



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2024 – 10:14 am GMT

PDB ID : 4CZ8  
Title : Structure of the sodium proton antiporter PaNhaP from *Pyrococcus abyssi* at pH 8.  
Authors : Woehlert, D.; Kuhlbrandt, W.; Yildiz, O.  
Deposited on : 2014-04-16  
Resolution : 3.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

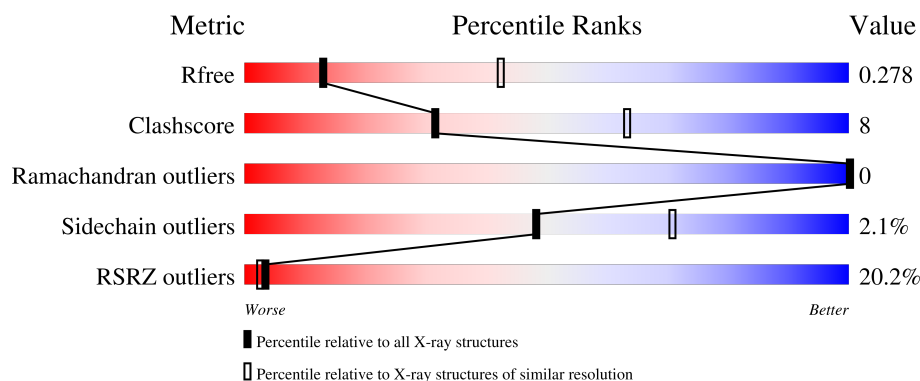
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	2168 (3.20-3.12)
Clashscore	180529	2333 (3.20-3.12)
Ramachandran outliers	177936	2266 (3.20-3.12)
Sidechain outliers	177891	2265 (3.20-3.12)
RSRZ outliers	164620	2169 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	422	<div> <div>21%</div> <div>79%</div> <div>21%</div> </div>
1	B	422	<div> <div>18%</div> <div>80%</div> <div>19%</div> </div>

## 2 Entry composition [i](#)

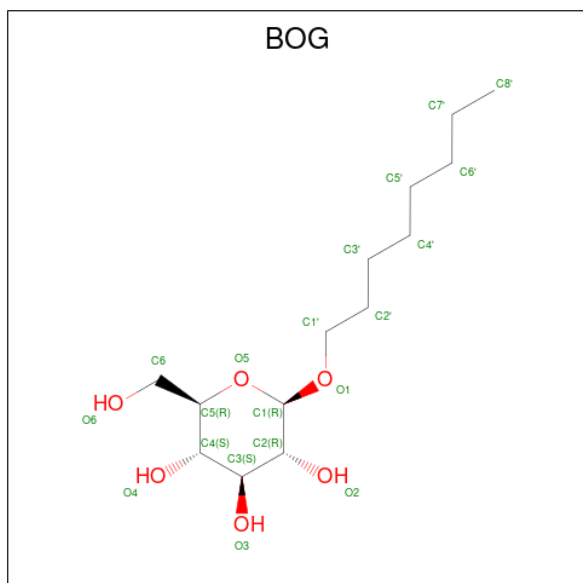
There are 6 unique types of molecules in this entry. The entry contains 6715 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 NA<sup>+</sup>/H<sup>+</sup> ANTIporter, PUTATIVE.

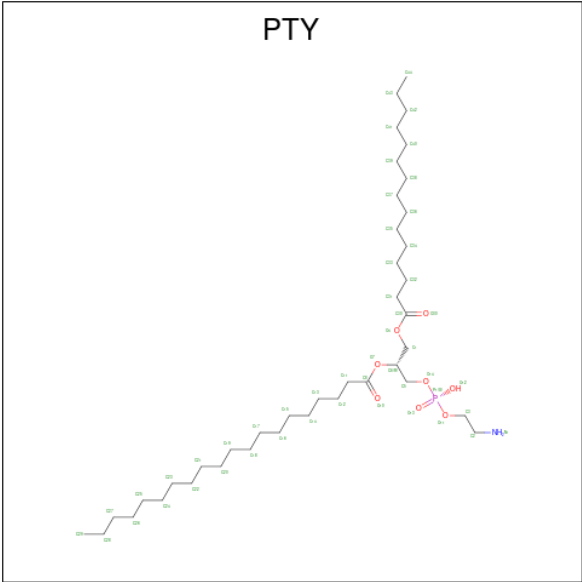
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	Se	0	0	0
			3295	2217	516	555	7			
1	B	421	Total	C	N	O	Se	0	0	0
			3287	2212	515	554	6			

- Molecule 2 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



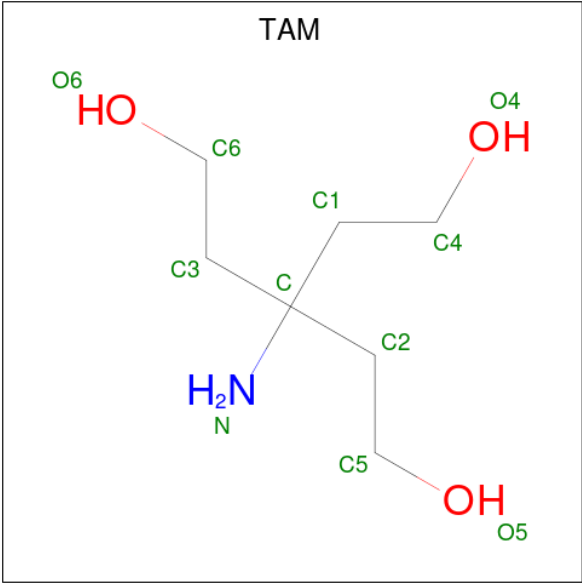
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: C<sub>40</sub>H<sub>80</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

- Molecule 4 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: C<sub>7</sub>H<sub>17</sub>NO<sub>3</sub>).



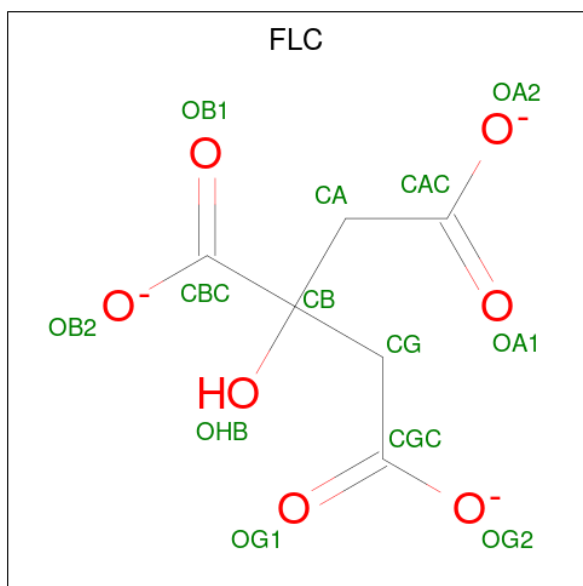
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			11	7	1	3		
4	A	1	Total	C	N	O	0	0
			11	7	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 5 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7^-$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			13	6	7		
5	B	1	Total	C	O	0	0
			13	6	7		

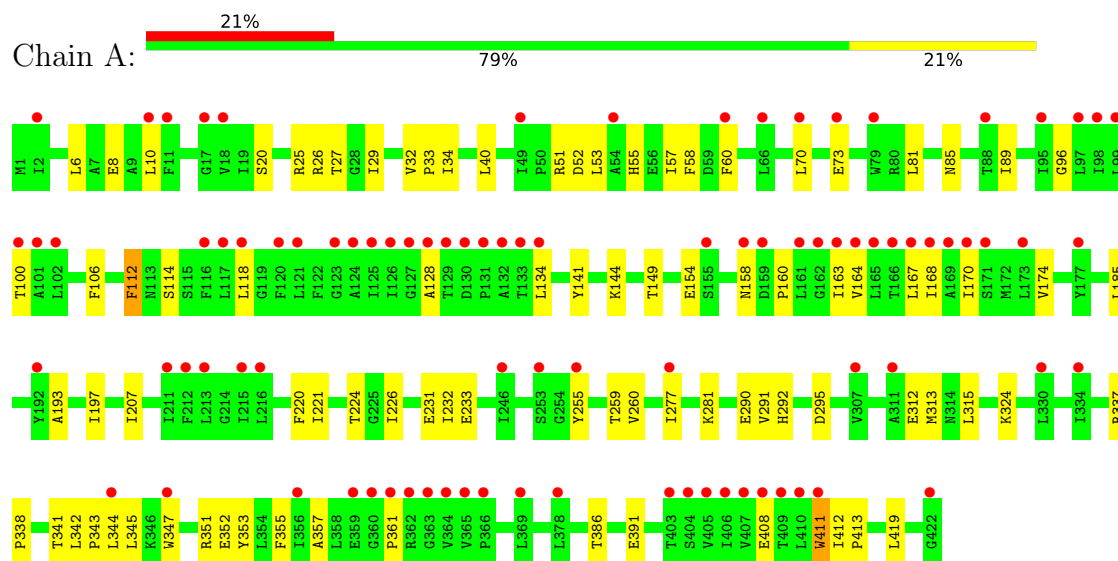
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		
6	B	2	Total	O	0	0
			2	2		

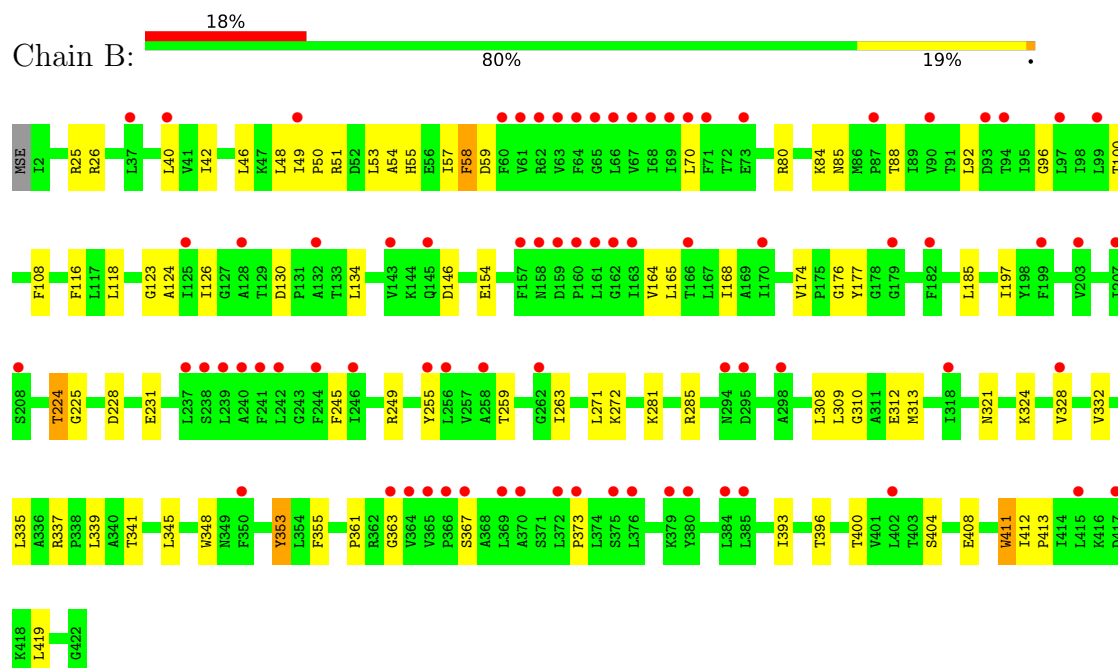
### 3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: NA<sup>+</sup>/H<sup>+</sup> ANTIPTORTER, PUTATIVE



- Molecule 1: NA<sup>+</sup>/H<sup>+</sup> ANTIPTORTER, PUTATIVE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.49Å 107.94Å 107.93Å 90.00° 95.19° 90.00°	Depositor
Resolution (Å)	48.49 – 3.15 48.49 – 3.15	Depositor EDS
% Data completeness (in resolution range)	96.7 (48.49-3.15) 97.6 (48.49-3.15)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 3.12Å)	Xtriage
Refinement program		Depositor
R, $R_{free}$	0.239 , 0.276 0.254 , 0.278	Depositor DCC
$R_{free}$ test set	1088 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	121.2	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 76.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	6715	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BOG, FLC, PTY, TAM

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	0.24	0/3362	0.42	0/4564
1	B	0.24	0/3354	0.42	0/4554
All	All	0.24	0/6716	0.42	0/9118

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

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	3295	0	3534	59	0
1	B	3287	0	3522	52	0
2	A	20	0	28	2	0
3	A	50	0	79	2	0
4	A	22	0	34	5	0
4	B	11	0	17	3	0
5	B	26	0	10	1	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
All	All	6715	0	7224	112	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 8.

All (112) 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:51:ARG:NH1	1:B:312:GLU:O	2.24	0.71
1:A:160:PRO:HG3	1:A:259:THR:HG21	1.73	0.70
1:B:174:VAL:HG12	1:B:176:GLY:H	1.58	0.69
1:A:6:LEU:HD13	1:A:53:LEU:HD11	1.78	0.65
1:A:221:ILE:HG23	1:A:226:ILE:HB	1.79	0.65
1:A:144:LYS:NZ	1:A:352:GLU:OE2	2.29	0.65
3:A:1424:PTY:H211	3:A:1424:PTY:H271	1.80	0.63
1:A:8:GLU:OE2	1:B:249:ARG:NH1	2.32	0.62
1:B:134:LEU:HD11	1:B:361:PRO:HD3	1.82	0.61
1:A:141:TYR:HE2	1:A:413:PRO:HB3	1.65	0.61
1:A:26:ARG:NH2	1:B:225:GLY:O	2.34	0.61
1:B:321:ASN:HA	1:B:324:LYS:HE3	1.84	0.60
1:A:185:LEU:HD23	1:A:197:ILE:HG23	1.83	0.60
1:B:355:PHE:HB2	1:B:419:LEU:HD13	1.84	0.59
1:A:338:PRO:O	1:A:353:TYR:OH	2.21	0.58
1:A:224:THR:HG23	1:A:226:ILE:HG13	1.86	0.57
1:A:163:ILE:O	1:A:167:LEU:N	2.37	0.57
1:A:10:LEU:HD21	1:A:57:ILE:HD12	1.86	0.56
1:A:337:ARG:O	1:A:341:THR:OG1	2.14	0.56
1:A:128:ALA:HA	1:A:158:ASN:HB3	1.86	0.56
1:A:26:ARG:NH2	1:B:224:THR:O	2.33	0.56
1:A:20:SER:HB3	1:A:34:ILE:HG22	1.87	0.56
1:A:342:LEU:N	1:A:343:PRO:HD2	2.21	0.56
1:A:26:ARG:NH1	1:B:231:GLU:OE2	2.40	0.55
1:B:185:LEU:HD23	1:B:197:ILE:HG23	1.89	0.55
1:B:123:GLY:HA2	1:B:126:ILE:HG22	1.87	0.54
1:B:310:GLY:HA2	1:B:313:MSE:HE3	1.89	0.54
1:B:88:THR:HG1	1:B:348:TRP:HE1	1.55	0.54
1:A:81:LEU:HB3	1:A:149:THR:HG21	1.90	0.53
1:A:112:PHE:HD2	1:A:324:LYS:HD3	1.74	0.53
1:B:54:ALA:O	1:B:58:PHE:HB2	2.08	0.53
1:A:207:ILE:HA	1:A:260:VAL:HG21	1.91	0.53
1:B:337:ARG:O	1:B:341:THR:OG1	2.19	0.53
1:A:292:HIS:HB2	2:A:1423:BOG:H3'2	1.91	0.52
1:A:351:ARG:HB3	1:A:419:LEU:HB2	1.92	0.52
1:B:408:GLU:OE1	1:B:411:TRP:NE1	2.43	0.52
1:A:55:HIS:ND1	1:A:312:GLU:OE2	2.42	0.52
1:A:25:ARG:NH1	1:B:228:ASP:OD2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LEU:HD12	1:B:255:TYR:HB3	1.92	0.51
4:B:1425:TAM:O5	4:B:1425:TAM:N	2.41	0.51
1:A:70:LEU:HD12	1:A:255:TYR:HB3	1.93	0.51
1:A:53:LEU:O	1:A:57:ILE:HG12	2.11	0.51
1:B:309:LEU:HD22	1:B:367:SER:HB3	1.91	0.51
1:A:141:TYR:CE2	1:A:413:PRO:HB3	2.47	0.50
5:B:1424:FLC:OHB	5:B:1424:FLC:OA2	2.27	0.50
1:B:55:HIS:ND1	1:B:312:GLU:OE2	2.40	0.49
1:A:51:ARG:NH2	1:A:391:GLU:OE2	2.38	0.49
1:B:59:ASP:O	4:B:1425:TAM:O5	2.31	0.49
1:A:295:ASP:OD1	4:A:1425:TAM:O6	2.19	0.48
1:B:228:ASP:OD1	1:B:228:ASP:N	2.41	0.48
1:B:335:LEU:O	1:B:339:LEU:HB2	2.14	0.48
1:A:164:VAL:O	1:A:168:ILE:HG12	2.14	0.48
1:B:396:THR:O	1:B:400:THR:HG22	2.13	0.47
4:A:1425:TAM:O6	4:A:1425:TAM:N	2.48	0.47
1:B:57:ILE:HG22	1:B:308:LEU:HD11	1.97	0.47
2:A:1423:BOG:O6	2:A:1423:BOG:O4	2.28	0.47
1:B:42:ILE:HD12	1:B:49:ILE:HD12	1.97	0.46
1:B:92:LEU:HB3	1:B:154:GLU:HG3	1.96	0.46
1:B:412:ILE:HG23	1:B:413:PRO:HD3	1.97	0.46
4:A:1425:TAM:H21	4:A:1425:TAM:H41	1.40	0.46
1:A:338:PRO:HB3	1:A:357:ALA:HB1	1.98	0.46
1:A:315:LEU:HD22	1:A:315:LEU:H	1.81	0.46
1:B:40:LEU:HD11	1:B:313:MSE:SE	2.66	0.45
1:B:404:SER:O	1:B:408:GLU:HG2	2.17	0.45
1:A:96:GLY:O	1:A:100:THR:OG1	2.25	0.45
1:B:124:ALA:HB1	1:B:165:LEU:HB3	1.99	0.45
1:B:46:LEU:HB3	1:B:48:LEU:HG	1.98	0.44
1:B:130:ASP:HB3	1:B:363:GLY:HA3	1.98	0.44
1:B:408:GLU:HA	1:B:411:TRP:CD1	2.52	0.44
1:A:233:GLU:HG3	1:A:290:GLU:HA	1.99	0.44
1:A:220:PHE:O	1:A:224:THR:HG22	2.17	0.44
1:B:50:PRO:HG2	1:B:53:LEU:HB3	1.99	0.44
1:A:85:ASN:O	1:A:89:ILE:HG12	2.18	0.43
1:B:164:VAL:O	1:B:168:ILE:HG12	2.19	0.43
1:B:373:PRO:HG3	1:B:393:ILE:HG21	2.01	0.43
4:B:1425:TAM:H11	4:B:1425:TAM:H62	1.67	0.43
1:A:277:ILE:O	1:A:281:LYS:HG2	2.19	0.43
1:B:361:PRO:HB3	1:B:408:GLU:HG3	2.01	0.43
1:A:32:VAL:HB	1:A:33:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:LEU:HD23	1:B:353:TYR:CD2	2.53	0.43
1:A:60:PHE:CD2	3:A:1424:PTY:H111	2.54	0.43
1:A:70:LEU:HB3	1:A:259:THR:HG22	2.00	0.43
1:A:408:GLU:HA	1:A:411:TRP:NE1	2.34	0.43
1:B:272:LYS:HA	1:B:272:LYS:HD3	1.76	0.43
1:B:245:PHE:O	1:B:249:ARG:HB2	2.19	0.42
1:A:291:VAL:O	1:A:295:ASP:HB2	2.20	0.42
1:B:324:LYS:O	1:B:328:VAL:HG23	2.19	0.42
1:A:70:LEU:HB3	1:A:259:THR:CG2	2.50	0.42
1:A:40:LEU:HD13	1:A:313:MSE:HE3	2.02	0.42
1:A:224:THR:O	1:B:26:ARG:NH2	2.41	0.42
1:B:281:LYS:O	1:B:285:ARG:HG2	2.19	0.42
1:A:114:SER:HB2	1:A:118:LEU:HD12	2.01	0.42
1:B:259:THR:O	1:B:263:ILE:HG13	2.20	0.42
1:A:27:THR:HB	1:A:29:ILE:HG13	2.01	0.42
1:B:85:ASN:ND2	1:B:146:ASP:OD1	2.53	0.42
1:A:170:ILE:O	1:A:174:VAL:HG22	2.19	0.41
1:A:408:GLU:HA	1:A:411:TRP:CD1	2.55	0.41
4:A:1426:TAM:H42	4:A:1426:TAM:H21	1.56	0.41
1:A:412:ILE:HG23	1:A:413:PRO:HD3	2.02	0.41
1:B:108:PHE:HE2	1:B:118:LEU:HD22	1.86	0.41
1:B:328:VAL:O	1:B:332:VAL:HG13	2.21	0.41
1:A:193:ALA:O	1:A:197:ILE:HG22	2.21	0.41
1:A:231:GLU:OE2	1:B:25:ARG:HD2	2.21	0.41
1:A:232:ILE:HG13	1:A:290:GLU:HB2	2.03	0.41
1:A:344:LEU:HD12	1:A:344:LEU:HA	1.83	0.41
1:A:355:PHE:HB2	1:A:419:LEU:HD22	2.03	0.41
1:A:134:LEU:HD11	1:A:361:PRO:HD3	2.02	0.41
1:A:73:GLU:HG2	4:A:1425:TAM:H52	2.03	0.40
1:A:154:GLU:CD	1:A:337:ARG:HH22	2.25	0.40
1:B:165:LEU:HD23	1:B:165:LEU:HA	1.92	0.40
1:B:80:ARG:O	1:B:84:LYS:HG2	2.22	0.40
1:B:96:GLY:O	1:B:100:THR:OG1	2.32	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	420/422 (100%)	398 (95%)	22 (5%)	0	100	100
1	B	419/422 (99%)	395 (94%)	24 (6%)	0	100	100
All	All	839/844 (99%)	793 (94%)	46 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	359/352 (102%)	351 (98%)	8 (2%)	47	70
1	B	358/352 (102%)	351 (98%)	7 (2%)	50	72
All	All	717/704 (102%)	702 (98%)	15 (2%)	48	71

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	58	PHE
1	A	106	PHE
1	A	112	PHE
1	A	345	LEU
1	A	347	TRP
1	A	386	THR
1	A	411	TRP

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Mol	Chain	Res	Type
1	B	58	PHE
1	B	116	PHE
1	B	177	TYR
1	B	224	THR
1	B	271	LEU
1	B	353	TYR
1	B	411	TRP

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	TAM	B	1425	-	7,10,10	1.27	1 (14%)	9,12,12	0.56	0
2	BOG	A	1423	-	20,20,20	0.49	0	25,25,25	0.79	1 (4%)
5	FLC	B	1424	-	12,12,12	1.27	0	17,17,17	1.52	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PTY	A	1424	-	49,49,49	1.01	3 (6%)	52,54,54	1.05	2 (3%)
5	FLC	B	1423	-	12,12,12	1.22	0	17,17,17	1.49	1 (5%)
4	TAM	A	1426	-	7,10,10	1.25	0	9,12,12	0.54	0
4	TAM	A	1425	-	7,10,10	1.27	1 (14%)	9,12,12	0.54	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
4	TAM	B	1425	-	-	3/12/12/12	-
2	BOG	A	1423	-	-	8/11/31/31	0/1/1/1
5	FLC	B	1424	-	-	11/16/16/16	-
3	PTY	A	1424	-	-	22/53/53/53	-
5	FLC	B	1423	-	-	7/16/16/16	-
4	TAM	A	1426	-	-	6/12/12/12	-
4	TAM	A	1425	-	-	7/12/12/12	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1424	PTY	O4-C30	3.71	1.44	1.33
3	A	1424	PTY	O7-C8	3.20	1.43	1.34
3	A	1424	PTY	O7-C6	-2.22	1.41	1.46
4	A	1425	TAM	C1-C4	-2.11	1.47	1.52
4	B	1425	TAM	C1-C4	-2.05	1.48	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1424	FLC	OB2-CBC-CB	4.01	120.02	113.05
5	B	1423	FLC	OB2-CBC-CB	3.91	119.84	113.05
3	A	1424	PTY	O7-C8-C11	3.60	119.26	111.50
3	A	1424	PTY	O4-C30-C31	2.47	119.66	111.91
2	A	1423	BOG	C1-O5-C5	-2.04	109.68	113.69

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1423	BOG	C2-C1-O1-C1'
2	A	1423	BOG	O5-C1-O1-C1'
3	A	1424	PTY	N1-C2-C3-O11
3	A	1424	PTY	C5-O14-P1-O11
3	A	1424	PTY	C5-O14-P1-O13
4	A	1425	TAM	C3-C-C1-C4
4	A	1425	TAM	N-C-C1-C4
4	A	1425	TAM	C1-C-C2-C5
4	A	1425	TAM	N-C-C2-C5
4	A	1426	TAM	C3-C-C1-C4
4	A	1426	TAM	N-C-C1-C4
4	A	1426	TAM	C1-C-C2-C5
4	A	1426	TAM	C3-C-C2-C5
4	A	1426	TAM	N-C-C2-C5
4	B	1425	TAM	C3-C-C1-C4
4	B	1425	TAM	N-C-C1-C4
5	B	1423	FLC	CG-CB-CBC-OB1
5	B	1423	FLC	CG-CB-CBC-OB2
5	B	1423	FLC	OHB-CB-CBC-OB1
5	B	1423	FLC	OHB-CB-CBC-OB2
5	B	1424	FLC	CG-CB-CBC-OB1
5	B	1424	FLC	CG-CB-CBC-OB2
5	B	1424	FLC	OHB-CB-CBC-OB2
2	A	1423	BOG	O5-C5-C6-O6
5	B	1424	FLC	CAC-CA-CB-CBC
5	B	1424	FLC	CAC-CA-CB-CG
3	A	1424	PTY	O4-C1-C6-O7
3	A	1424	PTY	C15-C16-C17-C18
3	A	1424	PTY	C13-C14-C15-C16
3	A	1424	PTY	C21-C22-C23-C24
3	A	1424	PTY	C40-C41-C42-C43
5	B	1423	FLC	CAC-CA-CB-CBC
4	A	1425	TAM	C2-C-C1-C4
4	A	1425	TAM	C3-C-C2-C5
4	A	1426	TAM	C2-C-C1-C4
3	A	1424	PTY	O4-C1-C6-C5
3	A	1424	PTY	C24-C25-C26-C27
4	A	1425	TAM	C-C2-C5-O5
5	B	1423	FLC	CAC-CA-CB-CG
5	B	1423	FLC	CAC-CA-CB-OHB
5	B	1424	FLC	CAC-CA-CB-OHB
2	A	1423	BOG	C1'-C2'-C3'-C4'
5	B	1424	FLC	CA-CB-CBC-OB2

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Mol	Chain	Res	Type	Atoms
3	A	1424	PTY	C18-C19-C20-C21
3	A	1424	PTY	C14-C15-C16-C17
2	A	1423	BOG	C3'-C4'-C5'-C6'
3	A	1424	PTY	C36-C37-C38-C39
5	B	1424	FLC	CA-CB-CBC-OB1
3	A	1424	PTY	C26-C27-C28-C29
3	A	1424	PTY	C41-C42-C43-C44
3	A	1424	PTY	C31-C32-C33-C34
3	A	1424	PTY	C3-O11-P1-O14
3	A	1424	PTY	C39-C40-C41-C42
2	A	1423	BOG	C4-C5-C6-O6
3	A	1424	PTY	C16-C17-C18-C19
5	B	1424	FLC	OHB-CB-CBC-OB1
4	B	1425	TAM	C2-C-C1-C4
2	A	1423	BOG	C2'-C3'-C4'-C5'
3	A	1424	PTY	C11-C12-C13-C14
5	B	1424	FLC	CB-CA-CAC-OA1
5	B	1424	FLC	CB-CA-CAC-OA2
2	A	1423	BOG	O1-C1'-C2'-C3'
3	A	1424	PTY	C2-C3-O11-P1
3	A	1424	PTY	O4-C30-C31-C32

There are no ring outliers.

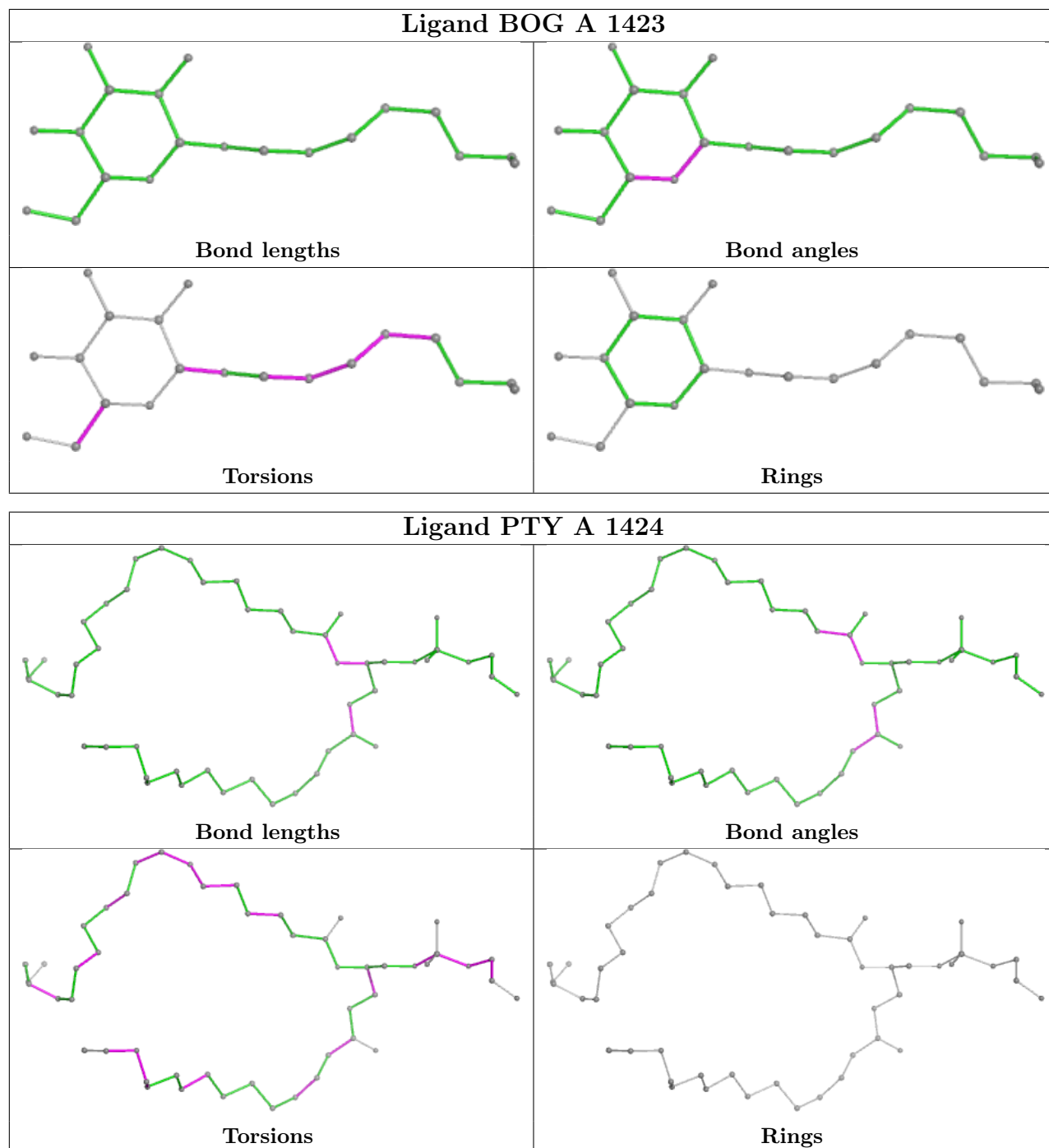
6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1425	TAM	3	0
2	A	1423	BOG	2	0
5	B	1424	FLC	1	0
3	A	1424	PTY	2	0
4	A	1426	TAM	1	0
4	A	1425	TAM	4	0

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	415/422 (98%)	1.37	90 (21%) 3 2	80, 131, 175, 200	0
1	B	415/422 (98%)	0.91	78 (18%) 4 3	75, 128, 175, 203	0
All	All	830/844 (98%)	1.14	168 (20%) 3 2	75, 130, 175, 203	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	ASP	15.9
1	A	130	ASP	13.8
1	A	125	ILE	13.0
1	A	169	ALA	11.4
1	A	129	THR	11.2
1	A	120	PHE	10.9
1	A	362	ARG	10.5
1	A	124	ALA	10.4
1	A	128	ALA	10.4
1	A	166	THR	10.3
1	A	163	ILE	10.2
1	A	170	ILE	10.1
1	A	117	LEU	9.8
1	A	361	PRO	9.1
1	A	121	LEU	9.1
1	A	407	VAL	8.6
1	A	127	GLY	8.2
1	B	255	TYR	7.9
1	A	363	GLY	7.8
1	A	162	GLY	7.6
1	A	406	ILE	7.5
1	B	94	THR	7.5
1	B	93	ASP	7.4
1	B	66	LEU	7.3

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Mol	Chain	Res	Type	RSRZ
1	A	365	VAL	7.2
1	B	161	LEU	7.2
1	B	241	PHE	7.2
1	A	126	ILE	7.1
1	A	168	ILE	6.9
1	A	404	SER	6.9
1	A	360	GLY	6.9
1	B	60	PHE	6.7
1	A	405	VAL	6.7
1	B	70	LEU	6.7
1	A	165	LEU	6.6
1	A	173	LEU	6.6
1	B	67	VAL	6.5
1	B	64	PHE	6.5
1	A	167	LEU	6.4
1	A	330	LEU	6.2
1	B	71	PHE	6.1
1	A	369	LEU	6.0
1	A	101	ALA	6.0
1	B	163	ILE	6.0
1	B	90	VAL	5.7
1	A	408	GLU	5.5
1	A	192	TYR	5.4
1	A	366	PRO	5.4
1	A	409	THR	5.3
1	A	99	LEU	5.3
1	B	376	LEU	5.2
1	A	132	ALA	5.2
1	B	237	LEU	5.1
1	A	171	SER	5.1
1	B	372	LEU	5.1
1	B	69	ILE	5.0
1	A	364	VAL	5.0
1	A	102	LEU	5.0
1	A	411	TRP	4.9
1	A	98	ILE	4.9
1	B	369	LEU	4.8
1	B	61	VAL	4.8
1	A	334	ILE	4.8
1	A	134	LEU	4.6
1	A	79	TRP	4.6
1	A	97	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	240	ALA	4.6
1	A	66	LEU	4.5
1	B	159	ASP	4.5
1	A	177	TYR	4.5
1	B	244	PHE	4.5
1	A	410	LEU	4.4
1	B	239	LEU	4.4
1	A	255	TYR	4.3
1	A	131	PRO	4.3
1	B	350	PHE	4.3
1	A	216	LEU	4.3
1	B	68	ILE	4.3
1	B	385	LEU	4.3
1	B	63	VAL	4.2
1	B	62	ARG	4.2
1	B	203	VAL	4.1
1	B	162	GLY	4.1
1	B	242	LEU	4.0
1	B	380	TYR	3.8
1	A	133	THR	3.7
1	A	158	ASN	3.7
1	B	295	ASP	3.6
1	B	256	LEU	3.6
1	A	116	PHE	3.6
1	A	164	VAL	3.6
1	A	403	THR	3.6
1	A	49	ILE	3.6
1	A	88	THR	3.5
1	A	123	GLY	3.5
1	B	364	VAL	3.5
1	B	258	ALA	3.5
1	A	100	THR	3.4
1	B	157	PHE	3.4
1	A	161	LEU	3.4
1	B	128	ALA	3.4
1	B	367	SER	3.4
1	A	155	SER	3.3
1	A	73	GLU	3.2
1	B	365	VAL	3.2
1	A	246	ILE	3.2
1	B	37	LEU	3.1
1	A	60	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	118	LEU	3.1
1	B	160	PRO	3.1
1	B	238	SER	3.1
1	B	375	SER	3.0
1	A	311	ALA	3.0
1	B	49	ILE	3.0
1	B	97	LEU	3.0
1	B	384	LEU	2.9
1	B	366	PRO	2.9
1	B	328	VAL	2.9
1	B	373	PRO	2.9
1	A	2	ILE	2.8
1	B	363	GLY	2.8
1	B	158	ASN	2.8
1	B	417	ASP	2.7
1	A	277	ILE	2.6
1	B	125	ILE	2.6
1	B	132	ALA	2.6
1	A	54	ALA	2.6
1	A	422	GLY	2.6
1	B	294	ASN	2.5
1	B	145	GLN	2.5
1	A	18	VAL	2.5
1	A	378	LEU	2.5
1	B	143	VAL	2.5
1	A	213	LEU	2.5
1	A	215	ILE	2.4
1	A	212	PHE	2.4
1	B	370	ALA	2.4
1	B	40	LEU	2.4
1	B	402	LEU	2.4
1	A	211	ILE	2.4
1	A	344	LEU	2.4
1	B	318	ILE	2.4
1	B	298	ALA	2.4
1	B	262	GLY	2.3
1	B	73	GLU	2.3
1	A	10	LEU	2.3
1	A	11	PHE	2.3
1	A	307	VAL	2.3
1	B	379	LYS	2.2
1	A	70	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	65	GLY	2.2
1	B	99	LEU	2.2
1	B	87	PRO	2.2
1	B	207	ILE	2.2
1	B	199	PHE	2.2
1	B	246	ILE	2.2
1	A	347	TRP	2.2
1	B	208	SER	2.2
1	B	415	LEU	2.1
1	B	182	PHE	2.1
1	A	359	GLU	2.1
1	B	166	THR	2.1
1	A	17	GLY	2.1
1	A	95	ILE	2.0
1	A	356	ILE	2.0
1	A	253	SER	2.0
1	B	170	ILE	2.0
1	B	179	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	FLC	B	1424	13/13	0.31	0.14	157,192,200,200	0
4	TAM	A	1426	11/11	0.66	0.24	121,144,158,164	0
2	BOG	A	1423	20/20	0.71	0.21	109,158,199,203	0
4	TAM	A	1425	11/11	0.73	0.19	93,116,137,139	0
5	FLC	B	1423	13/13	0.74	0.11	124,162,182,182	0

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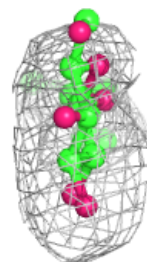
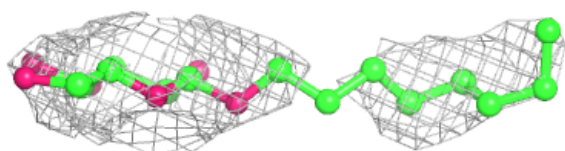
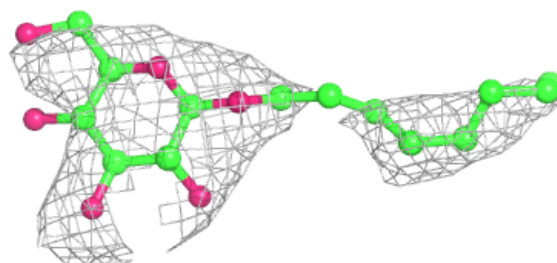
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	TAM	B	1425	11/11	0.86	0.12	120,136,142,148	0
3	PTY	A	1424	50/50	0.88	0.26	98,135,170,200	0

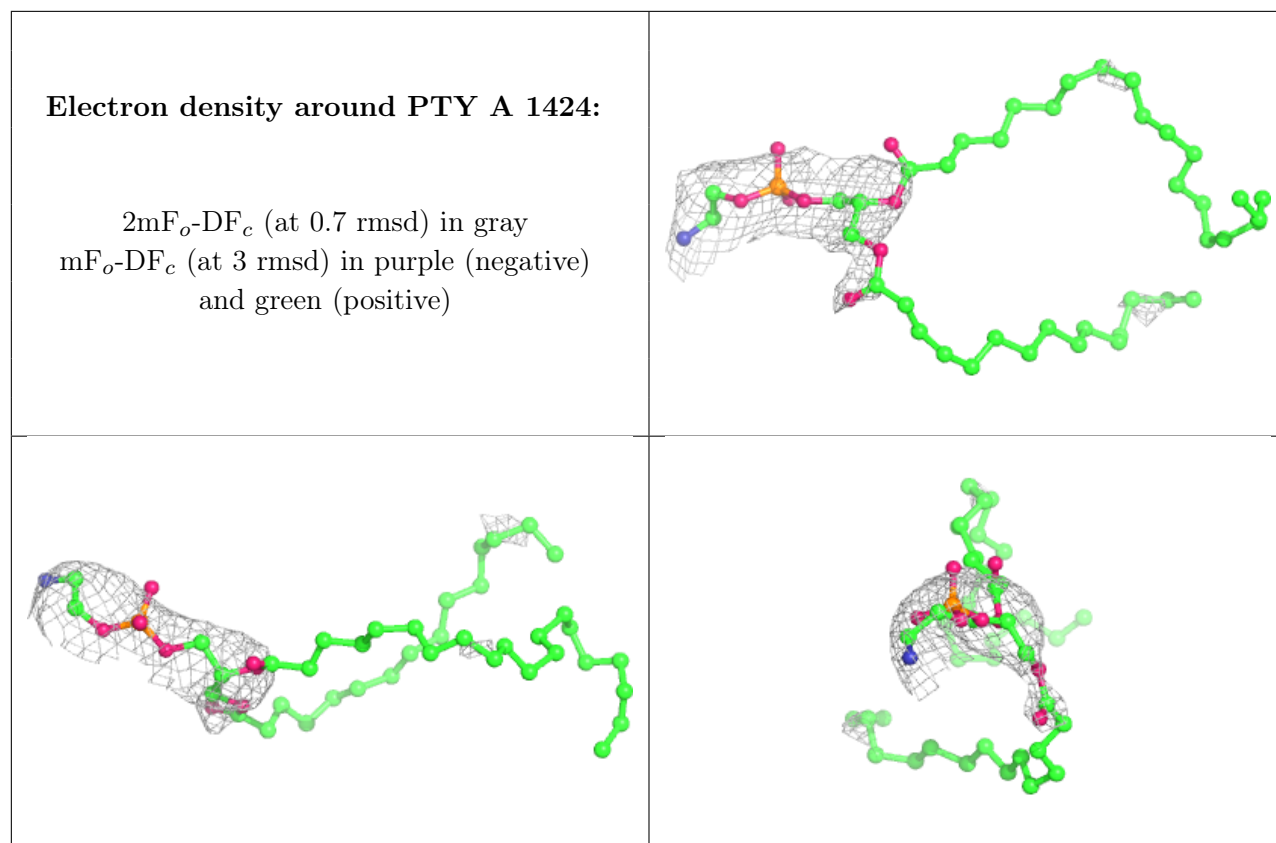
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around BOG A 1423:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)







## 6.5 Other polymers [i](#)

There are no such residues in this entry.