



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:51 PM BST

PDB ID : 3JAD  
EMDB ID: : EMD-6344  
Title : Structure of alpha-1 glycine receptor by single particle electron cryo-microscopy, strychnine-bound state  
Authors : Du, J.; Lu, W.; Wu, S.P.; Cheng, Y.F.; Gouaux, E.  
Deposited on : 2015-06-08  
Resolution : 3.90 Å(reported)  
Based on PDB ID : 3RHW

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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) : trunk27241

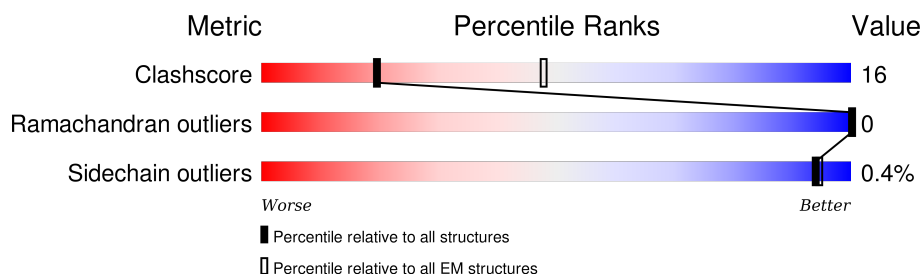
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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  $\geq 3$ , 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	342	70% 29% .
1	B	342	68% 30% .
1	C	342	68% 30% .
1	D	342	68% 30% .
1	E	342	69% 30% .

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12705 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.

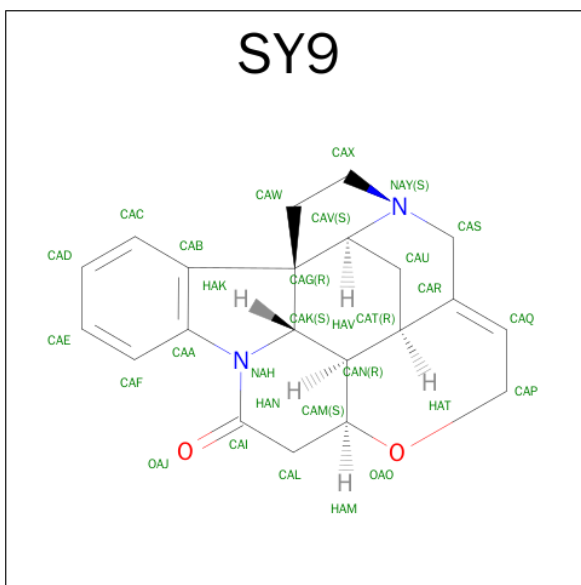
- Molecule 1 is a protein called Glycine receptor subunit alphaZ1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	337	Total	C	N	O	S	0	0
			2488	1624	414	437	13		
1	B	337	Total	C	N	O	S	0	0
			2488	1624	414	437	13		
1	C	337	Total	C	N	O	S	0	0
			2488	1624	414	437	13		
1	D	337	Total	C	N	O	S	0	0
			2488	1624	414	437	13		
1	E	337	Total	C	N	O	S	0	0
			2488	1624	414	437	13		

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				AltConf
2	A	2	Total	C	N	O	0
			28	16	2	10	
2	B	2	Total	C	N	O	0
			28	16	2	10	
2	C	2	Total	C	N	O	0
			28	16	2	10	
2	D	2	Total	C	N	O	0
			28	16	2	10	
2	E	2	Total	C	N	O	0
			28	16	2	10	

- Molecule 3 is STRYCHNINE (three-letter code: SY9) (formula: C<sub>21</sub>H<sub>22</sub>N<sub>2</sub>O<sub>2</sub>).

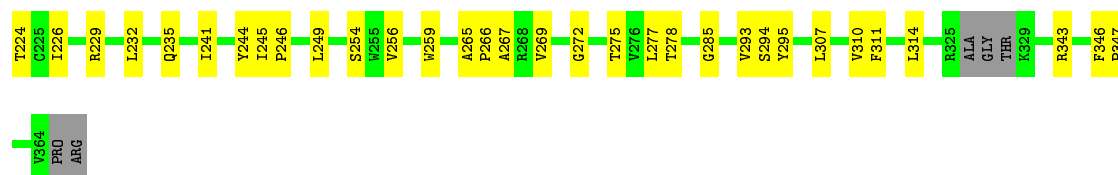


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total 25	C 21	N 2	O 2	0
3	B	1	Total 25	C 21	N 2	O 2	0
3	C	1	Total 25	C 21	N 2	O 2	0
3	D	1	Total 25	C 21	N 2	O 2	0
3	E	1	Total 25	C 21	N 2	O 2	0



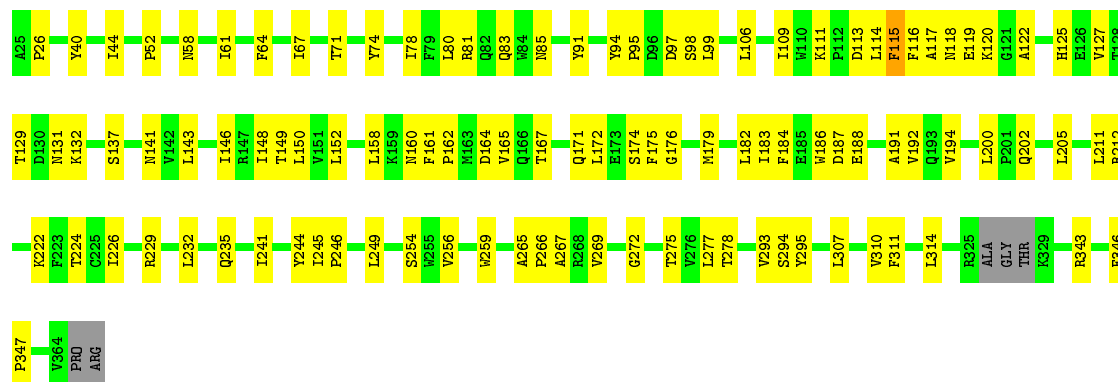
- Molecule 1: Glycine receptor subunit alphaZ1





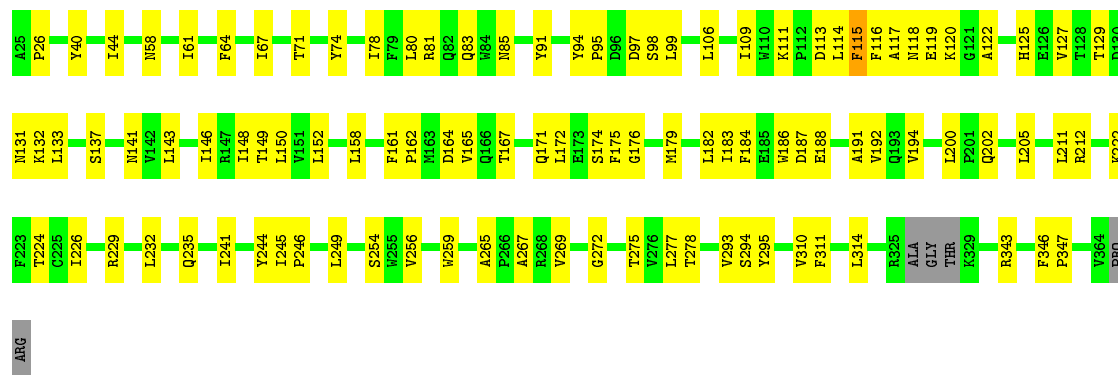
- Molecule 1: Glycine receptor subunit alphaZ1

Chain D:



- Molecule 1: Glycine receptor subunit alphaZ1

Chain E:



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	37094	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-3000	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 (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: SY9, NAG

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	0.31	0/2553	0.50	0/3498
1	B	0.31	0/2553	0.50	0/3498
1	C	0.31	0/2553	0.50	0/3498
1	D	0.31	0/2553	0.50	0/3498
1	E	0.31	0/2553	0.50	0/3498
All	All	0.31	0/12765	0.50	0/17490

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	2488	0	2274	86	0
1	B	2488	0	2274	100	0
1	C	2488	0	2274	95	0
1	D	2488	0	2274	96	0
1	E	2488	0	2274	90	0
2	A	28	0	25	1	0
2	B	28	0	25	1	0
2	C	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	28	0	25	1	0
2	E	28	0	25	0	0
3	A	25	0	22	4	0
3	B	25	0	22	6	0
3	C	25	0	22	5	0
3	D	25	0	22	5	0
3	E	25	0	22	5	0
All	All	12705	0	11605	399	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.

All (399) 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:D:183:ILE:HA	1:D:224:THR:HG21	1.67	0.76
1:E:81:ARG:HD2	3:E:401:SY9:HAL2	1.68	0.76
1:A:183:ILE:HA	1:A:224:THR:HG21	1.67	0.75
1:E:183:ILE:HA	1:E:224:THR:HG21	1.67	0.75
1:C:183:ILE:HA	1:C:224:THR:HG21	1.67	0.75
1:C:81:ARG:HD2	3:C:401:SY9:HAL2	1.69	0.75
1:B:183:ILE:HA	1:B:224:THR:HG21	1.67	0.74
1:A:64:PHE:HB2	1:A:200:LEU:HD11	1.70	0.73
1:C:64:PHE:HB2	1:C:200:LEU:HD11	1.70	0.72
1:B:64:PHE:HB2	1:B:200:LEU:HD11	1.70	0.72
1:B:81:ARG:HD2	3:B:401:SY9:HAL2	1.71	0.72
1:D:64:PHE:HB2	1:D:200:LEU:HD11	1.70	0.72
1:E:64:PHE:HB2	1:E:200:LEU:HD11	1.70	0.71
1:C:143:LEU:HD21	3:C:401:SY9:HAF	1.74	0.69
1:D:81:ARG:HD2	3:D:401:SY9:HAL2	1.75	0.69
1:E:143:LEU:HD21	3:E:401:SY9:HAF	1.74	0.68
1:B:311:PHE:HB2	1:C:249:LEU:HD21	1.77	0.66
1:B:143:LEU:HD21	3:B:401:SY9:HAF	1.77	0.65
1:A:212:ARG:HH22	1:A:229:ARG:HH11	1.45	0.64
1:E:212:ARG:HH22	1:E:229:ARG:HH11	1.45	0.64
1:B:212:ARG:HH22	1:B:229:ARG:HH11	1.46	0.64
1:B:98:SER:HA	1:B:137:SER:HA	1.80	0.63
1:D:212:ARG:HH22	1:D:229:ARG:HH11	1.45	0.63
1:B:44:ILE:HD11	1:C:26:PRO:HG2	1.81	0.63
1:C:212:ARG:HH22	1:C:229:ARG:HH11	1.45	0.63
1:C:98:SER:HA	1:C:137:SER:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:SER:HA	1:E:137:SER:HA	1.80	0.62
1:D:98:SER:HA	1:D:137:SER:HA	1.80	0.62
1:A:98:SER:HA	1:A:137:SER:HA	1.80	0.62
1:D:311:PHE:HB2	1:E:249:LEU:HD21	1.82	0.61
1:D:143:LEU:HD21	3:D:401:SY9:HAF	1.82	0.61
1:D:44:ILE:HD11	1:E:26:PRO:HG2	1.83	0.59
1:B:311:PHE:CG	1:C:249:LEU:HD11	2.37	0.59
1:B:295:TYR:HB3	1:C:235:GLN:NE2	2.18	0.59
1:D:295:TYR:HB3	1:E:235:GLN:NE2	2.18	0.59
1:E:115:PHE:CE2	1:E:175:PHE:HD1	2.21	0.58
1:D:115:PHE:CE2	1:D:175:PHE:HD1	2.21	0.58
3:A:503:SY9:HAX1	1:E:175:PHE:CD1	2.39	0.58
1:B:275:THR:HG22	1:B:310:VAL:HG13	1.86	0.58
1:C:113:ASP:HB2	1:D:129:THR:HG21	1.85	0.58
1:D:175:PHE:CD1	3:E:401:SY9:HAX1	2.39	0.58
1:A:175:PHE:CD1	3:B:401:SY9:HAX1	2.39	0.58
1:A:115:PHE:CE2	1:A:175:PHE:HD1	2.21	0.58
1:C:67:ILE:HG12	1:C:74:TYR:HB3	1.87	0.57
1:C:175:PHE:CD1	3:D:401:SY9:HAX1	2.39	0.57
1:A:295:TYR:HB3	1:B:235:GLN:NE2	2.20	0.57
1:A:67:ILE:HG12	1:A:74:TYR:HB3	1.87	0.57
1:C:275:THR:HG22	1:C:310:VAL:HG13	1.86	0.57
1:C:115:PHE:CE2	1:C:175:PHE:HD1	2.21	0.57
1:B:115:PHE:CE2	1:B:175:PHE:HD1	2.21	0.57
1:A:275:THR:HG22	1:A:310:VAL:HG13	1.86	0.57
1:D:67:ILE:HG12	1:D:74:TYR:HB3	1.87	0.57
1:A:44:ILE:HD11	1:B:26:PRO:HG2	1.86	0.56
1:B:175:PHE:CD1	3:C:401:SY9:HAX1	2.39	0.56
1:B:67:ILE:HG12	1:B:74:TYR:HB3	1.86	0.56
1:A:311:PHE:HB2	1:B:249:LEU:HD21	1.87	0.56
1:A:113:ASP:HB2	1:B:129:THR:HG21	1.87	0.56
1:D:275:THR:HG22	1:D:310:VAL:HG13	1.86	0.56
1:E:275:THR:HG22	1:E:310:VAL:HG13	1.86	0.56
1:E:61:ILE:HD11	1:E:194:VAL:HG22	1.88	0.56
1:B:61:ILE:HD11	1:B:194:VAL:HG22	1.88	0.56
1:D:311:PHE:CD2	1:E:249:LEU:HD11	2.41	0.56
1:D:61:ILE:HG22	1:D:78:ILE:HG22	1.88	0.55
1:E:67:ILE:HG12	1:E:74:TYR:HB3	1.87	0.55
1:A:81:ARG:HD2	3:A:503:SY9:HAL2	1.87	0.55
1:A:61:ILE:HD11	1:A:194:VAL:HG22	1.88	0.55
1:C:61:ILE:HD11	1:C:194:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ILE:HG22	1:C:78:ILE:HG22	1.88	0.55
1:D:61:ILE:HD11	1:D:194:VAL:HG22	1.88	0.55
1:C:118:ASN:OD1	1:C:152:LEU:HD22	2.07	0.55
1:B:61:ILE:HG22	1:B:78:ILE:HG22	1.88	0.55
1:C:295:TYR:HB3	1:D:235:GLN:NE2	2.21	0.55
1:C:311:PHE:HB2	1:D:249:LEU:HD21	1.89	0.55
1:B:118:ASN:OD1	1:B:152:LEU:HD22	2.07	0.55
1:E:118:ASN:OD1	1:E:152:LEU:HD22	2.07	0.55
1:E:254:SER:HB3	1:E:275:THR:HG21	1.89	0.54
1:C:254:SER:HB3	1:C:275:THR:HG21	1.89	0.54
1:D:254:SER:HB3	1:D:275:THR:HG21	1.89	0.54
1:B:277:LEU:CD1	1:C:278:THR:HA	2.37	0.54
1:D:311:PHE:CG	1:E:249:LEU:HD11	2.41	0.54
1:A:254:SER:HB3	1:A:275:THR:HG21	1.89	0.54
1:A:61:ILE:HG22	1:A:78:ILE:HG22	1.88	0.54
1:D:311:PHE:CB	1:E:249:LEU:HD21	2.38	0.54
1:B:254:SER:HB3	1:B:275:THR:HG21	1.89	0.54
1:C:91:TYR:OH	1:C:98:SER:O	2.25	0.54
1:E:61:ILE:HG22	1:E:78:ILE:HG22	1.88	0.54
1:A:118:ASN:OD1	1:A:152:LEU:HD22	2.07	0.54
1:B:311:PHE:CB	1:C:249:LEU:HD21	2.37	0.53
1:C:58:ASN:HB2	1:C:191:ALA:O	2.09	0.53
1:D:118:ASN:OD1	1:D:152:LEU:HD22	2.07	0.53
1:E:106:LEU:HD11	1:E:111:LYS:HD3	1.91	0.53
1:A:58:ASN:HB2	1:A:191:ALA:O	2.09	0.53
1:C:346:PHE:HB2	1:C:347:PRO:HD3	1.91	0.53
1:B:58:ASN:HB2	1:B:191:ALA:O	2.09	0.53
1:E:346:PHE:HB2	1:E:347:PRO:HD3	1.91	0.53
1:E:58:ASN:HB2	1:E:191:ALA:O	2.09	0.53
1:B:122:ALA:HB3	1:C:127:VAL:HB	1.91	0.53
1:E:81:ARG:HD2	3:E:401:SY9:CAL	2.38	0.53
1:B:115:PHE:CE2	1:B:175:PHE:CD1	2.97	0.53
1:B:311:PHE:CD2	1:C:249:LEU:HD11	2.43	0.53
1:D:346:PHE:HB2	1:D:347:PRO:HD3	1.91	0.53
1:D:58:ASN:HB2	1:D:191:ALA:O	2.09	0.53
1:D:115:PHE:CE2	1:D:175:PHE:CD1	2.97	0.52
1:A:115:PHE:CE2	1:A:175:PHE:CD1	2.97	0.52
1:C:125:HIS:CE1	1:C:149:THR:HG1	2.26	0.52
1:A:91:TYR:OH	1:A:98:SER:O	2.25	0.52
1:B:295:TYR:HD2	1:C:235:GLN:HE22	1.58	0.52
1:A:106:LEU:HD11	1:A:111:LYS:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LEU:HD13	1:B:184:PHE:CE2	2.45	0.52
1:B:346:PHE:HB2	1:B:347:PRO:HD3	1.91	0.52
1:C:106:LEU:HD11	1:C:111:LYS:HD3	1.91	0.52
1:A:311:PHE:CD2	1:B:249:LEU:HD11	2.44	0.52
1:B:106:LEU:HD11	1:B:111:LYS:HD3	1.91	0.52
1:A:143:LEU:HD21	3:A:503:SY9:HAF	1.92	0.52
1:D:125:HIS:HB2	1:D:131:ASN:HD22	1.75	0.52
1:D:106:LEU:HD11	1:D:111:LYS:HD3	1.91	0.52
1:A:212:ARG:NH2	1:A:229:ARG:HH11	2.08	0.52
1:E:115:PHE:CE2	1:E:175:PHE:CD1	2.97	0.52
1:E:114:LEU:HD13	1:E:184:PHE:CE2	2.45	0.52
1:C:44:ILE:HD11	1:D:26:PRO:HG2	1.91	0.52
1:A:129:THR:HG21	1:E:113:ASP:HB2	1.92	0.51
1:A:346:PHE:HB2	1:A:347:PRO:HD3	1.91	0.51
1:D:113:ASP:HB2	1:E:129:THR:HG21	1.92	0.51
1:C:114:LEU:HD13	1:C:184:PHE:CE2	2.45	0.51
1:A:249:LEU:HD21	1:E:311:PHE:HB2	1.92	0.51
1:C:115:PHE:CE2	1:C:175:PHE:CD1	2.97	0.51
1:B:212:ARG:NH2	1:B:229:ARG:HH11	2.09	0.51
1:D:186:TRP:NE1	1:D:226:ILE:HB	2.26	0.51
1:B:307:LEU:HD21	1:C:246:PRO:HB3	1.93	0.51
1:B:186:TRP:NE1	1:B:226:ILE:HB	2.26	0.51
1:E:186:TRP:NE1	1:E:226:ILE:HB	2.26	0.51
1:A:114:LEU:HD13	1:A:184:PHE:CE2	2.45	0.51
1:E:116:PHE:CE2	1:E:150:LEU:HD21	2.46	0.51
1:D:114:LEU:HD13	1:D:184:PHE:CE2	2.45	0.51
1:A:125:HIS:HB2	1:A:131:ASN:HD22	1.75	0.51
1:D:277:LEU:CD1	1:E:278:THR:HA	2.41	0.51
1:C:186:TRP:NE1	1:C:226:ILE:HB	2.26	0.51
1:C:125:HIS:HB2	1:C:131:ASN:HD22	1.75	0.51
1:B:125:HIS:HB2	1:B:131:ASN:HD22	1.75	0.51
1:A:186:TRP:NE1	1:A:226:ILE:HB	2.26	0.51
1:A:161:PHE:HB3	1:A:162:PRO:HD3	1.93	0.50
1:C:212:ARG:NH2	1:C:229:ARG:HH11	2.08	0.50
1:E:125:HIS:HB2	1:E:131:ASN:HD22	1.75	0.50
1:D:161:PHE:HB3	1:D:162:PRO:HD3	1.93	0.50
1:E:161:PHE:HB3	1:E:162:PRO:HD3	1.93	0.50
1:A:116:PHE:CE2	1:A:150:LEU:HD21	2.46	0.50
1:D:122:ALA:HB3	1:E:127:VAL:HB	1.94	0.50
1:C:294:SER:OG	1:D:202:GLN:HG3	2.12	0.50
1:B:161:PHE:HB3	1:B:162:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:PRO:HG3	1:C:267:ALA:HB2	1.92	0.50
1:D:307:LEU:HD21	1:E:246:PRO:HB3	1.93	0.50
1:C:116:PHE:CE2	1:C:150:LEU:HD21	2.46	0.50
1:D:212:ARG:NH2	1:D:229:ARG:HH11	2.09	0.50
1:C:311:PHE:CD2	1:D:249:LEU:HD11	2.47	0.50
1:C:161:PHE:HB3	1:C:162:PRO:HD3	1.93	0.50
1:D:116:PHE:CE2	1:D:150:LEU:HD21	2.46	0.50
1:B:91:TYR:OH	1:B:98:SER:O	2.25	0.50
1:E:91:TYR:OH	1:E:98:SER:O	2.25	0.50
1:B:295:TYR:HD2	1:C:235:GLN:NE2	2.09	0.50
1:C:122:ALA:HB3	1:D:127:VAL:HB	1.94	0.50
1:B:116:PHE:CE2	1:B:150:LEU:HD21	2.46	0.50
1:A:311:PHE:CB	1:B:249:LEU:HD21	2.41	0.49
1:D:295:TYR:HD2	1:E:235:GLN:NE2	2.10	0.49
1:C:117:ALA:HB3	1:C:171:GLN:HG3	1.95	0.49
1:A:311:PHE:CG	1:B:249:LEU:HD11	2.48	0.49
1:B:125:HIS:CE1	1:B:149:THR:HG1	2.28	0.49
1:A:85:ASN:HB3	1:A:141:ASN:HA	1.95	0.49
1:B:85:ASN:HB3	1:B:141:ASN:HA	1.95	0.49
1:C:71:THR:HG22	1:C:120:LYS:HE3	1.94	0.49
1:A:122:ALA:HB3	1:B:127:VAL:HB	1.95	0.49
1:C:85:ASN:HB3	1:C:141:ASN:HA	1.95	0.49
1:C:311:PHE:CB	1:D:249:LEU:HD21	2.43	0.49
1:E:71:THR:HG22	1:E:120:LYS:HE3	1.95	0.49
1:D:85:ASN:HB3	1:D:141:ASN:HA	1.95	0.49
1:D:266:PRO:HG3	1:E:267:ALA:HB2	1.95	0.49
1:E:212:ARG:NH2	1:E:229:ARG:HH11	2.09	0.49
1:E:117:ALA:HB3	1:E:171:GLN:HG3	1.95	0.49
1:C:81:ARG:HD2	3:C:401:SY9:CAL	2.39	0.48
1:D:265:ALA:O	1:D:269:VAL:N	2.46	0.48
1:B:113:ASP:HB2	1:C:129:THR:HG21	1.94	0.48
1:D:117:ALA:HB3	1:D:171:GLN:HG3	1.95	0.48
1:A:186:TRP:CD1	1:A:211:LEU:HD13	2.49	0.48
1:C:186:TRP:CD1	1:C:211:LEU:HD13	2.49	0.48
1:A:71:THR:HG22	1:A:120:LYS:HE3	1.95	0.48
1:E:85:ASN:HB3	1:E:141:ASN:HA	1.95	0.48
1:C:265:ALA:O	1:C:269:VAL:N	2.46	0.48
1:A:307:LEU:HD21	1:B:246:PRO:HB3	1.95	0.48
1:D:186:TRP:CD1	1:D:211:LEU:HD13	2.49	0.48
1:A:117:ALA:HB3	1:A:171:GLN:HG3	1.95	0.48
1:A:294:SER:OG	1:B:202:GLN:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:PRO:HG2	1:E:44:ILE:HD11	1.94	0.48
1:D:71:THR:HG22	1:D:120:LYS:HE3	1.95	0.48
1:B:186:TRP:CD1	1:B:211:LEU:HD13	2.49	0.48
1:A:265:ALA:O	1:A:269:VAL:N	2.46	0.48
1:E:186:TRP:CD1	1:E:211:LEU:HD13	2.49	0.47
1:A:239:TYR:HE2	1:E:294:SER:HG	1.62	0.47
1:D:125:HIS:CE1	1:D:149:THR:HG1	2.28	0.47
1:E:265:ALA:O	1:E:269:VAL:N	2.46	0.47
1:B:71:THR:HG22	1:B:120:LYS:HE3	1.95	0.47
1:A:83:GLN:HE21	1:A:143:LEU:HD13	1.80	0.47
1:E:94:TYR:CD1	1:E:95:PRO:HD2	2.50	0.47
1:A:40:TYR:CE2	1:A:109:ILE:HA	2.50	0.47
1:D:83:GLN:HE21	1:D:143:LEU:HD13	1.79	0.47
1:B:294:SER:OG	1:C:202:GLN:HG3	2.14	0.47
1:D:295:TYR:HD2	1:E:235:GLN:HE22	1.61	0.47
1:C:311:PHE:CG	1:D:249:LEU:HD11	2.50	0.47
1:E:125:HIS:CE1	1:E:149:THR:HG1	2.29	0.47
1:B:265:ALA:O	1:B:269:VAL:N	2.46	0.47
1:B:117:ALA:HB3	1:B:171:GLN:HG3	1.95	0.47
1:D:40:TYR:CE2	1:D:109:ILE:HA	2.50	0.47
1:B:94:TYR:CD1	1:B:95:PRO:HD2	2.50	0.47
1:E:83:GLN:HE21	1:E:143:LEU:HD13	1.79	0.46
1:B:83:GLN:HE21	1:B:143:LEU:HD13	1.80	0.46
1:C:80:LEU:HD21	1:C:114:LEU:HD23	1.97	0.46
1:E:192:VAL:HG12	1:E:211:LEU:HD23	1.98	0.46
1:C:94:TYR:CD1	1:C:95:PRO:HD2	2.50	0.46
1:D:294:SER:OG	1:E:202:GLN:HG3	2.15	0.46
1:C:83:GLN:HE21	1:C:143:LEU:HD13	1.80	0.46
1:A:192:VAL:HG12	1:A:211:LEU:HD23	1.98	0.46
1:B:116:PHE:CD1	1:B:116:PHE:N	2.84	0.46
1:D:94:TYR:CD1	1:D:95:PRO:HD2	2.50	0.46
1:A:94:TYR:CD1	1:A:95:PRO:HD2	2.50	0.46
1:D:192:VAL:HG12	1:D:211:LEU:HD23	1.98	0.46
1:B:40:TYR:CE2	1:B:109:ILE:HA	2.50	0.46
1:D:91:TYR:OH	1:D:98:SER:O	2.25	0.46
1:B:277:LEU:CD1	1:C:278:THR:CA	2.94	0.46
1:D:119:GLU:HA	1:D:152:LEU:HA	1.98	0.46
1:A:80:LEU:HD21	1:A:114:LEU:HD23	1.97	0.46
1:C:192:VAL:HG12	1:C:211:LEU:HD23	1.97	0.46
1:A:116:PHE:CD1	1:A:116:PHE:N	2.84	0.46
1:B:119:GLU:HA	1:B:152:LEU:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:GLU:HA	1:E:152:LEU:HA	1.98	0.46
1:B:192:VAL:HG12	1:B:211:LEU:HD23	1.98	0.46
1:C:307:LEU:HD21	1:D:246:PRO:HB3	1.98	0.46
1:C:119:GLU:HA	1:C:152:LEU:HA	1.98	0.46
1:D:116:PHE:N	1:D:116:PHE:CD1	2.84	0.46
1:E:80:LEU:HD21	1:E:114:LEU:HD23	1.97	0.46
1:A:125:HIS:CE1	1:A:149:THR:HG1	2.31	0.46
1:E:40:TYR:CE2	1:E:109:ILE:HA	2.50	0.46
1:C:125:HIS:HB2	1:C:131:ASN:ND2	2.31	0.46
1:A:119:GLU:HA	1:A:152:LEU:HA	1.98	0.46
1:B:114:LEU:HD11	1:B:172:LEU:HB3	1.98	0.46
1:A:241:ILE:HD12	1:A:245:ILE:HD12	1.98	0.46
1:B:67:ILE:HG12	1:B:74:TYR:CB	2.46	0.46
1:E:114:LEU:HD11	1:E:172:LEU:HB3	1.98	0.46
1:D:80:LEU:HD21	1:D:114:LEU:HD23	1.97	0.46
1:D:174:SER:HB3	1:D:182:LEU:HD11	1.98	0.46
1:C:40:TYR:CE2	1:C:109:ILE:HA	2.50	0.46
1:A:125:HIS:HB2	1:A:131:ASN:ND2	2.31	0.45
1:D:241:ILE:HD12	1:D:245:ILE:HD12	1.98	0.45
1:A:277:LEU:CD1	1:B:278:THR:HA	2.46	0.45
1:C:174:SER:HB3	1:C:182:LEU:HD11	1.98	0.45
1:B:80:LEU:HD21	1:B:114:LEU:HD23	1.97	0.45
1:C:114:LEU:HD11	1:C:172:LEU:HB3	1.98	0.45
1:E:125:HIS:HB2	1:E:131:ASN:ND2	2.31	0.45
1:B:174:SER:HB3	1:B:182:LEU:HD11	1.98	0.45
1:E:174:SER:HB3	1:E:182:LEU:HD11	1.98	0.45
1:B:81:ARG:HD2	3:B:401:SY9:CAL	2.42	0.45
1:C:241:ILE:HD12	1:C:245:ILE:HD12	1.98	0.45
1:B:272:GLY:HA3	1:B:314:LEU:HD21	1.99	0.45
1:A:114:LEU:HD11	1:A:172:LEU:HB3	1.98	0.45
1:C:67:ILE:HG12	1:C:74:TYR:CB	2.46	0.45
1:B:241:ILE:HD12	1:B:245:ILE:HD12	1.98	0.45
1:E:116:PHE:N	1:E:116:PHE:CD1	2.84	0.45
1:A:127:VAL:HB	1:E:122:ALA:HB3	1.99	0.45
1:A:187:ASP:OD1	1:A:188:GLU:N	2.50	0.45
1:B:187:ASP:OD1	1:B:188:GLU:N	2.50	0.45
1:B:176:GLY:HA2	3:C:401:SY9:HAC	1.99	0.45
1:C:176:GLY:HA2	3:D:401:SY9:HAC	1.99	0.45
1:A:67:ILE:HG12	1:A:74:TYR:CB	2.46	0.45
1:D:125:HIS:HB2	1:D:131:ASN:ND2	2.31	0.45
1:A:40:TYR:HE2	1:A:109:ILE:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:ASP:OD1	1:C:188:GLU:N	2.50	0.45
1:B:175:PHE:CE2	1:C:133:LEU:HB2	2.52	0.45
1:C:40:TYR:HE2	1:C:109:ILE:HA	1.82	0.45
1:A:174:SER:HB3	1:A:182:LEU:HD11	1.99	0.45
1:B:125:HIS:HB2	1:B:131:ASN:ND2	2.31	0.44
1:C:116:PHE:CD1	1:C:116:PHE:N	2.84	0.44
1:D:67:ILE:HG12	1:D:74:TYR:CB	2.46	0.44
1:E:187:ASP:OD1	1:E:188:GLU:N	2.50	0.44
1:E:241:ILE:HD12	1:E:245:ILE:HD12	1.98	0.44
1:A:272:GLY:HA3	1:A:314:LEU:HD21	1.99	0.44
1:E:67:ILE:HG12	1:E:74:TYR:CB	2.46	0.44
1:A:266:PRO:HG3	1:B:267:ALA:HB2	1.99	0.44
1:D:187:ASP:OD1	1:D:188:GLU:N	2.50	0.44
1:A:114:LEU:HD21	1:A:172:LEU:HD23	1.99	0.44
1:C:132:LYS:HG2	1:C:146:ILE:HG22	2.00	0.44
1:C:114:LEU:HD21	1:C:172:LEU:HD23	1.99	0.44
1:D:272:GLY:HA3	1:D:314:LEU:HD21	1.99	0.44
1:A:176:GLY:HA2	3:B:401:SY9:HAC	1.99	0.44
1:B:294:SER:HB3	1:C:235:GLN:O	2.18	0.44
1:E:272:GLY:HA3	1:E:314:LEU:HD21	1.99	0.44
3:A:503:SY9:HAC	1:E:176:GLY:HA2	1.99	0.44
1:B:277:LEU:CD1	1:C:278:THR:CB	2.96	0.44
1:D:114:LEU:HD11	1:D:172:LEU:HB3	1.98	0.44
1:B:97:ASP:OD1	1:B:98:SER:N	2.51	0.43
1:C:97:ASP:OD1	1:C:98:SER:N	2.51	0.43
1:C:164:ASP:OD1	1:C:165:VAL:N	2.51	0.43
1:C:266:PRO:HG3	1:D:267:ALA:HB2	2.00	0.43
1:D:176:GLY:HA2	3:E:401:SY9:HAC	1.99	0.43
1:A:295:TYR:HD2	1:B:235:GLN:NE2	2.16	0.43
1:D:40:TYR:HE2	1:D:109:ILE:HA	1.82	0.43
1:D:132:LYS:HG2	1:D:146:ILE:HG22	2.00	0.43
1:D:114:LEU:HD21	1:D:172:LEU:HD23	1.99	0.43
1:B:162:PRO:HG2	1:B:244:TYR:OH	2.19	0.43
1:C:272:GLY:HA3	1:C:314:LEU:HD21	1.99	0.43
1:D:212:ARG:HH22	1:D:229:ARG:NH1	2.15	0.43
1:B:114:LEU:HD21	1:B:172:LEU:HD23	2.00	0.43
1:B:40:TYR:HE2	1:B:109:ILE:HA	1.82	0.43
1:C:277:LEU:CD1	1:D:278:THR:HA	2.48	0.43
1:E:114:LEU:HD21	1:E:172:LEU:HD23	1.99	0.43
1:A:162:PRO:HG2	1:A:244:TYR:OH	2.19	0.43
1:A:94:TYR:HA	1:A:95:PRO:HD3	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:TYR:HE2	1:E:109:ILE:HA	1.82	0.43
1:E:164:ASP:OD1	1:E:165:VAL:N	2.51	0.43
1:D:81:ARG:HD2	3:D:401:SY9:CAL	2.48	0.43
1:E:97:ASP:OD1	1:E:98:SER:N	2.51	0.43
1:E:162:PRO:HG2	1:E:244:TYR:OH	2.19	0.43
1:C:162:PRO:HG2	1:C:244:TYR:OH	2.19	0.43
1:D:164:ASP:OD1	1:D:165:VAL:N	2.51	0.43
1:A:235:GLN:NE2	1:E:295:TYR:HB3	2.33	0.43
1:D:205:LEU:HA	1:D:232:LEU:HD23	2.01	0.43
1:D:97:ASP:OD1	1:D:98:SER:N	2.51	0.43
1:A:97:ASP:OD1	1:A:98:SER:N	2.51	0.43
1:B:164:ASP:OD1	1:B:165:VAL:N	2.51	0.43
1:B:132:LYS:HG2	1:B:146:ILE:HG22	2.00	0.43
1:C:212:ARG:HH22	1:C:229:ARG:NH1	2.15	0.43
1:E:132:LYS:HG2	1:E:146:ILE:HG22	2.00	0.43
1:A:205:LEU:HA	1:A:232:LEU:HD23	2.01	0.43
1:B:205:LEU:HA	1:B:232:LEU:HD23	2.01	0.43
1:A:132:LYS:HG2	1:A:146:ILE:HG22	2.00	0.42
1:A:167:THR:HB	1:A:229:ARG:HH21	1.84	0.42
1:C:167:THR:HB	1:C:229:ARG:HH21	1.84	0.42
1:A:249:LEU:HD11	1:E:311:PHE:CG	2.54	0.42
1:A:164:ASP:OD1	1:A:165:VAL:N	2.51	0.42
1:C:259:TRP:HA	1:C:343:ARG:NH2	2.35	0.42
1:C:158:LEU:HD12	1:C:293:VAL:HG21	2.02	0.42
1:E:94:TYR:HA	1:E:95:PRO:HD3	1.91	0.42
1:C:205:LEU:HA	1:C:232:LEU:HD23	2.01	0.42
1:D:94:TYR:HA	1:D:95:PRO:HD3	1.91	0.42
1:E:158:LEU:HD12	1:E:293:VAL:HG21	2.02	0.42
1:B:158:LEU:HD12	1:B:293:VAL:HG21	2.02	0.42
1:D:259:TRP:HA	1:D:343:ARG:NH2	2.35	0.42
1:D:162:PRO:HG2	1:D:244:TYR:OH	2.19	0.42
1:B:259:TRP:HA	1:B:343:ARG:NH2	2.35	0.42
1:D:158:LEU:HD12	1:D:293:VAL:HG21	2.02	0.42
1:E:256:VAL:HA	1:E:259:TRP:HD1	1.85	0.42
1:A:259:TRP:HA	1:A:343:ARG:NH2	2.35	0.42
1:E:167:THR:HB	1:E:229:ARG:HH21	1.85	0.41
1:B:167:THR:HB	1:B:229:ARG:HH21	1.84	0.41
1:A:148:ILE:CG2	1:A:150:LEU:HD23	2.50	0.41
1:E:205:LEU:HA	1:E:232:LEU:HD23	2.01	0.41
1:A:158:LEU:HD12	1:A:293:VAL:HG21	2.02	0.41
1:D:148:ILE:CG2	1:D:150:LEU:HD23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:TYR:HA	1:B:95:PRO:HD3	1.91	0.41
1:C:256:VAL:HA	1:C:259:TRP:HD1	1.85	0.41
1:A:278:THR:HA	1:E:277:LEU:CD1	2.50	0.41
1:B:284:SER:OG	1:C:285:GLY:HA3	2.20	0.41
1:D:167:THR:HB	1:D:229:ARG:HH21	1.84	0.41
1:D:256:VAL:HA	1:D:259:TRP:HD1	1.85	0.41
1:A:115:PHE:CD1	1:A:115:PHE:C	2.94	0.41
1:E:212:ARG:HH22	1:E:229:ARG:NH1	2.15	0.41
1:C:148:ILE:CG2	1:C:150:LEU:HD23	2.50	0.41
1:E:148:ILE:CG2	1:E:150:LEU:HD23	2.50	0.41
1:B:148:ILE:CG2	1:B:150:LEU:HD23	2.50	0.41
1:E:259:TRP:HA	1:E:343:ARG:NH2	2.35	0.41
1:B:256:VAL:HA	1:B:259:TRP:HD1	1.85	0.41
1:D:115:PHE:C	1:D:115:PHE:CD1	2.94	0.41
1:B:115:PHE:CD1	1:B:115:PHE:C	2.94	0.41
1:B:293:VAL:HG12	1:B:295:TYR:H	1.86	0.41
1:A:295:TYR:HD2	1:B:235:GLN:HE22	1.68	0.41
1:E:115:PHE:CD1	1:E:115:PHE:C	2.94	0.41
1:A:293:VAL:HG12	1:A:295:TYR:H	1.86	0.41
1:D:116:PHE:N	1:D:116:PHE:HD1	2.19	0.41
1:C:115:PHE:CD1	1:C:115:PHE:C	2.94	0.41
1:B:212:ARG:HH22	1:B:229:ARG:NH1	2.15	0.41
1:D:245:ILE:N	1:D:246:PRO:HD2	2.36	0.41
1:D:98:SER:O	1:D:99:LEU:HB2	2.21	0.41
1:A:150:LEU:HD13	1:A:152:LEU:HD21	2.03	0.41
1:D:150:LEU:HD13	1:D:152:LEU:HD21	2.03	0.40
1:B:245:ILE:N	1:B:246:PRO:HD2	2.36	0.40
1:D:179:MET:HG2	1:D:222:LYS:O	2.21	0.40
1:B:52:PRO:O	2:B:402:NAG:H83	2.22	0.40
1:D:52:PRO:O	2:D:402:NAG:H83	2.22	0.40
1:D:175:PHE:CE2	1:E:133:LEU:HB2	2.56	0.40
1:C:245:ILE:N	1:C:246:PRO:HD2	2.36	0.40
1:E:245:ILE:N	1:E:246:PRO:HD2	2.36	0.40
1:D:160:ASN:N	1:D:160:ASN:OD1	2.54	0.40
1:E:98:SER:O	1:E:99:LEU:HB2	2.21	0.40
1:E:117:ALA:HB3	1:E:171:GLN:HE21	1.87	0.40
1:A:256:VAL:HA	1:A:259:TRP:HD1	1.85	0.40
1:B:179:MET:HG2	1:B:222:LYS:O	2.21	0.40
1:A:52:PRO:O	2:A:501:NAG:H83	2.21	0.40
1:A:175:PHE:CE1	3:B:401:SY9:HAX1	2.57	0.40
1:E:118:ASN:ND2	1:E:171:GLN:HG2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ALA:HB3	1:C:171:GLN:HE21	1.87	0.40
1:B:117:ALA:HB3	1:B:171:GLN:HE21	1.87	0.40
1:E:179:MET:HG2	1:E:222:LYS:O	2.21	0.40
1:C:179:MET:HG2	1:C:222:LYS:O	2.22	0.40

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	333/342 (97%)	324 (97%)	9 (3%)	0	100	100
1	B	333/342 (97%)	324 (97%)	9 (3%)	0	100	100
1	C	333/342 (97%)	324 (97%)	9 (3%)	0	100	100
1	D	333/342 (97%)	324 (97%)	9 (3%)	0	100	100
1	E	333/342 (97%)	324 (97%)	9 (3%)	0	100	100
All	All	1665/1710 (97%)	1620 (97%)	45 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	232/304 (76%)	231 (100%)	1 (0%)	93	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	232/304 (76%)	231 (100%)	1 (0%)	93	97
1	C	232/304 (76%)	231 (100%)	1 (0%)	93	97
1	D	232/304 (76%)	231 (100%)	1 (0%)	93	97
1	E	232/304 (76%)	231 (100%)	1 (0%)	93	97
All	All	1160/1520 (76%)	1155 (100%)	5 (0%)	94	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	PHE
1	B	115	PHE
1	C	115	PHE
1	D	115	PHE
1	E	115	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	131	ASN
1	A	235	GLN
1	B	83	GLN
1	B	131	ASN
1	B	235	GLN
1	B	282	GLN
1	C	83	GLN
1	C	85	ASN
1	C	131	ASN
1	C	235	GLN
1	C	282	GLN
1	D	54	ASN
1	D	83	GLN
1	D	85	ASN
1	D	131	ASN
1	D	235	GLN
1	E	83	GLN
1	E	85	ASN
1	E	131	ASN
1	E	235	GLN
1	E	282	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 ⓘ

10 carbohydrates 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	NAG	A	501	2	14,14,15	0.40	0	15,19,21	0.70	0
2	NAG	A	502	2	14,14,15	0.47	0	15,19,21	0.40	0
2	NAG	B	402	2	14,14,15	0.40	0	15,19,21	0.69	0
2	NAG	B	403	2	14,14,15	0.48	0	15,19,21	0.40	0
2	NAG	C	402	2	14,14,15	0.39	0	15,19,21	0.70	0
2	NAG	C	403	2	14,14,15	0.47	0	15,19,21	0.40	0
2	NAG	D	402	2	14,14,15	0.41	0	15,19,21	0.70	0
2	NAG	D	403	2	14,14,15	0.47	0	15,19,21	0.41	0
2	NAG	E	402	2	14,14,15	0.40	0	15,19,21	0.70	0
2	NAG	E	403	2	14,14,15	0.47	0	15,19,21	0.40	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	NAG	A	501	2	-	0/6/23/26	0/1/1/1
2	NAG	A	502	2	-	0/6/23/26	0/1/1/1
2	NAG	B	402	2	-	0/6/23/26	0/1/1/1
2	NAG	B	403	2	-	0/6/23/26	0/1/1/1
2	NAG	C	402	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	403	2	-	0/6/23/26	0/1/1/1
2	NAG	D	402	2	-	0/6/23/26	0/1/1/1
2	NAG	D	403	2	-	0/6/23/26	0/1/1/1
2	NAG	E	402	2	-	0/6/23/26	0/1/1/1
2	NAG	E	403	2	-	0/6/23/26	0/1/1/1

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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	1	0
2	B	402	NAG	1	0
2	D	402	NAG	1	0

## 5.6 Ligand geometry [i](#)

5 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	$\# Z  > 2$
3	SY9	A	503	-	31,31,31	2.61	14 (45%)	51,51,51	3.95	26 (50%)
3	SY9	B	401	-	31,31,31	2.60	14 (45%)	51,51,51	3.94	26 (50%)
3	SY9	C	401	-	31,31,31	2.60	14 (45%)	51,51,51	3.95	26 (50%)
3	SY9	D	401	-	31,31,31	2.60	14 (45%)	51,51,51	3.94	26 (50%)
3	SY9	E	401	-	31,31,31	2.60	14 (45%)	51,51,51	3.95	26 (50%)

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
3	SY9	A	503	-	-	0/0/74/74	0/0/7/7
3	SY9	B	401	-	-	0/0/74/74	0/0/7/7
3	SY9	C	401	-	-	0/0/74/74	0/0/7/7
3	SY9	D	401	-	-	0/0/74/74	0/0/7/7
3	SY9	E	401	-	-	0/0/74/74	0/0/7/7

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	401	SY9	CAW-CAG	-2.60	1.49	1.54
3	C	401	SY9	CAW-CAG	-2.59	1.49	1.54
3	B	401	SY9	CAW-CAG	-2.58	1.49	1.54
3	A	503	SY9	CAW-CAG	-2.55	1.49	1.54
3	D	401	SY9	CAW-CAG	-2.55	1.49	1.54
3	A	503	SY9	CAE-CAF	2.22	1.43	1.38
3	E	401	SY9	CAG-CAB	2.22	1.54	1.51
3	D	401	SY9	CAG-CAB	2.22	1.54	1.51
3	B	401	SY9	CAG-CAB	2.24	1.54	1.51
3	A	503	SY9	CAG-CAB	2.24	1.54	1.51
3	C	401	SY9	CAE-CAF	2.25	1.43	1.38
3	D	401	SY9	CAE-CAF	2.26	1.43	1.38
3	E	401	SY9	CAE-CAF	2.26	1.43	1.38
3	B	401	SY9	CAE-CAF	2.26	1.43	1.38
3	A	503	SY9	CAQ-CAR	2.27	1.37	1.33
3	C	401	SY9	CAG-CAB	2.28	1.55	1.51
3	B	401	SY9	CAQ-CAR	2.31	1.37	1.33
3	E	401	SY9	CAQ-CAR	2.31	1.37	1.33
3	D	401	SY9	CAQ-CAR	2.32	1.37	1.33
3	C	401	SY9	CAQ-CAR	2.33	1.37	1.33
3	C	401	SY9	CAL-CAI	2.46	1.54	1.51
3	A	503	SY9	CAL-CAI	2.47	1.54	1.51
3	D	401	SY9	CAL-CAI	2.49	1.54	1.51
3	B	401	SY9	CAL-CAI	2.50	1.55	1.51
3	E	401	SY9	CAL-CAI	2.50	1.55	1.51
3	C	401	SY9	CAG-CAV	2.55	1.59	1.54
3	A	503	SY9	CAG-CAV	2.56	1.59	1.54
3	B	401	SY9	CAG-CAV	2.57	1.59	1.54
3	D	401	SY9	CAG-CAV	2.58	1.59	1.54
3	D	401	SY9	CAN-CAM	2.59	1.57	1.53
3	E	401	SY9	CAG-CAV	2.60	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	SY9	CAN-CAM	2.61	1.57	1.53
3	A	503	SY9	CAN-CAM	2.63	1.57	1.53
3	C	401	SY9	CAN-CAM	2.63	1.57	1.53
3	E	401	SY9	CAN-CAM	2.63	1.57	1.53
3	C	401	SY9	CAA-NAH	2.72	1.46	1.41
3	D	401	SY9	CAA-NAH	2.74	1.46	1.41
3	A	503	SY9	CAA-NAH	2.75	1.46	1.41
3	B	401	SY9	CAA-NAH	2.75	1.46	1.41
3	E	401	SY9	CAA-NAH	2.75	1.46	1.41
3	C	401	SY9	CAL-CAM	2.99	1.60	1.53
3	A	503	SY9	CAL-CAM	3.00	1.60	1.53
3	E	401	SY9	CAL-CAM	3.00	1.60	1.53
3	D	401	SY9	CAL-CAM	3.01	1.60	1.53
3	B	401	SY9	CAL-CAM	3.01	1.60	1.53
3	B	401	SY9	CAP-CAQ	3.04	1.56	1.50
3	A	503	SY9	CAP-CAQ	3.04	1.56	1.50
3	E	401	SY9	CAP-CAQ	3.05	1.56	1.50
3	D	401	SY9	CAP-CAQ	3.05	1.56	1.50
3	C	401	SY9	CAP-CAQ	3.07	1.56	1.50
3	C	401	SY9	CAA-CAB	3.71	1.44	1.39
3	E	401	SY9	CAA-CAB	3.71	1.44	1.39
3	A	503	SY9	CAA-CAB	3.72	1.44	1.39
3	B	401	SY9	CAA-CAB	3.72	1.44	1.39
3	D	401	SY9	CAA-CAB	3.76	1.44	1.39
3	C	401	SY9	CAS-NAY	4.46	1.57	1.47
3	E	401	SY9	CAS-NAY	4.48	1.57	1.47
3	B	401	SY9	CAS-NAY	4.50	1.57	1.47
3	D	401	SY9	CAS-NAY	4.51	1.57	1.47
3	A	503	SY9	CAS-NAY	4.51	1.57	1.47
3	D	401	SY9	CAS-CAR	5.49	1.62	1.51
3	A	503	SY9	CAS-CAR	5.51	1.62	1.51
3	C	401	SY9	CAS-CAR	5.51	1.62	1.51
3	B	401	SY9	CAS-CAR	5.51	1.62	1.51
3	E	401	SY9	CAS-CAR	5.52	1.62	1.51
3	D	401	SY9	CAI-NAH	7.55	1.46	1.36
3	B	401	SY9	CAI-NAH	7.56	1.46	1.36
3	C	401	SY9	CAI-NAH	7.57	1.46	1.36
3	E	401	SY9	CAI-NAH	7.57	1.46	1.36
3	A	503	SY9	CAI-NAH	7.62	1.46	1.36

All (130) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	SY9	CAT-CAR-CAQ	-11.51	110.80	122.63
3	E	401	SY9	CAT-CAR-CAQ	-11.50	110.81	122.63
3	B	401	SY9	CAT-CAR-CAQ	-11.48	110.82	122.63
3	C	401	SY9	CAT-CAR-CAQ	-11.48	110.83	122.63
3	A	503	SY9	CAT-CAR-CAQ	-11.45	110.86	122.63
3	D	401	SY9	CAW-CAG-CAK	-8.92	101.94	111.23
3	C	401	SY9	CAW-CAG-CAK	-8.90	101.96	111.23
3	A	503	SY9	CAW-CAG-CAK	-8.89	101.97	111.23
3	B	401	SY9	CAW-CAG-CAK	-8.88	101.98	111.23
3	E	401	SY9	CAW-CAG-CAK	-8.84	102.02	111.23
3	C	401	SY9	CAG-CAK-CAN	-5.82	112.88	117.01
3	A	503	SY9	CAG-CAK-CAN	-5.81	112.89	117.01
3	B	401	SY9	CAG-CAK-CAN	-5.78	112.92	117.01
3	D	401	SY9	CAG-CAK-CAN	-5.77	112.92	117.01
3	E	401	SY9	CAG-CAK-CAN	-5.73	112.95	117.01
3	C	401	SY9	CAW-CAG-CAB	-5.65	102.10	112.40
3	D	401	SY9	CAW-CAG-CAB	-5.64	102.11	112.40
3	B	401	SY9	CAW-CAG-CAB	-5.63	102.13	112.40
3	E	401	SY9	CAW-CAG-CAB	-5.62	102.15	112.40
3	A	503	SY9	CAW-CAG-CAB	-5.62	102.15	112.40
3	E	401	SY9	CAT-CAN-CAM	-5.10	114.55	118.52
3	B	401	SY9	CAT-CAN-CAM	-5.09	114.55	118.52
3	A	503	SY9	CAT-CAN-CAM	-5.07	114.56	118.52
3	D	401	SY9	CAT-CAN-CAM	-5.06	114.58	118.52
3	C	401	SY9	CAT-CAN-CAM	-5.02	114.60	118.52
3	E	401	SY9	CAU-CAV-NAY	-4.81	103.65	111.44
3	D	401	SY9	CAU-CAV-NAY	-4.80	103.67	111.44
3	A	503	SY9	CAU-CAV-NAY	-4.80	103.67	111.44
3	B	401	SY9	CAU-CAV-NAY	-4.80	103.67	111.44
3	C	401	SY9	CAU-CAV-NAY	-4.79	103.68	111.44
3	C	401	SY9	CAF-CAA-CAB	-4.55	116.88	121.77
3	A	503	SY9	CAF-CAA-CAB	-4.54	116.88	121.77
3	D	401	SY9	CAF-CAA-CAB	-4.53	116.89	121.77
3	B	401	SY9	CAF-CAA-CAB	-4.52	116.90	121.77
3	E	401	SY9	CAF-CAA-CAB	-4.52	116.91	121.77
3	C	401	SY9	CAK-NAH-CAI	-3.67	115.15	119.29
3	A	503	SY9	CAK-NAH-CAI	-3.66	115.16	119.29
3	B	401	SY9	CAK-NAH-CAI	-3.65	115.17	119.29
3	D	401	SY9	CAK-NAH-CAI	-3.65	115.17	119.29
3	E	401	SY9	CAK-NAH-CAI	-3.65	115.17	119.29
3	E	401	SY9	CAX-NAY-CAV	-3.10	98.42	106.13
3	C	401	SY9	CAX-NAY-CAV	-3.09	98.42	106.13
3	D	401	SY9	CAX-NAY-CAV	-3.09	98.43	106.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	SY9	CAX-NAY-CAV	-3.08	98.44	106.13
3	A	503	SY9	CAX-NAY-CAV	-3.08	98.44	106.13
3	C	401	SY9	OAJ-CAI-NAH	-3.07	119.99	122.61
3	A	503	SY9	OAJ-CAI-NAH	-3.05	120.01	122.61
3	E	401	SY9	OAJ-CAI-NAH	-3.04	120.02	122.61
3	B	401	SY9	OAJ-CAI-NAH	-3.02	120.04	122.61
3	D	401	SY9	OAJ-CAI-NAH	-3.00	120.06	122.61
3	A	503	SY9	CAS-NAY-CAV	2.19	115.02	113.03
3	B	401	SY9	CAS-NAY-CAV	2.20	115.03	113.03
3	E	401	SY9	CAS-NAY-CAV	2.20	115.03	113.03
3	E	401	SY9	CAG-CAV-NAY	2.20	108.12	105.75
3	C	401	SY9	CAS-NAY-CAV	2.21	115.04	113.03
3	D	401	SY9	CAS-NAY-CAV	2.21	115.04	113.03
3	C	401	SY9	CAG-CAV-NAY	2.23	108.14	105.75
3	B	401	SY9	CAG-CAV-NAY	2.23	108.15	105.75
3	A	503	SY9	CAG-CAV-NAY	2.24	108.16	105.75
3	D	401	SY9	CAG-CAV-NAY	2.26	108.18	105.75
3	D	401	SY9	CAR-CAS-NAY	2.90	118.39	112.92
3	C	401	SY9	CAR-CAS-NAY	2.92	118.42	112.92
3	B	401	SY9	CAR-CAS-NAY	2.92	118.42	112.92
3	A	503	SY9	CAR-CAS-NAY	2.93	118.44	112.92
3	E	401	SY9	CAR-CAS-NAY	2.93	118.45	112.92
3	C	401	SY9	OAD-CAM-CAN	3.05	116.63	114.44
3	A	503	SY9	OAD-CAM-CAN	3.11	116.67	114.44
3	D	401	SY9	OAD-CAM-CAN	3.12	116.68	114.44
3	C	401	SY9	CAN-CAT-CAR	3.12	116.69	114.40
3	E	401	SY9	OAD-CAM-CAN	3.12	116.68	114.44
3	B	401	SY9	OAD-CAM-CAN	3.13	116.68	114.44
3	B	401	SY9	CAN-CAT-CAR	3.14	116.70	114.40
3	E	401	SY9	CAN-CAT-CAR	3.14	116.71	114.40
3	D	401	SY9	CAN-CAT-CAR	3.15	116.71	114.40
3	A	503	SY9	CAN-CAT-CAR	3.17	116.73	114.40
3	C	401	SY9	CAN-CAK-NAH	3.83	109.01	106.09
3	D	401	SY9	CAN-CAK-NAH	3.83	109.01	106.09
3	A	503	SY9	CAN-CAK-NAH	3.84	109.02	106.09
3	B	401	SY9	CAN-CAK-NAH	3.84	109.02	106.09
3	E	401	SY9	CAN-CAK-NAH	3.84	109.02	106.09
3	E	401	SY9	CAB-CAG-CAV	3.97	125.08	115.30
3	B	401	SY9	CAB-CAG-CAV	3.98	125.12	115.30
3	D	401	SY9	CAB-CAG-CAV	3.99	125.13	115.30
3	C	401	SY9	CAB-CAG-CAV	3.99	125.14	115.30
3	A	503	SY9	CAB-CAG-CAV	4.00	125.15	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	SY9	CAK-CAG-CAV	4.09	118.03	113.91
3	E	401	SY9	CAK-CAG-CAV	4.10	118.04	113.91
3	B	401	SY9	CAK-CAG-CAV	4.12	118.06	113.91
3	A	503	SY9	CAK-CAG-CAV	4.13	118.07	113.91
3	C	401	SY9	CAK-CAG-CAV	4.13	118.07	113.91
3	B	401	SY9	CAU-CAT-CAN	4.22	111.97	106.68
3	A	503	SY9	CAU-CAT-CAN	4.22	111.97	106.68
3	E	401	SY9	CAU-CAT-CAN	4.22	111.97	106.68
3	C	401	SY9	CAU-CAT-CAN	4.23	111.98	106.68
3	D	401	SY9	CAU-CAT-CAN	4.24	112.00	106.68
3	B	401	SY9	CAU-CAV-CAG	4.58	118.76	113.86
3	A	503	SY9	CAU-CAV-CAG	4.58	118.76	113.86
3	E	401	SY9	CAU-CAV-CAG	4.58	118.77	113.86
3	D	401	SY9	CAU-CAV-CAG	4.58	118.77	113.86
3	C	401	SY9	CAU-CAV-CAG	4.60	118.79	113.86
3	D	401	SY9	CAS-NAY-CAX	4.65	120.13	112.56
3	B	401	SY9	CAS-NAY-CAX	4.66	120.14	112.56
3	A	503	SY9	CAS-NAY-CAX	4.67	120.16	112.56
3	C	401	SY9	CAS-NAY-CAX	4.68	120.18	112.56
3	E	401	SY9	CAS-NAY-CAX	4.69	120.20	112.56
3	D	401	SY9	OAO-CAM-CAL	5.22	110.31	104.41
3	B	401	SY9	OAO-CAM-CAL	5.25	110.34	104.41
3	A	503	SY9	OAO-CAM-CAL	5.26	110.36	104.41
3	E	401	SY9	OAO-CAM-CAL	5.26	110.36	104.41
3	C	401	SY9	OAO-CAM-CAL	5.28	110.38	104.41
3	D	401	SY9	CAP-OAO-CAM	5.72	120.39	114.93
3	B	401	SY9	CAP-OAO-CAM	5.77	120.44	114.93
3	C	401	SY9	CAP-OAO-CAM	5.78	120.45	114.93
3	A	503	SY9	CAP-OAO-CAM	5.79	120.46	114.93
3	E	401	SY9	CAP-OAO-CAM	5.81	120.47	114.93
3	C	401	SY9	CAM-CAN-CAK	6.34	112.61	107.47
3	A	503	SY9	CAM-CAN-CAK	6.36	112.63	107.47
3	E	401	SY9	CAM-CAN-CAK	6.38	112.65	107.47
3	B	401	SY9	CAM-CAN-CAK	6.38	112.65	107.47
3	D	401	SY9	CAM-CAN-CAK	6.40	112.66	107.47
3	C	401	SY9	CAS-CAR-CAQ	8.17	132.59	122.99
3	D	401	SY9	CAS-CAR-CAQ	8.17	132.59	122.99
3	B	401	SY9	CAS-CAR-CAQ	8.17	132.60	122.99
3	A	503	SY9	CAS-CAR-CAQ	8.18	132.60	122.99
3	E	401	SY9	CAS-CAR-CAQ	8.20	132.63	122.99
3	D	401	SY9	CAA-NAH-CAI	8.52	134.18	125.40
3	A	503	SY9	CAA-NAH-CAI	8.52	134.18	125.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	401	SY9	CAA-NAH-CAI	8.54	134.20	125.40
3	B	401	SY9	CAA-NAH-CAI	8.54	134.20	125.40
3	C	401	SY9	CAA-NAH-CAI	8.59	134.26	125.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	SY9	4	0
3	B	401	SY9	6	0
3	C	401	SY9	5	0
3	D	401	SY9	5	0
3	E	401	SY9	5	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.