



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

Nov 1, 2017 – 11:45 PM EDT

PDB ID : 5VHW  
EMDB ID: : EMD-8685  
Title : GluA2-0xGSG1L bound to ZK  
Authors : Twomey, E.C.; Yelshanskaya, M.V.; Grassucci, R.A.; Frank, J.; Sobolevsky, A.I.  
Deposited on : unknown  
Resolution : 7.80 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-20030345

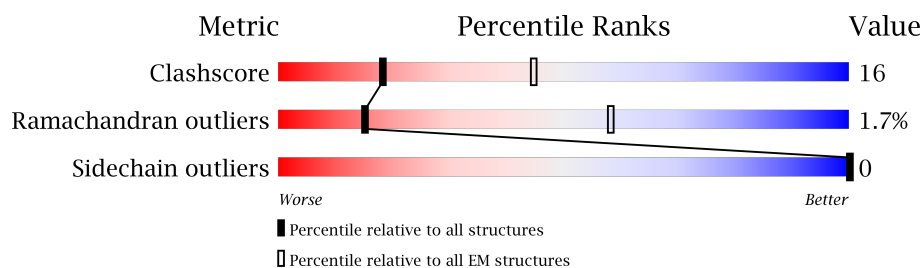
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.80 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	1057	
1	B	1057	
1	C	1057	
1	D	1057	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24756 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, Germ cell-specific gene 1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	783	Total	C	N	O	S	0	0
			6159	3950	1023	1156	30		
1	B	780	Total	C	N	O	S	0	0
			6137	3938	1017	1152	30		
1	C	783	Total	C	N	O	S	0	0
			6159	3950	1023	1156	30		
1	D	780	Total	C	N	O	S	0	0
			6137	3938	1017	1152	30		

There are 56 discrepancies between the modelled and reference sequences:

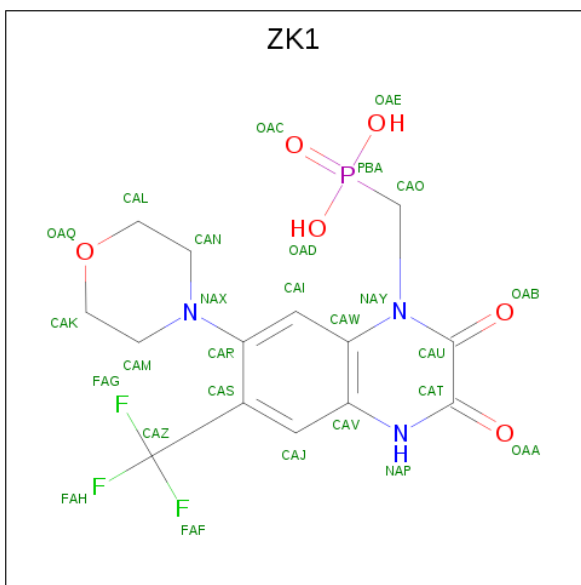
Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	827	GLY	-	linker	UNP P19491
A	828	THR	-	linker	UNP P19491
A	829	GLY	-	linker	UNP P19491
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491

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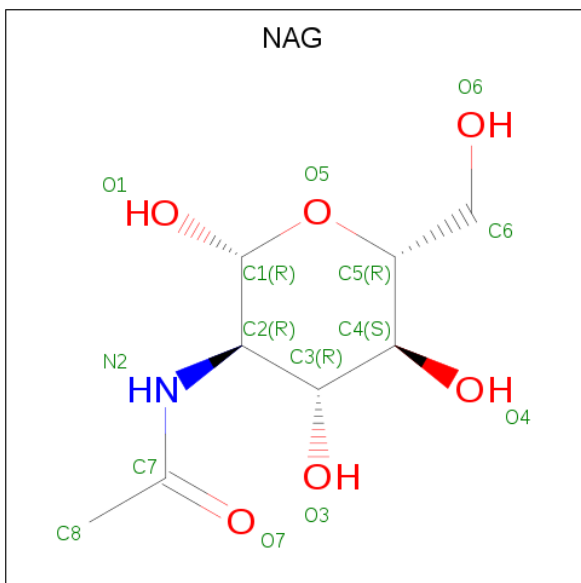
Chain	Residue	Modelled	Actual	Comment	Reference
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	827	GLY	-	linker	UNP P19491
B	828	THR	-	linker	UNP P19491
B	829	GLY	-	linker	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	827	GLY	-	linker	UNP P19491
C	828	THR	-	linker	UNP P19491
C	829	GLY	-	linker	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	829	GLY	-	linker	UNP P19491

- Molecule 2 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: C<sub>14</sub>H<sub>15</sub>F<sub>3</sub>N<sub>3</sub>O<sub>6</sub>P).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	B	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	C	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	D	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

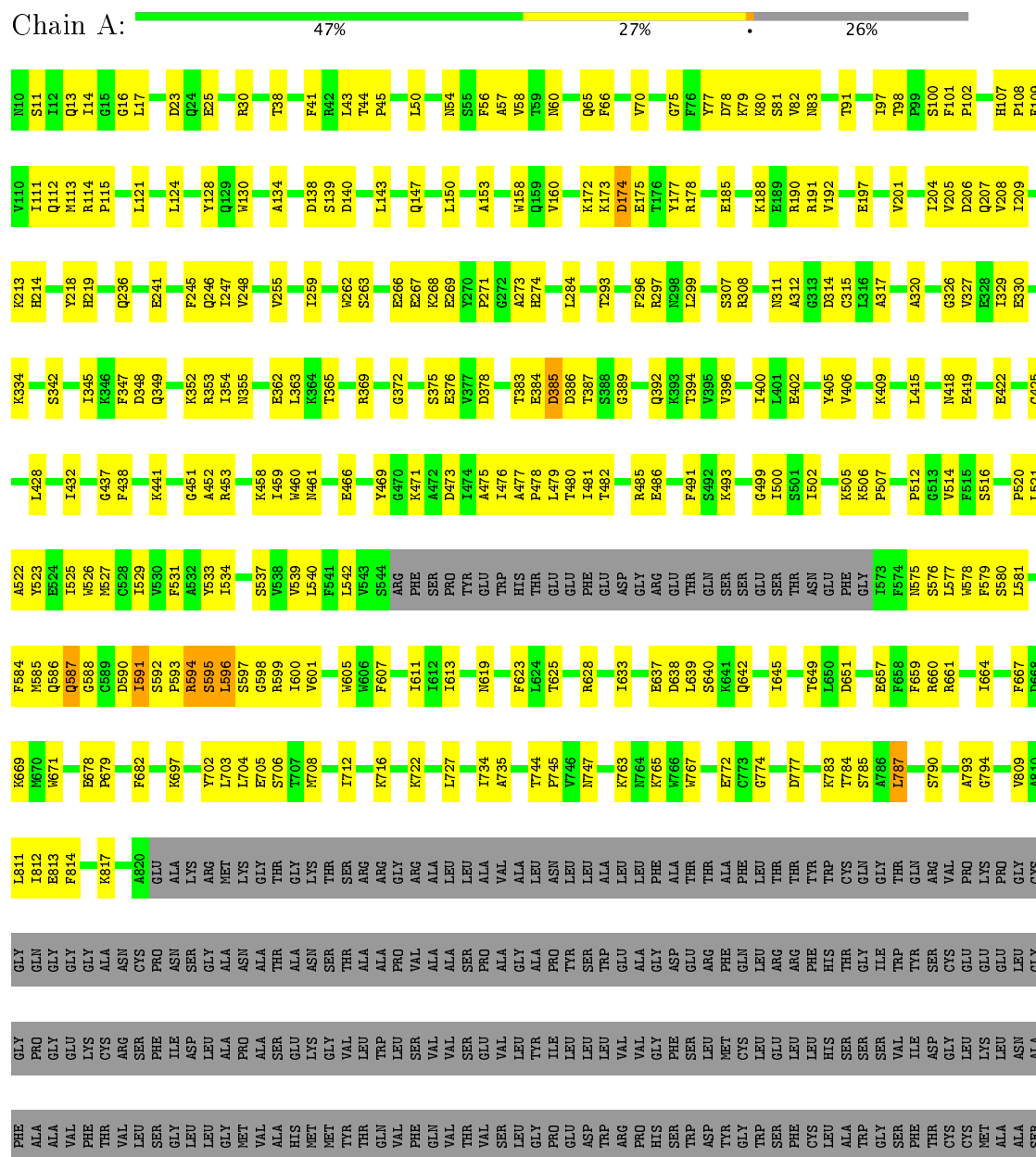


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	

### 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 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 2, Germ cell-specific gene 1-like protein









SER	GLU	ARG	THR	P478	S403
	LEU	THR	GLU		
PHE	LEU	PHE	TRP	T480	Y405
CYS	HIS	HIS	TRP	K485	Y406
ALA	SER	THR	GLN	R485	M407
TRP	SER	GLY	GLY	F574	M408
GLY	SER	ILE	GLY	N575	K409
SER	VAL	TRP	THR	F682	K410
PHE	ILE	TRP	THR	F683	M411
THR	ASP	THR	GLN	L577	H412
CYS	ASP	SER	ARG	M578	E413
GLY	GLY	CYS	VAL	F579	M414
LEU	LEU	GLU	PRO	S580	E419
LYS	LYS	THR	PRO	L581	
ALA	ALA	LEU	PRO	F582	E422
ALA	ASN	LEU	GLY	A583	C425
SER	GLY	GLY	CYS	P512	
VAL	PHE	GLY	PRO	G513	Y426
THR	ALA	PRO	GLN	V514	D427
THR	ALA	GLY	GLY	F515	L428
LEU	VAL	GLU	GLY	P520	E431
LEU	PHE	GLY	GLY	S587	
ASN	THR	THR	GLY	G588	I432
SER	PHE	CYS	ALA	D590	H435
THR	VAL	ARG	ASN	I591	
LEU	LEU	SER	CYS	F592	G436
LYS	SER	SER	PRO	P593	G437
THR	PHE	ILE	ASN	R594	F438
THR	GLY	ILE	ASN	S595	K439
VAL	LEU	ASP	SER	L596	
GLY	LEU	LEU	GLY	S597	L442
ILE	GLY	ALA	ALA	G598	
GLU	GLY	ALA	MET	Y711	T443
JGU	MET	PRO	ASN	L712	Y444
PHE	VAL	ALA	LYS	I713	
PHE	VAL	ALA	GLY	E713	V445
	ALA	SER	THR	Q714	
HIS	ALA	GLY	ALA	R715	G451
MET	MET	LYS	ASN	L716	A452
MET	GLY	GLY	ASN	THR	R453
THR	THR	VAL	THR	SER	D454
THR	LEU	LEU	ALA	ARG	K458
GLN	GLN	TRP	ALA	F608	
VAL	VAL	LEU	ALA	F607	I459
VAL	VAL	LEU	ALA	F608	M460
PHE	THR	LEU	PRO	T609	M461
GLN	VAL	SER	VAL	L610	G462
VAL	VAL	VAL	ALA	I611	M463
THR	THR	SER	LEU	I612	
THR	THR	VAL	THR	A622	V464
VAL	VAL	GLU	PRO	F623	G465
SER	VAL	VAL	ALA	L624	
LEU	LEU	GLY	GLY	T625	A466
GLY	THR	THR	ALA	P745	L467
PRO	ILE	PRO	ASN	V746	V468
GLU	LEU	LEU	LEU	R628	K471
ASP	ASP	LEU	LEU	M629	
TRP	TRP	LEU	TRP	V630	A472
ARG	VAL	VAL	GLU	E637	D473
PRO	PRO	VAL	LEU	L753	I474
HIS	HIS	GLY	GLY	E755	A475
SER	PHE	GLY	GLY	THR	L476
TRP	THR	ASP	ASP	K641	I477
ASP	LEU	LEU	THR	Q642	A478
TYR	MET	THR	THR	W766	L479
GLY	CYS	ALA	ALA	W767	I480
TRP	THR	THR	LEU	W769	A481

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	14372	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 ( $e^-/\text{\AA}^2$ )	80	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: NAG, ZK1

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	0.33	0/6287	0.46	0/8493
1	B	0.32	0/6265	0.45	0/8464
1	C	0.32	0/6287	0.45	0/8493
1	D	0.32	0/6265	0.45	0/8464
All	All	0.32	0/25104	0.45	0/33914

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	6159	0	6155	216	0
1	B	6137	0	6132	217	0
1	C	6159	0	6155	214	0
1	D	6137	0	6132	234	0
2	A	27	0	13	4	0
2	B	27	0	13	2	0
2	C	27	0	13	3	0
2	D	27	0	13	2	0
3	A	14	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	13	0	0
3	C	14	0	13	2	0
3	D	14	0	13	3	0
All	All	24756	0	24678	814	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 16.

The worst 5 of 814 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:337:GLN:HG3	1:C:346:LYS:HG2	1.58	0.82
1:B:595:SER:HA	1:B:599:ARG:HB2	1.63	0.81
1:A:190:ARG:HE	1:A:469:TYR:HB3	1.46	0.81
1:A:188:LYS:HD2	1:A:190:ARG:HH22	1.46	0.80
1:B:209:ILE:HA	1:B:214:HIS:HD2	1.46	0.80

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	779/1057 (74%)	729 (94%)	35 (4%)	15 (2%)	9	47
1	B	776/1057 (73%)	728 (94%)	37 (5%)	11 (1%)	13	54
1	C	779/1057 (74%)	726 (93%)	38 (5%)	15 (2%)	9	47
1	D	776/1057 (73%)	728 (94%)	35 (4%)	13 (2%)	11	50
All	All	3110/4228 (74%)	2911 (94%)	145 (5%)	54 (2%)	15	50

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	385	ASP
1	A	591	ILE
1	B	395	VAL
1	B	512	PRO
1	C	591	ILE

### 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	666/888 (75%)	666 (100%)	0	100	100
1	B	664/888 (75%)	664 (100%)	0	100	100
1	C	666/888 (75%)	666 (100%)	0	100	100
1	D	664/888 (75%)	664 (100%)	0	100	100
All	All	2660/3552 (75%)	2660 (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 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	587	GLN
1	C	83	ASN
1	D	587	GLN
1	B	642	GLN
1	C	112	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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	ZK1	A	1101	-	28,29,29	3.11	10 (35%)	36,45,45	1.66	7 (19%)
3	NAG	A	1102	-	14,14,15	0.26	0	15,19,21	0.40	0
2	ZK1	B	1101	-	28,29,29	3.15	10 (35%)	36,45,45	1.60	6 (16%)
3	NAG	B	1102	-	14,14,15	0.20	0	15,19,21	0.49	0
2	ZK1	C	1101	-	28,29,29	3.11	11 (39%)	36,45,45	1.64	7 (19%)
3	NAG	C	1102	-	14,14,15	0.20	0	15,19,21	0.49	0
2	ZK1	D	1101	-	28,29,29	3.15	11 (39%)	36,45,45	1.61	7 (19%)
3	NAG	D	1102	-	14,14,15	0.18	0	15,19,21	0.49	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	ZK1	A	1101	-	-	0/13/23/23	0/3/3/3
3	NAG	A	1102	-	-	0/6/23/26	0/1/1/1
2	ZK1	B	1101	-	-	0/13/23/23	0/3/3/3
3	NAG	B	1102	-	-	0/6/23/26	0/1/1/1
2	ZK1	C	1101	-	-	0/13/23/23	0/3/3/3
3	NAG	C	1102	-	-	0/6/23/26	0/1/1/1
2	ZK1	D	1101	-	-	0/13/23/23	0/3/3/3
3	NAG	D	1102	-	-	0/6/23/26	0/1/1/1

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	ZK1	PBA-OAD	-3.71	1.46	1.54
2	B	1101	ZK1	PBA-OAD	-3.68	1.46	1.54
2	C	1101	ZK1	PBA-OAD	-3.67	1.46	1.54
2	D	1101	ZK1	PBA-OAD	-3.65	1.46	1.54
2	C	1101	ZK1	CAU-NAY	-2.09	1.35	1.38

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	ZK1	CAI-CAR-NAX	-3.32	118.15	122.69
2	B	1101	ZK1	CAI-CAR-NAX	-3.16	118.37	122.69
2	A	1101	ZK1	CAI-CAR-NAX	-3.03	118.55	122.69
2	C	1101	ZK1	CAI-CAR-NAX	-2.92	118.69	122.69
2	A	1101	ZK1	FAG-CAZ-CAS	-2.43	108.33	112.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	ZK1	4	0
3	A	1102	NAG	2	0
2	B	1101	ZK1	2	0
2	C	1101	ZK1	3	0
3	C	1102	NAG	2	0
2	D	1101	ZK1	2	0
3	D	1102	NAG	3	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.