



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2016 – 01:35 AM EDT

PDB ID : 5CUX  
Title : Crystal structure of N-terminal domain truncated Trypanosoma cruzi Vacuolar Soluble Pyrophosphatases in complex with PPI  
Authors : Liu, W.D.; Yang, Y.Y.; Ko, T.P.; Zheng, Y.Y.; Chen, C.C.; Guo, R.T.  
Deposited on : 2015-07-25  
Resolution : 2.80 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

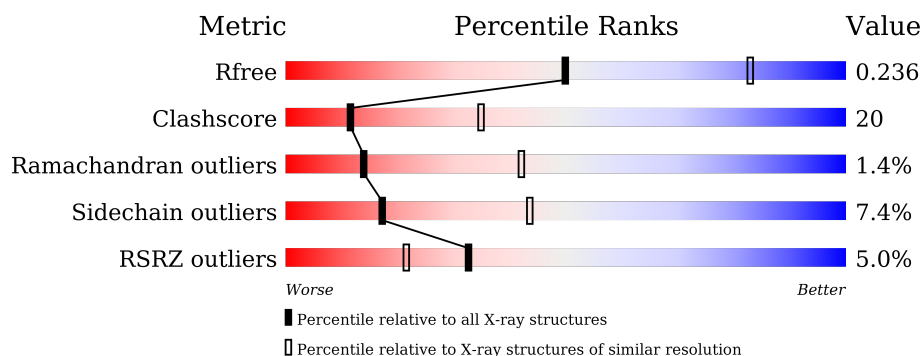
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	263	<div> <div>5%</div> <div> <div></div> <div>66%</div> <div>27%</div> <div>6%</div> </div> </div>
1	B	263	<div> <div>5%</div> <div> <div></div> <div>62%</div> <div>31%</div> <div>• •</div> </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	POP	B	501	-	-	-	X
3	PO4	A	804	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4434 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.

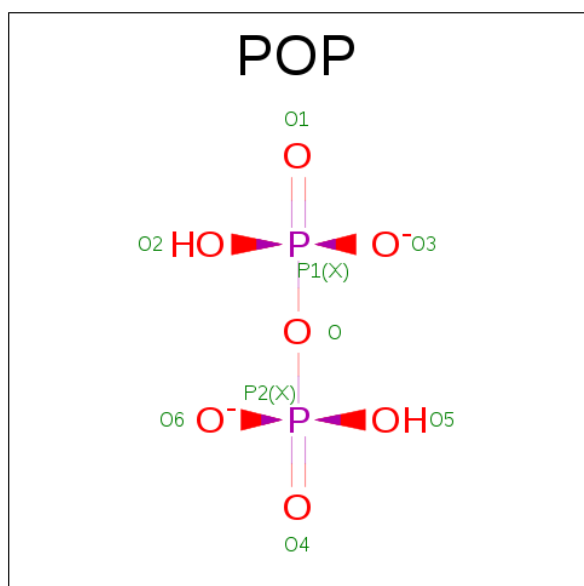
- Molecule 1 is a protein called Acidocalcisomal pyrophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2152	1397	357	382	16			
1	B	257	Total	C	N	O	S	0	0	0
			2102	1364	349	374	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	MET	-	initiating methionine	UNP Q4JH30
B	146	MET	-	initiating methionine	UNP Q4JH30

- Molecule 2 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $\text{H}_2\text{O}_7\text{P}_2$ ).



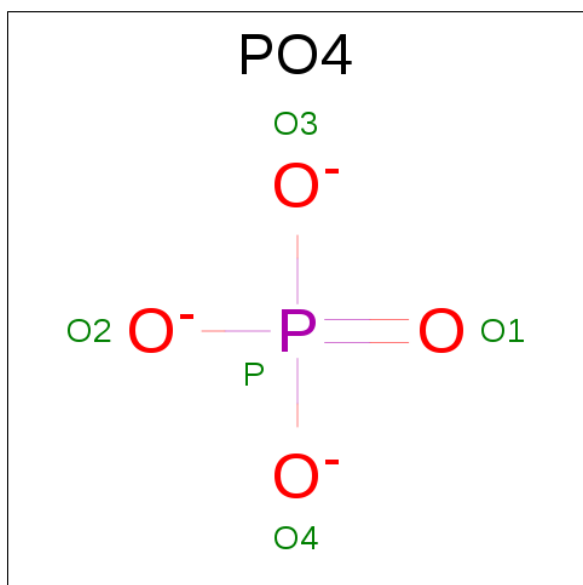
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			9	7	2		
2	B	1	Total	O	P	0	0
			9	7	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

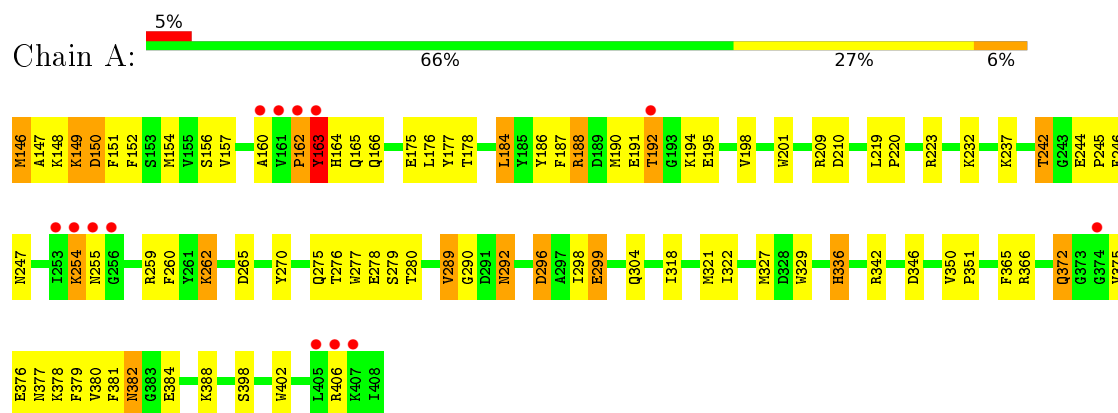
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	60	Total 60	O 60	0	0
4	B	58	Total 58	O 58	0	0

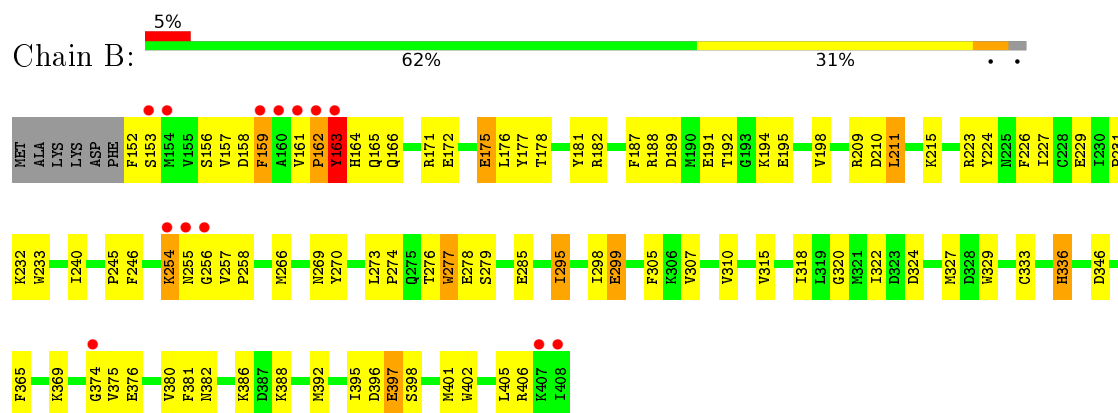
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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: Acidocalcisomal pyrophosphatase



#### • Molecule 1: Acidocalcisomal pyrophosphatase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.89Å 122.89Å 127.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.80 24.83 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (25.00-2.80) 96.5 (24.83-2.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.11 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.198 , 0.233 0.196 , 0.236	Depositor DCC
$R_{free}$ test set	1309 reflections (4.86%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.7	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.6	EDS
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 26977 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4434	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: PO4, POP

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	0.81	1/2216 (0.0%)	0.93	2/2999 (0.1%)
1	B	0.77	1/2165 (0.0%)	0.90	2/2933 (0.1%)
All	All	0.79	2/4381 (0.0%)	0.91	4/5932 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	397	GLU	CG-CD	5.55	1.60	1.51
1	A	146	MET	CG-SD	5.15	1.94	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	GLY	N-CA-C	-6.92	95.81	113.10
1	A	151	PHE	N-CA-C	-5.56	95.99	111.00
1	A	296	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	B	266	MET	N-CA-C	-5.05	97.36	111.00

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	2152	0	2103	100	0
1	B	2102	0	2050	99	0
2	A	18	0	0	1	0
2	B	9	0	0	1	0
3	A	20	0	0	0	0
3	B	15	0	0	0	0
4	A	60	0	0	0	0
4	B	58	0	0	3	0
All	All	4434	0	4153	173	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 20.

All (173) 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:148:LYS:C	1:A:149:LYS:HD2	1.73	1.08
1:B:255:ASN:HB3	1:B:257:VAL:HG12	1.33	1.06
1:B:279:SER:H	1:B:401:MET:CE	1.69	1.06
1:A:149:LYS:HD2	1:A:149:LYS:N	1.72	1.03
1:B:298:ILE:HD11	1:B:365:PHE:HE2	1.20	1.01
1:A:147:ALA:O	1:A:148:LYS:HD3	1.60	1.01
1:B:298:ILE:HD11	1:B:365:PHE:CE2	2.03	0.94
1:A:157:VAL:HG11	1:B:198:VAL:HG12	1.50	0.93
1:B:279:SER:H	1:B:401:MET:HE2	1.34	0.92
1:A:188:ARG:HH11	1:A:188:ARG:HG3	1.40	0.86
1:A:165:GLN:O	1:A:190:MET:HG3	1.80	0.82
1:A:254:LYS:HD3	1:A:255:ASN:N	1.97	0.79
1:A:149:LYS:CD	1:A:149:LYS:N	2.45	0.79
1:B:327:MET:HA	1:B:327:MET:HE2	1.66	0.76
1:A:292:ASN:HD22	1:B:152:PHE:HZ	1.31	0.75
1:A:402:TRP:CZ2	1:A:406:ARG:HD2	2.21	0.75
1:B:223:ARG:HG2	1:B:336:HIS:NE2	2.00	0.75
1:B:255:ASN:HB3	1:B:257:VAL:CG1	2.16	0.75
1:A:192:THR:OG1	1:A:194:LYS:HD3	1.87	0.75
1:B:157:VAL:HG13	1:B:157:VAL:O	1.87	0.75
1:A:198:VAL:HG12	1:B:157:VAL:HG11	1.69	0.74
1:A:223:ARG:HE	1:A:336:HIS:CE1	2.05	0.74
1:A:210:ASP:HA	1:B:210:ASP:HA	1.70	0.73
1:B:381:PHE:O	1:B:382:ASN:HB2	1.88	0.73
1:A:166:GLN:HE21	1:A:187:PHE:HB3	1.55	0.71
1:A:406:ARG:HH11	1:A:406:ARG:HG2	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:LYS:HD2	4:B:637:HOH:O	1.90	0.70
1:B:279:SER:N	1:B:401:MET:CE	2.51	0.69
1:B:254:LYS:HG2	1:B:257:VAL:HG13	1.75	0.68
1:A:223:ARG:HG3	1:A:336:HIS:NE2	2.09	0.68
1:B:279:SER:H	1:B:401:MET:HE3	1.56	0.68
1:A:292:ASN:ND2	1:B:152:PHE:CZ	2.62	0.66
1:B:346:ASP:OD1	1:B:388:LYS:HG2	1.96	0.66
1:A:154:MET:CE	1:B:406:ARG:HG2	2.26	0.66
1:A:163:TYR:HB2	1:B:162:PRO:HG3	1.78	0.65
1:A:198:VAL:HG12	1:B:157:VAL:CG1	2.26	0.65
1:A:188:ARG:NH1	1:A:188:ARG:HG3	2.12	0.64
1:B:163:TYR:HD1	1:B:164:HIS:H	1.44	0.64
1:A:375:VAL:HG12	1:A:376:GLU:H	1.63	0.63
1:B:298:ILE:CD1	1:B:365:PHE:HE2	2.05	0.62
1:B:172:GLU:OE2	1:B:181:TYR:HE1	1.81	0.62
1:A:381:PHE:O	1:A:382:ASN:HB2	1.99	0.62
1:B:211:LEU:HD23	1:B:211:LEU:N	2.15	0.62
1:B:172:GLU:OE2	1:B:181:TYR:CE1	2.53	0.61
1:A:406:ARG:HG2	1:A:406:ARG:NH1	2.16	0.61
1:A:219:LEU:HD12	1:A:220:PRO:HD2	1.83	0.61
1:A:237:LYS:HE3	1:A:259:ARG:HG2	1.82	0.60
1:B:406:ARG:HG2	1:B:406:ARG:HH11	1.65	0.60
1:B:273:LEU:HD12	1:B:295:ILE:HG21	1.83	0.60
1:B:401:MET:HG2	4:B:632:HOH:O	2.01	0.59
1:A:237:LYS:HE3	1:A:259:ARG:CG	2.33	0.59
1:A:245:PRO:HA	1:B:153:SER:OG	2.00	0.59
1:B:223:ARG:HG2	1:B:336:HIS:CD2	2.37	0.59
1:A:375:VAL:HG12	1:A:376:GLU:N	2.17	0.59
1:B:171:ARG:NH2	1:B:195:GLU:OE1	2.35	0.59
1:A:223:ARG:NE	1:A:336:HIS:CE1	2.70	0.59
1:A:237:LYS:HE3	1:A:259:ARG:CD	2.33	0.59
1:A:157:VAL:CG1	1:B:198:VAL:HG12	2.29	0.58
1:B:318:ILE:HD11	1:B:329:TRP:HB3	1.86	0.58
1:A:298:ILE:HD11	1:A:365:PHE:CE2	2.39	0.58
1:B:395:ILE:O	1:B:398:SER:HB3	2.03	0.58
1:A:163:TYR:H	1:B:162:PRO:HG3	1.68	0.57
1:A:209:ARG:HD3	1:B:165:GLN:OE1	2.04	0.57
1:A:157:VAL:O	1:A:157:VAL:HG13	2.04	0.57
1:A:210:ASP:HB2	1:B:209:ARG:O	2.04	0.57
1:A:175:GLU:HB3	1:A:178:THR:HG21	1.87	0.56
1:B:157:VAL:O	1:B:159:PHE:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ARG:HE	1:A:336:HIS:CG	2.24	0.56
1:B:401:MET:CG	4:B:632:HOH:O	2.52	0.56
1:B:278:GLU:HA	1:B:401:MET:HE1	1.88	0.56
1:A:262:LYS:HE2	1:A:372:GLN:NE2	2.22	0.55
1:B:227:ILE:HD11	1:B:274:PRO:HB3	1.87	0.55
1:A:166:GLN:NE2	1:A:187:PHE:HB3	2.21	0.54
1:B:215:LYS:HE3	2:B:501:POP:O2	2.08	0.54
1:A:259:ARG:HG3	1:A:260:PHE:N	2.23	0.54
1:A:219:LEU:HD12	1:A:220:PRO:CD	2.39	0.53
1:B:224:TYR:OH	1:B:392:MET:HG2	2.08	0.53
1:B:166:GLN:HE21	1:B:187:PHE:HB3	1.74	0.53
1:A:245:PRO:O	1:A:246:PHE:HB2	2.09	0.53
1:A:242:THR:HA	1:A:247:ASN:HD22	1.74	0.52
1:A:350:VAL:HB	1:A:351:PRO:HD3	1.91	0.52
1:A:299:GLU:O	1:A:299:GLU:HG3	2.07	0.52
1:B:176:LEU:HG	1:B:177:TYR:CD2	2.44	0.52
1:A:175:GLU:HB3	1:A:178:THR:CG2	2.39	0.52
1:A:223:ARG:NE	1:A:336:HIS:ND1	2.50	0.52
1:A:277:TRP:CZ3	1:A:279:SER:HB2	2.45	0.52
1:A:322:ILE:HD11	1:A:380:VAL:HG13	1.92	0.52
1:A:254:LYS:C	1:A:254:LYS:HD3	2.30	0.51
1:B:276:THR:HB	1:B:398:SER:OG	2.10	0.51
1:A:201:TRP:CZ3	1:A:242:THR:HG22	2.46	0.51
1:A:289:VAL:HG23	1:A:290:GLY:O	2.10	0.51
1:B:232:LYS:HD3	1:B:233:TRP:CZ2	2.46	0.51
1:B:279:SER:N	1:B:401:MET:HE3	2.22	0.50
1:A:162:PRO:HG3	1:B:163:TYR:HB2	1.94	0.49
1:A:163:TYR:HB2	1:B:162:PRO:CG	2.40	0.49
1:B:164:HIS:CG	1:B:191:GLU:HG3	2.48	0.49
1:A:336:HIS:CE1	1:A:342:ARG:NH2	2.81	0.48
1:A:237:LYS:CD	1:A:259:ARG:HG2	2.43	0.48
1:A:154:MET:HE1	1:B:406:ARG:HG2	1.95	0.48
1:B:269:ASN:HB2	1:B:299:GLU:HG3	1.96	0.48
1:A:292:ASN:ND2	1:B:152:PHE:CE2	2.82	0.48
1:B:232:LYS:HD3	1:B:233:TRP:CE2	2.49	0.48
1:B:187:PHE:O	1:B:195:GLU:HA	2.13	0.47
1:A:162:PRO:HG2	1:B:162:PRO:HG2	1.95	0.47
1:A:380:VAL:HG23	1:A:381:PHE:CD2	2.50	0.47
1:B:161:VAL:HG13	1:B:211:LEU:HD13	1.97	0.47
1:B:188:ARG:HH11	1:B:188:ARG:HG3	1.80	0.47
1:A:254:LYS:HD3	1:A:255:ASN:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ASP:HB2	1:A:329:TRP:O	2.15	0.47
1:B:182:ARG:HH11	1:B:182:ARG:HG2	1.79	0.47
1:A:150:ASP:HB3	1:A:152:PHE:CE2	2.50	0.47
1:B:245:PRO:O	1:B:246:PHE:HB2	2.14	0.47
1:A:318:ILE:HD11	1:A:329:TRP:HB3	1.97	0.46
1:A:162:PRO:HG3	1:B:163:TYR:H	1.79	0.46
1:B:406:ARG:HG2	1:B:406:ARG:NH1	2.31	0.46
1:B:224:TYR:CD1	1:B:315:VAL:HG23	2.50	0.46
1:A:150:ASP:HB3	1:A:152:PHE:HE2	1.81	0.45
1:A:298:ILE:CD1	1:A:365:PHE:HE2	2.29	0.45
1:A:321:MET:HB2	1:A:379:PHE:CE1	2.51	0.45
1:B:157:VAL:O	1:B:157:VAL:CG1	2.59	0.45
1:A:232:LYS:HB3	1:A:304:GLN:HB2	1.99	0.45
1:B:322:ILE:HD11	1:B:380:VAL:HG13	1.97	0.45
1:A:184:LEU:HD12	1:A:186:TYR:OH	2.17	0.45
1:A:276:THR:HB	1:A:398:SER:OG	2.16	0.45
1:B:270:TYR:CE1	1:B:365:PHE:HZ	2.35	0.45
1:A:160:ALA:O	1:A:162:PRO:HD3	2.17	0.45
1:B:229:GLU:OE2	1:B:240:ILE:HG13	2.16	0.45
1:A:162:PRO:HD3	1:B:163:TYR:HD2	1.81	0.45
1:A:176:LEU:O	1:A:177:TYR:HB2	2.17	0.44
1:A:164:HIS:CG	1:A:191:GLU:HG3	2.52	0.44
1:B:396:ASP:O	1:B:397:GLU:C	2.53	0.44
1:B:277:TRP:CD2	1:B:405:LEU:HD22	2.53	0.44
2:A:802:POP:O2	2:A:802:POP:O6	2.36	0.44
1:A:244:GLU:O	1:B:153:SER:HB3	2.18	0.44
1:B:231:PRO:HB3	1:B:305:PHE:O	2.18	0.44
1:A:270:TYR:HD1	1:A:298:ILE:HG12	1.83	0.43
1:B:166:GLN:NE2	1:B:187:PHE:HB3	2.33	0.43
1:B:346:ASP:CG	1:B:388:LYS:HG2	2.39	0.43
1:A:154:MET:CE	1:B:406:ARG:HH11	2.31	0.43
1:A:378:LYS:HA	1:A:378:LYS:HD3	1.66	0.43
1:A:275:GLN:HG2	1:A:402:TRP:CZ2	2.54	0.43
1:A:237:LYS:HE3	1:A:259:ARG:HD2	2.00	0.43
1:A:298:ILE:CD1	1:A:365:PHE:CE2	3.02	0.43
1:B:277:TRP:O	1:B:401:MET:HE1	2.18	0.43
1:B:187:PHE:CG	1:B:198:VAL:HG11	2.54	0.42
1:A:346:ASP:OD1	1:A:388:LYS:HG2	2.19	0.42
1:A:154:MET:HE2	1:B:406:ARG:HG2	2.02	0.42
1:B:402:TRP:CZ2	1:B:406:ARG:CD	3.02	0.42
1:A:162:PRO:HG2	1:B:162:PRO:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:VAL:HG12	1:B:376:GLU:H	1.85	0.42
1:B:402:TRP:CE2	1:B:406:ARG:HD2	2.55	0.42
1:A:366:ARG:CG	1:A:366:ARG:O	2.68	0.41
1:B:380:VAL:HG23	1:B:381:PHE:CD2	2.55	0.41
1:A:377:ASN:HD22	1:A:377:ASN:HA	1.61	0.41
1:A:382:ASN:HA	1:A:382:ASN:HD22	1.71	0.41
1:B:189:ASP:OD1	1:B:192:THR:HG23	2.20	0.41
1:B:381:PHE:CE1	1:B:386:LYS:HE2	2.55	0.41
1:A:157:VAL:CG1	1:A:157:VAL:O	2.69	0.41
1:A:237:LYS:CE	1:A:259:ARG:HG2	2.49	0.41
1:B:226:PHE:O	1:B:310:VAL:HA	2.20	0.41
1:B:299:GLU:HA	1:B:333:CYS:O	2.20	0.41
1:B:320:GLY:HA3	1:B:380:VAL:HG22	2.02	0.41
1:A:166:GLN:OE1	1:B:159:PHE:CE2	2.74	0.41
1:A:381:PHE:O	1:A:384:GLU:HB2	2.21	0.41
1:B:175:GLU:HB3	1:B:178:THR:CG2	2.51	0.41
1:B:231:PRO:HD3	1:B:307:VAL:HG22	2.03	0.41
1:A:146:MET:O	1:A:149:LYS:HE3	2.21	0.40
1:A:187:PHE:O	1:A:195:GLU:HA	2.21	0.40
1:A:166:GLN:OE1	1:B:159:PHE:HE2	2.04	0.40
1:B:254:LYS:CG	1:B:255:ASN:N	2.83	0.40
1:A:166:GLN:CD	1:B:159:PHE:HE2	2.24	0.40
1:B:254:LYS:HG2	1:B:257:VAL:CG1	2.47	0.40
1:A:164:HIS:HB3	1:A:191:GLU:HG2	2.04	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 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	261/263 (99%)	242 (93%)	17 (6%)	2 (1%)	24 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	255/263 (97%)	236 (92%)	14 (6%)	5 (2%)	9	30
All	All	516/526 (98%)	478 (93%)	31 (6%)	7 (1%)	14	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	PRO
1	B	158	ASP
1	B	162	PRO
1	B	163	TYR
1	A	163	TYR
1	B	374	GLY
1	B	285	GLU

### 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	233/233 (100%)	213 (91%)	20 (9%)	13	36
1	B	228/233 (98%)	214 (94%)	14 (6%)	23	55
All	All	461/466 (99%)	427 (93%)	34 (7%)	17	43

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	LYS
1	A	150	ASP
1	A	156	SER
1	A	163	TYR
1	A	184	LEU
1	A	188	ARG
1	A	192	THR
1	A	242	THR
1	A	254	LYS

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Mol	Chain	Res	Type
1	A	262	LYS
1	A	265	ASP
1	A	278	GLU
1	A	280	THR
1	A	289	VAL
1	A	292	ASN
1	A	299	GLU
1	A	327	MET
1	A	336	HIS
1	A	372	GLN
1	A	382	ASN
1	B	156	SER
1	B	159	PHE
1	B	163	TYR
1	B	175	GLU
1	B	194	LYS
1	B	211	LEU
1	B	254	LYS
1	B	258	PRO
1	B	277	TRP
1	B	295	ILE
1	B	299	GLU
1	B	324	ASP
1	B	336	HIS
1	B	369	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	372	GLN
1	A	377	ASN
1	A	382	ASN
1	B	166	GLN
1	B	263	HIS
1	B	377	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

10 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	POP	A	801	-	8,8,8	1.45	2 (25%)	13,13,13	1.39	2 (15%)
2	POP	A	802	-	8,8,8	1.73	2 (25%)	13,13,13	1.56	1 (7%)
3	PO4	A	803	-	4,4,4	1.52	0	6,6,6	0.23	0
3	PO4	A	804	-	4,4,4	1.30	0	6,6,6	0.23	0
3	PO4	A	805	-	4,4,4	1.21	0	6,6,6	0.23	0
3	PO4	A	806	-	4,4,4	1.22	0	6,6,6	0.23	0
2	POP	B	501	-	8,8,8	1.44	2 (25%)	13,13,13	1.32	2 (15%)
3	PO4	B	502	-	4,4,4	1.25	0	6,6,6	0.23	0
3	PO4	B	503	-	4,4,4	1.32	0	6,6,6	0.24	0
3	PO4	B	504	-	4,4,4	1.30	0	6,6,6	0.23	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	POP	A	801	-	-	0/6/6/6	0/0/0/0
2	POP	A	802	-	-	0/6/6/6	0/0/0/0
3	PO4	A	803	-	-	0/0/0/0	0/0/0/0
3	PO4	A	804	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	A	805	-	-	0/0/0/0	0/0/0/0
3	PO4	A	806	-	-	0/0/0/0	0/0/0/0
2	POP	B	501	-	-	0/6/6/6	0/0/0/0
3	PO4	B	502	-	-	0/0/0/0	0/0/0/0
3	PO4	B	503	-	-	0/0/0/0	0/0/0/0
3	PO4	B	504	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	POP	P1-O	-3.01	1.54	1.61
2	A	802	POP	P2-O	-2.91	1.54	1.61
2	A	801	POP	P2-O	-2.41	1.55	1.61
2	B	501	POP	P2-O	-2.40	1.55	1.61
2	A	801	POP	P1-O	-2.22	1.55	1.61
2	B	501	POP	P1-O	-2.19	1.55	1.61

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	802	POP	P2-O-P1	-4.65	119.18	132.51
2	A	801	POP	P2-O-P1	-2.69	124.81	132.51
2	B	501	POP	P2-O-P1	-2.30	125.92	132.51
2	B	501	POP	O2-P1-O	2.03	110.71	104.29
2	A	801	POP	O2-P1-O	2.08	110.86	104.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	802	POP	1	0
2	B	501	POP	1	0

## 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	263/263 (100%)	-0.12	13 (4%) 33 22	36, 56, 88, 116	0
1	B	257/263 (97%)	-0.10	13 (5%) 32 21	42, 57, 94, 126	0
All	All	520/526 (98%)	-0.11	26 (5%) 32 21	36, 56, 93, 126	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	ALA	6.7
1	B	153	SER	4.6
1	B	162	PRO	3.5
1	A	407	LYS	3.3
1	A	255	ASN	3.3
1	A	406	ARG	3.2
1	A	162	PRO	3.2
1	B	161	VAL	3.1
1	A	254	LYS	3.1
1	B	163	TYR	2.9
1	B	408	ILE	2.8
1	A	256	GLY	2.8
1	B	254	LYS	2.8
1	A	160	ALA	2.7
1	A	163	TYR	2.7
1	A	374	GLY	2.5
1	B	159	PHE	2.5
1	A	161	VAL	2.5
1	B	256	GLY	2.4
1	A	192	THR	2.3
1	B	154	MET	2.2
1	B	255	ASN	2.2
1	B	407	LYS	2.1
1	B	374	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	253	ILE	2.0
1	A	405	LEU	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
3	PO4	A	804	5/5	0.91	0.43	11.31	101,101,102,103	0
2	POP	B	501	9/9	0.86	0.35	3.22	94,96,105,106	0
3	PO4	A	803	5/5	0.94	0.20	1.87	88,89,90,91	0
2	POP	A	801	9/9	0.86	0.30	1.74	89,90,101,101	0
3	PO4	B	502	5/5	0.95	0.13	-0.16	89,90,90,91	0
3	PO4	B	503	5/5	0.89	0.19	-0.40	89,90,90,91	0
2	POP	A	802	9/9	0.88	0.18	-0.74	107,108,115,116	0
3	PO4	B	504	5/5	0.83	0.18	-	136,136,137,137	0
3	PO4	A	805	5/5	0.87	0.22	-	113,113,115,115	0
3	PO4	A	806	5/5	0.85	0.25	-	115,116,116,116	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.