

# wwPDB EM Validation Summary Report (i)

#### Dec 24, 2022 – 12:49 PM EST

PDB ID : 7UUY

EMDB ID : EMD-26806

Title: Structure of the sodium/iodide symporter (NIS)

Authors: Ravera, S.; Nicola, J.P.; Salazar-De Simone, G.; Sigworth, F.; Karakas, E.;

Amzel, L.M.; Bianchet, M.; Carrasco, N.

Deposited on : 2022-04-29

Resolution : 3.30 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (1)) were used in the production of this report:

EMDB validation analysis : FAILED

Mogul : 1.8.5 (274361), CSD as541be (2020)

MolProbity : 4.02b-467 buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

MapQ : FAILED

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

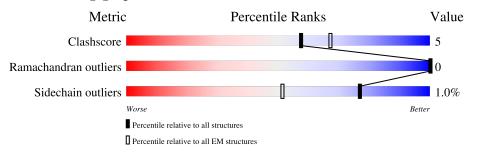
Validation Pipeline (wwPDB-VP) : 2.31.2

## 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 3.30 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 $(\# \mathrm{Entries})$	${ m EM~structures} \ (\#{ m Entries})$	
Clashscore	158937	4297	
Ramachandran outliers	154571	4023	
Sidechain outliers	154315	3826	

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 <=5%

Mol	Chain	Length	Quality of chain					
1	A	694	64%	9%	28%			



## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3809 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 Sodium/iodide cotransporter.

$\mathbf{Mol}$	Chain	Residues	Atoms				AltConf	Trace	
1	A	503	Total 3767	C 2479	N 601	O 660	S 27	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP Q63008
A	-14	TYR	-	expression tag	UNP Q63008
A	-13	PRO	-	expression tag	UNP Q63008
A	-12	TYR	-	expression tag	UNP Q63008
A	-11	ASP	-	expression tag	UNP Q63008
A	-10	VAL	-	expression tag	UNP Q63008
A	-9	PRO	-	expression tag	UNP Q63008
A	-8	ASP	-	expression tag	UNP Q63008
A	-7	TYR	-	expression tag	UNP Q63008
A	-6	ALA	-	expression tag	UNP Q63008
A	-5	GLU	-	expression tag	UNP Q63008
A	-4	ASN	-	expression tag	UNP Q63008
A	-3	LEU	-	expression tag	UNP Q63008
A	-2	TYR	-	expression tag	UNP Q63008
A	-1	PHE	-	expression tag	UNP Q63008
A	0	GLN	-	expression tag	UNP Q63008
A	1	SER	-	expression tag	UNP Q63008
A	225	GLN	ASN	engineered mutation	UNP Q63008
A	485	GLN	ASN	engineered mutation	UNP Q63008
A	497	GLN	ASN	engineered mutation	UNP Q63008
A	619	SER	-	expression tag	UNP Q63008
A	620	GLY	-	expression tag	UNP Q63008
A	621	GLY	-	expression tag	UNP Q63008
A	622	GLY	-	expression tag	UNP Q63008
A	623	GLY	-	expression tag	UNP Q63008
A	624	ALA	-	expression tag	UNP Q63008
A	625	LEU	-	expression tag	UNP Q63008



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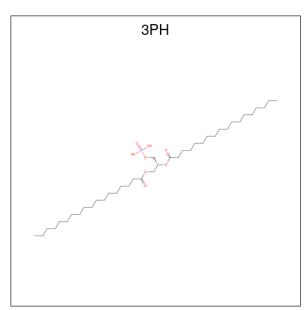
A         626         GLU         -         expression tag         UNP Q6           A         627         VAL         -         expression tag         UNP Q6           A         628         LEU         -         expression tag         UNP Q6           A         629         PHE         -         expression tag         UNP Q6           A         630         GLN         -         expression tag         UNP Q6           A         631         GLY         -         expression tag         UNP Q6           A         632         PRO         -         expression tag         UNP Q6           A         633         HIS         -         expression tag         UNP Q6           A         634         HIS         -         expression tag         UNP Q6           A         635         HIS         -         expression tag         UNP Q6           A         636         HIS         -         expression tag         UNP Q6           A         638         HIS         -         expression tag         UNP Q6           A         639         HIS         -         expression tag         UNP Q6           A	nce
A         628         LEU         -         expression tag         UNP QC           A         629         PHE         -         expression tag         UNP QC           A         630         GLN         -         expression tag         UNP QC           A         631         GLY         -         expression tag         UNP QC           A         632         PRO         -         expression tag         UNP QC           A         633         HIS         -         expression tag         UNP QC           A         634         HIS         -         expression tag         UNP QC           A         635         HIS         -         expression tag         UNP QC           A         636         HIS         -         expression tag         UNP QC           A         638         HIS         -         expression tag         UNP QC           A         639         HIS         -         expression tag         UNP QC           A         640         HIS         -         expression tag         UNP QC           A         641         MET         -         expression tag         UNP QC           A	3008
A         629         PHE         -         expression tag         UNP Q6           A         630         GLN         -         expression tag         UNP Q6           A         631         GLY         -         expression tag         UNP Q6           A         632         PRO         -         expression tag         UNP Q6           A         633         HIS         -         expression tag         UNP Q6           A         634         HIS         -         expression tag         UNP Q6           A         635         HIS         -         expression tag         UNP Q6           A         636         HIS         -         expression tag         UNP Q6           A         637         HIS         -         expression tag         UNP Q6           A         638         HIS         -         expression tag         UNP Q6           A         638         HIS         -         expression tag         UNP Q6           A         639         HIS         -         expression tag         UNP Q6           A         640         HIS         -         expression tag         UNP Q6           A	3008
A         630         GLN         -         expression tag         UNP Q6           A         631         GLY         -         expression tag         UNP Q6           A         632         PRO         -         expression tag         UNP Q6           A         633         HIS         -         expression tag         UNP Q6           A         634         HIS         -         expression tag         UNP Q6           A         635         HIS         -         expression tag         UNP Q6           A         636         HIS         -         expression tag         UNP Q6           A         637         HIS         -         expression tag         UNP Q6           A         638         HIS         -         expression tag         UNP Q6           A         639         HIS         -         expression tag         UNP Q6           A         640         HIS         -         expression tag         UNP Q6           A         641         MET         -         expression tag         UNP Q6           A         642         ASP         -         expression tag         UNP Q6           A	3008
A         631         GLY         -         expression tag         UNP Q6           A         632         PRO         -         expression tag         UNP Q6           A         633         HIS         -         expression tag         UNP Q6           A         634         HIS         -         expression tag         UNP Q6           A         635         HIS         -         expression tag         UNP Q6           A         636         HIS         -         expression tag         UNP Q6           A         637         HIS         -         expression tag         UNP Q6           A         638         HIS         -         expression tag         UNP Q6           A         639         HIS         -         expression tag         UNP Q6           A         640         HIS         -         expression tag         UNP Q6           A         641         MET         -         expression tag         UNP Q6           A         642         ASP         -         expression tag         UNP Q6           A         643         GLU         -         expression tag         UNP Q6           A	3008
A 632 PRO - expression tag UNP Q6 A 633 HIS - expression tag UNP Q6 A 634 HIS - expression tag UNP Q6 A 635 HIS - expression tag UNP Q6 A 636 HIS - expression tag UNP Q6 A 637 HIS - expression tag UNP Q6 A 638 HIS - expression tag UNP Q6 A 639 HIS - expression tag UNP Q6 A 640 HIS - expression tag UNP Q6 A 641 MET - expression tag UNP Q6 A 642 ASP - expression tag UNP Q6 A 643 GLU - expression tag UNP Q6 A 644 LYS - expression tag UNP Q6 A 645 THR - expression tag UNP Q6 A 646 THR - expression tag UNP Q6 A 647 GLY - expression tag UNP Q6 A 648 TRP - expression tag UNP Q6 A 650 GLY - expression tag UNP Q6 A 651 GLY - expression tag UNP Q6 A 655 GLU - expression tag UNP Q6 A 656 GLY - expression tag UNP Q6 A 657 LEU - expression tag UNP Q6 A 657 LEU - expression tag UNP Q6 A 658 ALA - expression tag UNP Q6	3008
A 633 HIS - expression tag UNP Q6 A 634 HIS - expression tag UNP Q6 A 635 HIS - expression tag UNP Q6 A 636 HIS - expression tag UNP Q6 A 637 HIS - expression tag UNP Q6 A 638 HIS - expression tag UNP Q6 A 639 HIS - expression tag UNP Q6 A 640 HIS - expression tag UNP Q6 A 641 MET - expression tag UNP Q6 A 642 ASP - expression tag UNP Q6 A 643 GLU - expression tag UNP Q6 A 644 LYS - expression tag UNP Q6 A 645 THR - expression tag UNP Q6 A 646 THR - expression tag UNP Q6 A 647 GLY - expression tag UNP Q6 A 648 TRP - expression tag UNP Q6 A 650 GLY - expression tag UNP Q6 A 651 GLY - expression tag UNP Q6 A 655 GLU - expression tag UNP Q6 A 656 GLY - expression tag UNP Q6 A 657 LEU - expression tag UNP Q6 A 657 LEU - expression tag UNP Q6 A 658 ALA - expression tag UNP Q6	3008
A         634         HIS         -         expression tag         UNP Q6           A         635         HIS         -         expression tag         UNP Q6           A         636         HIS         -         expression tag         UNP Q6           A         637         HIS         -         expression tag         UNP Q6           A         638         HIS         -         expression tag         UNP Q6           A         639         HIS         -         expression tag         UNP Q6           A         640         HIS         -         expression tag         UNP Q6           A         641         MET         -         expression tag         UNP Q6           A         641         MET         -         expression tag         UNP Q6           A         643         GLU         -         expression tag         UNP Q6           A         644         LYS         -         expression tag         UNP Q6           A         645         THR         -         expression tag         UNP Q6           A         646         THR         -         expression tag         UNP Q6           A	3008
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A         637         HIS         -         expression tag         UNP Q6           A         638         HIS         -         expression tag         UNP Q6           A         639         HIS         -         expression tag         UNP Q6           A         640         HIS         -         expression tag         UNP Q6           A         641         MET         -         expression tag         UNP Q6           A         642         ASP         -         expression tag         UNP Q6           A         643         GLU         -         expression tag         UNP Q6           A         644         LYS         -         expression tag         UNP Q6           A         645         THR         -         expression tag         UNP Q6           A         646         THR         -         expression tag         UNP Q6           A         647         GLY         -         expression tag         UNP Q6           A         649         ARG         -         expression tag         UNP Q6           A         650         GLY         -         expression tag         UNP Q6           A	3008
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A         644         LYS         -         expression tag         UNP Q6           A         645         THR         -         expression tag         UNP Q6           A         646         THR         -         expression tag         UNP Q6           A         647         GLY         -         expression tag         UNP Q6           A         648         TRP         -         expression tag         UNP Q6           A         649         ARG         -         expression tag         UNP Q6           A         650         GLY         -         expression tag         UNP Q6           A         651         GLY         -         expression tag         UNP Q6           A         652         HIS         -         expression tag         UNP Q6           A         653         VAL         -         expression tag         UNP Q6           A         654         VAL         -         expression tag         UNP Q6           A         655         GLU         -         expression tag         UNP Q6           A         656         GLY         -         expression tag         UNP Q6           A	3008
A         645         THR         -         expression tag         UNP Q6           A         646         THR         -         expression tag         UNP Q6           A         647         GLY         -         expression tag         UNP Q6           A         648         TRP         -         expression tag         UNP Q6           A         649         ARG         -         expression tag         UNP Q6           A         650         GLY         -         expression tag         UNP Q6           A         651         GLY         -         expression tag         UNP Q6           A         652         HIS         -         expression tag         UNP Q6           A         653         VAL         -         expression tag         UNP Q6           A         654         VAL         -         expression tag         UNP Q6           A         655         GLU         -         expression tag         UNP Q6           A         656         GLY         -         expression tag         UNP Q6           A         657         LEU         -         expression tag         UNP Q6           A	3008
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A         647         GLY         -         expression tag         UNP Q6           A         648         TRP         -         expression tag         UNP Q6           A         649         ARG         -         expression tag         UNP Q6           A         650         GLY         -         expression tag         UNP Q6           A         651         GLY         -         expression tag         UNP Q6           A         652         HIS         -         expression tag         UNP Q6           A         653         VAL         -         expression tag         UNP Q6           A         654         VAL         -         expression tag         UNP Q6           A         655         GLU         -         expression tag         UNP Q6           A         656         GLY         -         expression tag         UNP Q6           A         657         LEU         -         expression tag         UNP Q6           A         658         ALA         -         expression tag         UNP Q6	3008
A         648         TRP         -         expression tag         UNP Q6           A         649         ARG         -         expression tag         UNP Q6           A         650         GLY         -         expression tag         UNP Q6           A         651         GLY         -         expression tag         UNP Q6           A         652         HIS         -         expression tag         UNP Q6           A         653         VAL         -         expression tag         UNP Q6           A         654         VAL         -         expression tag         UNP Q6           A         655         GLU         -         expression tag         UNP Q6           A         656         GLY         -         expression tag         UNP Q6           A         657         LEU         -         expression tag         UNP Q6           A         658         ALA         -         expression tag         UNP Q6	3008
A         649         ARG         -         expression tag         UNP Q6           A         650         GLY         -         expression tag         UNP Q6           A         651         GLY         -         expression tag         UNP Q6           A         652         HIS         -         expression tag         UNP Q6           A         653         VAL         -         expression tag         UNP Q6           A         654         VAL         -         expression tag         UNP Q6           A         655         GLU         -         expression tag         UNP Q6           A         656         GLY         -         expression tag         UNP Q6           A         657         LEU         -         expression tag         UNP Q6           A         658         ALA         -         expression tag         UNP Q6	3008
A         650         GLY         -         expression tag         UNP Q6           A         651         GLY         -         expression tag         UNP Q6           A         652         HIS         -         expression tag         UNP Q6           A         653         VAL         -         expression tag         UNP Q6           A         654         VAL         -         expression tag         UNP Q6           A         655         GLU         -         expression tag         UNP Q6           A         656         GLY         -         expression tag         UNP Q6           A         657         LEU         -         expression tag         UNP Q6           A         658         ALA         -         expression tag         UNP Q6	3008
A         651         GLY         -         expression tag         UNP Q6           A         652         HIS         -         expression tag         UNP Q6           A         653         VAL         -         expression tag         UNP Q6           A         654         VAL         -         expression tag         UNP Q6           A         655         GLU         -         expression tag         UNP Q6           A         656         GLY         -         expression tag         UNP Q6           A         657         LEU         -         expression tag         UNP Q6           A         658         ALA         -         expression tag         UNP Q6	3008
A         652         HIS         -         expression tag         UNP Q6           A         653         VAL         -         expression tag         UNP Q6           A         654         VAL         -         expression tag         UNP Q6           A         655         GLU         -         expression tag         UNP Q6           A         656         GLY         -         expression tag         UNP Q6           A         657         LEU         -         expression tag         UNP Q6           A         658         ALA         -         expression tag         UNP Q6	3008
A         653         VAL         -         expression tag         UNP Q6           A         654         VAL         -         expression tag         UNP Q6           A         655         GLU         -         expression tag         UNP Q6           A         656         GLY         -         expression tag         UNP Q6           A         657         LEU         -         expression tag         UNP Q6           A         658         ALA         -         expression tag         UNP Q6	3008
A         654         VAL         -         expression tag         UNP Q6           A         655         GLU         -         expression tag         UNP Q6           A         656         GLY         -         expression tag         UNP Q6           A         657         LEU         -         expression tag         UNP Q6           A         658         ALA         -         expression tag         UNP Q6	3008
A         655         GLU         -         expression tag         UNP Q6           A         656         GLY         -         expression tag         UNP Q6           A         657         LEU         -         expression tag         UNP Q6           A         658         ALA         -         expression tag         UNP Q6	3008
A 656 GLY - expression tag UNP Q6 A 657 LEU - expression tag UNP Q6 A 658 ALA - expression tag UNP Q6	
A 657 LEU - expression tag UNP Q6 A 658 ALA - expression tag UNP Q6	3008
A 658 ALA - expression tag UNP Q6	
A 659 GLY - expression tag UNP Q6	
A 660 GLU - expression tag UNP Q6	3008
A 661 LEU - expression tag UNP Q6	3008
A 662 GLU - expression tag UNP Q6	3008
A 663 GLN - expression tag UNP Q6	
A 664 LEU - expression tag UNP Q6	3008
A 665 ARG - expression tag UNP Q6	3008
A 666 ALA - expression tag UNP Q6	3008
A 667 ARG - expression tag UNP Q6	3008



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Chain	Residue	Modelled	Actual	Comment	Reference
A	668	LEU	-	expression tag	UNP Q63008
A	669	GLU	-	expression tag	UNP Q63008
A	670	HIS	-	expression tag	UNP Q63008
A	671	HIS	-	expression tag	UNP Q63008
A	672	PRO	-	expression tag	UNP Q63008
A	673	GLN	-	expression tag	UNP Q63008
A	674	GLY	-	expression tag	UNP Q63008
A	675	GLN	-	expression tag	UNP Q63008
A	676	ARG	-	expression tag	UNP Q63008
A	677	GLU	-	expression tag	UNP Q63008
A	678	PRO	-	expression tag	UNP Q63008

• Molecule 2 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula:  $C_{39}H_{77}O_8P$ ) (labeled as "Ligand of Interest" by depositor).



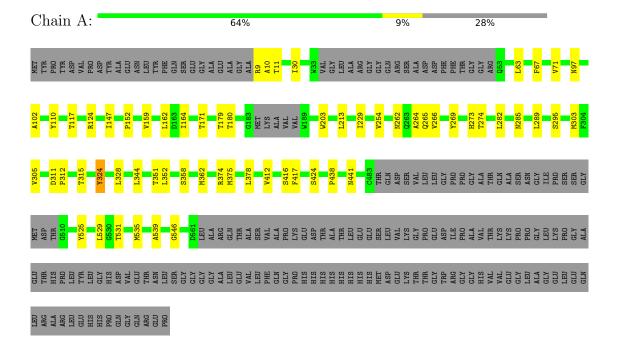
Mol	Chain	Residues	Atoms			AltConf	
2	A	1	Total	С	О	Р	0
_	11	1	42	33	8	1	



# 3 Residue-property plots (i)

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: Sodium/iodide cotransporter





# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	205030	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k 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: 3PH

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).

ſ	Mal	Chain	Bond	lengths	Bond angles		
	MOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
Ī	1	A	0.27	0/3856	0.46	0/5267	

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	3767	0	3878	39	0
2	A	42	0	57	0	0
All	All	3809	0	3935	39	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 5.

The worst 5 of 39 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
1:A:262:ASN:ND2	1:A:265:GLN:OE1	2.07	0.88
1:A:441:ASN:ND2	1:A:546:GLY:O	2.21	0.74



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Atom-1	Atom-2	$egin{aligned} &  ext{Interatomic} \ &  ext{distance} \ &  ext{(Å)} \end{aligned}$	Clash overlap (Å)
1:A:273:HIS:O	1:A:274:THR:OG1	2.10	0.70
1:A:162:LEU:O	1:A:162:LEU:HD23	1.98	0.64
1:A:117:THR:HG21	1:A:266:VAL:HG11	1.81	0.62

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	495/694 (71%)	468 (94%)	27 (6%)	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	397/544 (73%)	393 (99%)	4 (1%)	76 86	

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

Mol	Chain	Res	Type
1	A	97	ASN
1	A	110	TYR
1	A	324	TYR



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Mol	Chain	Res	Type
1	A	424	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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 monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

1 ligand is 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	Pog	Link	Bo	ond leng	$ ag{ths}$	В	ond ang	eles
MIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	3PH	A	701	-	41,41,47	0.66	1 (2%)	45,46,52	0.77	2 (4%)

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	3PH	A	701	-	-	13/43/43/49	-



All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
2	A	701	3PH	P-O14	2.85	1.65	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	701	3PH	O13-P-O12	3.28	123.51	110.68
2	A	701	3PH	O14-P-O11	-2.09	101.18	106.73

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

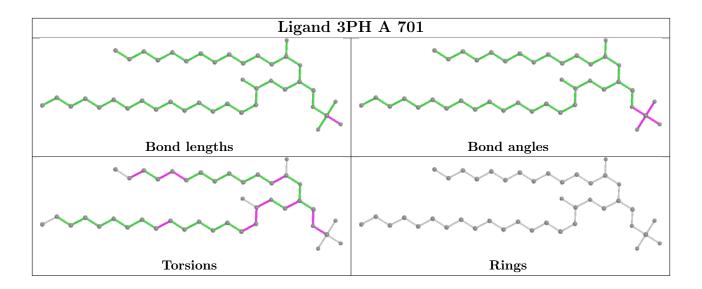
Mol	Chain	Res	Type	Atoms
2	A	701	3PH	C31-C32-C33-C34
2	A	701	3PH	C32-C31-O31-C3
2	A	701	3PH	O21-C2-C3-O31
2	A	701	3PH	O32-C31-O31-C3
2	A	701	3PH	C28-C29-C2A-C2B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





# 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.

