



Full wwPDB EM Validation Report ⓘ

Dec 24, 2022 – 12:50 PM EST

PDB ID : 7UV0
EMDB ID : EMD-26808
Title : Structure of the sodium/iodide symporter (NIS) in complex with iodide and sodium
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 : 3.10 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**
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

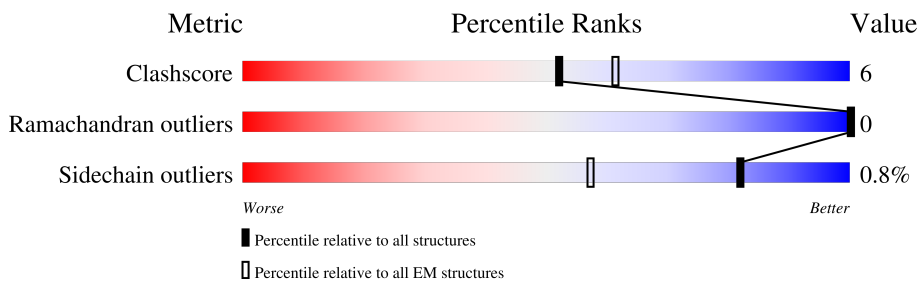
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	694	 62% 10% 28%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3784 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	501	3739	2461	594	657	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	626	GLU	-	expression tag	UNP Q63008
A	627	VAL	-	expression tag	UNP Q63008
A	628	LEU	-	expression tag	UNP Q63008
A	629	PHE	-	expression tag	UNP Q63008
A	630	GLN	-	expression tag	UNP Q63008
A	631	GLY	-	expression tag	UNP Q63008
A	632	PRO	-	expression tag	UNP Q63008
A	633	HIS	-	expression tag	UNP Q63008
A	634	HIS	-	expression tag	UNP Q63008
A	635	HIS	-	expression tag	UNP Q63008
A	636	HIS	-	expression tag	UNP Q63008
A	637	HIS	-	expression tag	UNP Q63008
A	638	HIS	-	expression tag	UNP Q63008
A	639	HIS	-	expression tag	UNP Q63008
A	640	HIS	-	expression tag	UNP Q63008
A	641	MET	-	expression tag	UNP Q63008
A	642	ASP	-	expression tag	UNP Q63008
A	643	GLU	-	expression tag	UNP Q63008
A	644	LYS	-	expression tag	UNP Q63008
A	645	THR	-	expression tag	UNP Q63008
A	646	THR	-	expression tag	UNP Q63008
A	647	GLY	-	expression tag	UNP Q63008
A	648	TRP	-	expression tag	UNP Q63008
A	649	ARG	-	expression tag	UNP Q63008
A	650	GLY	-	expression tag	UNP Q63008
A	651	GLY	-	expression tag	UNP Q63008
A	652	HIS	-	expression tag	UNP Q63008
A	653	VAL	-	expression tag	UNP Q63008
A	654	VAL	-	expression tag	UNP Q63008
A	655	GLU	-	expression tag	UNP Q63008
A	656	GLY	-	expression tag	UNP Q63008
A	657	LEU	-	expression tag	UNP Q63008
A	658	ALA	-	expression tag	UNP Q63008
A	659	GLY	-	expression tag	UNP Q63008
A	660	GLU	-	expression tag	UNP Q63008
A	661	LEU	-	expression tag	UNP Q63008
A	662	GLU	-	expression tag	UNP Q63008
A	663	GLN	-	expression tag	UNP Q63008
A	664	LEU	-	expression tag	UNP Q63008
A	665	ARG	-	expression tag	UNP Q63008
A	666	ALA	-	expression tag	UNP Q63008
A	667	ARG	-	expression tag	UNP Q63008

Continued on next page...

Continued from previous page...

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

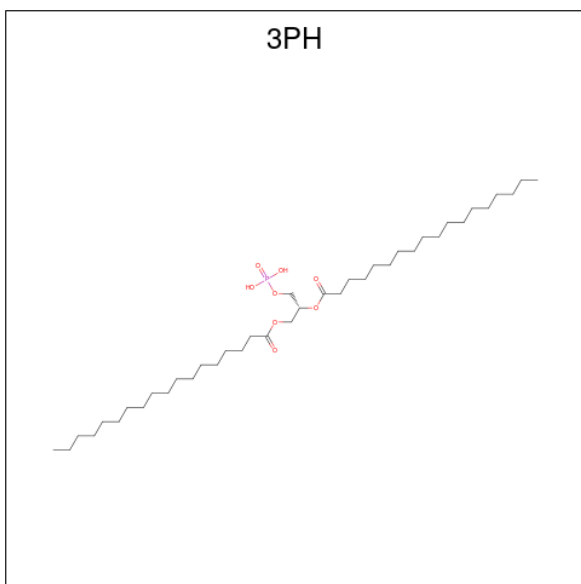
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	AltConf
2	A	2	Total Na 2 2	0

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total I 1 1	0

- Molecule 4 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: C₃₉H₇₇O₈P) (labeled as "Ligand of Interest" by depositor).

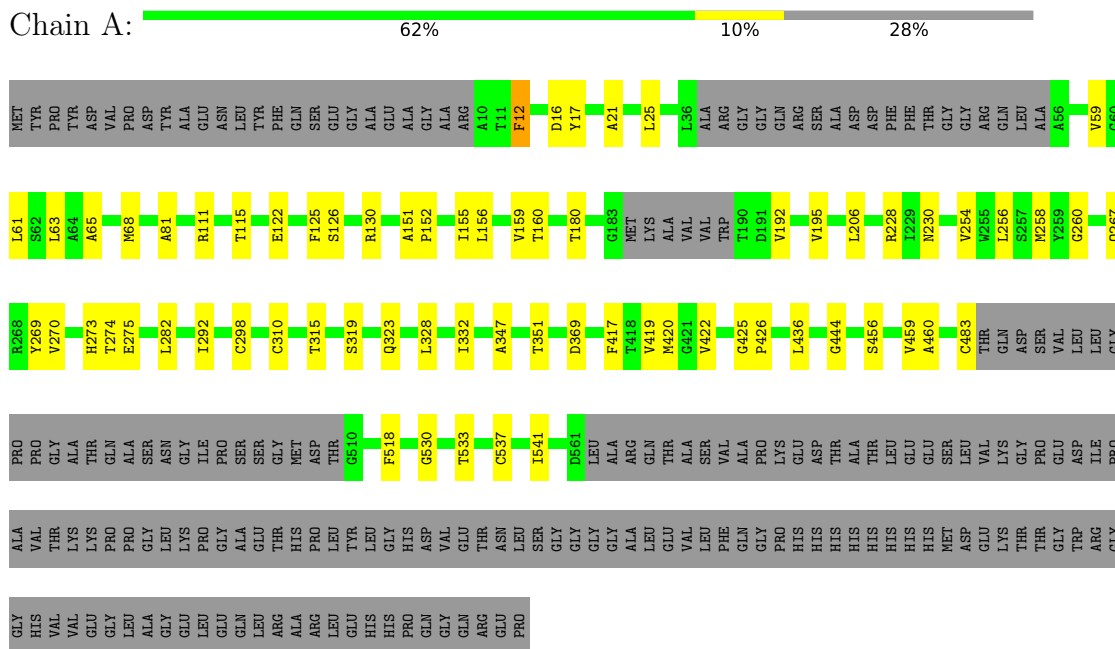


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
4	A	1	42	33	8	1	0

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

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	384418	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	-0.15	Depositor
Maximum defocus (nm)	-0.24	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: NA, IOD, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	0/3826	0.46	0/5226

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	3739	0	3854	44	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	42	0	57	0	0
All	All	3784	0	3911	44	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (44) 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:A:156:LEU:O	1:A:160:THR:HG22	1.96	0.64
1:A:65:ALA:HB2	1:A:195:VAL:HG23	1.84	0.60
1:A:115:THR:O	1:A:267:GLN:NE2	2.34	0.60
1:A:310:CYS:SG	1:A:483:CYS:N	2.75	0.59
1:A:111:ARG:NH1	1:A:275:GLU:OE1	2.36	0.58
1:A:125:PHE:O	1:A:126:SER:OG	2.16	0.57
1:A:122:GLU:OE1	1:A:130:ARG:NH1	2.38	0.56
1:A:530:GLY:O	1:A:533:THR:HG22	2.06	0.56
1:A:537:CYS:O	1:A:541:ILE:HG22	2.06	0.55
1:A:81:ALA:O	1:A:228:ARG:NE	2.39	0.54
1:A:17:TYR:OH	1:A:160:THR:O	2.26	0.53
1:A:328:LEU:HD11	1:A:332:ILE:HD11	1.93	0.51
1:A:444:GLY:HA2	1:A:541:ILE:HG23	1.92	0.50
1:A:152:PRO:HG3	1:A:351:THR:HG21	1.94	0.49
1:A:422:VAL:HG21	1:A:460:ALA:HB2	1.95	0.48
1:A:273:HIS:O	1:A:274:THR:HG22	2.14	0.47
1:A:319:SER:OG	1:A:323:GLN:NE2	2.42	0.47
1:A:254:VAL:HG11	1:A:417:PHE:HD1	1.80	0.46
1:A:273:HIS:C	1:A:274:THR:HG22	2.34	0.46
1:A:61:LEU:HD22	1:A:192:VAL:HG23	1.98	0.45
1:A:155:ILE:O	1:A:159:VAL:HG22	2.16	0.45
1:A:459:VAL:CG1	1:A:518:PHE:CZ	3.01	0.44
1:A:68:MET:HG3	1:A:292:ILE:HD13	2.00	0.44
1:A:270:VAL:HG12	1:A:270:VAL:O	2.17	0.44
1:A:315:THR:HG22	1:A:315:THR:O	2.18	0.43
1:A:63:LEU:HD21	1:A:269:TYR:CE1	2.53	0.43
1:A:206:LEU:HD11	1:A:298:CYS:HB3	2.00	0.42
1:A:422:VAL:HA	1:A:456:SER:OG	2.19	0.42
1:A:155:ILE:O	1:A:159:VAL:HG13	2.18	0.42
1:A:230:ASN:OD1	1:A:230:ASN:N	2.52	0.42
1:A:180:THR:HG22	1:A:180:THR:O	2.20	0.42
1:A:419:VAL:HG23	1:A:420:MET:N	2.34	0.42
1:A:65:ALA:CB	1:A:195:VAL:HG23	2.48	0.42
1:A:59:VAL:O	1:A:63:LEU:HD13	2.20	0.41
1:A:21:ALA:O	1:A:25:LEU:HG	2.21	0.41
1:A:12:PHE:CE1	1:A:159:VAL:HB	2.55	0.41
1:A:151:ALA:HB3	1:A:152:PRO:HD3	2.02	0.41
1:A:269:TYR:OH	1:A:282:LEU:HD13	2.20	0.41
1:A:425:GLY:N	1:A:426:PRO:HD2	2.36	0.41
1:A:152:PRO:HG3	1:A:351:THR:CG2	2.50	0.40
1:A:258:MET:CG	1:A:420:MET:HG2	2.51	0.40
1:A:256:LEU:O	1:A:260:GLY:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:PHE:CD2	1:A:16:ASP:HB3	2.57	0.40
1:A:347:ALA:O	1:A:351:THR:HG22	2.20	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	493/694 (71%)	455 (92%)	38 (8%)	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	395/544 (73%)	392 (99%)	3 (1%)	81 92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	PHE
1	A	369	ASP
1	A	436	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	GLN

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](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z > 2$
4	3PH	A	704	-	41,41,47	0.66	1 (2%)	45,46,52	0.75	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
4	3PH	A	704	-	-	16/43/43/49	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	704	3PH	P-O13	2.86	1.65	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	704	3PH	O14-P-O12	3.37	123.88	110.68
4	A	704	3PH	O13-P-O11	-2.01	101.39	106.73

There are no chirality outliers.

All (16) torsion outliers are listed below:

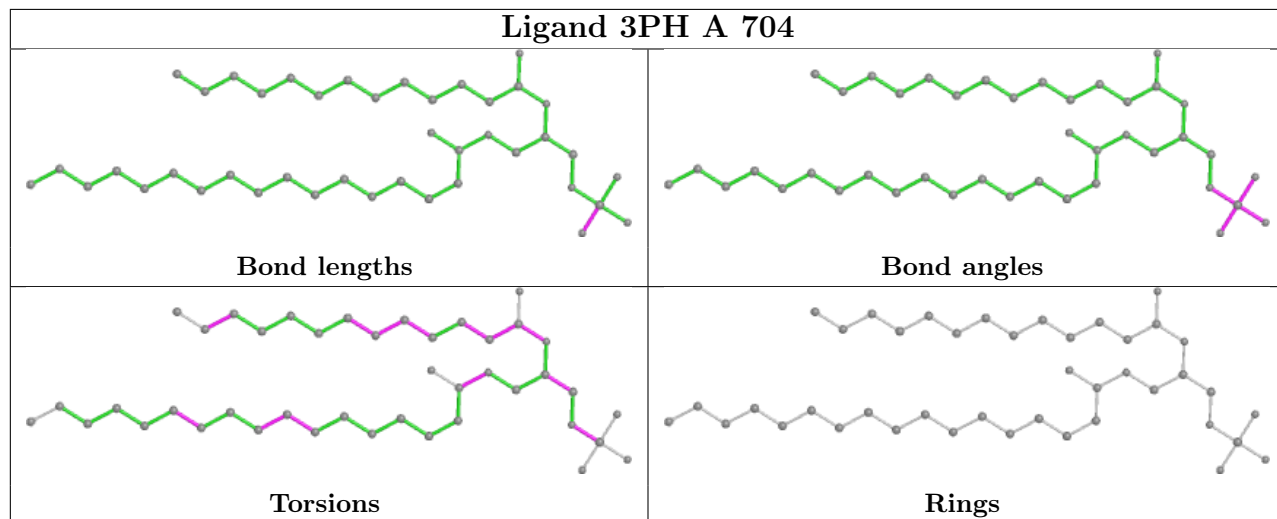
Mol	Chain	Res	Type	Atoms
4	A	704	3PH	C22-C21-O21-C2
4	A	704	3PH	O22-C21-O21-C2
4	A	704	3PH	C32-C31-O31-C3
4	A	704	3PH	O32-C31-O31-C3
4	A	704	3PH	C21-C22-C23-C24
4	A	704	3PH	C3A-C3B-C3C-C3D
4	A	704	3PH	C25-C26-C27-C28
4	A	704	3PH	C1-O11-P-O12
4	A	704	3PH	C24-C25-C26-C27
4	A	704	3PH	C2A-C2B-C2C-C2D
4	A	704	3PH	C36-C37-C38-C39
4	A	704	3PH	C23-C24-C25-C26
4	A	704	3PH	C37-C38-C39-C3A
4	A	704	3PH	O11-C1-C2-O21
4	A	704	3PH	O21-C21-C22-C23
4	A	704	3PH	O22-C21-C22-C23

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 than 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.