



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 21, 2018 – 04:00 pm GMT

PDB ID : 5W3S
EMDB ID: : EMD-8764
Title : Cryo-electron microscopy structure of a TRPML3 ion channel
Authors : Hirschi, M.; Herzik, M.A.; Wie, J.; Suo, Y.; Borschel, W.F.; Ren, D.; Lander, G.C.; Lee, S.Y.
Deposited on : 2017-06-08
Resolution : 2.94 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 ⓘ 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) : trunk30686

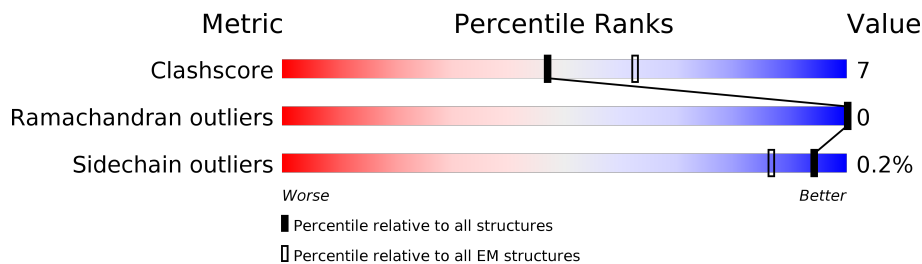
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.94 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	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	561	<div> <div>75%</div> <div>11%</div> <div>14%</div> </div>
1	B	561	<div> <div>75%</div> <div>11%</div> <div>14%</div> </div>
1	C	561	<div> <div>75%</div> <div>11%</div> <div>14%</div> </div>
1	D	561	<div> <div>75%</div> <div>12%</div> <div>14%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31486 atoms, of which 15288 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-3 isoform 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	485	Total	C	H	N	O	S	0	0
			7749	2574	3822	627	696	30		
1	B	485	Total	C	H	N	O	S	0	0
			7749	2574	3822	627	696	30		
1	C	485	Total	C	H	N	O	S	0	0
			7749	2574	3822	627	696	30		
1	D	485	Total	C	H	N	O	S	0	0
			7749	2574	3822	627	696	30		

There are 36 discrepancies between the modelled and reference sequences:

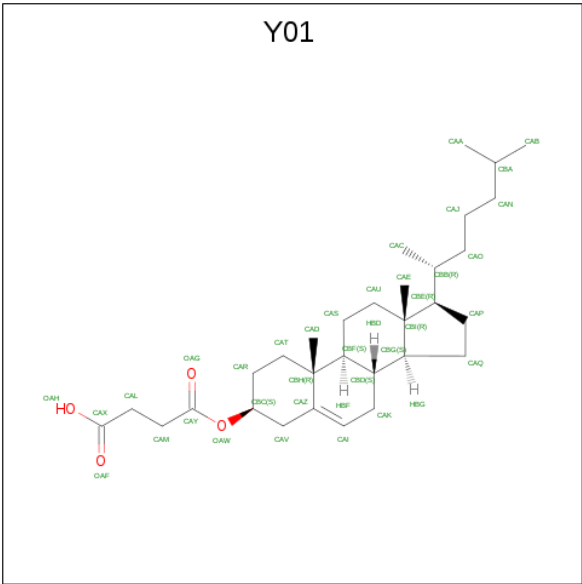
Chain	Residue	Modelled	Actual	Comment	Reference
A	138	GLN	ASN	engineered mutation	UNP F6RG56
A	554	SER	-	expression tag	UNP F6RG56
A	555	ASN	-	expression tag	UNP F6RG56
A	556	LEU	-	expression tag	UNP F6RG56
A	557	GLU	-	expression tag	UNP F6RG56
A	558	VAL	-	expression tag	UNP F6RG56
A	559	LEU	-	expression tag	UNP F6RG56
A	560	PHE	-	expression tag	UNP F6RG56
A	561	GLN	-	expression tag	UNP F6RG56
B	138	GLN	ASN	engineered mutation	UNP F6RG56
B	554	SER	-	expression tag	UNP F6RG56
B	555	ASN	-	expression tag	UNP F6RG56
B	556	LEU	-	expression tag	UNP F6RG56
B	557	GLU	-	expression tag	UNP F6RG56
B	558	VAL	-	expression tag	UNP F6RG56
B	559	LEU	-	expression tag	UNP F6RG56
B	560	PHE	-	expression tag	UNP F6RG56
B	561	GLN	-	expression tag	UNP F6RG56
C	138	GLN	ASN	engineered mutation	UNP F6RG56
C	554	SER	-	expression tag	UNP F6RG56
C	555	ASN	-	expression tag	UNP F6RG56
C	556	LEU	-	expression tag	UNP F6RG56

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Chain	Residue	Modelled	Actual	Comment	Reference
C	557	GLU	-	expression tag	UNP F6RG56
C	558	VAL	-	expression tag	UNP F6RG56
C	559	LEU	-	expression tag	UNP F6RG56
C	560	PHE	-	expression tag	UNP F6RG56
C	561	GLN	-	expression tag	UNP F6RG56
D	138	GLN	ASN	engineered mutation	UNP F6RG56
D	554	SER	-	expression tag	UNP F6RG56
D	555	ASN	-	expression tag	UNP F6RG56
D	556	LEU	-	expression tag	UNP F6RG56
D	557	GLU	-	expression tag	UNP F6RG56
D	558	VAL	-	expression tag	UNP F6RG56
D	559	LEU	-	expression tag	UNP F6RG56
D	560	PHE	-	expression tag	UNP F6RG56
D	561	GLN	-	expression tag	UNP F6RG56

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C₃₁H₅₀O₄).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			102	92	10	
2	A	1	Total	C	O	0
			102	92	10	
2	A	1	Total	C	O	0
			102	92	10	
2	B	1	Total	C	O	0
			102	92	10	

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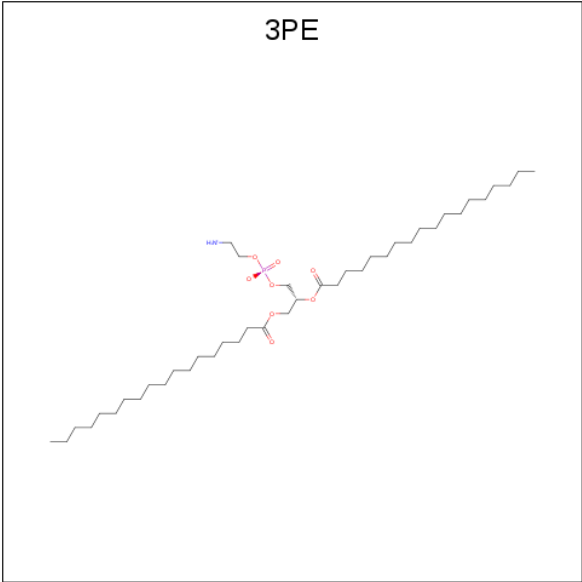
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Mol	Chain	Residues	Atoms			AltConf
2	B	1	Total	C	O	0
			102	92	10	
2	B	1	Total	C	O	0
			102	92	10	
2	C	1	Total	C	O	0
			102	92	10	
2	C	1	Total	C	O	0
			102	92	10	
2	C	1	Total	C	O	0
			102	92	10	
2	D	1	Total	C	O	0
			102	92	10	
2	D	1	Total	C	O	0
			102	92	10	
2	D	1	Total	C	O	0
			102	92	10	

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Na	0
			2	2	
3	D	1	Total	Na	0
			1	1	
3	C	3	Total	Na	0
			3	3	

- Molecule 4 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	C	0
			18	18	
4	B	1	Total	C	0
			18	18	
4	C	1	Total	C	0
			18	18	
4	D	1	Total	C	0
			18	18	

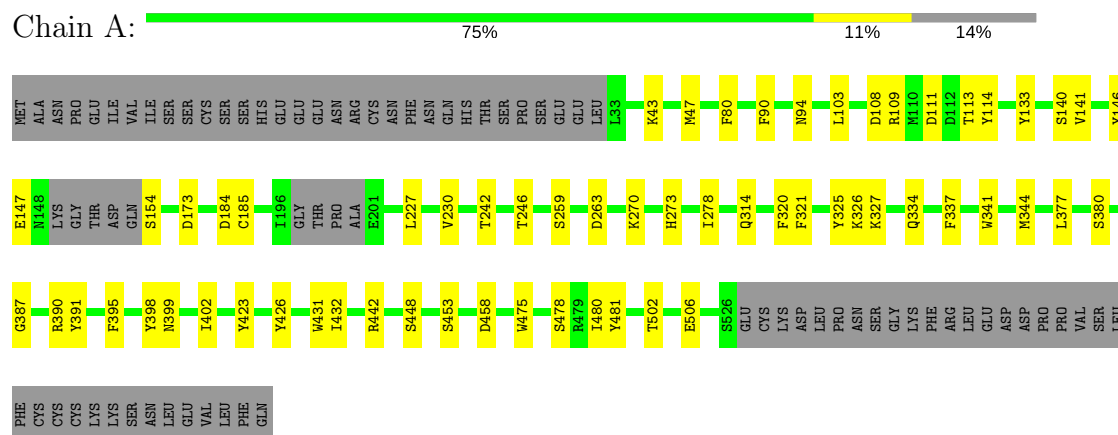
- Molecule 5 is water.

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

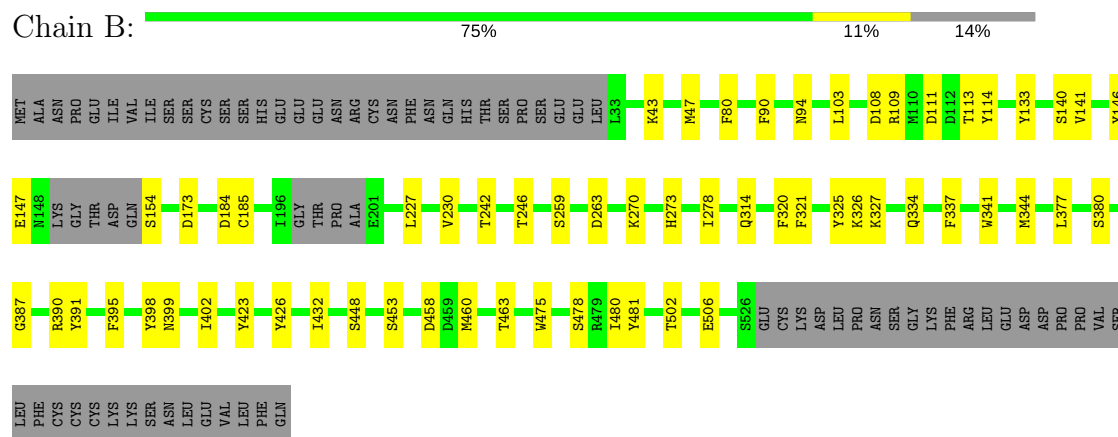
3 Residue-property plots

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.

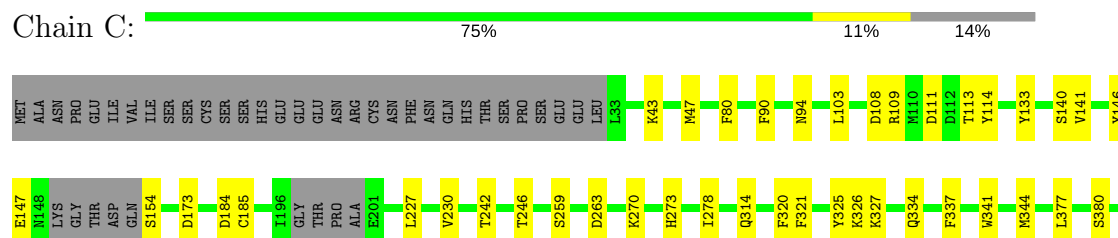
• Molecule 1: Mucolipin-3 isoform 1

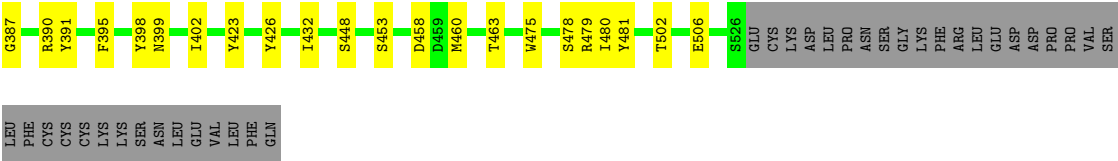


• Molecule 1: Mucolipin-3 isoform 1

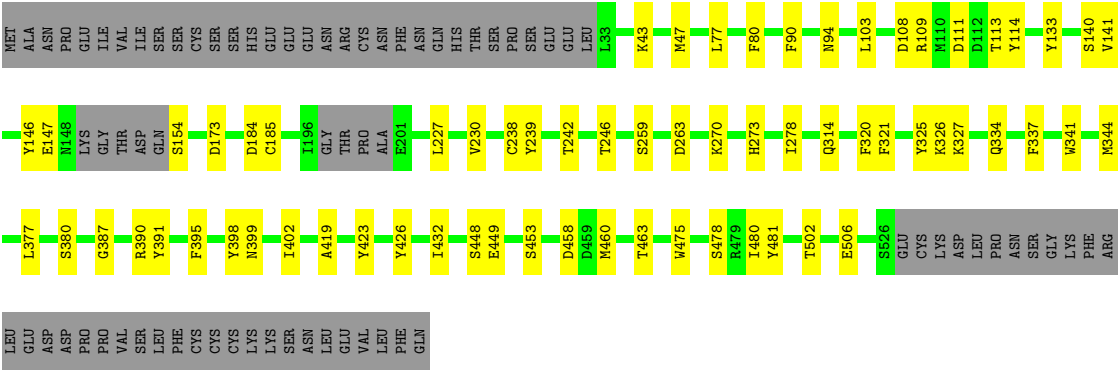


• Molecule 1: Mucolipin-3 isoform 1





● Molecule 1: Mucolipin-3 isoform 1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	104084	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 ($e^-/\text{\AA}^2$)	63	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, Y01, 3PE

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	0.35	0/4018	0.54	0/5441
1	B	0.35	0/4018	0.54	0/5441
1	C	0.35	0/4018	0.54	0/5441
1	D	0.35	0/4018	0.54	0/5441
All	All	0.35	0/16072	0.54	0/21764

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	3927	3822	3904	54	0
1	B	3927	3822	3904	55	0
1	C	3927	3822	3904	55	0
1	D	3927	3822	3904	58	0
2	A	102	0	145	16	0
2	B	102	0	145	15	0
2	C	102	0	145	18	0
2	D	102	0	145	18	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3	0	0	0	0
3	D	1	0	0	0	0
4	A	18	0	35	0	0
4	B	18	0	35	0	0
4	C	18	0	35	0	0
4	D	18	0	35	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	16198	15288	16336	229	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (229) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:LYS:O	1:C:47:MET:HG3	1.77	0.85
1:C:341:TRP:CE3	1:C:344:MET:HE2	2.12	0.84
1:D:43:LYS:O	1:D:47:MET:HG3	1.77	0.84
1:A:43:LYS:O	1:A:47:MET:HG3	1.77	0.84
1:C:391:TYR:O	2:C:602:Y01:HAR1	1.77	0.83
1:B:43:LYS:O	1:B:47:MET:HG3	1.77	0.83
1:A:341:TRP:CE3	1:A:344:MET:HE2	2.15	0.81
1:A:80:PHE:CD2	1:B:432:ILE:HD11	2.17	0.80
1:B:314:GLN:HE21	1:B:337:PHE:HB2	1.48	0.79
1:D:341:TRP:CE3	1:D:344:MET:HE2	2.17	0.79
1:A:314:GLN:HE21	1:A:337:PHE:HB2	1.48	0.79
1:B:80:PHE:CD2	1:D:432:ILE:HD11	2.17	0.79
1:D:314:GLN:HE21	1:D:337:PHE:HB2	1.48	0.78
1:B:341:TRP:CE3	1:B:344:MET:HE2	2.20	0.77
1:C:314:GLN:HE21	1:C:337:PHE:HB2	1.48	0.77
1:D:242:THR:OG1	1:D:263:ASP:O	2.05	0.75
1:D:391:TYR:O	2:D:604:Y01:HAR1	1.87	0.74
1:A:432:ILE:HD11	1:C:80:PHE:CD2	2.23	0.74
1:C:242:THR:OG1	1:C:263:ASP:O	2.05	0.74
2:A:606:Y01:HBA	2:C:606:Y01:HAC2	1.70	0.73
2:B:602:Y01:HAC2	2:D:602:Y01:HBA	1.70	0.72
1:B:341:TRP:CE3	1:B:344:MET:CE	2.74	0.70
1:B:391:TYR:O	2:B:604:Y01:HAR1	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:TRP:CE3	1:D:344:MET:CE	2.74	0.70
1:C:341:TRP:CE3	1:C:344:MET:CE	2.74	0.70
1:A:341:TRP:CE3	1:A:344:MET:CE	2.74	0.70
1:C:341:TRP:HE3	1:C:344:MET:HE2	1.57	0.69
1:A:242:THR:OG1	1:A:263:ASP:O	2.05	0.69
2:A:601:Y01:HAC2	2:B:601:Y01:HBA	1.75	0.69
2:C:607:Y01:HBA	2:D:605:Y01:HAC2	1.75	0.69
1:A:391:TYR:O	2:A:605:Y01:HAR1	1.93	0.68
1:A:80:PHE:HD2	1:B:432:ILE:HD11	1.59	0.68
1:B:242:THR:OG1	1:B:263:ASP:O	2.05	0.67
1:D:475:TRP:O	1:D:478:SER:OG	2.12	0.67
1:B:426:TYR:O	1:B:481:TYR:OH	2.12	0.66
1:B:80:PHE:HD2	1:D:432:ILE:HD11	1.61	0.66
1:C:387:GLY:O	1:C:390:ARG:HB3	1.96	0.65
1:B:387:GLY:O	1:B:390:ARG:HB3	1.96	0.65
1:C:432:ILE:HD11	1:D:80:PHE:CD2	2.31	0.65
1:B:475:TRP:O	1:B:478:SER:OG	2.12	0.65
1:A:387:GLY:O	1:A:390:ARG:HB3	1.96	0.65
1:A:426:TYR:O	1:A:481:TYR:OH	2.12	0.65
1:B:80:PHE:CE2	1:D:432:ILE:HD11	2.32	0.64
1:D:387:GLY:O	1:D:390:ARG:HB3	1.96	0.64
1:A:475:TRP:O	1:A:478:SER:OG	2.12	0.64
1:D:426:TYR:O	1:D:481:TYR:OH	2.12	0.64
1:C:133:TYR:O	1:C:146:TYR:OH	2.16	0.64
1:B:133:TYR:O	1:B:146:TYR:OH	2.16	0.64
1:B:341:TRP:HE3	1:B:344:MET:HE2	1.61	0.63
1:A:341:TRP:HE3	1:A:344:MET:CE	2.12	0.63
1:A:326:LYS:O	1:A:326:LYS:HG2	1.99	0.63
1:C:341:TRP:HE3	1:C:344:MET:CE	2.12	0.63
1:A:80:PHE:CE2	1:B:432:ILE:HD11	2.34	0.63
1:B:341:TRP:HE3	1:B:344:MET:CE	2.12	0.62
1:B:326:LYS:O	1:B:326:LYS:HG2	1.99	0.62
1:C:326:LYS:O	1:C:326:LYS:HG2	1.99	0.62
1:D:341:TRP:HE3	1:D:344:MET:HE2	1.60	0.62
1:A:133:TYR:O	1:A:146:TYR:OH	2.16	0.62
1:D:133:TYR:O	1:D:146:TYR:OH	2.16	0.62
1:D:341:TRP:HE3	1:D:344:MET:CE	2.12	0.62
1:D:326:LYS:O	1:D:326:LYS:HG2	1.99	0.62
1:A:432:ILE:HD11	1:C:80:PHE:HD2	1.64	0.61
1:A:341:TRP:HE3	1:A:344:MET:HE2	1.59	0.61
1:C:426:TYR:O	1:C:481:TYR:OH	2.12	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:TRP:O	1:C:478:SER:OG	2.12	0.60
1:C:453:SER:HB3	1:C:458:ASP:HB3	1.85	0.59
1:C:432:ILE:HD11	1:D:80:PHE:HD2	1.68	0.59
1:A:453:SER:HB3	1:A:458:ASP:HB3	1.85	0.59
1:C:480:ILE:HG23	2:C:607:Y01:HAC1	1.84	0.59
1:D:453:SER:HB3	1:D:458:ASP:HB3	1.85	0.59
1:B:453:SER:HB3	1:B:458:ASP:HB3	1.85	0.59
1:B:341:TRP:CZ3	1:B:344:MET:HE1	2.39	0.58
1:B:423:TYR:OH	1:B:448:SER:O	2.22	0.57
1:A:227:LEU:O	1:A:230:VAL:HG22	2.04	0.57
1:C:246:THR:OG1	1:C:259:SER:OG	2.22	0.57
1:A:246:THR:OG1	1:A:259:SER:OG	2.22	0.57
1:D:475:TRP:HZ3	2:D:602:Y01:HAL2	1.69	0.57
1:C:423:TYR:CE2	2:C:606:Y01:HAE2	2.39	0.57
1:A:432:ILE:HD11	1:C:80:PHE:CE2	2.39	0.57
1:D:227:LEU:O	1:D:230:VAL:HG22	2.04	0.57
1:A:423:TYR:OH	1:A:448:SER:O	2.22	0.57
1:D:246:THR:OG1	1:D:259:SER:OG	2.22	0.57
1:D:423:TYR:OH	1:D:448:SER:O	2.22	0.56
1:C:227:LEU:O	1:C:230:VAL:HG22	2.04	0.56
1:B:314:GLN:NE2	1:B:334:GLN:O	2.39	0.56
1:D:314:GLN:NE2	1:D:334:GLN:O	2.39	0.56
1:C:423:TYR:OH	1:C:448:SER:O	2.22	0.56
1:B:227:LEU:O	1:B:230:VAL:HG22	2.04	0.56
1:C:314:GLN:NE2	1:C:334:GLN:O	2.39	0.55
1:C:475:TRP:HZ3	2:C:607:Y01:HAL2	1.70	0.55
1:B:475:TRP:HZ3	2:B:601:Y01:HAL2	1.71	0.55
1:A:314:GLN:NE2	1:A:334:GLN:O	2.39	0.55
1:A:108:ASP:O	1:A:109:ARG:HB3	2.07	0.54
1:B:423:TYR:CE2	2:B:602:Y01:HAE2	2.42	0.54
1:A:423:TYR:CE2	2:A:601:Y01:HAE2	2.43	0.54
1:B:108:ASP:O	1:B:109:ARG:CB	2.55	0.54
1:B:108:ASP:O	1:B:109:ARG:HB3	2.07	0.54
1:C:113:THR:HG22	1:C:113:THR:O	2.08	0.54
1:A:108:ASP:O	1:A:109:ARG:CB	2.55	0.54
1:A:475:TRP:HZ3	2:A:606:Y01:HAL2	1.72	0.54
1:D:108:ASP:O	1:D:109:ARG:HB3	2.07	0.54
1:D:341:TRP:CZ3	1:D:344:MET:HE1	2.42	0.54
1:B:113:THR:O	1:B:113:THR:HG22	2.08	0.53
1:A:173:ASP:HB2	1:C:270:LYS:NZ	2.22	0.53
1:D:113:THR:HG22	1:D:113:THR:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:GLU:OE2	1:C:154:SER:N	2.42	0.53
1:C:108:ASP:O	1:C:109:ARG:HB3	2.07	0.53
1:A:147:GLU:OE2	1:A:154:SER:N	2.42	0.53
1:A:113:THR:O	1:A:113:THR:HG22	2.08	0.53
1:D:108:ASP:O	1:D:109:ARG:CB	2.55	0.53
1:B:109:ARG:O	1:B:109:ARG:HG3	2.09	0.52
1:B:246:THR:OG1	1:B:259:SER:OG	2.22	0.52
1:C:109:ARG:HG3	1:C:109:ARG:O	2.09	0.52
1:B:147:GLU:OE2	1:B:154:SER:N	2.42	0.52
1:C:108:ASP:O	1:C:109:ARG:CB	2.55	0.52
1:D:109:ARG:HG3	1:D:109:ARG:O	2.09	0.52
1:D:502:THR:O	1:D:506:GLU:HG2	2.10	0.52
1:B:270:LYS:NZ	1:D:173:ASP:HB2	2.24	0.52
1:A:109:ARG:O	1:A:109:ARG:HG3	2.09	0.52
1:D:147:GLU:OE2	1:D:154:SER:N	2.42	0.52
1:C:502:THR:O	1:C:506:GLU:HG2	2.10	0.52
1:A:341:TRP:CZ3	1:A:344:MET:HE1	2.46	0.51
1:D:273:HIS:NE2	1:D:278:ILE:HG12	2.25	0.51
1:B:502:THR:O	1:B:506:GLU:HG2	2.10	0.51
1:A:502:THR:O	1:A:506:GLU:HG2	2.10	0.51
1:B:273:HIS:NE2	1:B:278:ILE:HG12	2.25	0.51
1:C:273:HIS:NE2	1:C:278:ILE:HG12	2.25	0.51
1:A:273:HIS:NE2	1:A:278:ILE:HG12	2.25	0.50
1:C:320:PHE:C	1:C:320:PHE:CD2	2.86	0.49
1:A:320:PHE:CD2	1:A:320:PHE:C	2.86	0.49
1:D:320:PHE:C	1:D:320:PHE:CD2	2.86	0.49
1:A:270:LYS:NZ	1:B:173:ASP:HB2	2.27	0.49
1:A:90:PHE:O	1:A:94:ASN:ND2	2.46	0.49
1:D:90:PHE:O	1:D:94:ASN:ND2	2.46	0.49
1:B:90:PHE:O	1:B:94:ASN:ND2	2.46	0.48
1:D:423:TYR:CE2	2:D:605:Y01:HAE2	2.48	0.48
2:D:604:Y01:HAV1	2:D:604:Y01:CAL	2.43	0.48
2:A:605:Y01:CAL	2:A:605:Y01:HAV1	2.44	0.48
1:B:320:PHE:C	1:B:320:PHE:CD2	2.86	0.48
2:B:604:Y01:CAL	2:B:604:Y01:HAV1	2.43	0.48
1:B:377:LEU:O	1:B:380:SER:OG	2.27	0.48
1:B:480:ILE:HG23	2:B:601:Y01:HAC1	1.95	0.48
1:C:475:TRP:CZ3	2:C:607:Y01:HAL2	2.47	0.48
2:C:602:Y01:CAL	2:C:602:Y01:HAV1	2.43	0.48
1:C:90:PHE:O	1:C:94:ASN:ND2	2.46	0.48
1:B:321:PHE:CD2	1:B:327:LYS:O	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:PHE:CD2	1:A:327:LYS:O	2.67	0.48
1:C:321:PHE:CD2	1:C:327:LYS:O	2.67	0.48
1:A:140:SER:OG	1:A:141:VAL:N	2.47	0.47
1:C:391:TYR:HB3	2:C:602:Y01:HAT1	1.97	0.47
1:B:140:SER:OG	1:B:141:VAL:N	2.47	0.47
1:D:475:TRP:CZ3	2:D:602:Y01:HAL2	2.50	0.47
1:D:480:ILE:HG23	2:D:602:Y01:HAC1	1.96	0.47
1:D:321:PHE:CD2	1:D:327:LYS:O	2.67	0.47
2:A:605:Y01:HAO2	2:A:605:Y01:HAP1	1.39	0.47
1:C:423:TYR:CD2	2:C:606:Y01:HAE2	2.49	0.47
1:B:395:PHE:O	1:B:399:ASN:HB2	2.15	0.47
1:B:460:MET:O	1:B:463:THR:OG1	2.20	0.46
2:C:602:Y01:HAP1	2:C:602:Y01:HAO2	1.37	0.46
2:B:604:Y01:HAP1	2:B:604:Y01:HAO2	1.37	0.46
1:D:377:LEU:O	1:D:380:SER:OG	2.27	0.46
1:B:341:TRP:CE3	1:B:344:MET:HE1	2.50	0.46
1:D:140:SER:OG	1:D:141:VAL:N	2.47	0.46
1:A:423:TYR:CD2	2:A:601:Y01:HAE2	2.50	0.46
1:C:140:SER:OG	1:C:141:VAL:N	2.47	0.46
1:A:480:ILE:HG23	2:A:606:Y01:HAC1	1.97	0.46
1:B:475:TRP:CZ3	2:B:601:Y01:HAL2	2.50	0.46
1:C:395:PHE:O	1:C:399:ASN:HB2	2.16	0.46
1:D:395:PHE:O	1:D:399:ASN:HB2	2.16	0.45
1:C:341:TRP:CZ3	1:C:344:MET:HE1	2.51	0.45
2:C:607:Y01:HAA3	2:D:605:Y01:HAN2	1.97	0.45
1:A:395:PHE:O	1:A:399:ASN:HB2	2.16	0.45
1:C:432:ILE:HD12	1:D:77:LEU:HG	1.99	0.45
1:D:460:MET:O	1:D:463:THR:OG1	2.20	0.45
2:A:606:Y01:HAM1	2:C:606:Y01:OAG	2.17	0.45
1:B:184:ASP:OD1	1:B:185:CYS:N	2.50	0.45
2:D:604:Y01:HAJ1	2:D:604:Y01:HAC3	1.79	0.44
2:A:601:Y01:HAN2	2:B:601:Y01:HAA3	1.99	0.44
1:B:423:TYR:CD2	2:B:602:Y01:HAE2	2.52	0.44
1:A:475:TRP:CZ3	2:A:606:Y01:HAL2	2.51	0.44
2:A:606:Y01:HAA3	2:C:606:Y01:HAN2	2.00	0.44
1:C:432:ILE:HD11	1:D:80:PHE:CE2	2.52	0.44
1:D:423:TYR:CD2	2:D:605:Y01:HAE2	2.53	0.43
1:C:460:MET:O	1:C:463:THR:OG1	2.20	0.43
2:B:602:Y01:OAG	2:D:602:Y01:HAM1	2.19	0.43
1:B:398:TYR:O	1:B:402:ILE:HD12	2.19	0.43
1:D:184:ASP:OD1	1:D:185:CYS:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:TYR:HB3	2:D:604:Y01:HAT1	2.01	0.43
2:A:601:Y01:HAP1	2:A:601:Y01:HAO1	1.62	0.43
2:A:605:Y01:HAC3	2:A:605:Y01:HAJ1	1.77	0.43
1:D:419:ALA:HB3	2:D:605:Y01:HAA2	2.00	0.43
2:B:602:Y01:HAN2	2:D:602:Y01:HAA3	2.01	0.42
2:D:605:Y01:HAP1	2:D:605:Y01:HAO1	1.63	0.42
2:C:606:Y01:HAO1	2:C:606:Y01:HAP1	1.66	0.42
2:C:607:Y01:HAB1	2:C:607:Y01:HAJ1	1.79	0.42
1:D:398:TYR:O	1:D:402:ILE:HD12	2.19	0.42
1:B:341:TRP:HZ3	1:B:344:MET:HE1	1.83	0.42
1:A:184:ASP:OD1	1:A:185:CYS:N	2.50	0.42
1:C:103:LEU:HD12	1:C:114:TYR:OH	2.19	0.42
1:C:184:ASP:OD1	1:C:185:CYS:N	2.50	0.42
1:A:398:TYR:O	1:A:402:ILE:HD12	2.19	0.42
1:B:109:ARG:C	1:B:111:ASP:H	2.23	0.42
2:B:602:Y01:HAO1	2:B:602:Y01:HAP1	1.66	0.42
1:C:398:TYR:O	1:C:402:ILE:HD12	2.19	0.42
1:A:103:LEU:HD12	1:A:114:TYR:OH	2.19	0.42
1:A:341:TRP:CZ3	1:A:344:MET:CE	3.03	0.42
1:A:80:PHE:HD2	1:B:432:ILE:CD1	2.30	0.42
1:A:109:ARG:C	1:A:111:ASP:H	2.23	0.42
1:A:431:TRP:NE1	1:A:442:ARG:O	2.48	0.42
2:C:602:Y01:HAC3	2:C:602:Y01:HAJ1	1.79	0.42
1:C:173:ASP:HB2	1:D:270:LYS:NZ	2.35	0.42
2:D:604:Y01:HAO2	2:D:604:Y01:HAP1	1.37	0.42
1:B:103:LEU:HD12	1:B:114:TYR:OH	2.19	0.41
1:D:109:ARG:C	1:D:111:ASP:N	2.74	0.41
1:D:103:LEU:HD12	1:D:114:TYR:OH	2.19	0.41
1:D:341:TRP:CZ3	1:D:344:MET:CE	3.03	0.41
1:C:479:ARG:NH2	1:D:449:GLU:OE2	2.53	0.41
2:A:601:Y01:OAG	2:B:601:Y01:HAM1	2.20	0.41
1:C:341:TRP:CZ3	1:C:344:MET:CE	3.03	0.41
1:A:109:ARG:C	1:A:111:ASP:N	2.74	0.41
1:B:109:ARG:C	1:B:111:ASP:N	2.74	0.41
1:C:377:LEU:O	1:C:380:SER:OG	2.27	0.41
1:D:109:ARG:C	1:D:111:ASP:H	2.23	0.41
1:D:238:CYS:SG	1:D:239:TYR:N	2.94	0.41
1:C:109:ARG:C	1:C:111:ASP:H	2.23	0.41
2:C:607:Y01:HAM1	2:D:605:Y01:OAG	2.20	0.41
1:A:173:ASP:HB2	1:C:270:LYS:HZ2	1.85	0.40
1:A:377:LEU:O	1:A:380:SER:OG	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:PHE:HD2	1:D:432:ILE:CD1	2.30	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	479/561 (85%)	459 (96%)	20 (4%)	0	100	100
1	B	479/561 (85%)	459 (96%)	20 (4%)	0	100	100
1	C	479/561 (85%)	459 (96%)	20 (4%)	0	100	100
1	D	479/561 (85%)	459 (96%)	20 (4%)	0	100	100
All	All	1916/2244 (85%)	1836 (96%)	80 (4%)	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	431/515 (84%)	430 (100%)	1 (0%)	94	98
1	B	431/515 (84%)	430 (100%)	1 (0%)	94	98
1	C	431/515 (84%)	430 (100%)	1 (0%)	94	98
1	D	431/515 (84%)	430 (100%)	1 (0%)	94	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1724/2060 (84%)	1720 (100%)	4 (0%)	94 98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	325	TYR
1	B	325	TYR
1	C	325	TYR
1	D	325	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	314	GLN
1	B	314	GLN
1	C	314	GLN
1	D	314	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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
2	Y01	A	601	-	35,38,38	0.63	0	54,57,57	0.74	0
4	3PE	A	604	-	17,17,50	0.90	1 (5%)	16,16,55	0.85	0
2	Y01	A	605	-	35,35,38	0.65	0	53,53,57	0.80	0
2	Y01	A	606	-	35,38,38	0.66	0	54,57,57	0.82	0
2	Y01	B	601	-	35,38,38	0.67	0	54,57,57	0.83	0
2	Y01	B	602	-	35,38,38	0.63	0	54,57,57	0.75	0
4	3PE	B	603	-	17,17,50	0.90	1 (5%)	16,16,55	0.85	0
2	Y01	B	604	-	35,35,38	0.65	0	53,53,57	0.79	0
4	3PE	C	601	-	17,17,50	0.90	1 (5%)	16,16,55	0.85	0
2	Y01	C	602	-	35,35,38	0.65	0	53,53,57	0.79	0
2	Y01	C	606	-	35,38,38	0.62	0	54,57,57	0.75	0
2	Y01	C	607	-	35,38,38	0.66	0	54,57,57	0.83	0
2	Y01	D	602	-	35,38,38	0.66	0	54,57,57	0.82	0
4	3PE	D	603	-	17,17,50	0.89	1 (5%)	16,16,55	0.85	0
2	Y01	D	604	-	35,35,38	0.65	0	53,53,57	0.79	0
2	Y01	D	605	-	35,38,38	0.62	0	54,57,57	0.75	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	Y01	A	601	-	-	0/17/77/77	0/4/4/4
4	3PE	A	604	-	-	0/15/15/54	0/0/0/0
2	Y01	A	605	-	-	0/16/74/77	0/4/4/4
2	Y01	A	606	-	-	0/17/77/77	0/4/4/4
2	Y01	B	601	-	-	0/17/77/77	0/4/4/4
2	Y01	B	602	-	-	0/17/77/77	0/4/4/4
4	3PE	B	603	-	-	0/15/15/54	0/0/0/0
2	Y01	B	604	-	-	0/16/74/77	0/4/4/4
4	3PE	C	601	-	-	0/15/15/54	0/0/0/0
2	Y01	C	602	-	-	0/16/74/77	0/4/4/4
2	Y01	C	606	-	-	0/17/77/77	0/4/4/4
2	Y01	C	607	-	-	0/17/77/77	0/4/4/4
2	Y01	D	602	-	-	0/17/77/77	0/4/4/4
4	3PE	D	603	-	-	0/15/15/54	0/0/0/0
2	Y01	D	604	-	-	0/16/74/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Y01	D	605	-	-	0/17/77/77	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	3PE	C3A-C39	-2.77	1.35	1.51
4	A	604	3PE	C3A-C39	-2.77	1.35	1.51
4	B	603	3PE	C3A-C39	-2.77	1.35	1.51
4	D	603	3PE	C3A-C39	-2.75	1.36	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	Y01	6	0
2	A	605	Y01	4	0
2	A	606	Y01	6	0
2	B	601	Y01	6	0
2	B	602	Y01	6	0
2	B	604	Y01	3	0
2	C	602	Y01	5	0
2	C	606	Y01	6	0
2	C	607	Y01	7	0
2	D	602	Y01	6	0
2	D	604	Y01	5	0
2	D	605	Y01	7	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.