



Full wwPDB EM Validation Report ⓘ

Nov 4, 2025 – 02:58 PM JST

PDB ID : 9JF7 / pdb_00009jf7
EMDB ID : EMD-61429
Title : The structure of PDPNaC1 at APO state
Authors : Yuan, L.; Shang, J.; Dong, W.
Deposited on : 2024-09-04
Resolution : 3.03 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

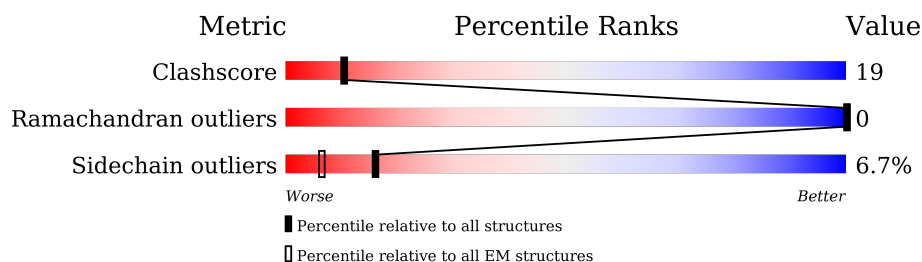
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.03 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	421	
1	B	421	
1	C	421	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14580 atoms, of which 5988 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.

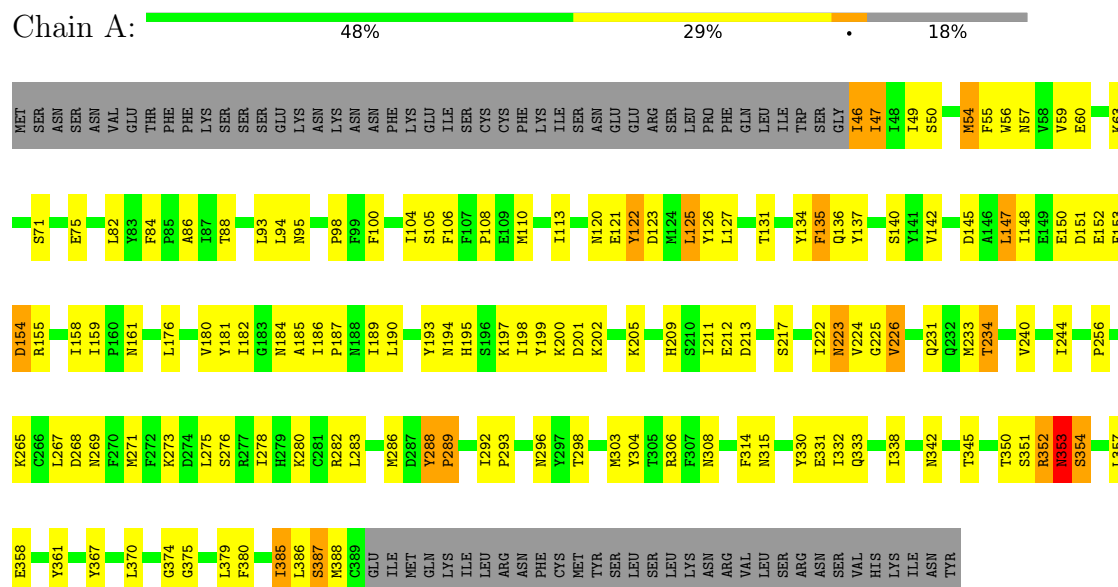
- Molecule 1 is a protein called proton dissociation permeative sodium channel (PDPNaC1).

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	344	Total	C	H	N	O	S	0	0
			4860	1871	1996	443	528	22		
1	B	344	Total	C	H	N	O	S	0	0
			4860	1871	1996	443	528	22		
1	C	344	Total	C	H	N	O	S	0	0
			4860	1871	1996	443	528	22		

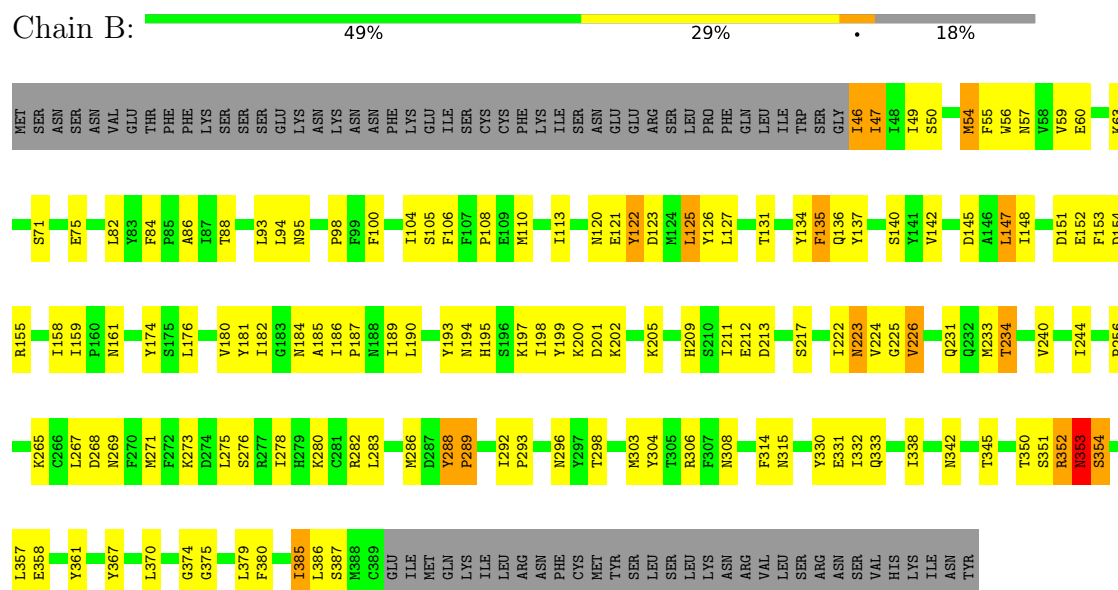
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: proton dissociation permeative sodium channel (PDPNaC1)

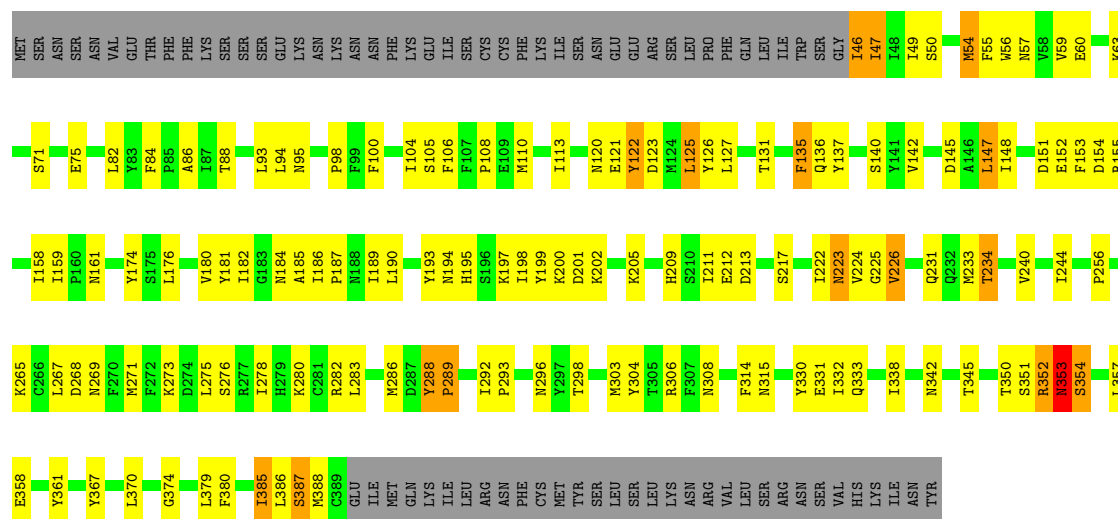


- Molecule 1: proton dissociation permeative sodium channel (PDPNaC1)



- Molecule 1: proton dissociation permeative sodium channel (PDPNaC1)

Chain C:  49% 29% 18%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	121831	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 ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/2945	0.75	17/3993 (0.4%)
1	B	0.45	0/2945	0.75	17/3993 (0.4%)
1	C	0.45	0/2945	0.75	17/3993 (0.4%)
All	All	0.45	0/8835	0.75	51/11979 (0.4%)

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
All	All	0	3

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	288	TYR	N-CA-C	11.25	127.43	112.35
1	A	288	TYR	N-CA-C	11.24	127.41	112.35
1	B	288	TYR	N-CA-C	11.24	127.42	112.35
1	A	289	PRO	N-CA-C	-9.78	98.77	110.70
1	B	289	PRO	N-CA-C	-9.74	98.82	110.70
1	C	289	PRO	N-CA-C	-9.69	98.88	110.70
1	C	122	TYR	N-CA-C	8.63	123.84	110.20
1	A	122	TYR	N-CA-C	8.61	123.81	110.20
1	B	122	TYR	N-CA-C	8.62	123.81	110.20
1	A	123	ASP	N-CA-C	-7.51	98.70	109.96
1	C	123	ASP	N-CA-C	-7.50	98.71	109.96
1	B	123	ASP	N-CA-C	-7.47	98.76	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	ASN	N-CA-C	6.89	119.61	109.69
1	C	353	ASN	N-CA-C	6.88	119.59	109.69
1	B	353	ASN	N-CA-C	6.82	119.52	109.69
1	B	385	ILE	N-CA-C	-6.74	103.76	110.30
1	A	385	ILE	N-CA-C	-6.67	103.83	110.30
1	C	385	ILE	N-CA-C	-6.65	103.85	110.30
1	B	120	ASN	N-CA-C	-6.35	99.54	109.25
1	C	120	ASN	N-CA-C	-6.32	99.58	109.25
1	A	120	ASN	N-CA-C	-6.32	99.59	109.25
1	A	288	TYR	CB-CA-C	-6.25	102.85	113.04
1	C	288	TYR	CB-CA-C	-6.25	102.86	113.04
1	B	288	TYR	CB-CA-C	-6.22	102.90	113.04
1	A	122	TYR	N-CA-CB	6.17	119.37	110.06
1	B	122	TYR	N-CA-CB	6.13	119.31	110.06
1	C	122	TYR	N-CA-CB	6.10	119.28	110.06
1	B	126	TYR	N-CA-C	-5.82	105.02	111.36
1	C	126	TYR	N-CA-C	-5.79	105.05	111.36
1	A	126	TYR	N-CA-C	-5.77	105.07	111.36
1	B	288	TYR	CA-C-N	-5.76	114.44	120.38
1	B	288	TYR	C-N-CA	-5.76	114.44	120.38
1	C	288	TYR	CA-C-N	-5.74	114.46	120.38
1	C	288	TYR	C-N-CA	-5.74	114.46	120.38
1	A	288	TYR	CA-C-N	-5.74	114.47	120.38
1	A	288	TYR	C-N-CA	-5.74	114.47	120.38
1	C	125	LEU	N-CA-CB	5.72	119.11	110.30
1	A	125	LEU	N-CA-CB	5.71	119.10	110.30
1	B	125	LEU	N-CA-CB	5.69	119.06	110.30
1	A	234	THR	OG1-CB-CG2	5.56	120.42	109.30
1	B	125	LEU	CB-CA-C	5.55	121.71	110.38
1	B	234	THR	OG1-CB-CG2	5.55	120.40	109.30
1	A	125	LEU	CB-CA-C	5.55	121.69	110.38
1	C	125	LEU	CB-CA-C	5.54	121.68	110.38
1	C	234	THR	OG1-CB-CG2	5.52	120.34	109.30
1	A	293	PRO	N-CA-C	5.31	119.66	111.21
1	C	293	PRO	N-CA-C	5.31	119.65	111.21
1	B	293	PRO	N-CA-C	5.30	119.64	111.21
1	C	161	ASN	CB-CA-C	5.07	119.47	110.85
1	A	161	ASN	CB-CA-C	5.04	119.42	110.85
1	B	161	ASN	CB-CA-C	5.02	119.39	110.85

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	LEU	Mainchain
1	B	94	LEU	Mainchain
1	C	94	LEU	Mainchain

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	2864	1996	2771	131	0
1	B	2864	1996	2771	126	0
1	C	2864	1996	2771	128	0
All	All	8592	5988	8313	314	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 19.

All (314) 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:104:ILE:HD11	1:B:108:PRO:HG3	1.18	1.18
1:A:104:ILE:HD11	1:A:108:PRO:HG3	1.18	1.15
1:C:104:ILE:HD11	1:C:108:PRO:HG3	1.18	1.15
1:A:60:GLU:HG3	1:C:367:TYR:CD1	2.07	0.89
1:A:104:ILE:CD1	1:A:108:PRO:HG3	2.04	0.88
1:B:181:TYR:OH	1:C:315:ASN:HB2	1.74	0.88
1:A:367:TYR:CD1	1:B:60:GLU:HG3	2.10	0.87
1:B:104:ILE:CD1	1:B:108:PRO:HG3	2.04	0.86
1:B:275:LEU:HB3	1:B:303:MET:HE1	1.56	0.86
1:A:181:TYR:OH	1:B:315:ASN:HB2	1.75	0.86
1:C:275:LEU:HB3	1:C:303:MET:HE1	1.56	0.85
1:A:275:LEU:HB3	1:A:303:MET:HE1	1.56	0.85
1:A:315:ASN:HB2	1:C:181:TYR:OH	1.76	0.85
1:C:104:ILE:CD1	1:C:108:PRO:HG3	2.04	0.84
1:B:296:ASN:OD1	1:B:298:THR:OG1	1.95	0.83
1:A:296:ASN:OD1	1:A:298:THR:OG1	1.95	0.83
1:C:147:LEU:HD23	1:C:147:LEU:H	1.43	0.83
1:C:296:ASN:OD1	1:C:298:THR:OG1	1.95	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ASN:CB	1:C:181:TYR:OH	2.27	0.82
1:B:181:TYR:OH	1:C:315:ASN:CB	2.28	0.82
1:A:181:TYR:OH	1:B:315:ASN:CB	2.27	0.82
1:A:147:LEU:HD23	1:A:147:LEU:H	1.43	0.82
1:B:367:TYR:CD1	1:C:60:GLU:HG3	2.15	0.82
1:B:147:LEU:H	1:B:147:LEU:HD23	1.43	0.81
1:A:226:VAL:HG23	1:A:332:ILE:HD13	1.66	0.77
1:B:226:VAL:HG23	1:B:332:ILE:HD13	1.66	0.77
1:C:226:VAL:HG23	1:C:332:ILE:HD13	1.66	0.75
1:A:367:TYR:CE1	1:B:60:GLU:HG3	2.22	0.75
1:A:75:GLU:HA	1:B:358:GLU:OE2	1.85	0.74
1:B:75:GLU:HA	1:C:358:GLU:OE2	1.89	0.73
1:A:60:GLU:HG3	1:C:367:TYR:CE1	2.24	0.72
1:A:358:GLU:OE2	1:C:75:GLU:HA	1.88	0.72
1:C:82:LEU:HD11	1:C:240:VAL:HG21	1.72	0.72
1:A:385:ILE:N	1:B:379:LEU:O	2.21	0.72
1:B:82:LEU:HD11	1:B:240:VAL:HG21	1.72	0.72
1:A:379:LEU:O	1:C:385:ILE:N	2.22	0.71
1:A:82:LEU:HD11	1:A:240:VAL:HG21	1.72	0.71
1:B:280:LYS:HE2	1:B:292:ILE:HD12	1.72	0.70
1:A:280:LYS:HE2	1:A:292:ILE:HD12	1.72	0.70
1:C:280:LYS:HE2	1:C:292:ILE:HD12	1.72	0.70
1:A:151:ASP:O	1:A:152:GLU:HG2	1.94	0.68
1:B:151:ASP:O	1:B:152:GLU:HG2	1.94	0.67
1:B:367:TYR:CE1	1:C:60:GLU:HG3	2.28	0.67
1:A:213:ASP:O	1:A:217:SER:HB2	1.95	0.67
1:C:151:ASP:O	1:C:152:GLU:HG2	1.94	0.67
1:C:213:ASP:O	1:C:217:SER:HB2	1.95	0.66
1:A:88:THR:OG1	1:A:209:HIS:NE2	2.29	0.66
1:B:275:LEU:HB3	1:B:303:MET:CE	2.26	0.66
1:B:213:ASP:O	1:B:217:SER:HB2	1.95	0.66
1:C:88:THR:OG1	1:C:209:HIS:NE2	2.29	0.66
1:B:88:THR:OG1	1:B:209:HIS:NE2	2.29	0.65
1:B:135:PHE:HB2	1:B:193:TYR:CD1	2.32	0.65
1:C:135:PHE:HB2	1:C:193:TYR:CD1	2.32	0.65
1:A:142:VAL:HG22	1:A:189:ILE:HG12	1.79	0.65
1:B:385:ILE:N	1:C:379:LEU:O	2.29	0.65
1:A:135:PHE:HB2	1:A:193:TYR:CD1	2.32	0.65
1:C:142:VAL:HG22	1:C:189:ILE:HG12	1.78	0.65
1:B:142:VAL:HG22	1:B:189:ILE:HG12	1.78	0.64
1:A:314:PHE:O	1:C:184:ASN:ND2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:SER:OG	1:B:331:GLU:OE2	2.14	0.64
1:A:57:ASN:HD21	1:C:370:LEU:HB2	1.62	0.64
1:B:184:ASN:ND2	1:C:314:PHE:O	2.29	0.64
1:A:331:GLU:OE2	1:C:354:SER:OG	2.15	0.64
1:B:354:SER:OG	1:C:331:GLU:OE2	2.16	0.64
1:A:275:LEU:HB3	1:A:303:MET:CE	2.26	0.63
1:C:197:LYS:HG3	1:C:198:ILE:N	2.15	0.62
1:C:275:LEU:HB3	1:C:303:MET:CE	2.26	0.62
1:B:197:LYS:HG3	1:B:198:ILE:N	2.15	0.61
1:A:104:ILE:HD11	1:A:108:PRO:CG	2.12	0.61
1:A:197:LYS:HG3	1:A:198:ILE:N	2.15	0.61
1:A:184:ASN:ND2	1:B:314:PHE:O	2.29	0.61
1:A:142:VAL:HG23	1:A:158:ILE:HD11	1.82	0.61
1:A:226:VAL:CG2	1:A:332:ILE:HD13	2.31	0.60
1:B:142:VAL:HG23	1:B:158:ILE:HD11	1.82	0.60
1:C:142:VAL:HG23	1:C:158:ILE:HD11	1.82	0.60
1:C:226:VAL:CG2	1:C:332:ILE:HD13	2.31	0.60
1:B:271:MET:O	1:B:275:LEU:HG	2.02	0.60
1:B:244:ILE:HD13	1:B:357:LEU:HD11	1.83	0.60
1:C:244:ILE:HD13	1:C:357:LEU:HD11	1.83	0.60
1:A:271:MET:O	1:A:275:LEU:HG	2.02	0.59
1:A:244:ILE:HD13	1:A:357:LEU:HD11	1.83	0.59
1:B:226:VAL:CG2	1:B:332:ILE:HD13	2.31	0.59
1:C:271:MET:O	1:C:275:LEU:HG	2.02	0.59
1:A:225:GLY:O	1:C:352:ARG:NH2	2.36	0.59
1:A:370:LEU:HB2	1:B:57:ASN:HD21	1.67	0.58
1:B:56:TRP:CZ2	1:B:60:GLU:OE2	2.57	0.58
1:A:352:ARG:NH2	1:B:225:GLY:O	2.36	0.58
1:B:197:LYS:HG3	1:B:198:ILE:H	1.67	0.58
1:C:98:PRO:HG3	1:C:202:LYS:HD2	1.86	0.58
1:A:56:TRP:CZ2	1:A:60:GLU:OE2	2.57	0.58
1:B:352:ARG:NH2	1:C:225:GLY:O	2.37	0.58
1:B:98:PRO:HG3	1:B:202:LYS:HD2	1.85	0.58
1:C:197:LYS:HG3	1:C:198:ILE:H	1.67	0.58
1:C:200:LYS:C	1:C:200:LYS:HD3	2.29	0.57
1:A:98:PRO:HG3	1:A:202:LYS:HD2	1.85	0.57
1:A:197:LYS:HG3	1:A:198:ILE:H	1.67	0.57
1:B:104:ILE:HD11	1:B:108:PRO:CG	2.13	0.57
1:C:56:TRP:CZ2	1:C:60:GLU:OE2	2.57	0.57
1:B:200:LYS:HD3	1:B:200:LYS:C	2.29	0.57
1:B:280:LYS:O	1:B:280:LYS:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:LYS:HG3	1:C:280:LYS:O	2.04	0.57
1:C:289:PRO:HB2	1:C:292:ILE:HB	1.87	0.57
1:B:370:LEU:HB2	1:C:57:ASN:HD21	1.70	0.57
1:A:280:LYS:O	1:A:280:LYS:HG3	2.04	0.57
1:C:104:ILE:HD11	1:C:108:PRO:CG	2.13	0.57
1:A:289:PRO:HB2	1:A:292:ILE:HB	1.87	0.56
1:A:50:SER:OG	1:C:386:LEU:CD1	2.53	0.56
1:A:200:LYS:HD3	1:A:200:LYS:C	2.29	0.56
1:A:231:GLN:HB3	1:A:342:ASN:O	2.05	0.56
1:B:289:PRO:HB2	1:B:292:ILE:HB	1.87	0.56
1:C:231:GLN:HB3	1:C:342:ASN:O	2.05	0.56
1:B:231:GLN:HB3	1:B:342:ASN:O	2.05	0.56
1:C:182:ILE:O	1:C:182:ILE:HG22	2.05	0.56
1:A:182:ILE:HG22	1:A:182:ILE:O	2.05	0.56
1:A:333:GLN:HG3	1:A:353:ASN:OD1	2.06	0.56
1:C:276:SER:HA	1:C:280:LYS:HA	1.88	0.56
1:A:276:SER:HA	1:A:280:LYS:HA	1.88	0.55
1:B:182:ILE:HG22	1:B:182:ILE:O	2.05	0.55
1:B:333:GLN:HG3	1:B:353:ASN:OD1	2.06	0.55
1:A:54:MET:HE2	1:A:55:PHE:HA	1.89	0.55
1:C:212:GLU:HG2	1:C:256:PRO:HB2	1.89	0.55
1:C:333:GLN:HG3	1:C:353:ASN:OD1	2.06	0.55
1:B:180:VAL:HG21	1:B:187:PRO:HG2	1.89	0.55
1:A:142:VAL:HG21	1:A:176:LEU:HD11	1.89	0.55
1:B:142:VAL:HG21	1:B:176:LEU:HD11	1.89	0.55
1:B:212:GLU:HG2	1:B:256:PRO:HB2	1.88	0.55
1:A:222:ILE:HD12	1:C:147:LEU:HB3	1.89	0.54
1:B:276:SER:HA	1:B:280:LYS:HA	1.88	0.54
1:C:180:VAL:HG21	1:C:187:PRO:HG2	1.89	0.54
1:C:54:MET:HE2	1:C:55:PHE:HA	1.89	0.54
1:B:54:MET:HE2	1:B:55:PHE:HA	1.89	0.54
1:A:180:VAL:HG21	1:A:187:PRO:HG2	1.89	0.54
1:B:46:ILE:HG22	1:B:47:ILE:HD12	1.90	0.54
1:C:142:VAL:HG21	1:C:176:LEU:HD11	1.89	0.54
1:A:386:LEU:HD13	1:B:380:PHE:O	2.08	0.53
1:A:212:GLU:HG2	1:A:256:PRO:HB2	1.89	0.53
1:C:280:LYS:HE2	1:C:292:ILE:CD1	2.39	0.53
1:B:174:TYR:HH	1:B:193:TYR:HH	1.57	0.53
1:A:379:LEU:HB2	1:C:374:GLY:CA	2.39	0.53
1:B:147:LEU:HB3	1:C:222:ILE:HD12	1.90	0.53
1:B:152:GLU:HG3	1:B:153:PHE:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:LEU:HD22	1:B:271:MET:HE2	1.91	0.52
1:C:152:GLU:HG3	1:C:153:PHE:CE1	2.45	0.52
1:A:267:LEU:HD22	1:A:271:MET:HE2	1.91	0.52
1:A:147:LEU:HB3	1:B:222:ILE:HD12	1.91	0.52
1:A:152:GLU:HG3	1:A:153:PHE:CE1	2.45	0.52
1:B:280:LYS:HE2	1:B:292:ILE:CD1	2.39	0.52
1:C:267:LEU:HD22	1:C:271:MET:HE2	1.91	0.52
1:A:95:ASN:HA	1:A:113:ILE:HG13	1.93	0.52
1:A:380:PHE:O	1:C:386:LEU:HD13	2.10	0.52
1:C:182:ILE:HG23	1:C:186:ILE:HG13	1.92	0.51
1:C:231:GLN:N	1:C:345:THR:OG1	2.38	0.51
1:B:233:MET:HG2	1:B:338:ILE:HB	1.92	0.51
1:A:186:ILE:HD12	1:A:186:ILE:H	1.75	0.51
1:B:140:SER:HA	1:B:190:LEU:O	2.10	0.51
1:A:233:MET:HG2	1:A:338:ILE:HB	1.91	0.51
1:C:140:SER:HA	1:C:190:LEU:O	2.10	0.51
1:A:231:GLN:N	1:A:345:THR:OG1	2.38	0.51
1:B:182:ILE:HG23	1:B:186:ILE:HG13	1.92	0.51
1:C:186:ILE:HD12	1:C:186:ILE:H	1.75	0.51
1:A:93:LEU:HD22	1:C:147:LEU:HA	1.92	0.51
1:C:233:MET:HG2	1:C:338:ILE:HB	1.91	0.51
1:A:140:SER:HA	1:A:190:LEU:O	2.10	0.50
1:A:182:ILE:HG23	1:A:186:ILE:HG13	1.92	0.50
1:B:275:LEU:HD13	1:B:283:LEU:HD12	1.92	0.50
1:B:186:ILE:HD12	1:B:186:ILE:H	1.75	0.50
1:A:275:LEU:HD13	1:A:283:LEU:HD12	1.92	0.50
1:B:386:LEU:HD13	1:C:380:PHE:O	2.12	0.50
1:C:275:LEU:HD13	1:C:283:LEU:HD12	1.92	0.50
1:B:127:LEU:O	1:B:131:THR:HG23	2.12	0.50
1:C:127:LEU:O	1:C:131:THR:HG23	2.12	0.50
1:A:386:LEU:CD1	1:B:50:SER:OG	2.60	0.50
1:B:95:ASN:HA	1:B:113:ILE:HG13	1.93	0.50
1:A:282:ARG:HA	1:A:286:MET:HE2	1.94	0.49
1:A:100:PHE:CZ	1:A:127:LEU:HD11	2.48	0.49
1:A:223:ASN:HB2	1:C:185:ALA:CB	2.42	0.49
1:C:95:ASN:HA	1:C:113:ILE:HG13	1.93	0.49
1:C:282:ARG:HA	1:C:286:MET:HE2	1.94	0.49
1:A:127:LEU:O	1:A:131:THR:HG23	2.12	0.49
1:A:181:TYR:OH	1:B:315:ASN:HB3	2.11	0.49
1:A:280:LYS:HE2	1:A:292:ILE:CD1	2.39	0.49
1:B:100:PHE:CZ	1:B:127:LEU:HD11	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LEU:H	1:B:147:LEU:CD2	2.21	0.49
1:B:244:ILE:CD1	1:B:357:LEU:HD11	2.43	0.49
1:B:282:ARG:HA	1:B:286:MET:HE2	1.94	0.49
1:C:100:PHE:CZ	1:C:127:LEU:HD11	2.48	0.49
1:C:104:ILE:HD12	1:C:106:PHE:CZ	2.48	0.49
1:C:142:VAL:HG22	1:C:189:ILE:CG1	2.42	0.49
1:A:110:MET:HG2	1:C:148:ILE:HG23	1.93	0.49
1:B:142:VAL:HG22	1:B:189:ILE:CG1	2.42	0.49
1:B:386:LEU:CD1	1:C:50:SER:OG	2.61	0.49
1:A:315:ASN:HB3	1:C:181:TYR:OH	2.10	0.49
1:C:244:ILE:CD1	1:C:357:LEU:HD11	2.43	0.49
1:A:60:GLU:HG3	1:C:367:TYR:CG	2.46	0.48
1:A:142:VAL:HG22	1:A:189:ILE:CG1	2.42	0.48
1:B:71:SER:OG	1:B:361:TYR:CE1	2.66	0.48
1:A:185:ALA:CB	1:B:223:ASN:HB2	2.43	0.48
1:A:385:ILE:HG12	1:B:379:LEU:O	2.13	0.48
1:B:374:GLY:CA	1:C:379:LEU:HB2	2.42	0.48
1:C:71:SER:OG	1:C:361:TYR:CE1	2.66	0.48
1:A:71:SER:OG	1:A:361:TYR:CE1	2.66	0.48
1:C:147:LEU:H	1:C:147:LEU:CD2	2.22	0.48
1:A:147:LEU:HA	1:B:93:LEU:HD22	1.95	0.48
1:A:200:LYS:HD3	1:A:201:ASP:HB2	1.95	0.48
1:B:200:LYS:HD3	1:B:201:ASP:HB2	1.95	0.48
1:C:59:VAL:HG12	1:C:63:LYS:HE2	1.96	0.48
1:C:205:LYS:NZ	1:C:222:ILE:O	2.43	0.48
1:B:104:ILE:HD12	1:B:106:PHE:CZ	2.48	0.48
1:A:104:ILE:HD12	1:A:106:PHE:CZ	2.48	0.48
1:A:304:TYR:CZ	1:C:147:LEU:HD12	2.48	0.48
1:C:200:LYS:HD3	1:C:201:ASP:HB2	1.95	0.48
1:A:244:ILE:CD1	1:A:357:LEU:HD11	2.43	0.47
1:C:46:ILE:HG22	1:C:47:ILE:HD12	1.95	0.47
1:A:148:ILE:HG23	1:B:110:MET:HG2	1.95	0.47
1:B:148:ILE:HG23	1:C:110:MET:HG2	1.96	0.47
1:B:231:GLN:N	1:B:345:THR:OG1	2.38	0.47
1:A:136:GLN:HB3	1:A:194:ASN:O	2.15	0.47
1:C:136:GLN:HB3	1:C:194:ASN:O	2.15	0.47
1:A:59:VAL:HG12	1:A:63:LYS:HE2	1.96	0.47
1:A:46:ILE:HG22	1:A:47:ILE:HD12	1.96	0.47
1:C:268:ASP:HB3	1:C:288:TYR:CB	2.45	0.47
1:A:147:LEU:HD12	1:B:304:TYR:CZ	2.50	0.47
1:A:375:GLY:O	1:C:374:GLY:HA3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:TYR:HA	1:C:193:TYR:CD1	2.51	0.46
1:B:195:HIS:ND1	1:B:231:GLN:HG3	2.30	0.46
1:A:268:ASP:HB3	1:A:288:TYR:CB	2.45	0.46
1:B:59:VAL:HG12	1:B:63:LYS:HE2	1.96	0.46
1:A:240:VAL:HG22	1:A:330:TYR:CD1	2.51	0.46
1:B:268:ASP:HB3	1:B:288:TYR:CB	2.45	0.46
1:A:195:HIS:ND1	1:A:231:GLN:HG3	2.30	0.46
1:B:240:VAL:HG22	1:B:330:TYR:CD1	2.51	0.46
1:C:195:HIS:ND1	1:C:231:GLN:HG3	2.30	0.46
1:B:136:GLN:HB3	1:B:194:ASN:O	2.15	0.46
1:A:195:HIS:CE1	1:A:231:GLN:HG3	2.51	0.46
1:B:195:HIS:CE1	1:B:231:GLN:HG3	2.51	0.46
1:B:181:TYR:OH	1:C:315:ASN:HB3	2.13	0.46
1:C:195:HIS:CE1	1:C:231:GLN:HG3	2.51	0.46
1:A:50:SER:OG	1:C:386:LEU:HD11	2.16	0.45
1:A:137:TYR:HA	1:A:193:TYR:CD1	2.51	0.45
1:C:240:VAL:HG22	1:C:330:TYR:CD1	2.51	0.45
1:B:137:TYR:HA	1:B:193:TYR:CD1	2.51	0.45
1:A:374:GLY:HA3	1:B:375:GLY:O	2.16	0.45
1:C:186:ILE:HD12	1:C:186:ILE:N	2.32	0.45
1:A:205:LYS:NZ	1:A:222:ILE:O	2.43	0.45
1:A:269:ASN:O	1:A:273:LYS:HG3	2.17	0.45
1:B:265:LYS:O	1:B:269:ASN:OD1	2.36	0.44
1:A:374:GLY:CA	1:B:379:LEU:HB2	2.47	0.44
1:B:186:ILE:HD12	1:B:186:ILE:N	2.32	0.44
1:B:367:TYR:CG	1:C:60:GLU:HG3	2.52	0.44
1:A:186:ILE:HD12	1:A:186:ILE:N	2.32	0.44
1:B:269:ASN:O	1:B:273:LYS:HG3	2.17	0.44
1:C:136:GLN:O	1:C:136:GLN:CG	2.66	0.44
1:A:136:GLN:CG	1:A:136:GLN:O	2.66	0.44
1:C:265:LYS:O	1:C:269:ASN:OD1	2.36	0.44
1:B:136:GLN:O	1:B:136:GLN:CG	2.66	0.44
1:C:269:ASN:O	1:C:273:LYS:HG3	2.17	0.44
1:A:265:LYS:O	1:A:269:ASN:OD1	2.36	0.44
1:B:185:ALA:CB	1:C:223:ASN:HB2	2.48	0.44
1:B:147:LEU:HA	1:C:93:LEU:HD22	1.98	0.43
1:B:385:ILE:HG12	1:C:379:LEU:O	2.19	0.43
1:A:86:ALA:HB2	1:A:211:ILE:HD13	2.00	0.43
1:A:273:LYS:NZ	1:A:273:LYS:HB3	2.34	0.43
1:A:367:TYR:CG	1:B:60:GLU:HG3	2.50	0.43
1:B:198:ILE:O	1:B:198:ILE:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:LYS:NZ	1:C:273:LYS:HB3	2.34	0.43
1:C:86:ALA:HB2	1:C:211:ILE:HD13	2.01	0.42
1:C:198:ILE:O	1:C:198:ILE:HG22	2.19	0.42
1:A:280:LYS:O	1:A:280:LYS:CG	2.67	0.42
1:A:379:LEU:O	1:C:385:ILE:HG12	2.20	0.42
1:A:152:GLU:HG3	1:A:153:PHE:CD1	2.55	0.42
1:C:268:ASP:HB3	1:C:288:TYR:HB2	2.01	0.42
1:B:273:LYS:NZ	1:B:273:LYS:HB3	2.34	0.42
1:C:278:ILE:HG13	1:C:306:ARG:HG2	2.01	0.42
1:A:147:LEU:HD21	1:B:308:ASN:HA	2.02	0.42
1:A:278:ILE:HG13	1:A:306:ARG:HG2	2.01	0.42
1:B:86:ALA:HB2	1:B:211:ILE:HD13	2.01	0.42
1:B:200:LYS:HD3	1:B:201:ASP:CB	2.50	0.42
1:B:268:ASP:HB3	1:B:288:TYR:HB2	2.01	0.42
1:B:385:ILE:O	1:B:386:LEU:C	2.63	0.42
1:A:198:ILE:HG22	1:A:198:ILE:O	2.19	0.42
1:A:268:ASP:HB3	1:A:288:TYR:HB2	2.01	0.42
1:A:379:LEU:HB2	1:C:374:GLY:HA2	2.02	0.41
1:B:147:LEU:HD12	1:C:304:TYR:CZ	2.54	0.41
1:B:224:VAL:HG12	1:B:224:VAL:O	2.21	0.41
1:C:152:GLU:HG3	1:C:153:PHE:CD1	2.55	0.41
1:B:278:ILE:HG13	1:B:306:ARG:HG2	2.01	0.41
1:C:199:TYR:H	1:C:231:GLN:HE22	1.68	0.41
1:C:200:LYS:HD3	1:C:201:ASP:CB	2.50	0.41
1:B:152:GLU:HG3	1:B:153:PHE:CD1	2.55	0.41
1:C:174:TYR:HH	1:C:193:TYR:HH	1.61	0.41
1:A:200:LYS:HD3	1:A:201:ASP:CB	2.50	0.41
1:A:84:PHE:HD2	1:A:189:ILE:HD12	1.86	0.41
1:A:387:SER:O	1:A:388:MET:C	2.64	0.41
1:A:134:TYR:CE2	1:A:135:PHE:HE1	2.39	0.41
1:A:224:VAL:HG12	1:A:224:VAL:O	2.21	0.41
1:A:303:MET:HE3	1:A:303:MET:HB3	2.01	0.41
1:B:84:PHE:HD2	1:B:189:ILE:HD12	1.86	0.41
1:C:224:VAL:HG12	1:C:224:VAL:O	2.21	0.41
1:A:186:ILE:HD13	1:A:351:SER:O	2.21	0.41
1:A:385:ILE:O	1:A:386:LEU:C	2.63	0.41
1:B:374:GLY:HA3	1:C:379:LEU:HB2	2.03	0.41
1:A:275:LEU:HD12	1:A:286:MET:SD	2.62	0.40
1:B:186:ILE:HD13	1:B:351:SER:O	2.21	0.40
1:B:205:LYS:NZ	1:B:222:ILE:O	2.43	0.40
1:C:186:ILE:HD13	1:C:351:SER:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:PHE:HD2	1:C:189:ILE:HD12	1.86	0.40
1:B:134:TYR:CE2	1:B:135:PHE:HE1	2.39	0.40
1:B:199:TYR:H	1:B:231:GLN:HE22	1.68	0.40
1:C:275:LEU:HD12	1:C:286:MET:SD	2.62	0.40
1:A:308:ASN:HA	1:C:147:LEU:HD21	2.03	0.40
1:B:147:LEU:HD21	1:C:308:ASN:HA	2.04	0.40
1:A:150:GLU:HB3	1:A:154:ASP:OD1	2.22	0.40
1:A:199:TYR:H	1:A:231:GLN:HE22	1.68	0.40
1:C:387:SER:O	1:C:388:MET:C	2.64	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	342/421 (81%)	327 (96%)	15 (4%)	0	100	100
1	B	342/421 (81%)	327 (96%)	15 (4%)	0	100	100
1	C	342/421 (81%)	327 (96%)	15 (4%)	0	100	100
All	All	1026/1263 (81%)	981 (96%)	45 (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	328/404 (81%)	306 (93%)	22 (7%)	13	40
1	B	328/404 (81%)	306 (93%)	22 (7%)	13	40
1	C	328/404 (81%)	306 (93%)	22 (7%)	13	40
All	All	984/1212 (81%)	918 (93%)	66 (7%)	16	40

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	47	ILE
1	A	49	ILE
1	A	54	MET
1	A	105	SER
1	A	121	GLU
1	A	122	TYR
1	A	125	LEU
1	A	135	PHE
1	A	145	ASP
1	A	147	LEU
1	A	154	ASP
1	A	155	ARG
1	A	159	ILE
1	A	223	ASN
1	A	226	VAL
1	A	234	THR
1	A	350	THR
1	A	352	ARG
1	A	353	ASN
1	A	354	SER
1	A	387	SER
1	B	46	ILE
1	B	47	ILE
1	B	49	ILE
1	B	54	MET
1	B	105	SER
1	B	121	GLU
1	B	122	TYR
1	B	125	LEU
1	B	135	PHE
1	B	145	ASP
1	B	147	LEU
1	B	154	ASP

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Mol	Chain	Res	Type
1	B	155	ARG
1	B	159	ILE
1	B	223	ASN
1	B	226	VAL
1	B	234	THR
1	B	350	THR
1	B	352	ARG
1	B	353	ASN
1	B	354	SER
1	B	387	SER
1	C	46	ILE
1	C	47	ILE
1	C	49	ILE
1	C	54	MET
1	C	105	SER
1	C	121	GLU
1	C	122	TYR
1	C	125	LEU
1	C	135	PHE
1	C	145	ASP
1	C	147	LEU
1	C	154	ASP
1	C	155	ARG
1	C	159	ILE
1	C	223	ASN
1	C	226	VAL
1	C	234	THR
1	C	350	THR
1	C	352	ARG
1	C	353	ASN
1	C	354	SER
1	C	387	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	97	ASN
1	A	237	ASN
1	B	57	ASN
1	B	97	ASN
1	B	136	GLN

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Mol	Chain	Res	Type
1	B	172	HIS
1	C	57	ASN
1	C	97	ASN
1	C	136	GLN
1	C	172	HIS
1	C	237	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.