



wwPDB EM Map/Model Validation Report ⓘ

Jul 13, 2016 – 01:58 PM EDT

PDB ID : 5KBV
EMDB ID: : EMD-8232
Title : Cryo-EM structure of GluA2 bound to antagonist ZK200775 at 6.8 Angstrom resolution
Authors : Twomey, E.C.; Yelshanskaya, M.V.; Grassucci, R.G.; Frank, J.; Sobolevsky, A.I.
Deposited on : 2016-06-03
Resolution : 6.80 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-20027790

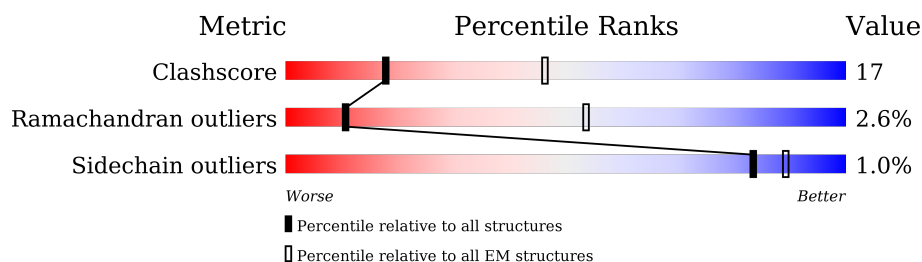
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.80 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	822	
1	B	822	
1	C	822	
1	D	822	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22637 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	782	Total	C	N	O	S	0	0
			5626	3620	898	1081	27		
1	B	779	Total	C	N	O	S	0	0
			5647	3635	902	1083	27		
1	C	779	Total	C	N	O	S	0	0
			5600	3605	891	1077	27		
1	D	779	Total	C	N	O	S	0	0
			5600	3605	891	1077	27		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	engineered mutation	UNP P19491
A	382	LEU	VAL	engineered mutation	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	engineered mutation	UNP P19491
A	385	ASP	ASN	engineered mutation	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	758	LEU	VAL	engineered mutation	UNP P19491
A	827	GLY	-	expression tag	UNP P19491
A	828	LEU	-	expression tag	UNP P19491
A	829	VAL	-	expression tag	UNP P19491
A	830	PRO	-	expression tag	UNP P19491
A	831	ARG	-	expression tag	UNP P19491
B	241	GLU	ASN	engineered mutation	UNP P19491
B	382	LEU	VAL	engineered mutation	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491

Continued on next page...

Continued from previous page...

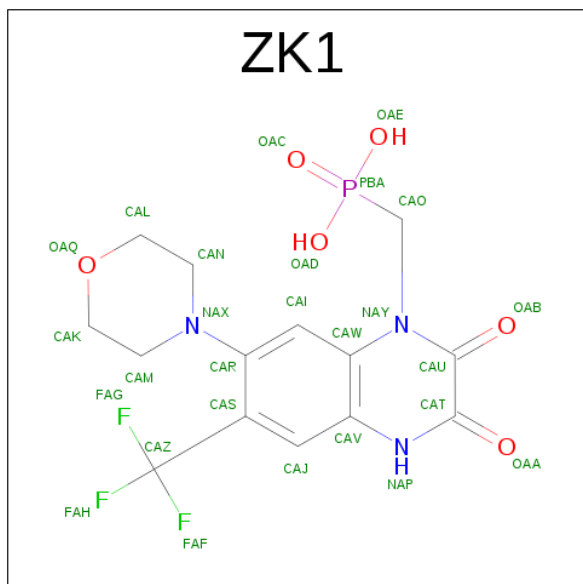
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	engineered mutation	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	758	LEU	VAL	engineered mutation	UNP P19491
B	827	GLY	-	expression tag	UNP P19491
B	828	LEU	-	expression tag	UNP P19491
B	829	VAL	-	expression tag	UNP P19491
B	830	PRO	-	expression tag	UNP P19491
B	831	ARG	-	expression tag	UNP P19491
C	241	GLU	ASN	engineered mutation	UNP P19491
C	382	LEU	VAL	engineered mutation	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	engineered mutation	UNP P19491
C	385	ASP	ASN	engineered mutation	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	758	LEU	VAL	engineered mutation	UNP P19491
C	827	GLY	-	expression tag	UNP P19491
C	828	LEU	-	expression tag	UNP P19491
C	829	VAL	-	expression tag	UNP P19491
C	830	PRO	-	expression tag	UNP P19491
C	831	ARG	-	expression tag	UNP P19491
D	241	GLU	ASN	engineered mutation	UNP P19491
D	382	LEU	VAL	engineered mutation	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	engineered mutation	UNP P19491
D	385	ASP	ASN	engineered mutation	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	758	LEU	VAL	engineered mutation	UNP P19491
D	827	GLY	-	expression tag	UNP P19491

Continued on next page...

Continued from previous page...

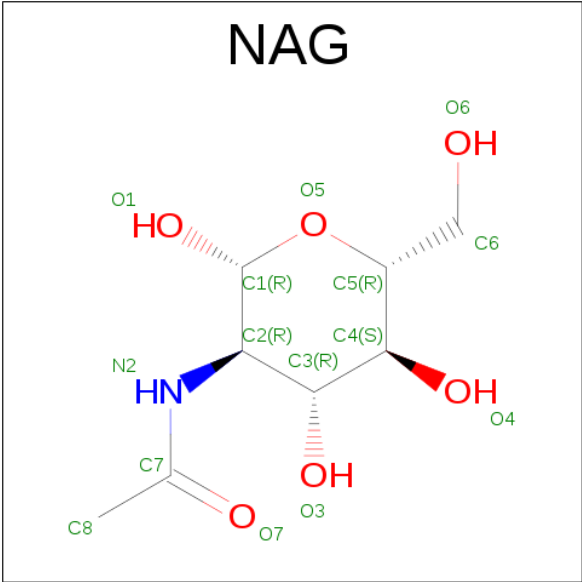
Chain	Residue	Modelled	Actual	Comment	Reference
D	828	LEU	-	expression tag	UNP P19491
D	829	VAL	-	expression tag	UNP P19491
D	830	PRO	-	expression tag	UNP P19491
D	831	ARG	-	expression tag	UNP P19491

- 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: C₁₄H₁₅F₃N₃O₆P).

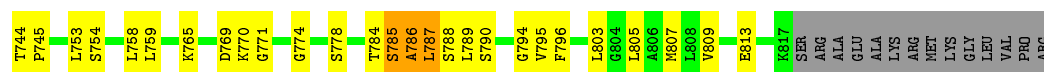


Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	B	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	C	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	D	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).

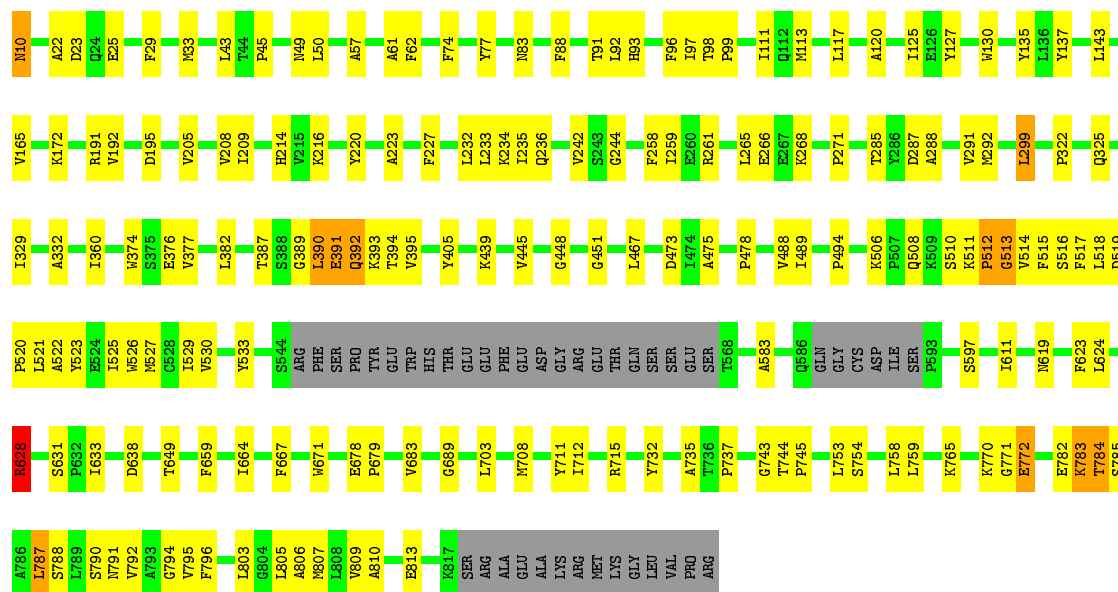


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	



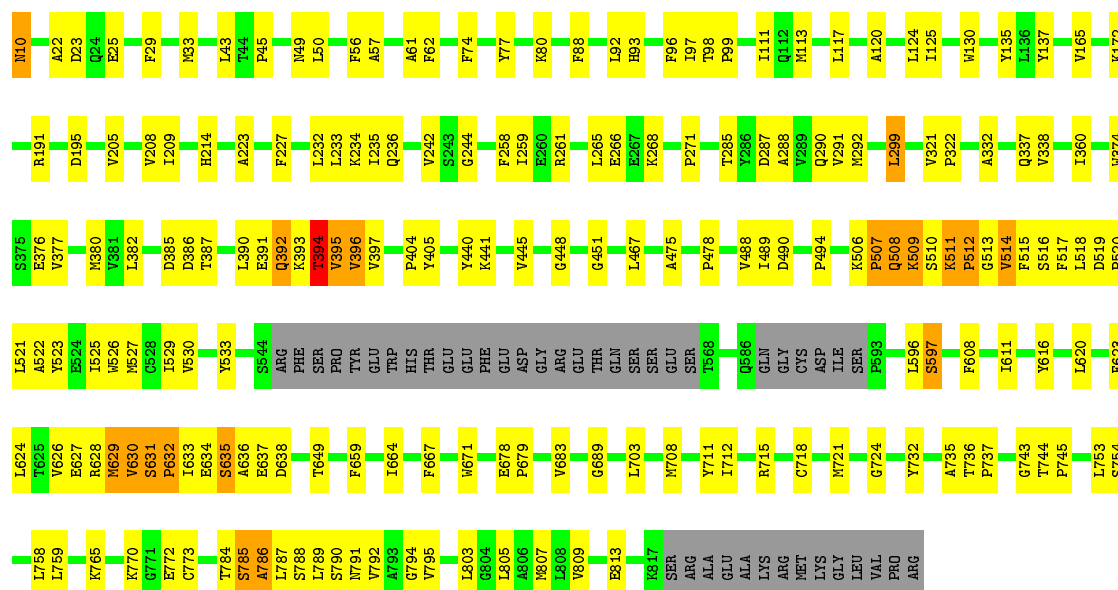
• Molecule 1: Glutamate receptor 2

Chain C: 73% 20% 5%



• Molecule 1: Glutamate receptor 2

Chain D: 71% 21% 5%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	33152	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	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: 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	0.25	1/5747 (0.0%)	0.53	5/7870 (0.1%)
1	B	0.24	0/5768	0.37	2/7888 (0.0%)
1	C	0.24	0/5721	0.43	6/7837 (0.1%)
1	D	0.24	0/5721	0.37	1/7837 (0.0%)
All	All	0.24	1/22957 (0.0%)	0.43	14/31432 (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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	787	LEU	C-N	-5.16	1.22	1.34

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	787	LEU	O-C-N	-28.18	77.61	122.70
1	C	628	ARG	NE-CZ-NH1	-13.79	113.41	120.30
1	A	628	ARG	NE-CZ-NH2	-12.50	114.05	120.30
1	C	628	ARG	NE-CZ-NH2	11.88	126.24	120.30
1	A	628	ARG	NE-CZ-NH1	11.00	125.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	787	LEU	Mainchain

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	5626	0	5105	208	0
1	B	5647	0	5177	225	0
1	C	5600	0	5073	182	0
1	D	5600	0	5072	214	0
2	A	27	0	13	1	0
2	B	27	0	13	1	0
2	C	27	0	13	1	0
2	D	27	0	13	1	0
3	A	14	0	13	2	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	2	0
All	All	22637	0	20531	753	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 17.

The worst 5 of 753 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:512:PRO:HB3	1:C:790:SER:CB	1.19	1.65
1:C:512:PRO:CB	1:C:790:SER:HB2	1.23	1.61
1:D:514:VAL:HG22	1:D:794:GLY:CA	1.29	1.61
1:C:611:ILE:HD12	1:D:517:PHE:CE1	1.36	1.54
1:D:512:PRO:CB	1:D:790:SER:HB2	1.45	1.46

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	776/822 (94%)	701 (90%)	56 (7%)	19 (2%)	7	47
1	B	773/822 (94%)	699 (90%)	56 (7%)	18 (2%)	8	48
1	C	773/822 (94%)	701 (91%)	57 (7%)	15 (2%)	10	52
1	D	773/822 (94%)	692 (90%)	54 (7%)	27 (4%)	4	39
All	All	3095/3288 (94%)	2793 (90%)	223 (7%)	79 (3%)	11	45

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	LYS
1	A	385	ASP
1	A	387	THR
1	A	389	GLY
1	A	511	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	537/702 (76%)	532 (99%)	5 (1%)	84	93
1	B	546/702 (78%)	540 (99%)	6 (1%)	80	91
1	C	534/702 (76%)	529 (99%)	5 (1%)	84	93
1	D	534/702 (76%)	529 (99%)	5 (1%)	84	93
All	All	2151/2808 (77%)	2130 (99%)	21 (1%)	83	92

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	633	ILE
1	C	10	ASN
1	D	299	LEU
1	B	631	SER
1	D	394	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	619	ASN
1	D	344	ASN
1	C	83	ASN
1	B	83	ASN
1	D	337	GLN

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](#)

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	3.23	14 (50%)	35,45,45	1.53	3 (8%)
3	NAG	A	1102	-	14,14,15	0.46	0	15,19,21	0.72	0
2	ZK1	B	1101	-	28,29,29	3.22	14 (50%)	35,45,45	1.52	3 (8%)
3	NAG	B	1102	-	14,14,15	0.48	0	15,19,21	0.65	0
2	ZK1	C	1101	-	28,29,29	3.21	14 (50%)	35,45,45	1.53	3 (8%)
3	NAG	C	1102	-	14,14,15	0.45	0	15,19,21	0.89	1 (6%)
2	ZK1	D	1101	-	28,29,29	3.22	14 (50%)	35,45,45	1.53	3 (8%)
3	NAG	D	1102	-	14,14,15	0.49	0	15,19,21	0.68	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 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	ZK1	PBA-OAD	-3.38	1.46	1.54
2	A	1101	ZK1	PBA-OAD	-3.36	1.46	1.54
2	D	1101	ZK1	PBA-OAD	-3.36	1.46	1.54
2	B	1101	ZK1	PBA-OAD	-3.34	1.46	1.54
2	A	1101	ZK1	CAN-NAX	2.06	1.49	1.46

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	ZK1	CAI-CAR-NAX	-2.58	118.98	122.62
2	B	1101	ZK1	CAI-CAR-NAX	-2.58	118.98	122.62
2	C	1101	ZK1	CAI-CAR-NAX	-2.56	119.01	122.62
2	D	1101	ZK1	CAI-CAR-NAX	-2.52	119.06	122.62
3	C	1102	NAG	C1-O5-C5	2.02	115.11	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	ZK1	1	0
3	A	1102	NAG	2	0
2	B	1101	ZK1	1	0
2	C	1101	ZK1	1	0
2	D	1101	ZK1	1	0
3	D	1102	NAG	2	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.