Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Sep 27, 2018 – 05:17 PM EDT

PDB ID	:	6E1N
EMDB ID:	:	EMD-8958
Title	:	Structure of AtTPC1(DDE) in state 1
Authors	:	Kintzer, A.F.; Green, E.M.; Cheng, Y.; Stroud, R.M.
Deposited on	:	2018-07-10
Resolution	:	3.70 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

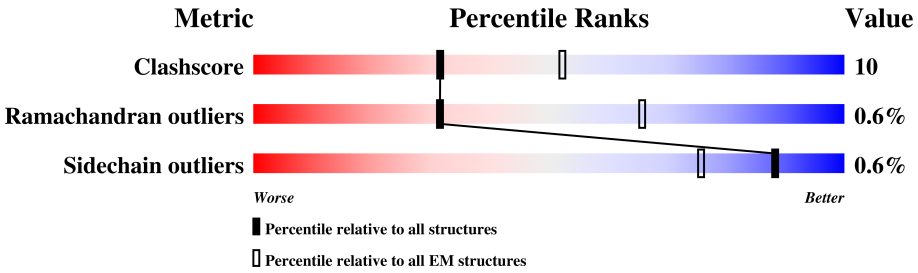
MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031172

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	727	67% 20% 12%
1	B	727	68% 19% • 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PLM	A	811	-	-	X	-
3	PLM	B	809	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10682 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 Two pore calcium channel protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	639	Total	C	N	O	P	S	0	0
			5145	3415	788	916	3	23		
1	B	639	Total	C	N	O	P	S	0	0
			5145	3415	788	916	3	23		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	initiating methionine	UNP Q94KI8
A	12	GLY	-	expression tag	UNP Q94KI8
A	13	GLY	-	expression tag	UNP Q94KI8
A	14	GLY	-	expression tag	UNP Q94KI8
A	15	GLY	-	expression tag	UNP Q94KI8
A	16	THR	-	expression tag	UNP Q94KI8
A	17	ASP	-	expression tag	UNP Q94KI8
A	18	ARG	-	expression tag	UNP Q94KI8
A	19	VAL	-	expression tag	UNP Q94KI8
A	20	ARG	-	expression tag	UNP Q94KI8
A	21	ARG	-	expression tag	UNP Q94KI8
A	23	GLU	-	expression tag	UNP Q94KI8
A	24	ALA	-	expression tag	UNP Q94KI8
A	25	ILE	-	expression tag	UNP Q94KI8
A	27	HIS	-	expression tag	UNP Q94KI8
A	28	GLY	-	expression tag	UNP Q94KI8
A	240	ASN	ASP	engineered mutation	UNP Q94KI8
A	454	ASN	ASP	engineered mutation	UNP Q94KI8
A	528	GLN	GLU	engineered mutation	UNP Q94KI8
A	734	LEU	-	expression tag	UNP Q94KI8
A	735	VAL	-	expression tag	UNP Q94KI8
A	736	PRO	-	expression tag	UNP Q94KI8
A	737	ARG	-	expression tag	UNP Q94KI8
B	11	MET	-	initiating methionine	UNP Q94KI8
B	12	GLY	-	expression tag	UNP Q94KI8
B	13	GLY	-	expression tag	UNP Q94KI8

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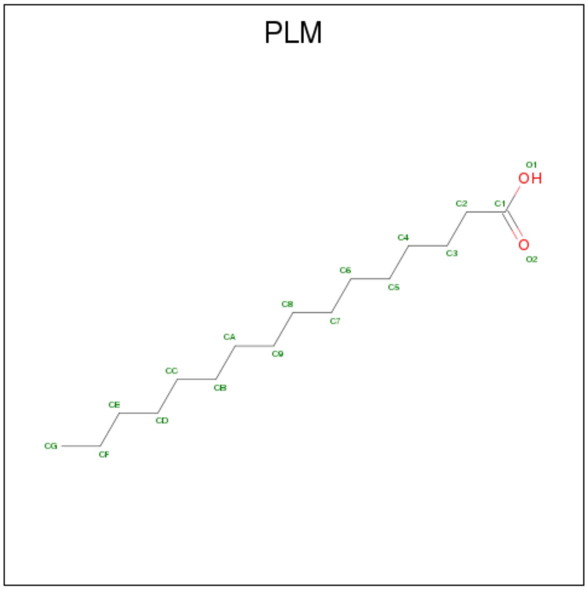
Chain	Residue	Modelled	Actual	Comment	Reference
B	14	GLY	-	expression tag	UNP Q94KI8
B	15	GLY	-	expression tag	UNP Q94KI8
B	16	THR	-	expression tag	UNP Q94KI8
B	17	ASP	-	expression tag	UNP Q94KI8
B	18	ARG	-	expression tag	UNP Q94KI8
B	19	VAL	-	expression tag	UNP Q94KI8
B	20	ARG	-	expression tag	UNP Q94KI8
B	21	ARG	-	expression tag	UNP Q94KI8
B	23	GLU	-	expression tag	UNP Q94KI8
B	24	ALA	-	expression tag	UNP Q94KI8
B	25	ILE	-	expression tag	UNP Q94KI8
B	27	HIS	-	expression tag	UNP Q94KI8
B	28	GLY	-	expression tag	UNP Q94KI8
B	240	ASN	ASP	engineered mutation	UNP Q94KI8
B	454	ASN	ASP	engineered mutation	UNP Q94KI8
B	528	GLN	GLU	engineered mutation	UNP Q94KI8
B	734	LEU	-	expression tag	UNP Q94KI8
B	735	VAL	-	expression tag	UNP Q94KI8
B	736	PRO	-	expression tag	UNP Q94KI8
B	737	ARG	-	expression tag	UNP Q94KI8

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
2	B	3	Total Ca 3 3	0
2	A	3	Total Ca 3 3	0

- Molecule 3 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total 144	C 128	O 16	0
3	A	1	Total 144	C 128	O 16	0
3	A	1	Total 144	C 128	O 16	0
3	A	1	Total 144	C 128	O 16	0
3	A	1	Total 144	C 128	O 16	0
3	A	1	Total 144	C 128	O 16	0
3	A	1	Total 144	C 128	O 16	0
3	A	1	Total 144	C 128	O 16	0
3	B	1	Total 144	C 128	O 16	0
3	B	1	Total 144	C 128	O 16	0
3	B	1	Total 144	C 128	O 16	0
3	B	1	Total 144	C 128	O 16	0
3	B	1	Total 144	C 128	O 16	0
3	B	1	Total 144	C 128	O 16	0

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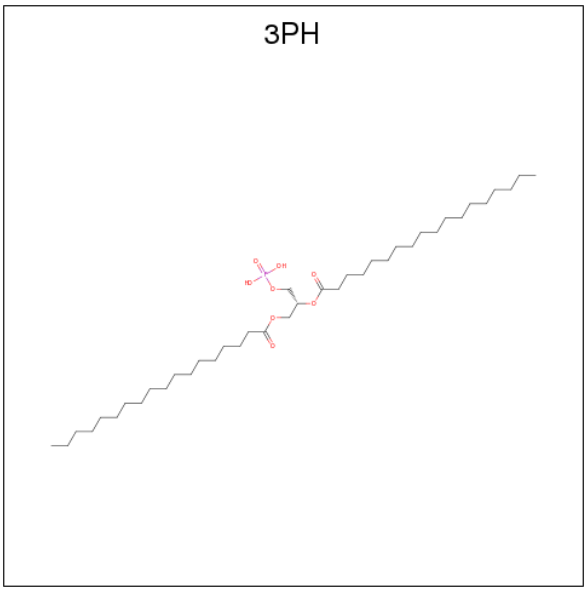
Mol	Chain	Residues	Atoms			AltConf
3	B	1	Total 144	C 128	O 16	0
3	B	1	Total 144	C 128	O 16	0

- Molecule 4 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 48	C 39	O 8	P 1	0
4	B	1	Total 48	C 39	O 8	P 1	0

- Molecule 5 is water.

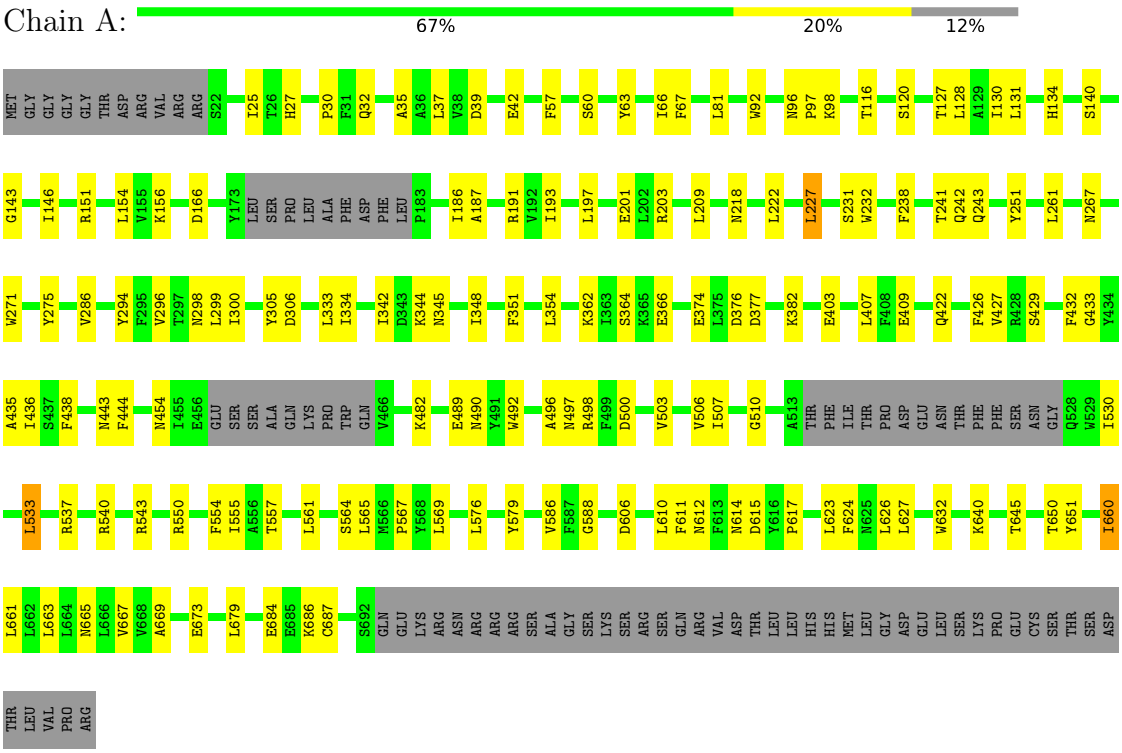
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total 1	O 1	0
5	B	1	Total 1	O 1	0

3 Residue-property plots (i)

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.

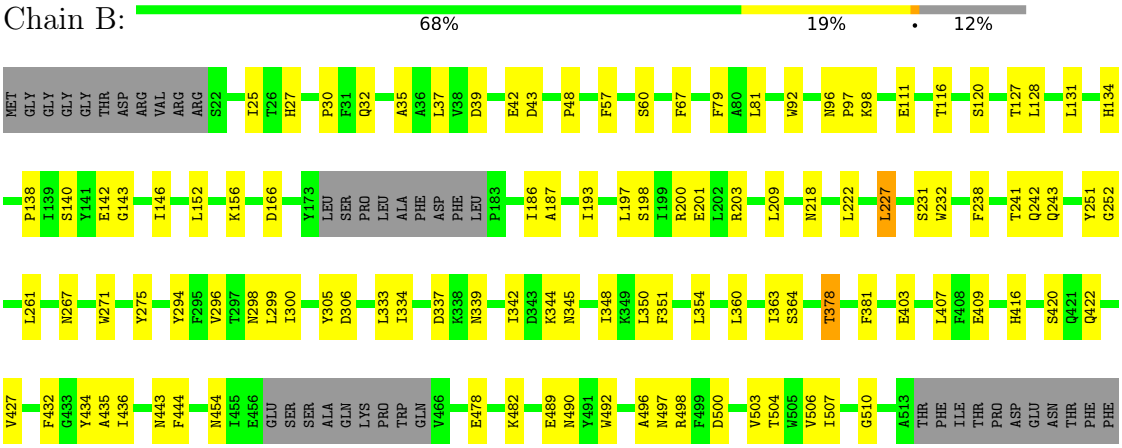
• Molecule 1: Two pore calcium channel protein 1

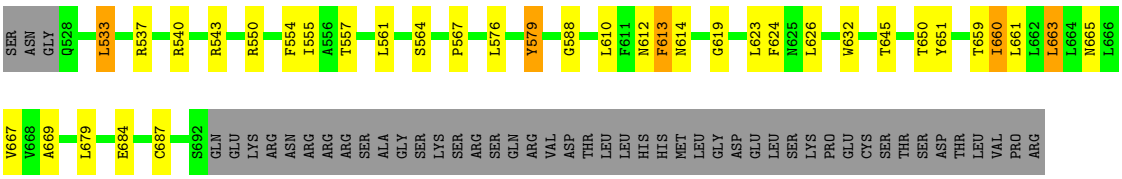
Chain A:



• Molecule 1: Two pore calcium channel protein 1

Chain B:




SER ASN GLY Q528 L533 R537 R540 R543 R550 F554 I555 A556 T557 L561 S564 P567 L576 Y579 G588 L610 F611 N612 F613 N614 G619 L623 F624 W625 L626 W632 T645 T650 Y651 T659 I660 L661 L662 L663 L664 N665 L666
V667 V668 A669 L679 E684 C687 S692 GLN GLU LYS ARG ASN ARG ARG ARG SER ALA GLY SER LYS SER ARG SER GLN ARG VAL ASP THR LEU LEU HIS HIS MET LEU GLY ASP GLU LEU SER LYS PRO GLU CYS SER THR SER ASP THR LEU VAL PRO ARG

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	44353	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	41132	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: TPO, 3PH, CA, PLM, SEP

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	0.71	1/5245 (0.0%)	0.74	6/7138 (0.1%)
1	B	0.70	2/5245 (0.0%)	0.73	6/7138 (0.1%)
All	All	0.70	3/10490 (0.0%)	0.73	12/14276 (0.1%)

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	5
1	B	0	6
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	TRP	CB-CG	-5.18	1.41	1.50
1	B	579	TYR	CD1-CE1	-5.09	1.31	1.39
1	A	92	TRP	CB-CG	-5.06	1.41	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	533	LEU	CB-CG-CD2	-5.87	101.02	111.00
1	B	663	LEU	CB-CG-CD1	-5.72	101.28	111.00
1	B	533	LEU	CB-CG-CD2	-5.67	101.36	111.00
1	B	555	ILE	CG1-CB-CG2	-5.61	99.07	111.40
1	A	555	ILE	CG1-CB-CG2	-5.60	99.08	111.40
1	B	222	LEU	CB-CG-CD2	-5.54	101.58	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	227	LEU	CB-CG-CD1	-5.47	101.70	111.00
1	A	227	LEU	CB-CG-CD1	-5.40	101.81	111.00
1	A	261	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	A	222	LEU	CB-CG-CD2	-5.28	102.03	111.00
1	A	354	LEU	CA-CB-CG	5.25	127.36	115.30
1	B	261	LEU	CB-CG-CD1	-5.22	102.13	111.00

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	ILE	Peptide
1	A	409	GLU	Peptide
1	A	611	PHE	Peptide
1	A	660	ILE	Peptide
1	A	665	ASN	Peptide
1	B	186	ILE	Peptide
1	B	378	THR	Peptide
1	B	409	GLU	Peptide
1	B	612	ASN	Peptide
1	B	660	ILE	Peptide
1	B	665	ASN	Peptide

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	5145	0	5020	98	0
1	B	5145	0	5020	93	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	144	0	237	33	0
3	B	144	0	237	31	0
4	A	48	0	70	2	0
4	B	48	0	70	5	0
5	A	1	0	0	1	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10682	0	10654	221	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 10.

All (221) 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:B:496:ALA:HB3	1:B:543:ARG:HH12	1.34	0.92
1:A:496:ALA:HB3	1:A:543:ARG:HH12	1.37	0.90
1:A:197:LEU:O	1:A:203:ARG:NH1	2.06	0.89
1:B:197:LEU:O	1:B:203:ARG:NH1	2.05	0.89
1:A:444:PHE:HA	1:A:537:ARG:HH11	1.37	0.89
1:B:444:PHE:HA	1:B:537:ARG:HH11	1.36	0.88
3:B:804:PLM:H21	3:B:808:PLM:H22	1.67	0.77
3:A:811:PLM:H21	3:B:809:PLM:H52	1.66	0.75
3:A:805:PLM:H41	3:A:810:PLM:H52	1.68	0.73
1:B:497:ASN:HA	1:B:540:ARG:HH12	1.54	0.72
3:A:804:PLM:H21	3:A:808:PLM:H22	1.71	0.72
1:B:344:LYS:NZ	1:B:364:SER:OG	2.21	0.70
3:A:809:PLM:HG2	3:B:811:PLM:HD1	1.74	0.70
1:A:134:HIS:CD2	1:A:156:LYS:HZ3	2.10	0.69
1:A:497:ASN:HA	1:A:540:ARG:HH12	1.59	0.68
1:A:667:VAL:HG11	1:B:294:TYR:HB3	1.75	0.68
1:B:650:THR:HG23	3:B:810:PLM:HE2	1.76	0.66
1:A:294:TYR:HB3	1:B:667:VAL:HG11	1.78	0.66
1:A:435:ALA:HA	1:A:438:PHE:HB2	1.77	0.65
1:A:650:THR:HG23	3:A:810:PLM:HE2	1.79	0.63
3:A:811:PLM:H41	3:B:809:PLM:C7	2.29	0.63
1:B:294:TYR:O	1:B:298:ASN:ND2	2.32	0.62
1:B:238:PHE:HB3	1:B:243:GLN:HB3	1.82	0.61
1:B:576:LEU:HD22	1:B:623:LEU:HB3	1.81	0.61
1:A:32:GLN:H	1:A:35:ALA:HB3	1.65	0.61
1:A:294:TYR:O	1:A:298:ASN:ND2	2.33	0.60
1:B:403:GLU:OE2	1:B:490:ASN:ND2	2.35	0.60
1:A:238:PHE:HB3	1:A:243:GLN:HB3	1.82	0.59
1:B:267:ASN:O	1:B:271:TRP:NE1	2.36	0.59
1:B:500:ASP:HB2	1:B:540:ARG:HH12	1.67	0.59
3:A:811:PLM:H41	3:B:809:PLM:C8	2.33	0.59
1:B:496:ALA:O	1:B:540:ARG:NH2	2.36	0.58
1:A:496:ALA:O	1:A:540:ARG:NH2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:O	1:A:231:SER:N	2.34	0.58
1:A:267:ASN:O	1:A:271:TRP:NE1	2.36	0.58
1:A:500:ASP:HB2	1:A:540:ARG:HH12	1.68	0.58
1:A:576:LEU:HD22	1:A:623:LEU:HB3	1.85	0.58
1:A:403:GLU:OE2	1:A:490:ASN:ND2	2.37	0.57
1:A:334:ILE:HG21	1:A:342:ILE:HD12	1.85	0.57
1:A:627:LEU:HD21	3:A:811:PLM:HF1	1.86	0.57
1:B:227:LEU:O	1:B:231:SER:N	2.34	0.57
1:B:496:ALA:HB3	1:B:543:ARG:NH1	2.14	0.57
3:A:804:PLM:H21	3:A:808:PLM:H52	1.87	0.56
1:A:588:GLY:O	1:A:614:ASN:ND2	2.36	0.56
1:B:360:LEU:HD23	1:B:363:ILE:HD12	1.86	0.56
1:A:201:GLU:HB3	1:A:567:PRO:HB3	1.87	0.55
1:B:334:ILE:HG21	1:B:342:ILE:HD12	1.89	0.55
1:A:612:ASN:ND2	1:A:614:ASN:OD1	2.38	0.55
1:B:588:GLY:O	1:B:614:ASN:ND2	2.38	0.55
1:B:143:GLY:H	1:B:146:ILE:HD12	1.70	0.55
1:A:496:ALA:HB3	1:A:543:ARG:NH1	2.16	0.55
1:B:500:ASP:HB2	1:B:540:ARG:NH1	2.22	0.54
1:B:201:GLU:HB3	1:B:567:PRO:HB3	1.89	0.54
1:B:152:LEU:HD11	1:B:203:ARG:HD2	1.90	0.54
1:A:362:LYS:O	1:A:366:GLU:N	2.40	0.54
1:A:624:PHE:CD1	3:A:811:PLM:HC2	2.42	0.54
1:B:351:PHE:HE2	1:B:364:SER:HB3	1.72	0.54
1:A:507:ILE:HG12	1:A:533:LEU:HD21	1.89	0.53
1:A:241:THR:OG1	1:A:242:GLN:N	2.40	0.53
1:B:32:GLN:H	1:B:35:ALA:HB3	1.73	0.53
1:A:679:LEU:HG	1:B:306:ASP:OD2	2.09	0.53
3:A:809:PLM:HG1	1:B:624:PHE:HD1	1.73	0.53
1:A:500:ASP:HB2	1:A:540:ARG:NH1	2.24	0.52
1:B:344:LYS:HZ2	1:B:364:SER:HG	1.54	0.52
1:A:586:VAL:HG11	3:A:807:PLM:H31	1.91	0.52
1:B:241:THR:OG1	1:B:242:GLN:N	2.40	0.52
1:B:345:ASN:HA	1:B:348:ILE:HB	1.91	0.52
1:A:351:PHE:HE2	1:A:364:SER:HB3	1.74	0.52
3:B:804:PLM:H21	3:B:808:PLM:H52	1.90	0.52
1:A:306:ASP:OD2	1:B:679:LEU:HG	2.09	0.52
1:B:344:LYS:O	1:B:348:ILE:N	2.43	0.52
1:B:351:PHE:HB3	1:B:360:LEU:HD13	1.92	0.52
1:A:81:LEU:HD21	1:A:127:THR:HA	1.92	0.52
3:B:804:PLM:C2	3:B:808:PLM:H22	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:809:PLM:HC2	3:B:809:PLM:H82	1.91	0.52
1:A:561:LEU:HD13	1:A:564:SER:HB2	1.91	0.51
1:A:557:THR:HG21	1:B:299:LEU:HD21	1.92	0.51
3:A:805:PLM:H72	3:A:810:PLM:H72	1.91	0.51
1:B:443:ASN:O	1:B:537:ARG:NH1	2.44	0.51
1:B:561:LEU:HD13	1:B:564:SER:HB2	1.91	0.51
1:A:166:ASP:OD2	1:A:187:ALA:HB2	2.10	0.51
1:A:345:ASN:HA	1:A:348:ILE:HB	1.93	0.51
1:B:81:LEU:HD21	1:B:127:THR:HA	1.93	0.51
1:A:443:ASN:O	1:A:537:ARG:NH1	2.44	0.50
3:B:805:PLM:H41	3:B:810:PLM:H52	1.93	0.50
1:A:344:LYS:O	1:A:348:ILE:N	2.41	0.50
1:B:296:VAL:O	1:B:300:ILE:N	2.42	0.50
3:A:811:PLM:H32	3:B:809:PLM:H61	1.93	0.50
1:A:299:LEU:HD21	1:B:557:THR:HG21	1.93	0.50
1:A:299:LEU:HB3	1:B:554:PHE:CE1	2.48	0.49
1:A:624:PHE:HD1	3:A:811:PLM:HC2	1.78	0.49
1:B:166:ASP:OD2	1:B:187:ALA:HB2	2.13	0.49
1:B:39:ASP:HA	1:B:42:GLU:HB3	1.94	0.49
1:A:209:LEU:HD22	1:A:661:LEU:HD21	1.94	0.49
3:A:805:PLM:HB1	3:A:805:PLM:HE2	1.62	0.49
1:B:337:ASP:OD2	1:B:339:ASN:ND2	2.45	0.49
1:B:209:LEU:HD22	1:B:661:LEU:HD21	1.95	0.48
1:B:334:ILE:HD13	1:B:342:ILE:HD12	1.94	0.48
1:A:128:LEU:HD23	1:A:131:LEU:HD12	1.95	0.48
1:B:232:TRP:HA	1:B:251:TYR:HE1	1.78	0.48
1:A:626:LEU:HD23	1:A:632:TRP:HB2	1.95	0.48
1:A:116:THR:O	1:A:120:SER:N	2.47	0.48
3:A:809:PLM:H21	1:B:111:GLU:HB3	1.96	0.48
3:A:804:PLM:C2	3:A:808:PLM:H22	2.40	0.48
1:B:128:LEU:HD23	1:B:131:LEU:HD12	1.96	0.48
1:A:241:THR:HG23	1:A:243:GLN:H	1.78	0.48
1:B:193:ILE:HD11	3:B:806:PLM:HG3	1.95	0.48
1:A:554:PHE:CE1	1:B:299:LEU:HB3	2.49	0.48
1:B:436:ILE:HG21	1:B:482:LYS:HD3	1.96	0.48
1:B:116:THR:O	1:B:120:SER:N	2.46	0.47
1:B:37:LEU:HD13	1:B:333:LEU:HB3	1.96	0.47
1:A:232:TRP:HA	1:A:251:TYR:HE1	1.79	0.47
1:B:138:PRO:O	1:B:142:GLU:N	2.47	0.47
1:A:344:LYS:NZ	1:A:364:SER:OG	2.41	0.47
1:A:296:VAL:O	1:A:300:ILE:N	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:THR:HG23	1:B:243:GLN:H	1.79	0.47
3:B:806:PLM:HA1	3:B:806:PLM:H72	1.59	0.47
3:A:807:PLM:H52	3:A:807:PLM:H81	1.35	0.47
1:A:96:ASN:OD1	1:A:96:ASN:N	2.45	0.47
1:A:376:ASP:H	1:A:382:LYS:HE2	1.80	0.47
1:A:97:PRO:HG2	1:A:98:LYS:HD3	1.97	0.47
1:B:626:LEU:HD23	1:B:632:TRP:HB2	1.96	0.47
1:A:57:PHE:HB2	1:A:60:SER:HA	1.98	0.47
1:A:334:ILE:HD13	1:A:342:ILE:HD12	1.97	0.46
1:B:613:PHE:HB3	1:B:619:GLY:HA3	1.95	0.46
1:A:193:ILE:HD11	3:A:806:PLM:HG3	1.97	0.46
3:A:805:PLM:H41	3:A:810:PLM:C5	2.40	0.46
3:A:811:PLM:H41	3:B:809:PLM:C6	2.45	0.46
1:A:377:ASP:H	1:A:382:LYS:HD3	1.80	0.46
1:B:350:LEU:O	1:B:354:LEU:N	2.49	0.46
1:B:684:GLU:HA	1:B:687:CYS:HB2	1.97	0.46
1:A:37:LEU:HD13	1:A:333:LEU:HB3	1.97	0.46
3:B:804:PLM:H42	3:B:805:PLM:H42	1.97	0.46
1:A:550:ARG:HH11	1:B:218:ASN:ND2	2.13	0.46
1:B:57:PHE:HB2	1:B:60:SER:HA	1.97	0.46
1:A:426:PHE:O	1:A:429:SER:OG	2.31	0.46
1:A:606:ASP:OD2	5:A:901:HOH:O	2.20	0.46
1:A:684:GLU:HA	1:A:687:CYS:HB2	1.98	0.46
1:B:252:GLY:HA3	3:B:805:PLM:H51	1.99	0.45
1:A:39:ASP:HA	1:A:42:GLU:HB3	1.98	0.45
1:B:507:ILE:HG12	1:B:533:LEU:HD21	1.98	0.45
1:A:151:ARG:HA	1:A:154:LEU:HD12	1.98	0.45
3:B:805:PLM:H72	3:B:805:PLM:H41	1.64	0.45
3:B:811:PLM:HA1	3:B:811:PLM:H72	1.74	0.45
1:A:143:GLY:H	1:A:146:ILE:HD12	1.82	0.45
1:A:530:ILE:HA	1:A:533:LEU:HB3	1.98	0.45
3:B:811:PLM:CC	4:B:812:3PH:H2D2	2.47	0.45
1:A:218:ASN:ND2	1:B:550:ARG:HH11	2.15	0.44
1:A:374:GLU:HG2	1:A:376:ASP:H	1.81	0.44
1:B:200:ARG:H	4:B:812:3PH:H332	1.83	0.44
1:B:96:ASN:N	1:B:96:ASN:OD1	2.44	0.44
3:A:805:PLM:H82	3:A:805:PLM:H51	1.56	0.44
1:B:134:HIS:CD2	1:B:156:LYS:NZ	2.86	0.44
1:A:436:ILE:HD13	1:A:482:LYS:HD3	2.00	0.44
3:A:811:PLM:H21	3:B:809:PLM:C5	2.43	0.44
1:A:436:ILE:HG21	1:A:482:LYS:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:VAL:HG12	1:B:507:ILE:HD11	2.00	0.44
4:A:812:3PH:H361	4:A:812:3PH:H332	1.59	0.43
3:B:804:PLM:H21	3:B:808:PLM:C5	2.48	0.43
1:B:97:PRO:HG2	1:B:98:LYS:HD3	2.00	0.43
1:B:497:ASN:HA	1:B:540:ARG:NH1	2.27	0.43
1:B:67:PHE:HD2	1:B:140:SER:HB3	1.83	0.43
1:A:645:THR:OG1	3:A:810:PLM:O1	2.36	0.43
1:B:416:HIS:O	1:B:420:SER:N	2.51	0.43
1:B:478:GLU:O	1:B:482:LYS:NZ	2.52	0.43
3:B:809:PLM:HF1	3:B:809:PLM:HB2	1.99	0.43
1:A:275:TYR:HE2	1:B:610:LEU:HB3	1.84	0.43
3:B:806:PLM:H81	3:B:806:PLM:H51	1.83	0.43
1:A:579:TYR:O	1:A:651:TYR:OH	2.32	0.43
1:B:43:ASP:HA	1:B:48:PRO:HD2	1.99	0.43
1:A:561:LEU:HA	1:A:564:SER:HB2	2.01	0.43
1:B:663:LEU:HA	1:B:663:LEU:HD23	1.80	0.43
1:A:503:VAL:HG12	1:A:507:ILE:HD11	2.01	0.42
1:A:615:ASP:HB3	1:A:617:PRO:HD2	2.01	0.42
3:A:811:PLM:C2	3:B:809:PLM:H41	2.48	0.42
1:A:286:VAL:HG21	3:A:809:PLM:HB2	2.01	0.42
1:B:305:TYR:HD1	1:B:669:ALA:HB1	1.84	0.42
1:A:663:LEU:HD23	1:A:663:LEU:HA	1.79	0.42
1:B:506:VAL:O	1:B:510:GLY:N	2.44	0.42
1:A:565:LEU:HA	1:A:565:LEU:HD23	1.81	0.42
1:B:432:PHE:HA	1:B:435:ALA:HB3	1.99	0.42
3:B:808:PLM:HC1	3:B:808:PLM:HF1	1.82	0.42
1:B:427:VAL:HA	1:B:432:PHE:CD2	2.55	0.42
3:B:805:PLM:H41	3:B:810:PLM:C5	2.50	0.42
1:A:489:GLU:HA	1:A:492:TRP:HB2	2.00	0.42
1:A:63:TYR:HA	1:A:66:ILE:HD12	2.00	0.42
1:B:492:TRP:CE3	1:B:498:ARG:HG3	2.55	0.42
3:A:806:PLM:HA1	3:A:806:PLM:H72	1.52	0.42
1:A:427:VAL:HA	1:A:432:PHE:CD2	2.54	0.42
1:A:492:TRP:CE3	1:A:498:ARG:HG3	2.55	0.42
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.87	0.42
1:B:504:THR:HA	1:B:507:ILE:HD12	2.02	0.42
1:B:79:PHE:HD2	4:B:812:3PH:H381	1.72	0.42
1:B:378:THR:OG1	1:B:381:PHE:O	2.38	0.41
1:B:489:GLU:HA	1:B:492:TRP:HB2	2.01	0.41
1:A:610:LEU:HB3	1:B:275:TYR:HE2	1.85	0.41
3:A:804:PLM:H21	3:A:808:PLM:C5	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:645:THR:OG1	3:B:810:PLM:O1	2.38	0.41
3:B:811:PLM:H51	4:B:812:3PH:C3I	2.50	0.41
3:B:811:PLM:HC1	4:B:812:3PH:H2D2	2.02	0.41
3:A:808:PLM:HC1	3:A:808:PLM:HF1	1.80	0.41
1:A:686:LYS:HD2	1:A:686:LYS:HA	1.81	0.41
1:A:81:LEU:HG	1:A:130:ILE:HB	2.02	0.41
1:B:561:LEU:HA	1:B:564:SER:HB2	2.01	0.41
1:A:67:PHE:HD2	1:A:140:SER:HB3	1.85	0.41
3:A:811:PLM:C1	3:B:809:PLM:H41	2.50	0.41
1:A:187:ALA:CB	1:A:191:ARG:HH11	2.34	0.41
1:A:506:VAL:O	1:A:510:GLY:N	2.44	0.41
1:B:660:ILE:HG23	1:B:660:ILE:HD12	1.82	0.41
4:A:812:3PH:H271	4:A:812:3PH:H241	1.96	0.40
1:A:640:LYS:HE3	1:A:640:LYS:HB3	1.92	0.40
1:A:305:TYR:HE1	1:A:673:GLU:HG2	1.85	0.40
1:B:156:LYS:NZ	1:B:198:SER:OG	2.54	0.40
1:A:433:GLY:HA2	1:A:436:ILE:HD12	2.03	0.40
1:A:305:TYR:HD1	1:A:669:ALA:HB1	1.86	0.40
3:A:805:PLM:HD2	3:A:810:PLM:HC1	2.03	0.40
1:A:569:LEU:HA	1:A:569:LEU:HD23	1.93	0.40
1:A:660:ILE:HD12	1:A:660:ILE:HG23	1.81	0.40
1:B:579:TYR:O	1:B:651:TYR:OH	2.33	0.40
1:B:659:THR:O	1:B:663:LEU:N	2.40	0.40
3:A:811:PLM:H52	3:B:809:PLM:H81	2.03	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	629/727 (86%)	575 (91%)	50 (8%)	4 (1%)	27 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	629/727 (86%)	572 (91%)	53 (8%)	4 (1%)	27 68
All	All	1258/1454 (86%)	1147 (91%)	103 (8%)	8 (1%)	31 68

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	B	30	PRO
1	A	407	LEU
1	A	27	HIS
1	B	27	HIS
1	B	407	LEU
1	A	25	ILE
1	B	25	ILE

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	537/648 (83%)	535 (100%)	2 (0%)	92 97
1	B	537/648 (83%)	533 (99%)	4 (1%)	85 93
All	All	1074/1296 (83%)	1068 (99%)	6 (1%)	88 94

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	422	GLN
1	A	454	ASN
1	B	422	GLN
1	B	434	TYR
1	B	454	ASN
1	B	613	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	HIS
1	A	218	ASN
1	A	257	GLN
1	A	454	ASN
1	A	618	ASN
1	B	218	ASN
1	B	257	GLN
1	B	454	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)

6 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	SEP	A	22	1	9,9,10	1.63	2 (22%)	9,12,14	1.57	1 (11%)
1	TPO	A	26	1	9,10,11	1.47	1 (11%)	11,14,16	1.81	1 (9%)
1	TPO	A	29	1	9,10,11	1.50	1 (11%)	11,14,16	1.80	2 (18%)
1	SEP	B	22	1	9,9,10	1.61	2 (22%)	9,12,14	1.48	1 (11%)
1	TPO	B	26	1	9,10,11	1.47	1 (11%)	11,14,16	1.85	1 (9%)
1	TPO	B	29	1	9,10,11	1.45	1 (11%)	11,14,16	1.79	2 (18%)

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
1	SEP	A	22	1	-	0/5/8/10	0/0/0/0
1	TPO	A	26	1	-	0/8/11/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	29	1	-	0/8/11/13	0/0/0/0
1	SEP	B	22	1	-	0/5/8/10	0/0/0/0
1	TPO	B	26	1	-	0/8/11/13	0/0/0/0
1	TPO	B	29	1	-	0/8/11/13	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	22	SEP	CA-C	2.35	1.53	1.50
1	A	22	SEP	CA-C	2.46	1.53	1.50
1	A	26	TPO	P-O1P	3.08	1.61	1.50
1	B	26	TPO	P-O1P	3.10	1.61	1.50
1	A	22	SEP	P-O1P	3.21	1.61	1.50
1	B	22	SEP	P-O1P	3.21	1.61	1.50
1	B	29	TPO	CA-C	3.26	1.54	1.50
1	A	29	TPO	CA-C	3.46	1.54	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	26	TPO	P-OG1-CB	-5.41	106.87	123.21
1	A	26	TPO	P-OG1-CB	-5.34	107.07	123.21
1	B	29	TPO	P-OG1-CB	-4.78	108.76	123.21
1	A	29	TPO	P-OG1-CB	-4.72	108.96	123.21
1	A	29	TPO	O-C-CA	-2.88	118.39	125.09
1	B	29	TPO	O-C-CA	-2.84	118.47	125.09
1	B	22	SEP	OG-CB-CA	2.99	111.11	108.17
1	A	22	SEP	OG-CB-CA	3.39	111.51	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 for Mogul analysis.

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	PLM	A	804	-	14,17,17	0.20	0	13,17,17	0.35	0
3	PLM	A	805	-	14,17,17	0.21	0	13,17,17	0.40	0
3	PLM	A	806	-	14,17,17	0.19	0	13,17,17	0.49	0
3	PLM	A	807	-	14,17,17	0.20	0	13,17,17	0.60	0
3	PLM	A	808	-	14,17,17	0.25	0	13,17,17	0.39	0
3	PLM	A	809	1,3	14,17,17	0.14	0	13,17,17	0.90	1 (7%)
3	PLM	A	810	1	14,17,17	0.25	0	13,17,17	0.38	0
3	PLM	A	811	1,3	14,17,17	0.24	0	13,17,17	0.33	0
4	3PH	A	812	1	47,47,47	0.92	1 (2%)	51,52,52	1.04	2 (3%)
3	PLM	B	804	-	14,17,17	0.22	0	13,17,17	0.31	0
3	PLM	B	805	-	14,17,17	0.23	0	13,17,17	0.31	0
3	PLM	B	806	-	14,17,17	0.21	0	13,17,17	0.40	0
3	PLM	B	807	-	14,17,17	0.21	0	13,17,17	0.58	0
3	PLM	B	808	-	14,17,17	0.25	0	13,17,17	0.38	0
3	PLM	B	809	1,3	14,17,17	0.28	0	13,17,17	0.48	0
3	PLM	B	810	1	14,17,17	0.24	0	13,17,17	0.40	0
3	PLM	B	811	1,3	14,17,17	0.39	0	13,17,17	0.30	0
4	3PH	B	812	1	47,47,47	0.91	1 (2%)	51,52,52	1.02	2 (3%)

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	PLM	A	804	-	-	0/13/15/15	0/0/0/0
3	PLM	A	805	-	-	0/13/15/15	0/0/0/0
3	PLM	A	806	-	-	0/13/15/15	0/0/0/0
3	PLM	A	807	-	-	0/13/15/15	0/0/0/0
3	PLM	A	808	-	-	0/13/15/15	0/0/0/0
3	PLM	A	809	1,3	-	0/13/15/15	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLM	A	810	1	-	0/13/15/15	0/0/0/0
3	PLM	A	811	1,3	-	0/13/15/15	0/0/0/0
4	3PH	A	812	1	-	1/49/49/49	0/0/0/0
3	PLM	B	804	-	-	0/13/15/15	0/0/0/0
3	PLM	B	805	-	-	0/13/15/15	0/0/0/0
3	PLM	B	806	-	-	0/13/15/15	0/0/0/0
3	PLM	B	807	-	-	0/13/15/15	0/0/0/0
3	PLM	B	808	-	-	0/13/15/15	0/0/0/0
3	PLM	B	809	1,3	-	0/13/15/15	0/0/0/0
3	PLM	B	810	1	-	0/13/15/15	0/0/0/0
3	PLM	B	811	1,3	-	0/13/15/15	0/0/0/0
4	3PH	B	812	1	-	0/49/49/49	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	812	3PH	O31-C31	2.60	1.40	1.33
4	A	812	3PH	O31-C31	2.78	1.41	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	809	PLM	CE-CD-CC	-2.01	103.52	114.41
4	B	812	3PH	O31-C31-C32	3.25	121.31	111.92
4	A	812	3PH	O31-C31-C32	3.39	121.72	111.92
4	A	812	3PH	O21-C21-C22	4.17	120.34	111.55
4	B	812	3PH	O21-C21-C22	4.19	120.39	111.55

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	812	3PH	C2-O21-C21-C22

There are no ring outliers.

17 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	PLM	4	0
3	A	805	PLM	6	0
3	A	806	PLM	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	807	PLM	2	0
3	A	808	PLM	5	0
3	A	809	PLM	4	0
3	A	810	PLM	6	0
3	A	811	PLM	12	0
4	A	812	3PH	2	0
3	B	804	PLM	5	0
3	B	805	PLM	5	0
3	B	806	PLM	3	0
3	B	808	PLM	5	0
3	B	809	PLM	11	0
3	B	810	PLM	4	0
3	B	811	PLM	5	0
4	B	812	3PH	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.