



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:38 PM 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

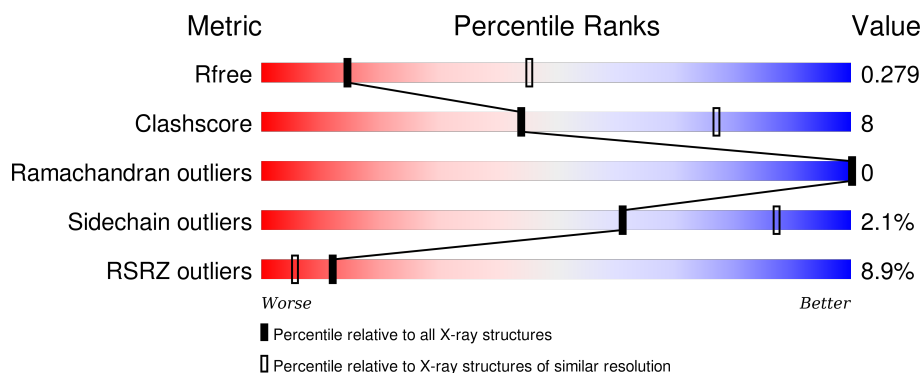
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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>8%</div> <div>79%</div> <div>21%</div> </div>
1	B	422	<div> <div>9%</div> <div>80%</div> <div>19%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BOG	A	1423	-	-	-	X
3	PTY	A	1424	-	-	-	X
4	TAM	A	1425	-	-	-	X
4	TAM	A	1426	-	-	-	X

## 2 Entry composition [i](#)

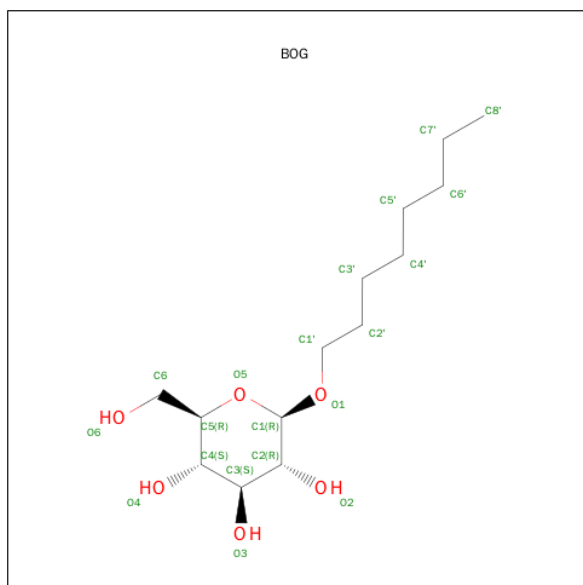
There are 6 unique types of molecules in this entry. The entry contains 6715 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

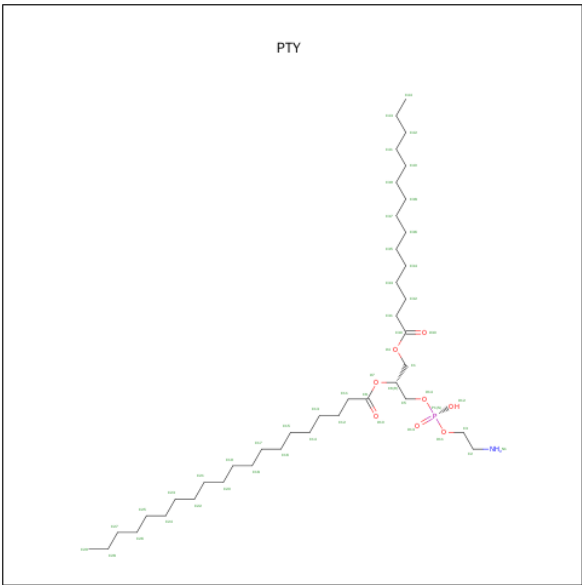
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	Se	0	0	0
			3295	2217	516	555	7			
1	B	421	Total	C	N	O	Se	0	0	0
			3287	2212	515	554	6			

- Molecule 2 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



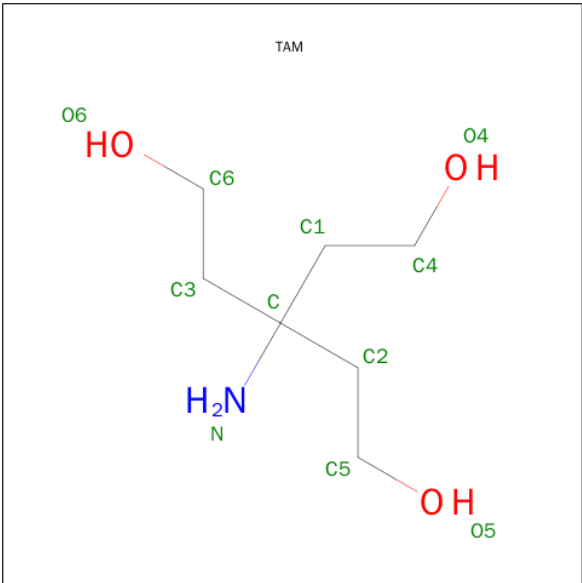
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		

- 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>).



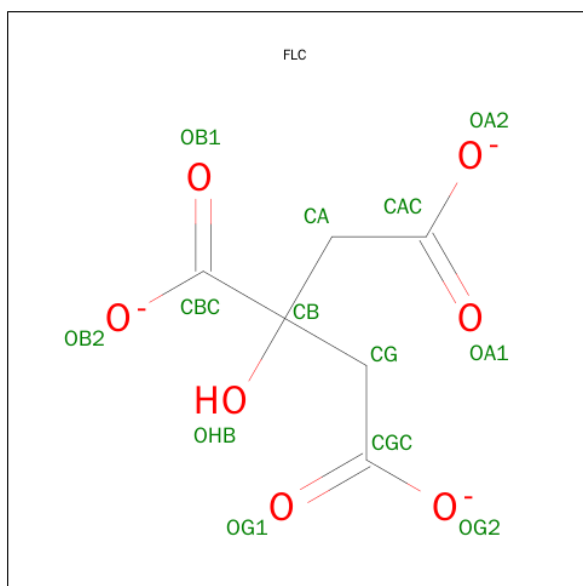
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			11	7	1	3		
4	A	1	Total	C	N	O	0	0
			11	7	1	3		

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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		

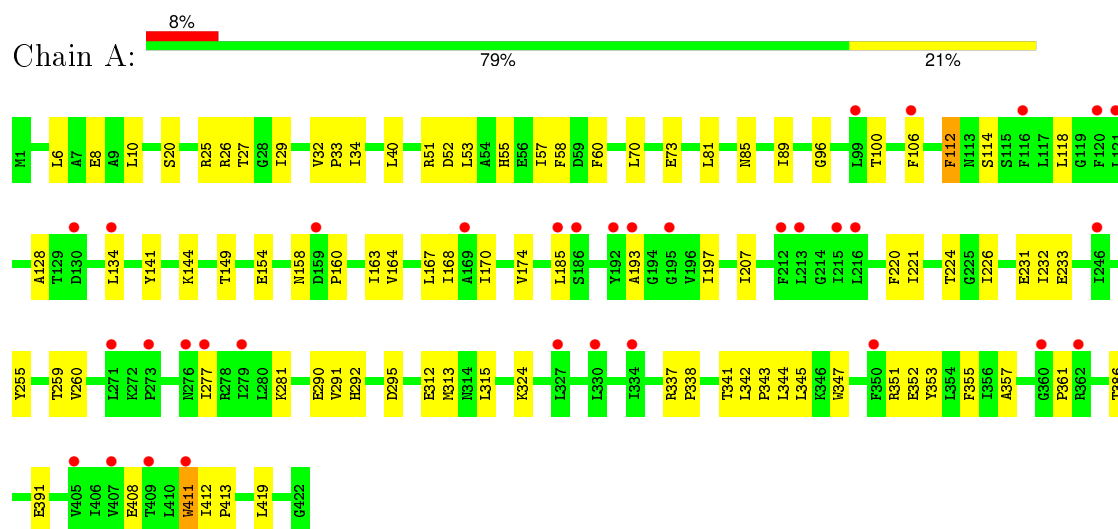
- Molecule 6 is water.

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

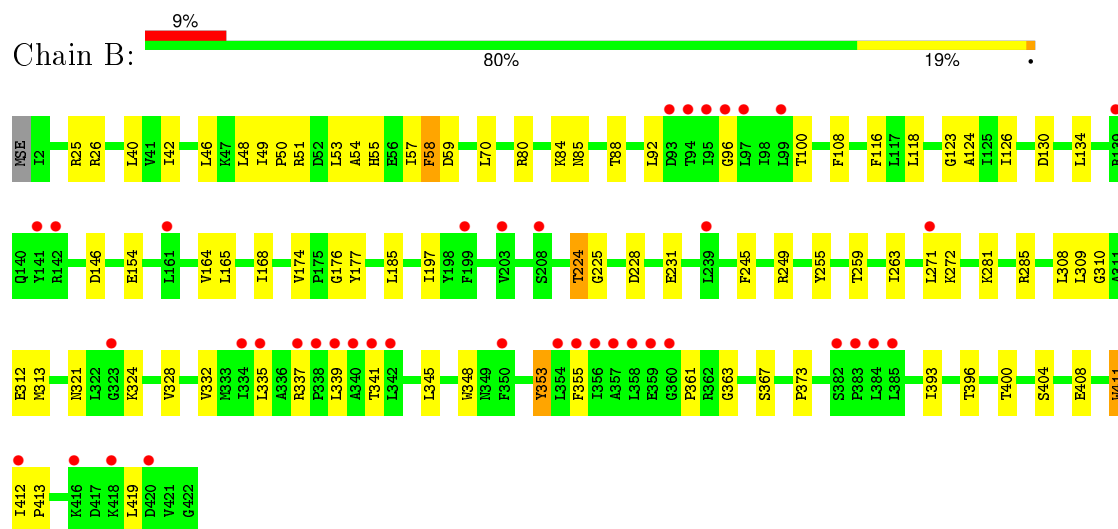
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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> ANTIporter, PUTATIVE



- Molecule 1: NA<sup>+</sup>/H<sup>+</sup> ANTIporter, 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	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.239 , 0.276 0.255 , 0.279	Depositor DCC
$R_{free}$ test set	1088 reflections (5.42%)	DCC
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> )	0.28 , 98.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 21145 reflections (0.005%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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: TAM, FLC, PTY, BOG

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:B:337:ARG:O	1:B:341:THR:OG1	2.19	0.53
1:A:207:ILE:HA	1:A:260:VAL:HG21	1.91	0.53
1:A:351:ARG:HB3	1:A:419:LEU:HB2	1.92	0.52
1:A:292:HIS:HB2	2:A:1423:BOG:H3'2	1.91	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)
4:B:1425:TAM:O5	4:B:1425:TAM:N	2.41	0.51
1:B:70:LEU:HD12	1:B:255:TYR:HB3	1.92	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:B:59:ASP:O	4:B:1425:TAM:O5	2.31	0.49
1:A:51:ARG:NH2	1:A:391:GLU:OE2	2.38	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:412:ILE:HG23	1:B:413:PRO:HD3	1.97	0.46
1:B:92:LEU:HB3	1:B:154:GLU:HG3	1.96	0.46
4:A:1425:TAM:H41	4:A:1425:TAM:H21	1.40	0.46
1:A:338:PRO:HB3	1:A:357:ALA:HB1	1.98	0.46
1:A:315:LEU:H	1:A:315:LEU:HD22	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:130:ASP:HB3	1:B:363:GLY:HA3	1.98	0.44
1:B:46:LEU:HB3	1:B:48:LEU:HG	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
4:B:1425:TAM:H62	4:B:1425:TAM:H11	1.67	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
1:B:361:PRO:HB3	1:B:408:GLU:HG3	2.01	0.43
1:A:277:ILE:O	1:A:281:LYS:HG2	2.19	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:70:LEU:HB3	1:A:259:THR:HG22	2.00	0.43
1:A:60:PHE:CD2	3:A:1424:PTY:H111	2.54	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:B:324:LYS:O	1:B:328:VAL:HG23	2.19	0.42
1:A:291:VAL:O	1:A:295:ASP:HB2	2.20	0.42
1:A:70:LEU:HB3	1:A:259:THR:CG2	2.50	0.42
1:A:224:THR:O	1:B:26:ARG:NH2	2.41	0.42
1:A:40:LEU:HD13	1:A:313:MSE:HE3	2.02	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:B:85:ASN:ND2	1:B:146:ASP:OD1	2.53	0.42
1:A:27:THR:HB	1:A:29:ILE:HG13	2.01	0.42
1:A:408:GLU:HA	1:A:411:TRP:CD1	2.55	0.41
1:A:170:ILE:O	1:A:174:VAL:HG22	2.19	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:355:PHE:HB2	1:A:419:LEU:HD22	2.03	0.41
1:A:232:ILE:HG13	1:A:290:GLU:HB2	2.03	0.41
1:A:231:GLU:OE2	1:B:25:ARG:HD2	2.21	0.41
1:A:344:LEU:HA	1:A:344:LEU:HD12	1.83	0.41
1:A:134:LEU:HD11	1:A:361:PRO:HD3	2.02	0.41
1:A:154:GLU:CD	1:A:337:ARG:HH22	2.25	0.40
1:A:73:GLU:HG2	4:A:1425:TAM:H52	2.03	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%)	60	87
1	B	358/352 (102%)	351 (98%)	7 (2%)	63	88
All	All	717/704 (102%)	702 (98%)	15 (2%)	61	87

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

Some 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 carbohydrates 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	$\# Z  > 2$
2	BOG	A	1423	-	20,20,20	0.48	0	25,25,25	0.79	1 (4%)
3	PTY	A	1424	-	48,49,49	0.99	3 (6%)	49,54,54	1.07	2 (4%)
4	TAM	A	1425	-	7,10,10	1.15	0	9,12,12	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	TAM	A	1426	-	7,10,10	1.14	0	9,12,12	0.57	0
5	FLC	B	1423	-	3,12,12	1.67	0	3,17,17	2.41	2 (66%)
5	FLC	B	1424	-	3,12,12	1.75	0	3,17,17	2.65	2 (66%)
4	TAM	B	1425	-	7,10,10	1.15	0	9,12,12	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BOG	A	1423	-	-	0/11/31/31	0/1/1/1
3	PTY	A	1424	-	-	0/53/53/53	0/0/0/0
4	TAM	A	1425	-	-	0/12/12/12	0/0/0/0
4	TAM	A	1426	-	-	0/12/12/12	0/0/0/0
5	FLC	B	1423	-	-	0/6/16/16	0/0/0/0
5	FLC	B	1424	-	-	0/6/16/16	0/0/0/0
4	TAM	B	1425	-	-	0/12/12/12	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1424	PTY	O7-C6	-2.16	1.41	1.46
3	A	1424	PTY	O7-C8	3.02	1.43	1.34
3	A	1424	PTY	O4-C30	3.61	1.44	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1424	FLC	CB-CG-CGC	-3.37	109.57	114.96
5	B	1424	FLC	CB-CA-CAC	-3.11	109.99	114.96
5	B	1423	FLC	CB-CG-CGC	-2.97	110.22	114.96
5	B	1423	FLC	CB-CA-CAC	-2.93	110.28	114.96
2	A	1423	BOG	C1-O5-C5	-2.10	109.68	113.75
3	A	1424	PTY	O4-C30-C31	2.55	119.66	111.90
3	A	1424	PTY	O7-C8-C11	3.56	119.26	111.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 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%)	0.25	34 (8%)	14 7	80, 131, 175, 200	0
1	B	415/422 (98%)	0.31	40 (9%)	10 5	75, 128, 175, 203	0
All	All	830/844 (98%)	0.28	74 (8%)	12 6	75, 130, 175, 203	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	TYR	6.8
1	B	358	LEU	6.0
1	B	93	ASP	5.7
1	B	354	LEU	5.3
1	B	99	LEU	4.8
1	A	277	ILE	4.5
1	B	420	ASP	4.5
1	B	335	LEU	4.1
1	B	385	LEU	3.9
1	B	350	PHE	3.9
1	B	356	ILE	3.8
1	B	334	ILE	3.7
1	B	323	GLY	3.7
1	B	94	THR	3.7
1	B	97	LEU	3.7
1	B	139	ARG	3.5
1	B	95	ILE	3.5
1	A	216	LEU	3.4
1	A	411	TRP	3.4
1	B	340	ALA	3.3
1	B	383	PRO	3.0
1	B	412	ILE	3.0
1	B	342	LEU	3.0
1	A	273	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	418	LYS	2.9
1	B	360	GLY	2.8
1	B	382	SER	2.8
1	B	337	ARG	2.8
1	A	195	GLY	2.8
1	A	193	ALA	2.8
1	A	407	VAL	2.8
1	B	384	LEU	2.7
1	B	141	TYR	2.7
1	A	116	PHE	2.7
1	A	276	ASN	2.6
1	A	130	ASP	2.6
1	A	330	LEU	2.6
1	B	96	GLY	2.6
1	B	338	PRO	2.6
1	A	212	PHE	2.6
1	A	215	ILE	2.6
1	A	362	ARG	2.6
1	A	159	ASP	2.5
1	A	99	LEU	2.5
1	A	334	ILE	2.5
1	A	185	LEU	2.5
1	A	405	VAL	2.5
1	B	341	THR	2.4
1	A	106	PHE	2.4
1	B	339	LEU	2.4
1	A	409	THR	2.4
1	A	213	LEU	2.3
1	B	359	GLU	2.3
1	A	279	ILE	2.3
1	A	169	ALA	2.3
1	B	357	ALA	2.3
1	B	208	SER	2.3
1	B	199	PHE	2.2
1	A	120	PHE	2.2
1	B	203	VAL	2.2
1	A	246	ILE	2.2
1	A	360	GLY	2.2
1	B	416	LYS	2.2
1	A	186	SER	2.1
1	B	142	ARG	2.1
1	B	355	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	121	LEU	2.1
1	B	271	LEU	2.1
1	A	271	LEU	2.1
1	A	134	LEU	2.0
1	A	327	LEU	2.0
1	B	239	LEU	2.0
1	B	161	LEU	2.0
1	A	350	PHE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	TAM	A	1426	11/11	0.61	0.80	8.98	121,144,158,164	0
2	BOG	A	1423	20/20	0.80	0.41	2.42	109,158,199,203	0
3	PTY	A	1424	50/50	0.74	0.39	2.40	98,135,170,200	0
4	TAM	A	1425	11/11	0.74	0.43	1.84	93,116,137,139	0
5	FLC	B	1423	13/13	0.64	0.31	1.46	124,162,182,182	0
4	TAM	B	1425	11/11	0.84	0.26	0.63	120,136,142,148	0
5	FLC	B	1424	13/13	0.52	0.29	-	157,192,200,200	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.