260
D	658	SER	ALA	engineered mutation	UNP P42260

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Chain	Residue	Modelled	Actual	Comment	Reference
D	690	SER	ASN	engineered mutation	UNP P42260
D	704	LEU	PHE	engineered mutation	UNP P42260

- Molecule 2 is 2S,4R-4-METHYLGLUTAMATE (three-letter code: SYM) (formula:  $C_6H_{10}NO_4$ ).

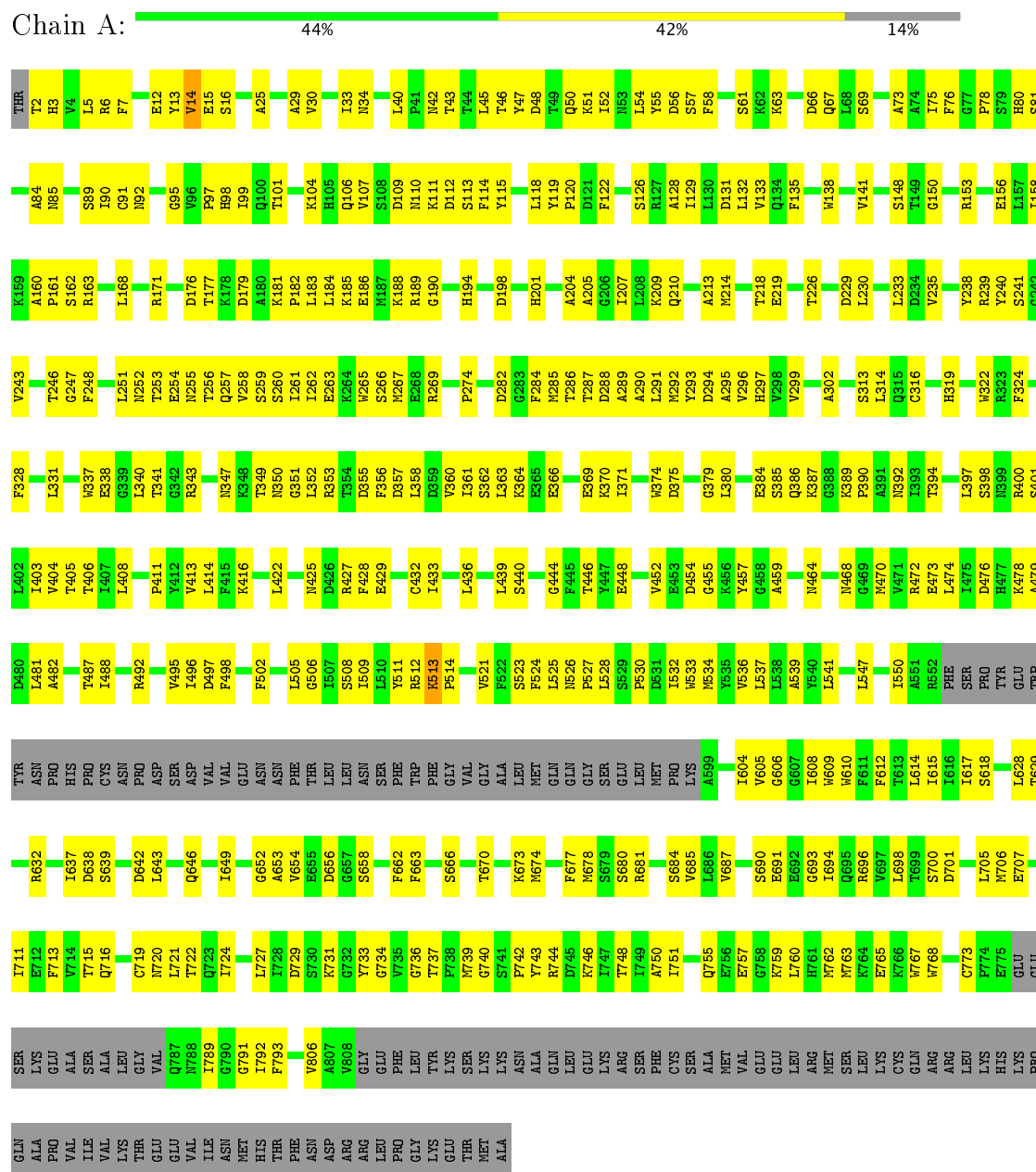


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			11	6	1	4	
2	B	1	Total	C	N	O	0
			11	6	1	4	
2	C	1	Total	C	N	O	0
			11	6	1	4	
2	D	1	Total	C	N	O	0
			11	6	1	4	

### 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 the various outlier classes 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 ionotropic, kainate 2



- Molecule 1: Glutamate receptor ionotropic, kainate 2

Chain B: 

THR	T2	V4	L5	R6	F7	G8	G9	I10	F11	E12	Y13	V14	E15	S16	M19	G20	E22	E23	L24	A25	F26	R27	F28	A29	V30	I33	N34	R35	L39	L40	P41	M42	T43	L44	L45	T46	Y47	D48	T49	Q50	K51	I52	N53	L54	Y55	F56	S57	F58	E59	A60	S61	K62	K63																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
	D66	Q67	L68		G71	V72	A73	A74	F75	F76		H80	S81	S82	S83	A84	N85		Q88	S89	I90	L91	L92	N92	A93	L94	F96	G95		H98	I99	Q100			W103	K104	H105	Q106	V107	S108	D109		D112	S113	F114	Y115	V116	S117	L118	Y119	P120	D121	F122	S123	S124	L125	K209	Q210	A211	L212	A213	F136	F137																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
	W138			V144	Y145	D146	D147		I152	R153		E156		P161	Y164		K169	I170	R171	Q172	L173	P174	A175	D176	T177			L183	L184	K185	E186	M187	K188	R189	G190	K191	E192	F193	H194		D198	C199	S200	S201	E202	M203	A204	A205	G206	L207	L208	L209	K209	Q210	A211	L212	A213	M214																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
	M217	T218	E219		E222	Y223	I224	T226		L230		L233	D234	V235	E236	K237	Y238	R239	Y240	S241	L173	G242	V243	I244	E245	T246	G247	F248																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			</

- Molecule 1: Glutamate receptor ionotropic, kainate 2

Chain C: 

THR																										N85																										K159																										R171																										D176																										P177																										K178																										D179																										A180																										P182																										L183																										L184																										K185																										E186																										M187																										K188																										R189																										G190																										H194																										D198																										E201																										A204																										A205																										G206																										I207																										L208																										K209																										Q210																										A213																										M214																										T218																										E219																										T226																										D229																										L230																										L233																										D234																										V235																										Y238																										R239																										Y240																										S241																										G242																									
	H2	T3	V4	L5	R6	F7	E12	Y13	V14	E15	S16	A25	A29	V30	I33	N34	L40	M42	T43	F44	L45	Y47	D48	T49	Q50		R51	I52	H53	L54	Y55	D56	S57	F58	S61	D66	Q67	L68	S69	A73	A74	I75	F76	H80	S81	A84	N85	S89	P91	C91	N92		A93	L94	G95	V96	P97	H98	I99	Q100	T101	K104	H105	Q106	L106	L107	S108	D109	K110	K111	D112	S113	F114	Y115	L118	Y119	P120		D121	F122	S126	R127	A128	I129	L130	D131	L132	V133	Q134	F135	W138	V141	S148	T149	G150	V153	R154	Q155	E156	L157	I158	K159	A160		S162	R163	L168	R171	D176	P177	K178	D179	A180	P182	L183	L184	K185	E186	M187	K188	R189	G190	H194	D198	E201	A204	A205	G206	I207		L208	K209	Q210	A213	M214	T218	E219	T226	D229	L230	L233	D234	V235	Y238	R239	Y240	S241	G242																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									

- Molecule 1: Glutamate receptor ionotropic, kainate 2






## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	62244	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 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: SYM

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	0.48	0/6050	0.58	1/8194 (0.0%)
1	B	0.48	0/6050	0.59	0/8194
1	C	0.48	0/6050	0.58	1/8194 (0.0%)
1	D	0.48	0/6050	0.59	0/8194
All	All	0.48	0/24200	0.58	2/32776 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	3
1	D	0	1
All	All	0	8

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	513	LYS	C-N-CD	-5.10	109.37	120.60
1	C	513	LYS	C-N-CD	-5.09	109.40	120.60

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	VAL	Peptide
1	A	380	LEU	Peptide
1	A	80	HIS	Peptide
1	B	35	ARG	Peptide
1	C	14	VAL	Peptide

## 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	5921	0	5917	324	0
1	B	5921	0	5917	360	0
1	C	5921	0	5917	332	0
1	D	5921	0	5917	364	0
2	A	11	0	9	5	0
2	B	11	0	9	6	0
2	C	11	0	9	5	0
2	D	11	0	9	7	0
All	All	23728	0	23704	1337	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 28.

The worst 5 of 1337 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:C:5:LEU:HB3	1:C:45:LEU:HD22	1.44	0.98
1:A:5:LEU:HB3	1:A:45:LEU:HD22	1.44	0.97
1:B:92:ASN:HD21	1:B:113:SER:H	0.98	0.96
1:D:92:ASN:HD21	1:D:113:SER:H	0.98	0.91
1:D:88:GLN:HE22	1:D:106:GLN:HE22	1.21	0.88

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	744/877 (85%)	627 (84%)	116 (16%)	1 (0%)	55	88
1	B	744/877 (85%)	630 (85%)	114 (15%)	0	100	100
1	C	744/877 (85%)	625 (84%)	118 (16%)	1 (0%)	55	88
1	D	744/877 (85%)	630 (85%)	114 (15%)	0	100	100
All	All	2976/3508 (85%)	2512 (84%)	462 (16%)	2 (0%)	58	88

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	C	15	GLU

### 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 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	649/767 (85%)	649 (100%)	0	100	100
1	B	649/767 (85%)	649 (100%)	0	100	100
1	C	649/767 (85%)	649 (100%)	0	100	100
1	D	648/767 (84%)	648 (100%)	0	100	100
All	All	2595/3068 (85%)	2595 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	526	ASN
1	C	92	ASN
1	D	526	ASN
1	B	716	GLN
1	A	515	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](#)

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	SYM	A	901	-	2,10,10	0.22	0	2,13,13	0.27	0
2	SYM	B	901	-	2,10,10	0.15	0	2,13,13	0.31	0
2	SYM	C	901	-	2,10,10	0.23	0	2,13,13	0.28	0
2	SYM	D	901	-	2,10,10	0.15	0	2,13,13	0.32	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	SYM	A	901	-	-	0/4/12/12	0/0/0/0
2	SYM	B	901	-	-	0/4/12/12	0/0/0/0
2	SYM	C	901	-	-	0/4/12/12	0/0/0/0
2	SYM	D	901	-	-	0/4/12/12	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.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	SYM	5	0
2	B	901	SYM	6	0
2	C	901	SYM	5	0
2	D	901	SYM	7	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.