



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 23, 2019 – 10:06 PM EST

PDB ID : 6I2K
EMDB ID: : EMD-0332
Title : Structure of EV71 complexed with its receptor SCARB2
Authors : Zhou, D.; Zhao, Y.; Kotecha, A.; Fry, E.E.; Kelly, J.; Wang, X.; Rao, Z.;
Rowlands, D.J.; Ren, J.; Stuart, D.I.
Deposited on : 2018-11-01
Resolution : 3.40 Å(reported)
Based on PDB ID : 3VBH, 4Q4B

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

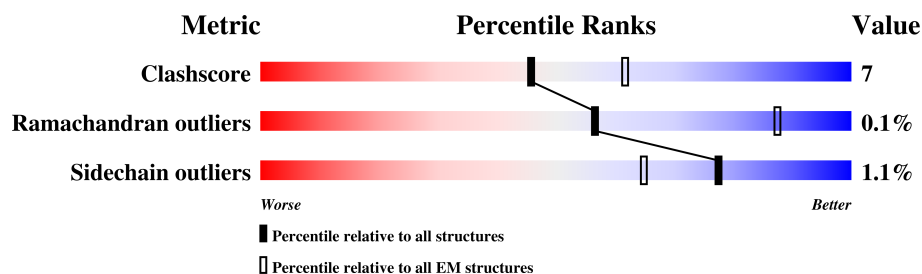
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY






The reported resolution of this entry is 3.40 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	297	 84% 14% .
2	B	254	 78% 18% .
3	C	242	 86% 14%
4	D	58	 84% 16%
5	E	416	 79% 14% . 6%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10035 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 Polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	290	Total	C	N	O	S	0	0
			2255	1420	386	435	14		

- Molecule 2 is a protein called Polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	245	Total	C	N	O	S	0	0
			1897	1215	313	360	9		

- Molecule 3 is a protein called Polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	242	Total	C	N	O	S	0	0
			1867	1199	311	345	12		

- Molecule 4 is a protein called Polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	58	Total	C	N	O	S	0	0
			449	279	73	96	1		

- Molecule 5 is a protein called Lysosome membrane protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	392	Total	C	N	O	S	0	0
			3175	2049	514	600	12		

There are 11 discrepancies between the modelled and reference sequences:

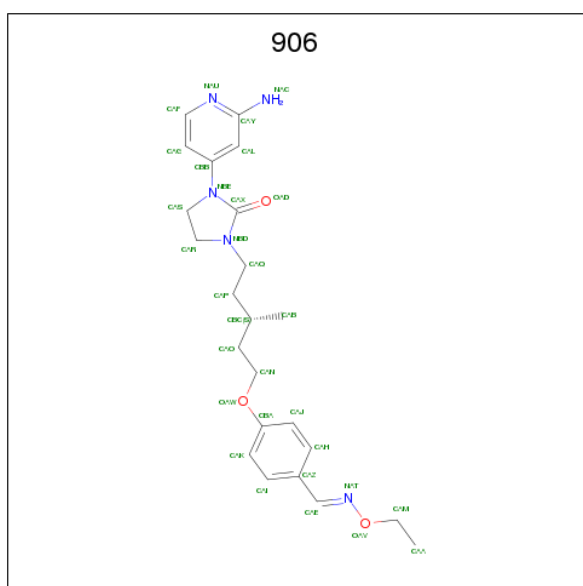
Chain	Residue	Modelled	Actual	Comment	Reference
E	25	GLU	-	expression tag	UNP Q14108
E	26	THR	-	expression tag	UNP Q14108
E	27	GLY	-	expression tag	UNP Q14108

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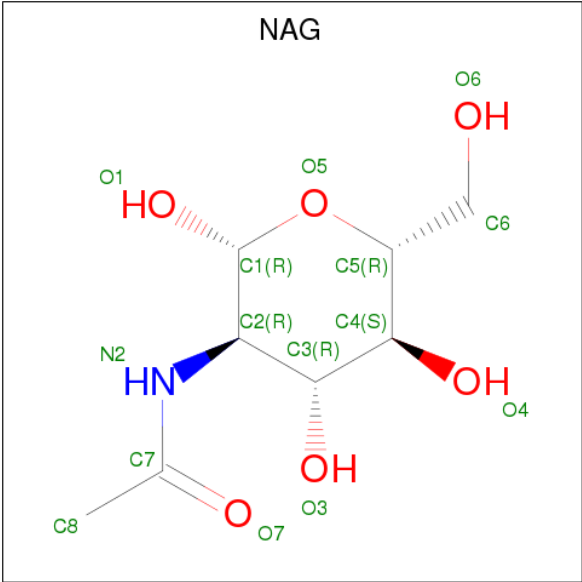
Chain	Residue	Modelled	Actual	Comment	Reference
E	433	GLY	-	expression tag	UNP Q14108
E	434	LYS	-	expression tag	UNP Q14108
E	435	HIS	-	expression tag	UNP Q14108
E	436	HIS	-	expression tag	UNP Q14108
E	437	HIS	-	expression tag	UNP Q14108
E	438	HIS	-	expression tag	UNP Q14108
E	439	HIS	-	expression tag	UNP Q14108
E	440	HIS	-	expression tag	UNP Q14108

- Molecule 6 is 1-(2-aminopyridin-4-yl)-3-[(3S)-5-{4-[(E)-(ethoxyimino)methyl]phenoxy}-3-methylpentyl]imidazolidin-2-one (three-letter code: 906) (formula: $C_{23}H_{31}N_5O_3$).



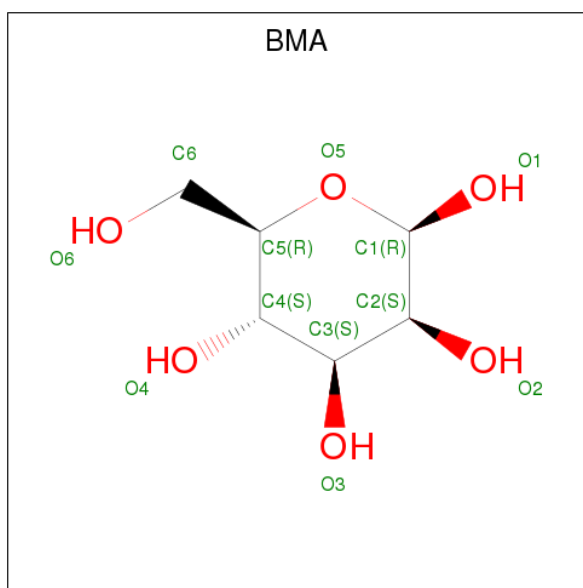
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			31	23	5	3	

- Molecule 7 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



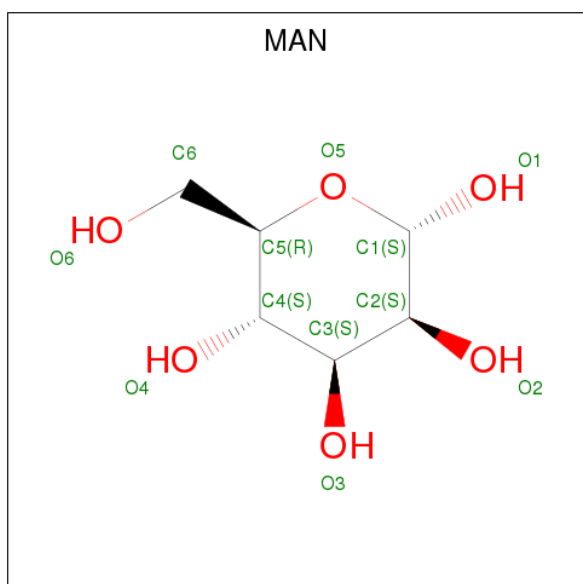
Mol	Chain	Residues	Atoms				AltConf
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	
7	E	1	Total	C	N	O	0
			196	112	14	70	

- Molecule 8 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			AltConf
8	E	1	Total	C	O	0
			44	24	20	
8	E	1	Total	C	O	0
			44	24	20	
8	E	1	Total	C	O	0
			44	24	20	
8	E	1	Total	C	O	0
			44	24	20	

- Molecule 9 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).

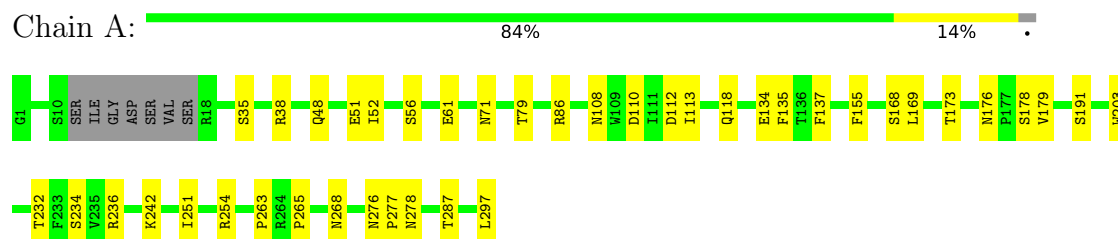


Mol	Chain	Residues	Atoms			AltConf
9	E	1	Total	C	O	0
			121	66	55	
9	E	1	Total	C	O	0
			121	66	55	
9	E	1	Total	C	O	0
			121	66	55	
9	E	1	Total	C	O	0
			121	66	55	
9	E	1	Total	C	O	0
			121	66	55	
9	E	1	Total	C	O	0
			121	66	55	
9	E	1	Total	C	O	0
			121	66	55	
9	E	1	Total	C	O	0
			121	66	55	
9	E	1	Total	C	O	0
			121	66	55	

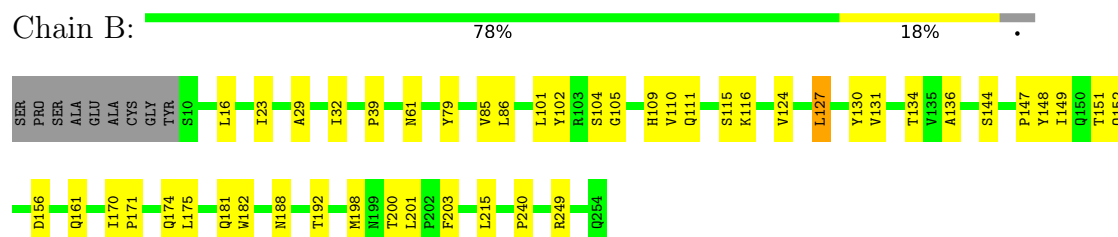
3 Residue-property plots

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.

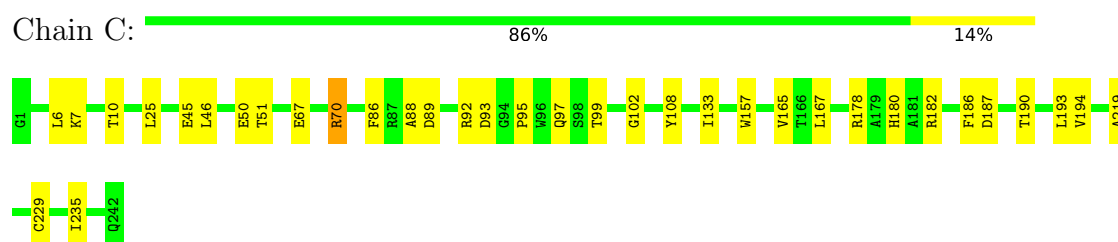
- Molecule 1: Polyprotein



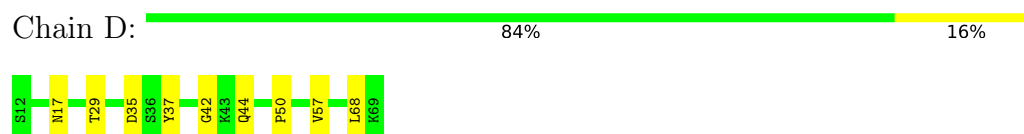
- Molecule 2: Polyprotein



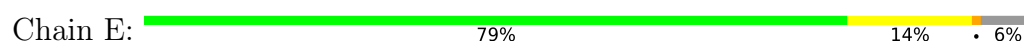
- Molecule 3: Polyprotein



- Molecule 4: Polyprotein



- Molecule 5: Lysosome membrane protein 2



N412	D418	T421	M428	ILE	ASN	THR	THR	GLY	LYS	HIS	HIS	HIS	HIS	HIS	HIS	GLU	THR	GLY	VAL	PHE	GLN	LYS	ALA	VAL	ASP	GLN	SER	I37	E48	V60	L76	R92	R95	S110	V118	V143	S147	L152	R153	E154	I155	M159	L160	Y163	H171	L176	D182	E183	I184	L187	V190	F191	R192	P193	D194	I195	E204
V214	F215	L216	E230	T235	W239	T261	V268	F269	P270	C274	R275	Q288	G289	L290	P291	R294	Y295	K296	N317	V326	K330	I335	I336	M337	D346	F349	E364	T365	F366	V367	N370	A379	A380	K381	R382	I385	N386	D400																			

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	10443	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	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: BMA, 906, NAG, MAN

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	0.56	0/2312	0.61	0/3146
2	B	0.58	0/1952	0.66	1/2678 (0.0%)
3	C	0.57	0/1920	0.61	0/2625
4	D	0.44	0/458	0.52	0/619
5	E	0.29	0/3258	0.51	0/4428
All	All	0.49	0/9900	0.58	1/13496 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	127	LEU	CA-CB-CG	5.15	127.15	115.30

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	2255	0	2189	37	0
2	B	1897	0	1830	46	0
3	C	1867	0	1841	22	0
4	D	449	0	425	7	0
5	E	3175	0	3079	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	31	0	31	10	0
7	E	196	0	172	2	0
8	E	44	0	35	0	0
9	E	121	0	104	0	0
All	All	10035	0	9706	143	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 7.

The worst 5 of 143 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)
5:E:326:VAL:HG23	5:E:335:ILE:HG23	1.21	1.18
1:A:278:ASN:ND2	2:B:134:THR:HG22	1.57	1.18
2:B:134:THR:HG21	2:B:144:SER:OG	1.57	1.04
2:B:149:ILE:HD11	5:E:159:MET:SD	1.99	1.01
1:A:179:VAL:HG23	6:A:301:906:HAAB	1.44	0.99

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	286/297 (96%)	273 (96%)	13 (4%)	0	100	100
2	B	243/254 (96%)	230 (95%)	13 (5%)	0	100	100
3	C	240/242 (99%)	226 (94%)	14 (6%)	0	100	100
4	D	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
5	E	390/416 (94%)	372 (95%)	17 (4%)	1 (0%)	43	77
All	All	1215/1267 (96%)	1151 (95%)	63 (5%)	1 (0%)	56	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	288	GLN

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	246/252 (98%)	242 (98%)	4 (2%)	65	85
2	B	209/215 (97%)	207 (99%)	2 (1%)	78	89
3	C	203/203 (100%)	202 (100%)	1 (0%)	90	95
4	D	49/49 (100%)	49 (100%)	0	100	100
5	E	353/374 (94%)	348 (99%)	5 (1%)	69	87
All	All	1060/1093 (97%)	1048 (99%)	12 (1%)	77	89

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	249	ARG
3	C	70	ARG
5	E	288	GLN
2	B	198	MET
5	E	275	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	181	GLN
4	D	44	GLN
5	E	370	ASN
2	B	161	GLN
5	E	341	HIS

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

30 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$
6	906	A	301	-	33,33,33	1.70	6 (18%)	41,43,43	2.10	11 (26%)
7	NAG	E	501	5	14,14,15	1.25	1 (7%)	17,19,21	1.45	1 (5%)
7	NAG	E	502	5,7	14,14,15	0.28	0	17,19,21	0.60	0
7	NAG	E	503	8,7	14,14,15	0.24	0	17,19,21	0.58	0
8	BMA	E	504	9,7	11,11,12	0.59	0	15,15,17	1.06	1 (6%)
9	MAN	E	505	8	11,11,12	0.90	0	15,15,17	1.40	2 (13%)
7	NAG	E	506	5,7	14,14,15	0.53	0	17,19,21	0.67	0
7	NAG	E	507	7	14,14,15	0.53	0	17,19,21	0.44	0
7	NAG	E	508	5	14,14,15	1.34	1 (7%)	17,19,21	1.47	1 (5%)
7	NAG	E	509	5,7	14,14,15	0.42	0	17,19,21	0.63	0
7	NAG	E	510	8,7	14,14,15	0.31	0	17,19,21	0.56	0
8	BMA	E	511	7	11,11,12	0.92	1 (9%)	15,15,17	1.04	1 (6%)
7	NAG	E	512	5,7	14,14,15	0.50	0	17,19,21	0.63	0
7	NAG	E	513	7	14,14,15	0.59	0	17,19,21	0.54	0
7	NAG	E	514	5,7	14,14,15	0.21	0	17,19,21	0.61	0
7	NAG	E	515	8,7	14,14,15	0.30	0	17,19,21	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BMA	E	516	9,7	11,11,12	0.84	0	15,15,17	0.86	0
9	MAN	E	517	9,8	11,11,12	0.90	1 (9%)	15,15,17	1.43	2 (13%)
9	MAN	E	518	9	11,11,12	0.85	0	15,15,17	1.02	1 (6%)
9	MAN	E	519	9	11,11,12	0.96	2 (18%)	15,15,17	1.66	2 (13%)
9	MAN	E	520	9	11,11,12	0.95	0	15,15,17	0.92	0
9	MAN	E	521	9	11,11,12	1.08	2 (18%)	15,15,17	1.25	3 (20%)
9	MAN	E	522	9,8	11,11,12	0.87	1 (9%)	15,15,17	1.11	2 (13%)
9	MAN	E	523	9	11,11,12	1.31	2 (18%)	15,15,17	1.52	3 (20%)
9	MAN	E	524	9	11,11,12	0.93	1 (9%)	15,15,17	1.18	2 (13%)
7	NAG	E	525	5,7	14,14,15	0.44	0	17,19,21	1.03	1 (5%)
7	NAG	E	526	8,7	14,14,15	0.32	0	17,19,21	0.52	0
8	BMA	E	527	9,7	11,11,12	0.69	0	15,15,17	1.06	1 (6%)
9	MAN	E	528	8	11,11,12	0.97	0	15,15,17	0.94	1 (6%)
9	MAN	E	529	8	11,11,12	1.07	1 (9%)	15,15,17	1.11	1 (6%)

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
6	906	A	301	-	-	0/20/33/33	0/3/3/3
7	NAG	E	501	5	-	0/6/23/26	0/1/1/1
7	NAG	E	502	5,7	-	0/6/23/26	0/1/1/1
7	NAG	E	503	8,7	-	0/6/23/26	0/1/1/1
8	BMA	E	504	9,7	-	0/2/19/22	0/1/1/1
9	MAN	E	505	8	-	0/2/19/22	1/1/1/1
7	NAG	E	506	5,7	-	0/6/23/26	0/1/1/1
7	NAG	E	507	7	-	0/6/23/26	0/1/1/1
7	NAG	E	508	5	-	0/6/23/26	0/1/1/1
7	NAG	E	509	5,7	-	0/6/23/26	0/1/1/1
7	NAG	E	510	8,7	-	0/6/23/26	0/1/1/1
8	BMA	E	511	7	-	0/2/19/22	0/1/1/1
7	NAG	E	512	5,7	-	0/6/23/26	0/1/1/1
7	NAG	E	513	7	-	0/6/23/26	0/1/1/1
7	NAG	E	514	5,7	-	0/6/23/26	0/1/1/1
7	NAG	E	515	8,7	-	0/6/23/26	0/1/1/1
8	BMA	E	516	9,7	-	0/2/19/22	0/1/1/1
9	MAN	E	517	9,8	-	0/2/19/22	0/1/1/1
9	MAN	E	518	9	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	E	519	9	-	0/2/19/22	0/1/1/1
9	MAN	E	520	9	-	0/2/19/22	0/1/1/1
9	MAN	E	521	9	-	0/2/19/22	0/1/1/1
9	MAN	E	522	9,8	-	0/2/19/22	0/1/1/1
9	MAN	E	523	9	-	0/2/19/22	0/1/1/1
9	MAN	E	524	9	-	0/2/19/22	0/1/1/1
7	NAG	E	525	5,7	-	0/6/23/26	0/1/1/1
7	NAG	E	526	8,7	-	0/6/23/26	0/1/1/1
8	BMA	E	527	9,7	-	0/2/19/22	0/1/1/1
9	MAN	E	528	8	-	0/2/19/22	0/1/1/1
9	MAN	E	529	8	-	0/2/19/22	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	301	906	CBB-NBE	-4.59	1.33	1.43
6	A	301	906	CAX-NBE	-4.03	1.33	1.38
6	A	301	906	CAZ-CAE	-3.83	1.39	1.47
9	E	519	MAN	O5-C5	2.04	1.47	1.43
8	E	511	BMA	C2-C3	2.07	1.55	1.52

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	301	906	CAS-NBE-CAX	-5.20	107.77	111.75
6	A	301	906	CAG-CAF-NAU	-3.66	119.47	123.92
6	A	301	906	OAD-CAX-NBD	-3.51	122.92	125.89
6	A	301	906	OAD-CAX-NBE	-2.89	123.99	126.85
6	A	301	906	CAN-OAW-CBA	-2.74	110.69	117.91

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	E	505	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	301	906	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	508	NAG	1	0
7	E	515	NAG	1	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.