



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 22, 2018 – 03:40 PM EST

PDB ID : 6E7Z  
EMDB ID: : EMD-9002  
Title : cryo-EM structure of human TRPML1 with ML-SA1 and PI35P2  
Authors : Schmiede, P.; Li, X.  
Deposited on : 2018-07-27  
Resolution : 3.73 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation 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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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

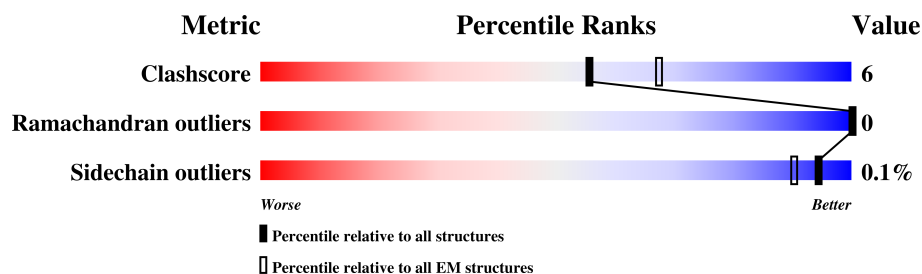
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.73 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  $\geq 3$ , 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	580	71% 11% 18%
1	B	580	71% 11% 18%
1	C	580	72% 10% 18%
1	D	580	71% 11% 18%

2 Entry composition ⓘ

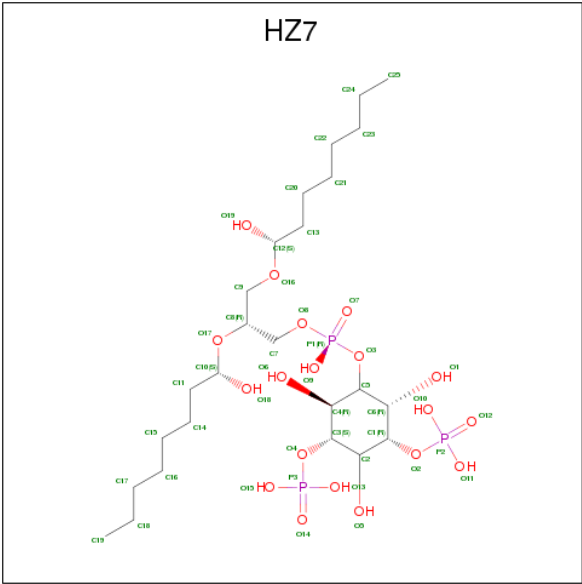
There are 3 unique types of molecules in this entry. The entry contains 15616 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Mucolipin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	475	Total	C	N	O	S	0	0
			3830	2501	640	664	25		
1	B	475	Total	C	N	O	S	0	0
			3830	2501	640	664	25		
1	C	475	Total	C	N	O	S	0	0
			3830	2501	640	664	25		
1	D	475	Total	C	N	O	S	0	0
			3830	2501	640	664	25		

- Molecule 2 is (1R,2S,3S,4R,5S,6R)-5-{[(R)-[(2R)-2,3-bis{[(1S)-1-hydroxyoctyl]oxy}propoxy](hydroxy)phosphoryl]oxy}-2,4,6-trihydroxycyclohexane-1,3-diyl bis[dihydrogen (phosphate)] (three-letter code: HZ7) (formula: C<sub>25</sub>H<sub>53</sub>O<sub>19</sub>P<sub>3</sub>).



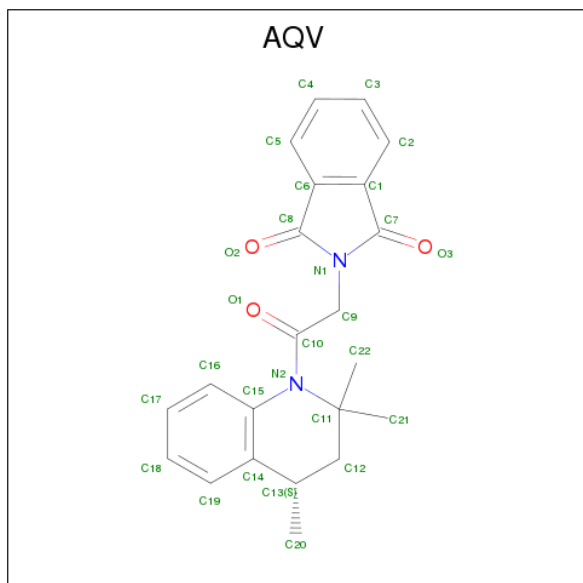
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			47	25	19	3	
2	B	1	Total	C	O	P	0
			47	25	19	3	

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Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	O	P	0
			47	25	19	3	
2	D	1	Total	C	O	P	0
			47	25	19	3	

- Molecule 3 is 2-{2-oxo-2-[(4S)-2,2,4-trimethyl-3,4-dihydroquinolin-1(2H)-yl]ethyl}-1H-isindole-1,3(2H)-dione (three-letter code: AQV) (formula: C<sub>22</sub>H<sub>22</sub>N<sub>2</sub>O<sub>3</sub>).

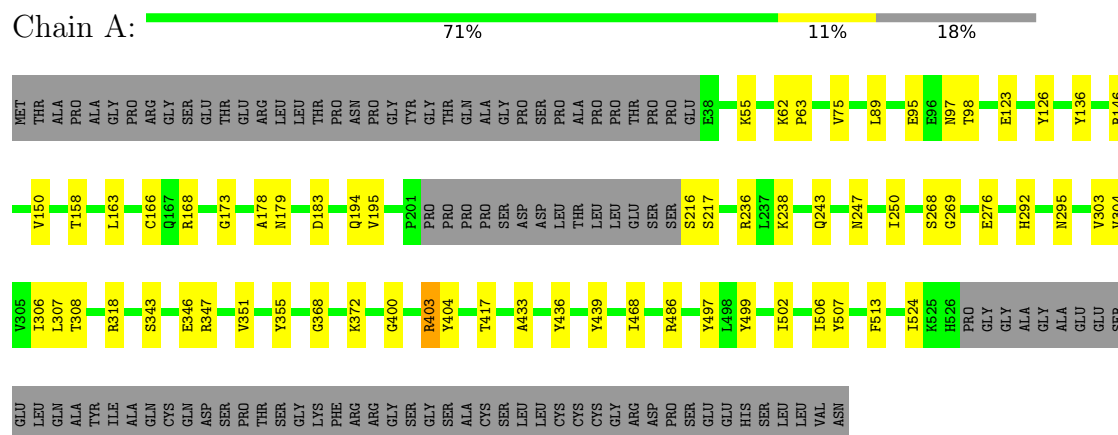


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			27	22	2	3	
3	B	1	Total	C	N	O	0
			27	22	2	3	
3	C	1	Total	C	N	O	0
			27	22	2	3	
3	D	1	Total	C	N	O	0
			27	22	2	3	

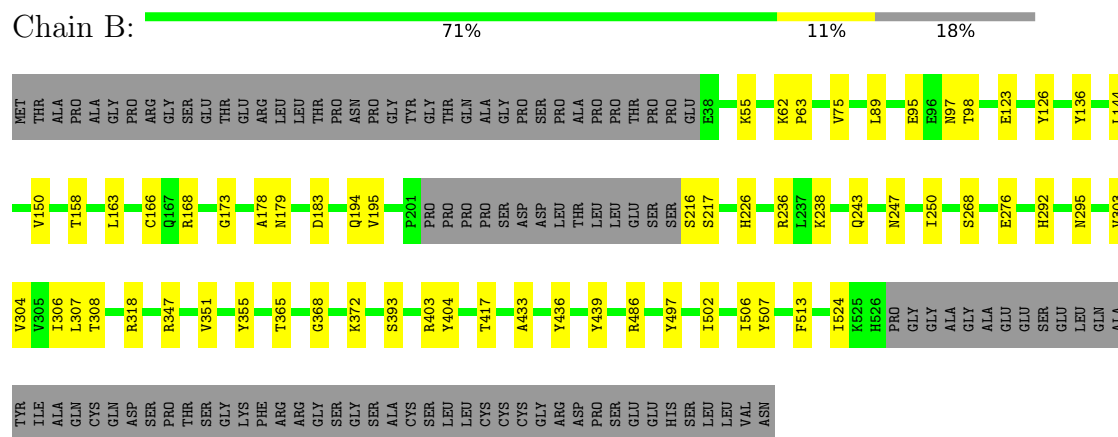
### 3 Residue-property plots

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.

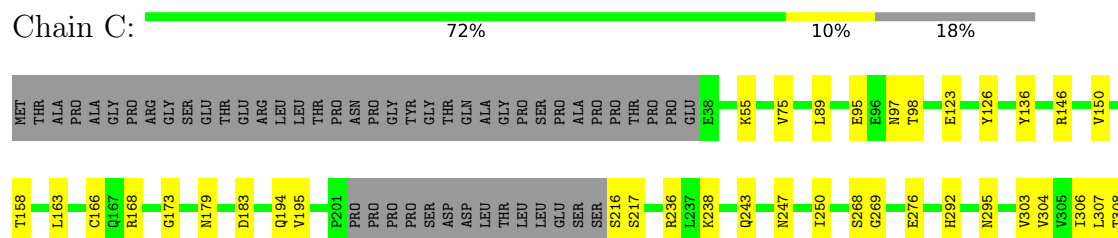
#### • Molecule 1: Mucolipin-1

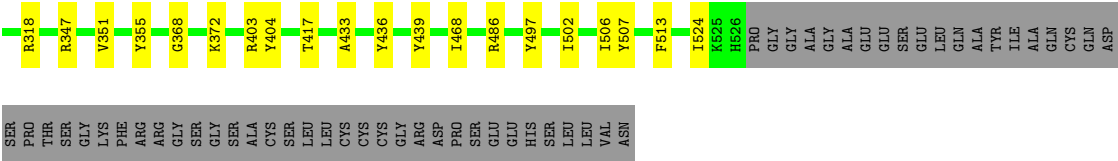


#### • Molecule 1: Mucolipin-1

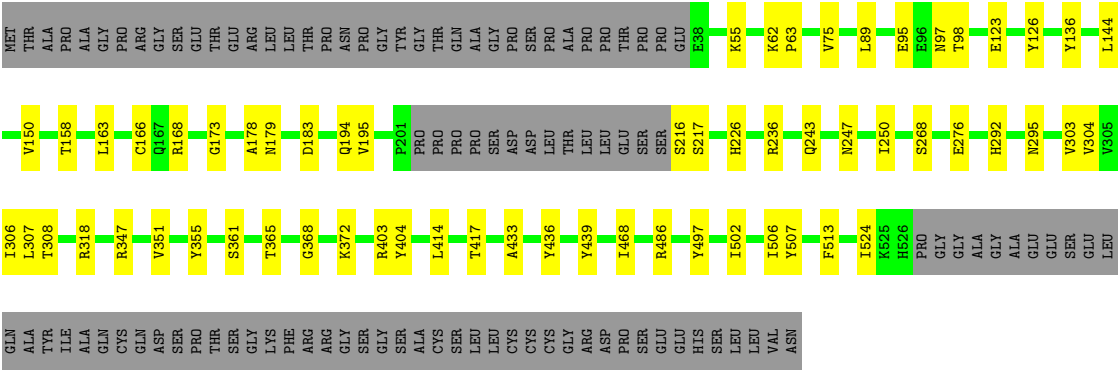


#### • Molecule 1: Mucolipin-1





● Molecule 1: Mucolipin-1



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	45481	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 ( $e^-/\text{\AA}^2$ )	1.6	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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HZ7, AQV

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	0.44	0/3925	0.60	0/5326
1	B	0.44	0/3925	0.60	0/5326
1	C	0.44	0/3925	0.60	0/5326
1	D	0.44	0/3925	0.60	0/5326
All	All	0.44	0/15700	0.60	0/21304

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
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	179	ASN	Peptide
1	B	179	ASN	Peptide
1	C	179	ASN	Peptide
1	D	179	ASN	Peptide



## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3830	0	3856	49	0
1	B	3830	0	3856	47	0
1	C	3830	0	3856	47	0
1	D	3830	0	3856	51	0
2	A	47	0	0	5	0
2	B	47	0	0	5	0
2	C	47	0	0	4	0
2	D	47	0	0	4	0
3	A	27	0	0	6	0
3	B	27	0	0	6	0
3	C	27	0	0	6	0
3	D	27	0	0	6	0
All	All	15616	0	15424	177	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 6.

All (177) 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:436:TYR:CB	3:D:802:AQV:O3	1.74	1.35
1:C:436:TYR:CB	3:C:802:AQV:O3	1.74	1.35
1:A:436:TYR:CB	3:A:802:AQV:O3	1.74	1.34
1:B:436:TYR:CB	3:B:802:AQV:O3	1.74	1.32
1:C:433:ALA:HB2	3:C:802:AQV:C17	1.71	1.21
1:D:433:ALA:HB2	3:D:802:AQV:C17	1.71	1.20
1:B:433:ALA:HB2	3:B:802:AQV:C17	1.71	1.20
1:A:433:ALA:HB2	3:A:802:AQV:C17	1.71	1.19
1:D:436:TYR:HB3	3:D:802:AQV:O3	1.38	1.15
1:B:436:TYR:HB3	3:B:802:AQV:O3	1.38	1.14
1:A:436:TYR:HB3	3:A:802:AQV:O3	1.38	1.12
1:C:436:TYR:HB3	3:C:802:AQV:O3	1.38	1.10
1:C:436:TYR:HB2	3:C:802:AQV:O3	1.56	1.05
1:A:436:TYR:HB2	3:A:802:AQV:O3	1.56	1.05
1:D:355:TYR:CE2	1:D:403:ARG:NH1	2.25	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:TYR:HB2	3:B:802:AQV:O3	1.56	1.04
1:D:436:TYR:HB2	3:D:802:AQV:O3	1.56	1.01
1:B:355:TYR:CE2	1:B:403:ARG:NH1	2.35	0.95
1:C:355:TYR:CE2	1:C:403:ARG:NH1	2.43	0.85
1:C:433:ALA:CB	3:C:802:AQV:C17	2.56	0.84
1:B:433:ALA:CB	3:B:802:AQV:C17	2.56	0.83
1:D:433:ALA:CB	3:D:802:AQV:C17	2.56	0.81
1:B:55:LYS:CE	2:B:801:HZ7:O7	2.29	0.81
1:A:55:LYS:CE	2:A:801:HZ7:O7	2.29	0.81
1:C:55:LYS:CE	2:C:801:HZ7:O7	2.29	0.80
1:D:55:LYS:CE	2:D:801:HZ7:O7	2.29	0.80
1:A:433:ALA:CB	3:A:802:AQV:C17	2.56	0.80
1:D:355:TYR:CZ	1:D:403:ARG:NH2	2.53	0.77
1:C:355:TYR:HE2	1:C:403:ARG:HH12	1.35	0.73
1:A:400:GLY:O	1:A:403:ARG:HG2	1.94	0.68
1:A:173:GLY:HA2	1:A:183:ASP:HB3	1.77	0.67
1:C:173:GLY:HA2	1:C:183:ASP:HB3	1.77	0.66
1:C:355:TYR:CZ	1:C:403:ARG:NH2	2.64	0.66
1:D:173:GLY:HA2	1:D:183:ASP:HB3	1.77	0.66
1:B:173:GLY:HA2	1:B:183:ASP:HB3	1.77	0.65
1:B:355:TYR:CZ	1:B:403:ARG:NH2	2.64	0.64
1:B:268:SER:O	1:C:97:ASN:ND2	2.32	0.63
1:B:486:ARG:HH21	1:C:276:GLU:HG3	1.64	0.62
1:A:403:ARG:HD3	1:A:404:TYR:CE2	2.34	0.61
1:C:486:ARG:HH21	1:D:276:GLU:HG3	1.66	0.60
1:A:486:ARG:HH21	1:B:276:GLU:HG3	1.68	0.59
1:B:436:TYR:CG	3:B:802:AQV:O3	2.55	0.59
1:D:55:LYS:NZ	2:D:801:HZ7:O7	2.36	0.59
1:D:436:TYR:CG	3:D:802:AQV:O3	2.55	0.59
1:A:55:LYS:NZ	2:A:801:HZ7:O7	2.36	0.58
1:C:55:LYS:NZ	2:C:801:HZ7:O7	2.36	0.58
1:A:97:ASN:ND2	1:D:268:SER:O	2.37	0.58
1:A:276:GLU:HG3	1:D:486:ARG:HH21	1.68	0.57
1:A:400:GLY:O	1:A:403:ARG:CG	2.51	0.57
1:C:436:TYR:CG	3:C:802:AQV:O3	2.55	0.57
1:D:355:TYR:HE2	1:D:403:ARG:HH12	1.37	0.57
1:B:55:LYS:NZ	2:B:801:HZ7:O7	2.36	0.57
1:C:268:SER:O	1:D:97:ASN:ND2	2.38	0.56
1:A:513:PHE:HE2	1:D:507:TYR:HB3	1.70	0.56
1:A:247:ASN:ND2	1:A:250:ILE:O	2.39	0.56
1:C:247:ASN:ND2	1:C:250:ILE:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:ASN:ND2	1:B:250:ILE:O	2.39	0.55
1:A:436:TYR:CG	3:A:802:AQV:O3	2.55	0.55
1:D:247:ASN:ND2	1:D:250:ILE:O	2.39	0.55
1:A:55:LYS:HE2	2:A:801:HZ7:O7	2.07	0.55
1:B:55:LYS:HE2	2:B:801:HZ7:O7	2.07	0.55
1:B:355:TYR:HE2	1:B:403:ARG:HH12	1.39	0.54
1:D:55:LYS:HE2	2:D:801:HZ7:O7	2.07	0.54
1:C:55:LYS:HE2	2:C:801:HZ7:O7	2.07	0.54
1:A:268:SER:O	1:B:97:ASN:ND2	2.41	0.53
1:D:355:TYR:CE1	1:D:403:ARG:NH2	2.66	0.51
1:D:292:HIS:HA	1:D:295:ASN:HB2	1.93	0.51
1:D:163:LEU:HB3	1:D:195:VAL:HG13	1.93	0.51
1:C:163:LEU:HB3	1:C:195:VAL:HG13	1.93	0.51
1:B:163:LEU:HB3	1:B:195:VAL:HG13	1.93	0.50
1:C:507:TYR:HB3	1:D:513:PHE:HE2	1.75	0.50
1:B:507:TYR:HB3	1:C:513:PHE:HE2	1.76	0.50
1:A:439:TYR:OH	1:A:497:TYR:O	2.30	0.50
1:B:292:HIS:HA	1:B:295:ASN:HB2	1.93	0.50
1:B:178:ALA:HB2	1:C:238:LYS:HD2	1.94	0.50
1:A:238:LYS:HD2	1:D:178:ALA:HB2	1.94	0.50
1:A:507:TYR:HB3	1:B:513:PHE:HE2	1.77	0.50
1:C:303:VAL:HA	1:C:306:ILE:HG22	1.93	0.50
1:A:292:HIS:HA	1:A:295:ASN:HB2	1.93	0.49
1:C:292:HIS:HA	1:C:295:ASN:HB2	1.93	0.49
1:C:75:VAL:HG21	1:C:308:THR:HG21	1.95	0.49
1:D:75:VAL:HG21	1:D:308:THR:HG21	1.94	0.49
1:D:303:VAL:HA	1:D:306:ILE:HG22	1.93	0.49
1:B:303:VAL:HA	1:B:306:ILE:HG22	1.93	0.49
1:B:439:TYR:OH	1:B:497:TYR:O	2.30	0.49
1:A:163:LEU:HB3	1:A:195:VAL:HG13	1.93	0.49
1:C:355:TYR:CE1	1:C:403:ARG:NH2	2.77	0.49
1:C:368:GLY:O	1:C:372:LYS:N	2.46	0.49
1:A:158:THR:HG23	1:A:194:GLN:HE22	1.78	0.49
1:A:303:VAL:HA	1:A:306:ILE:HG22	1.93	0.49
1:B:158:THR:HG23	1:B:194:GLN:HE22	1.78	0.49
1:A:368:GLY:O	1:A:372:LYS:N	2.46	0.48
1:B:75:VAL:HG21	1:B:308:THR:HG21	1.95	0.48
1:D:439:TYR:OH	1:D:497:TYR:O	2.30	0.48
1:B:368:GLY:O	1:B:372:LYS:N	2.46	0.48
1:D:368:GLY:O	1:D:372:LYS:N	2.46	0.48
1:A:95:GLU:O	1:A:98:THR:OG1	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:VAL:HG21	1:A:308:THR:HG21	1.94	0.48
1:A:318:ARG:NH1	2:A:801:HZ7:O14	2.41	0.48
1:C:158:THR:HG23	1:C:194:GLN:HE22	1.78	0.48
1:C:216:SER:OG	1:C:217:SER:N	2.47	0.48
1:D:158:THR:HG23	1:D:194:GLN:HE22	1.78	0.48
1:C:439:TYR:OH	1:C:497:TYR:O	2.30	0.48
1:A:355:TYR:CE2	1:A:403:ARG:NH1	2.73	0.48
1:B:216:SER:OG	1:B:217:SER:N	2.47	0.47
1:D:355:TYR:CD2	1:D:403:ARG:NH1	2.69	0.47
1:B:303:VAL:O	1:B:307:LEU:N	2.48	0.47
1:C:403:ARG:HD3	1:C:404:TYR:CE2	2.50	0.47
1:C:303:VAL:O	1:C:307:LEU:N	2.48	0.47
1:B:226:HIS:HB2	1:C:146:ARG:HD2	1.96	0.47
1:D:355:TYR:CE2	1:D:403:ARG:CZ	2.97	0.47
1:A:216:SER:OG	1:A:217:SER:N	2.47	0.47
1:C:417:THR:HG22	1:C:524:ILE:HG21	1.97	0.47
1:B:417:THR:HG22	1:B:524:ILE:HG21	1.97	0.46
1:A:303:VAL:O	1:A:307:LEU:N	2.48	0.46
1:D:303:VAL:O	1:D:307:LEU:N	2.48	0.46
1:A:417:THR:HG22	1:A:524:ILE:HG21	1.97	0.46
1:A:502:ILE:HB	1:A:506:ILE:HD12	1.98	0.46
1:D:361:SER:O	1:D:365:THR:OG1	2.28	0.45
1:D:502:ILE:HB	1:D:506:ILE:HD12	1.98	0.45
1:A:304:VAL:HA	1:A:307:LEU:HD12	1.99	0.45
1:B:318:ARG:NH1	2:B:801:HZ7:O14	2.41	0.45
1:C:347:ARG:O	1:C:351:VAL:N	2.49	0.45
1:C:318:ARG:NH1	2:C:801:HZ7:O14	2.41	0.45
1:D:304:VAL:HA	1:D:307:LEU:HD12	1.99	0.45
1:C:304:VAL:HA	1:C:307:LEU:HD12	1.99	0.45
1:B:304:VAL:HA	1:B:307:LEU:HD12	1.99	0.45
1:C:123:GLU:HA	1:C:126:TYR:HD2	1.82	0.45
1:C:355:TYR:CE2	1:C:403:ARG:NH2	2.85	0.45
1:D:417:THR:HG22	1:D:524:ILE:HG21	1.97	0.45
1:D:123:GLU:HA	1:D:126:TYR:HD2	1.82	0.45
1:B:123:GLU:HA	1:B:126:TYR:HD2	1.82	0.44
1:B:502:ILE:HB	1:B:506:ILE:HD12	1.98	0.44
1:A:123:GLU:HA	1:A:126:TYR:HD2	1.82	0.44
1:A:343:SER:OG	1:A:346:GLU:OE1	2.28	0.44
1:A:136:TYR:CE2	1:A:163:LEU:HB2	2.53	0.44
1:B:347:ARG:O	1:B:351:VAL:N	2.49	0.44
1:C:502:ILE:HB	1:C:506:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:SER:OG	1:D:217:SER:N	2.47	0.44
1:B:150:VAL:HG11	1:B:236:ARG:HB2	2.00	0.44
1:D:136:TYR:CE2	1:D:163:LEU:HB2	2.53	0.44
1:B:166:CYS:HB3	1:B:168:ARG:NH2	2.33	0.43
1:D:166:CYS:HB3	1:D:168:ARG:NH2	2.33	0.43
1:A:150:VAL:HG11	1:A:236:ARG:HB2	2.00	0.43
1:C:150:VAL:HG11	1:C:236:ARG:HB2	2.00	0.43
1:D:150:VAL:HG11	1:D:236:ARG:HB2	2.00	0.43
1:D:347:ARG:O	1:D:351:VAL:N	2.49	0.43
1:A:166:CYS:HB3	1:A:168:ARG:NH2	2.33	0.43
1:C:166:CYS:HB3	1:C:168:ARG:NH2	2.33	0.43
1:D:403:ARG:HD3	1:D:404:TYR:CE2	2.54	0.43
1:C:136:TYR:CE2	1:C:163:LEU:HB2	2.53	0.43
1:B:136:TYR:CE2	1:B:163:LEU:HB2	2.53	0.43
1:D:318:ARG:NH1	2:D:801:HZ7:O14	2.41	0.43
1:B:403:ARG:HD3	1:B:404:TYR:CE2	2.53	0.42
1:C:95:GLU:O	1:C:98:THR:OG1	2.30	0.42
1:D:95:GLU:O	1:D:98:THR:OG1	2.30	0.42
1:D:89:LEU:HD23	1:D:243:GLN:HB3	2.01	0.42
1:A:499:TYR:HD1	1:A:499:TYR:HA	1.75	0.42
1:A:269:GLY:HA2	1:B:144:LEU:HD12	2.00	0.42
1:B:62:LYS:HA	1:B:63:PRO:HD3	1.84	0.42
1:B:89:LEU:HD23	1:B:243:GLN:HB3	2.01	0.41
1:B:95:GLU:O	1:B:98:THR:OG1	2.30	0.41
1:A:89:LEU:HD23	1:A:243:GLN:HB3	2.01	0.41
1:A:62:LYS:HA	1:A:63:PRO:HD3	1.84	0.41
1:C:89:LEU:HD23	1:C:243:GLN:HB3	2.01	0.41
2:B:801:HZ7:O6	2:B:801:HZ7:O8	2.39	0.41
1:C:269:GLY:HA2	1:D:144:LEU:HD12	2.03	0.41
1:A:347:ARG:O	1:A:351:VAL:N	2.49	0.41
1:C:468:ILE:HA	1:C:506:ILE:HD11	2.03	0.41
1:A:178:ALA:HB2	1:B:238:LYS:HD2	2.03	0.40
1:D:468:ILE:HA	1:D:506:ILE:HD11	2.03	0.40
1:D:414:LEU:HD23	1:D:414:LEU:HA	1.89	0.40
1:D:62:LYS:HA	1:D:63:PRO:HD3	1.84	0.40
1:A:468:ILE:HA	1:A:506:ILE:HD11	2.03	0.40
2:A:801:HZ7:O6	2:A:801:HZ7:O8	2.39	0.40
1:B:365:THR:OG1	1:B:393:SER:OG	2.37	0.40
1:A:146:ARG:HD2	1:D:226:HIS:HB2	2.04	0.40

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	471/580 (81%)	420 (89%)	51 (11%)	0	100	100
1	B	471/580 (81%)	420 (89%)	51 (11%)	0	100	100
1	C	471/580 (81%)	420 (89%)	51 (11%)	0	100	100
1	D	471/580 (81%)	421 (89%)	50 (11%)	0	100	100
All	All	1884/2320 (81%)	1681 (89%)	203 (11%)	0	100	100

There are no Ramachandran outliers to report.

### 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	423/507 (83%)	422 (100%)	1 (0%)	94	98
1	B	423/507 (83%)	423 (100%)	0	100	100
1	C	423/507 (83%)	423 (100%)	0	100	100
1	D	423/507 (83%)	423 (100%)	0	100	100
All	All	1692/2028 (83%)	1691 (100%)	1 (0%)	94	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	403	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	97	ASN
1	A	234	HIS
1	A	469	ASN
1	B	69	GLN
1	B	97	ASN
1	B	234	HIS
1	B	247	ASN
1	B	469	ASN
1	C	69	GLN
1	C	97	ASN
1	C	234	HIS
1	C	469	ASN
1	D	69	GLN
1	D	97	ASN
1	D	234	HIS
1	D	247	ASN
1	D	469	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	HZ7	A	801	-	47,47,47	0.72	1 (2%)	59,65,65	0.98	4 (6%)
3	AQV	A	802	-	30,30,30	4.23	17 (56%)	40,46,46	3.31	17 (42%)
2	HZ7	B	801	-	47,47,47	0.71	1 (2%)	59,65,65	0.98	4 (6%)
3	AQV	B	802	-	30,30,30	4.24	17 (56%)	40,46,46	3.32	17 (42%)
2	HZ7	C	801	-	47,47,47	0.71	1 (2%)	59,65,65	0.98	4 (6%)
3	AQV	C	802	-	30,30,30	4.23	17 (56%)	40,46,46	3.31	17 (42%)
2	HZ7	D	801	-	47,47,47	0.71	1 (2%)	59,65,65	0.98	4 (6%)
3	AQV	D	802	-	30,30,30	4.23	17 (56%)	40,46,46	3.31	17 (42%)

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	HZ7	A	801	-	-	0/42/68/68	0/1/1/1
3	AQV	A	802	-	-	0/8/43/43	0/4/4/4
2	HZ7	B	801	-	-	0/42/68/68	0/1/1/1
3	AQV	B	802	-	-	0/8/43/43	0/4/4/4
2	HZ7	C	801	-	-	0/42/68/68	0/1/1/1
3	AQV	C	802	-	-	0/8/43/43	0/4/4/4
2	HZ7	D	801	-	-	0/42/68/68	0/1/1/1
3	AQV	D	802	-	-	0/8/43/43	0/4/4/4

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	AQV	C8-N1	-5.54	1.32	1.39
3	C	802	AQV	C8-N1	-5.49	1.32	1.39
3	D	802	AQV	C8-N1	-5.48	1.32	1.39
3	A	802	AQV	C8-N1	-5.47	1.32	1.39
3	D	802	AQV	C11-N2	-4.64	1.45	1.50
3	B	802	AQV	C11-N2	-4.62	1.45	1.50
3	A	802	AQV	C11-N2	-4.58	1.45	1.50
3	C	802	AQV	C11-N2	-4.56	1.45	1.50
3	A	802	AQV	C7-N1	-3.87	1.34	1.39
3	D	802	AQV	C7-N1	-3.86	1.34	1.39
3	B	802	AQV	C7-N1	-3.81	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	802	AQV	C7-N1	-3.81	1.34	1.39
3	B	802	AQV	C1-C7	-3.39	1.43	1.48
3	D	802	AQV	C1-C7	-3.37	1.43	1.48
3	C	802	AQV	C1-C7	-3.36	1.43	1.48
3	A	802	AQV	C1-C7	-3.35	1.43	1.48
3	A	802	AQV	C6-C8	-3.17	1.43	1.48
3	C	802	AQV	C6-C8	-3.14	1.43	1.48
3	B	802	AQV	C6-C8	-3.14	1.43	1.48
3	D	802	AQV	C6-C8	-3.09	1.43	1.48
3	C	802	AQV	O1-C10	-2.46	1.17	1.23
3	A	802	AQV	O1-C10	-2.45	1.17	1.23
3	D	802	AQV	O1-C10	-2.44	1.17	1.23
3	B	802	AQV	O1-C10	-2.44	1.17	1.23
3	A	802	AQV	C15-C14	2.05	1.42	1.40
2	C	801	HZ7	O18-C10	2.05	1.43	1.39
3	B	802	AQV	C15-C14	2.06	1.42	1.40
3	C	802	AQV	C15-C14	2.07	1.42	1.40
2	B	801	HZ7	O18-C10	2.07	1.43	1.39
3	D	802	AQV	C15-C14	2.10	1.42	1.40
2	D	801	HZ7	O18-C10	2.11	1.43	1.39
2	A	801	HZ7	O18-C10	2.11	1.43	1.39
3	C	802	AQV	C18-C17	2.15	1.43	1.38
3	B	802	AQV	C18-C17	2.15	1.43	1.38
3	D	802	AQV	C18-C17	2.16	1.43	1.38
3	A	802	AQV	C18-C17	2.18	1.43	1.38
3	C	802	AQV	C22-C11	2.31	1.58	1.53
3	D	802	AQV	C22-C11	2.34	1.58	1.53
3	A	802	AQV	C22-C11	2.35	1.58	1.53
3	B	802	AQV	C22-C11	2.36	1.58	1.53
3	D	802	AQV	C4-C5	2.53	1.43	1.38
3	A	802	AQV	C4-C5	2.54	1.43	1.38
3	B	802	AQV	C4-C5	2.56	1.43	1.38
3	C	802	AQV	C4-C5	2.58	1.44	1.38
3	D	802	AQV	C5-C6	3.30	1.45	1.39
3	A	802	AQV	C5-C6	3.31	1.45	1.39
3	B	802	AQV	C5-C6	3.34	1.45	1.39
3	C	802	AQV	C5-C6	3.35	1.45	1.39
3	D	802	AQV	C2-C1	3.89	1.46	1.39
3	B	802	AQV	C2-C1	3.93	1.46	1.39
3	C	802	AQV	C2-C1	3.95	1.46	1.39
3	A	802	AQV	C2-C1	4.01	1.46	1.39
3	A	802	AQV	C9-C10	4.60	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802	AQV	C9-C10	4.60	1.59	1.53
3	C	802	AQV	C9-C10	4.61	1.59	1.53
3	B	802	AQV	C9-C10	4.66	1.59	1.53
3	A	802	AQV	C15-N2	5.37	1.50	1.42
3	D	802	AQV	C15-N2	5.42	1.50	1.42
3	C	802	AQV	C15-N2	5.45	1.50	1.42
3	B	802	AQV	C15-N2	5.45	1.50	1.42
3	C	802	AQV	C10-N2	6.47	1.53	1.38
3	A	802	AQV	C10-N2	6.47	1.53	1.38
3	B	802	AQV	C10-N2	6.47	1.53	1.38
3	D	802	AQV	C10-N2	6.48	1.53	1.38
3	C	802	AQV	O2-C8	11.45	1.45	1.22
3	D	802	AQV	O2-C8	11.45	1.45	1.22
3	A	802	AQV	O2-C8	11.50	1.45	1.22
3	B	802	AQV	O2-C8	11.51	1.45	1.22
3	A	802	AQV	O3-C7	12.36	1.47	1.22
3	B	802	AQV	O3-C7	12.37	1.47	1.22
3	C	802	AQV	O3-C7	12.39	1.47	1.22
3	D	802	AQV	O3-C7	12.41	1.47	1.22

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	AQV	O1-C10-C9	-9.05	106.22	120.62
3	C	802	AQV	O1-C10-C9	-9.01	106.28	120.62
3	A	802	AQV	O1-C10-C9	-9.01	106.28	120.62
3	D	802	AQV	O1-C10-C9	-9.01	106.30	120.62
3	B	802	AQV	C21-C11-C22	-5.43	96.78	108.59
3	A	802	AQV	C21-C11-C22	-5.42	96.82	108.59
3	D	802	AQV	C21-C11-C22	-5.41	96.82	108.59
3	C	802	AQV	C21-C11-C22	-5.40	96.84	108.59
3	B	802	AQV	C1-C6-C8	-3.64	105.18	108.27
3	A	802	AQV	C1-C6-C8	-3.62	105.20	108.27
3	D	802	AQV	C1-C6-C8	-3.59	105.22	108.27
3	C	802	AQV	C1-C6-C8	-3.57	105.23	108.27
2	C	801	HZ7	C4-C5-C6	-2.59	107.09	110.84
2	B	801	HZ7	C4-C5-C6	-2.57	107.11	110.84
2	A	801	HZ7	C4-C5-C6	-2.56	107.12	110.84
2	D	801	HZ7	C4-C5-C6	-2.55	107.15	110.84
2	C	801	HZ7	C5-C4-C3	-2.52	103.71	108.94
2	D	801	HZ7	C5-C4-C3	-2.51	103.72	108.94
2	A	801	HZ7	C5-C4-C3	-2.51	103.73	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HZ7	C5-C4-C3	-2.50	103.75	108.94
2	B	801	HZ7	C14-C11-C10	-2.25	108.26	113.19
2	D	801	HZ7	C14-C11-C10	-2.25	108.27	113.19
2	A	801	HZ7	C14-C11-C10	-2.25	108.27	113.19
2	C	801	HZ7	C14-C11-C10	-2.24	108.29	113.19
3	C	802	AQV	C16-C15-C14	-2.15	117.23	120.05
3	A	802	AQV	C16-C15-C14	-2.15	117.23	120.05
3	D	802	AQV	C16-C15-C14	-2.15	117.23	120.05
3	B	802	AQV	C16-C15-C14	-2.11	117.28	120.05
3	A	802	AQV	C8-N1-C7	-2.03	110.33	112.02
3	C	802	AQV	C8-N1-C7	-2.02	110.35	112.02
3	D	802	AQV	C8-N1-C7	-2.01	110.35	112.02
3	B	802	AQV	C8-N1-C7	-2.01	110.35	112.02
3	B	802	AQV	C14-C15-N2	2.18	119.55	117.24
3	C	802	AQV	C2-C1-C7	2.22	133.07	129.63
3	D	802	AQV	C14-C15-N2	2.23	119.60	117.24
3	A	802	AQV	C2-C1-C7	2.23	133.09	129.63
3	A	802	AQV	C14-C15-N2	2.24	119.61	117.24
3	D	802	AQV	C20-C13-C12	2.24	113.52	110.16
3	C	802	AQV	C14-C15-N2	2.24	119.61	117.24
3	D	802	AQV	C2-C1-C7	2.25	133.13	129.63
3	B	802	AQV	C2-C1-C7	2.25	133.13	129.63
3	C	802	AQV	C20-C13-C12	2.27	113.57	110.16
3	A	802	AQV	C20-C13-C12	2.28	113.58	110.16
3	B	802	AQV	C20-C13-C12	2.28	113.58	110.16
3	D	802	AQV	C17-C16-C15	2.33	123.22	118.29
3	B	802	AQV	C17-C16-C15	2.34	123.23	118.29
3	A	802	AQV	C17-C16-C15	2.36	123.27	118.29
3	C	802	AQV	C17-C16-C15	2.36	123.27	118.29
3	D	802	AQV	C9-N1-C8	2.40	125.66	123.72
3	A	802	AQV	C9-N1-C8	2.40	125.66	123.72
3	B	802	AQV	C9-N1-C8	2.44	125.69	123.72
2	A	801	HZ7	C6-C1-C2	2.44	114.39	110.84
3	C	802	AQV	C9-N1-C8	2.45	125.70	123.72
2	D	801	HZ7	C6-C1-C2	2.46	114.41	110.84
2	C	801	HZ7	C6-C1-C2	2.46	114.42	110.84
2	B	801	HZ7	C6-C1-C2	2.46	114.42	110.84
3	C	802	AQV	C19-C14-C15	2.55	121.32	118.31
3	C	802	AQV	C1-C7-N1	2.56	107.67	105.88
3	B	802	AQV	C1-C7-N1	2.57	107.68	105.88
3	A	802	AQV	C1-C7-N1	2.57	107.68	105.88
3	B	802	AQV	C19-C14-C15	2.57	121.35	118.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	AQV	C19-C14-C15	2.58	121.35	118.31
3	D	802	AQV	C11-C12-C13	2.58	119.26	114.49
3	B	802	AQV	C11-C12-C13	2.59	119.27	114.49
3	D	802	AQV	C19-C14-C15	2.59	121.37	118.31
3	A	802	AQV	C11-C12-C13	2.60	119.28	114.49
3	C	802	AQV	C11-C12-C13	2.60	119.28	114.49
3	D	802	AQV	C1-C7-N1	2.62	107.72	105.88
3	D	802	AQV	C5-C6-C8	3.15	134.52	129.63
3	C	802	AQV	C5-C6-C8	3.16	134.53	129.63
3	B	802	AQV	C5-C6-C8	3.17	134.55	129.63
3	A	802	AQV	C5-C6-C8	3.18	134.57	129.63
3	D	802	AQV	C6-C8-N1	5.04	109.41	105.88
3	C	802	AQV	C6-C8-N1	5.06	109.43	105.88
3	B	802	AQV	C6-C8-N1	5.12	109.47	105.88
3	A	802	AQV	C6-C8-N1	5.12	109.47	105.88
3	C	802	AQV	C22-C11-N2	8.26	122.77	109.50
3	B	802	AQV	C22-C11-N2	8.28	122.80	109.50
3	A	802	AQV	C22-C11-N2	8.28	122.81	109.50
3	D	802	AQV	C22-C11-N2	8.29	122.82	109.50
3	C	802	AQV	C9-C10-N2	11.39	129.53	116.49
3	A	802	AQV	C9-C10-N2	11.41	129.55	116.49
3	B	802	AQV	C9-C10-N2	11.42	129.56	116.49
3	D	802	AQV	C9-C10-N2	11.44	129.59	116.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	HZ7	5	0
3	A	802	AQV	6	0
2	B	801	HZ7	5	0
3	B	802	AQV	6	0
2	C	801	HZ7	4	0
3	C	802	AQV	6	0
2	D	801	HZ7	4	0
3	D	802	AQV	6	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.