



wwPDB EM Map/Model Validation Report ⓘ

Sep 27, 2016 – 09:39 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 : 2016-07-13
Resolution : 3.80 Å(reported)

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) : rb-20027939

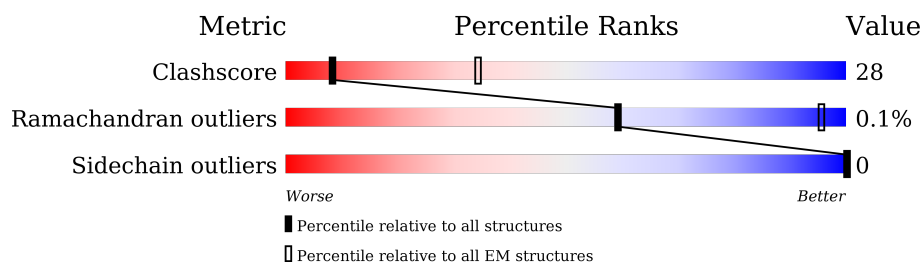
1 Overall quality at a glance

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	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	877	44% 42% 14%
1	B	877	41% 44% 14%
1	C	877	43% 42% 14%
1	D	877	41% 44% 14%

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:

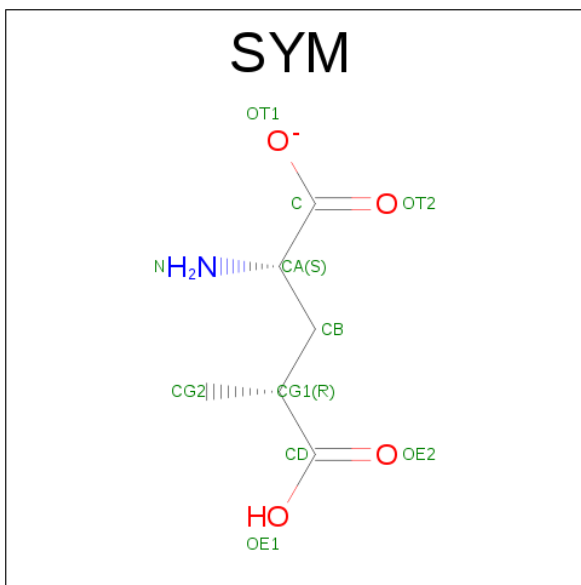
Chain	Residue	Modelled	Actual	Comment	Reference
A	487	THR	ALA	engineered mutation	UNP P42260
A	536	VAL	ILE	variant	UNP P42260
A	545	VAL	CYS	variant	UNP P42260
A	658	SER	ALA	engineered mutation	UNP P42260
A	690	SER	ASN	engineered mutation	UNP P42260
A	704	LEU	PHE	engineered mutation	UNP P42260
B	487	THR	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: $C_6H_{10}NO_4$).

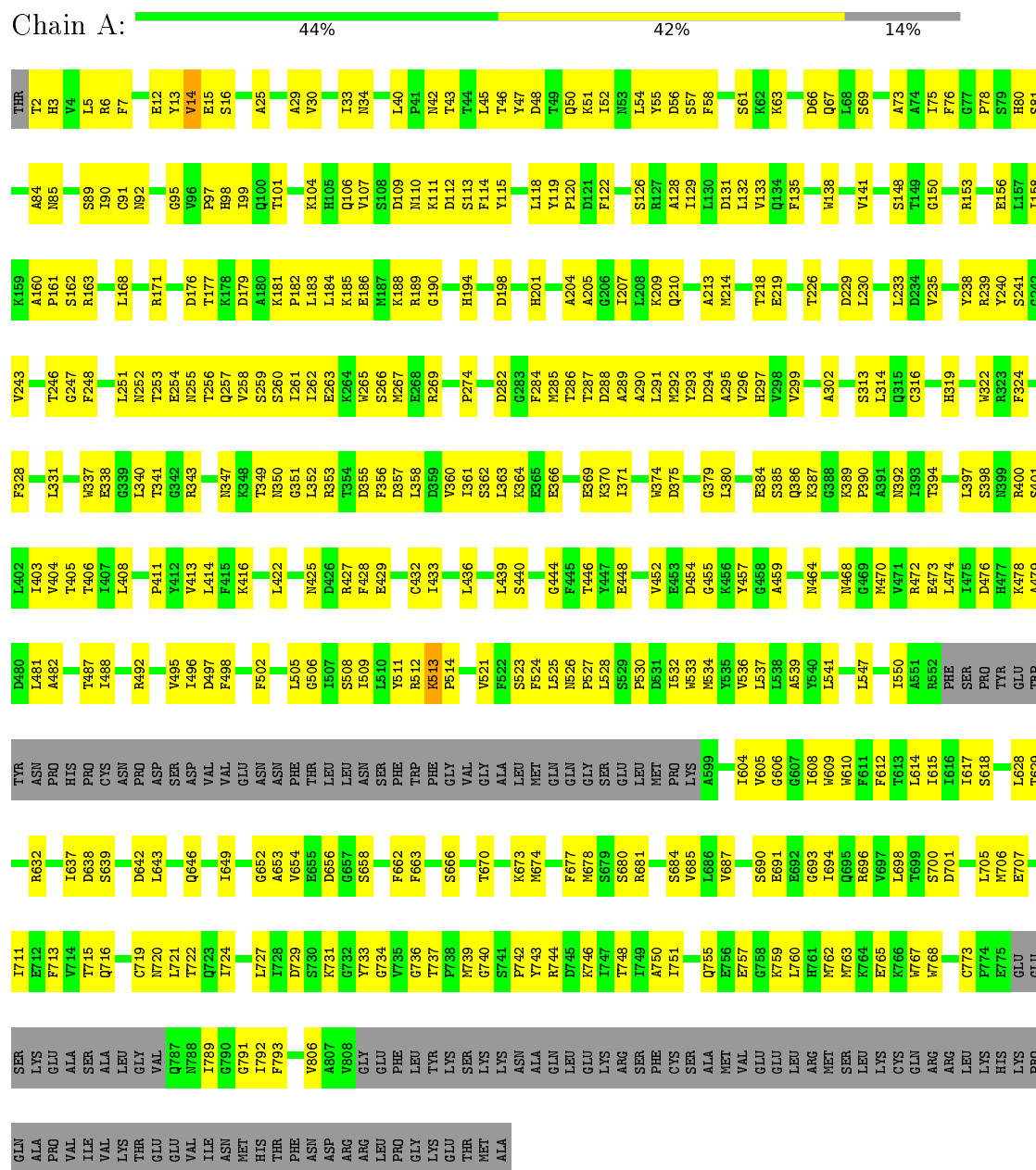


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			11	6	1	4	
2	B	1	Total	C	N	O	0
			11	6	1	4	
2	C	1	Total	C	N	O	0
			11	6	1	4	
2	D	1	Total	C	N	O	0
			11	6	1	4	

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 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 ionotropic, kainate 2



- Molecule 1: Glutamate receptor ionotropic, kainate 2

Chain B:  41% 44% 14%

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	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	O88	S89	C90	N91	N92	A93	L94	G95	H98	I99	Q100	M103	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	K137
	W138	V144	Y145	D146	D147	I152	R153	E156	P161	Y164	K169	I170	R171	Q172	L173	A175	D176	T177	K178	D179	A180	L183	L184	K185	E186	M187	K188	R189	G190	K191	E192	F193	H194	D198	C199	S200	E202	M203	A204	A205	Q206	L207	L208	K209	Q210	A211	L212	A213	M214	V206				
	M217	T218	E219	E222	Y223	I224	T226	L230	L233	D234	E236	Y237	Y238	R239	Y240	G242	N244	Y245	T246	G247	F248	T256	Q257	V258	S259	S260	L261	L262	E263	K264	W265	S266	M267	E268	R269	L270	D277	S278	G279	T286	T287	D288	A289	L290	L291	Y292	Y293	T405						
	H297	V298	M309	T310	V311	S312	L314	K322	R323	F324	F328	K329	E334	A335	H336	W337	L340	T341	N347	N350	R353	T354	D355	F356	D357	L358	D359	V360	E365	E366	E369	K370	L371	G372	L373	K374	D375	P376	A377	S378	A391	N392	S401	V404	T405	T406								
	E409	E410	P411	Y412	V413	L414	K415	M425	F428	E429	G430	C432	L433	D434	L435	L436	L439	L443	G444	T446	E447	E448	I449	R450	L451	V452	D453	G455	Y457	Q460	D461	M464	W467	N468	V471	R472	E473	L474	D480	L481	A482	P485	L486	T487	I488									
	T489	Y490	F492	E493	K494	V495	L496	D497	F498	S499	K500	T504	L505	G506	I507	S508	I509	R512	T517	N518	P519	S523	F524	L525	P527	L528	S529	D531	I532	W533	Y534	Y535	V536	A539	Y540	L541	G542	V545	V546	L547	F548	V549	I550	A551	R552	PHE	PRO	TYR	TRP					
TYR	ASN	PRO	HIS	PRO	CYS	ASN	PRO	ASP	ASP	ASP	VAL	VAL	GLU	ASN	ASN	PHE	THR	LEU	LEU	ASN	SER	PHE	TRP	PHE	GLY	VAL	GLY	ALA	ALA	MET	GLN	GLN	GLY	SER	GLU	LEU	MET	PRO	LYS	A599	L600	S601	I604	G607	I608	W609	N610	F611	L614	I615	L622	N623	L624	V625
	L628	T629	E630	E631	R632	E633	E634	S635	P636	D638	D642	Q646	K648	I649	E650	V654	E655	G657	S658	T659	P660	T661	F662	F663	K664	K665	I668	T670	Y671	D672	W675	M678	S679	S680	R681	V685	L686	V687	E691	E692	G693	I694	Q695	K696	V697	L698	T699							
	Y702	A703	L704	L705	M706	E707	S708	T709	T710	E711	E712	F713	V714	T715	Q716	Q719	T722	Q723	I724	I728	K731	G732	Y733	F734	T735	T736	T737	G740	R744	D745	K746	I747	T748	L752	Q753	L754	Q755	E756	E757	G758	K759	L760	H761	H762	M763	K764	E765	K766	K767	W768	C773	P774		
E775	GLU	GLU	SER	LYS	GLU	ALA	SER	ALA	ALA	GLY	VAL	Q787	F792	F793	L796	A797	F798	G799	L800	W801	L802	V808	GLY	GLU	PHE	LEU	TYR	LYS	LYS	ALA	ALA	GLN	LEU	GLU	LYS	ARG	SER	PHE	CYS	SER	ALA	MET	VAL	VAL	GLU	GLU	LEU	ARG	MET	SER	LEU	LYS	GLN	ARG
ARG	LEU	LYS	HIS	LYS	PRO	GLN	ALA	PRO	VAL	ILE	LYS	THR	GLU	GLU	VAL	ILE	ASN	MET	HIS	THR	PHE	ASN	ASP	ARG	ARG	ARG	GLY	PRO	GLY	GLY	LYS	GLU	THR	THR	SER	ARG	ARG	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA		

- Molecule 1: Glutamate receptor ionotropic, kainate 2

Chain C:  43% 42% 14%

THR																																																																																
	T2	H3	V4	L5	R6	F7	E12	Y13	V14	E15	S16	A25	A29	V30	I33	N34	L40	N42	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	I90	C91	N92	A93	L94	G95	V96	P97	H98	I99	Q100	T101	K104	H105	Q106	L106	L107	S108	M109	D110	K111	D112	S113	F114	Y115	L118	Y119	P120	D121	F122	S126	R127	A128	I129	L130	D131	L132	S133	Q134	F135	W138	V141	S148	T149	G150	V153	L154	Q155	L156	L157	I158																												
K159	A160	P161	S162	R163	L168	R171	D176	P177	K178	D179	A180	K181	P182	L183	L184	K185	E186	M187	K188	R189	G190	H194	D198	E201	A204	A205	G206	I207	L208	K209	Q210	A213	D214	T218	E219	T226	D229	L230	L233	D234	V235	Y238	R239	T240	S241	G242																																		

- Molecule 1: Glutamate receptor ionotropic, kainate 2

[illegible]




4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	62244	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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(°)	Ideal(°)
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 ⓘ

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 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%)	56	90
1	B	744/877 (85%)	630 (85%)	114 (15%)	0	100	100
1	C	744/877 (85%)	625 (84%)	118 (16%)	1 (0%)	56	90
1	D	744/877 (85%)	630 (85%)	114 (15%)	0	100	100
All	All	2976/3508 (85%)	2512 (84%)	462 (16%)	2 (0%)	59	90

All (2) Ramachandran outliers are listed below:

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

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	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	-	4,10,10	0.27	0	3,13,13	0.23	0
2	SYM	B	901	-	4,10,10	0.22	0	3,13,13	0.34	0
2	SYM	C	901	-	4,10,10	0.28	0	3,13,13	0.24	0
2	SYM	D	901	-	4,10,10	0.21	0	3,13,13	0.35	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.