



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:22 AM GMT

PDB ID : 4J13  
Title : Structural and functional characterization of 3'(2'),5'-bisphosphatenucleotidase2 from Entamoeba histolytica  
Authors : Tarique, K.F.; Abdul Rehman, S.A.; Betzel, C.; Gourinath, S.  
Deposited on : 2013-01-31  
Resolution : 2.55 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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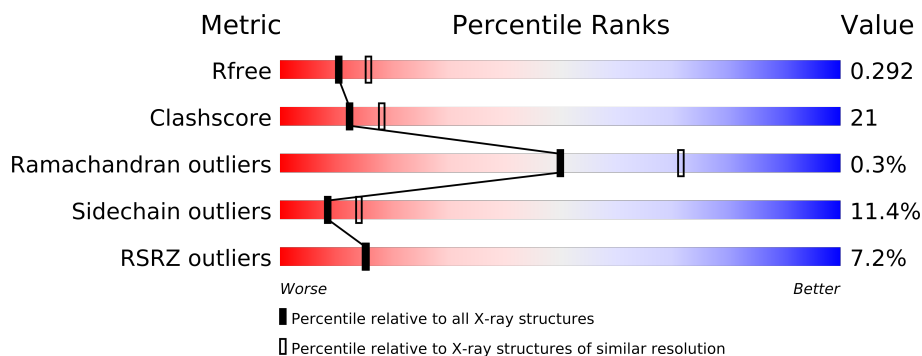
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.55 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))
$R_{free}$	66092	3413 (2.58-2.50)
Clashscore	79885	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)
RSRZ outliers	66119	3414 (2.58-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	293	
1	B	293	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	A	302	-	X
3	MG	B	302	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4619 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

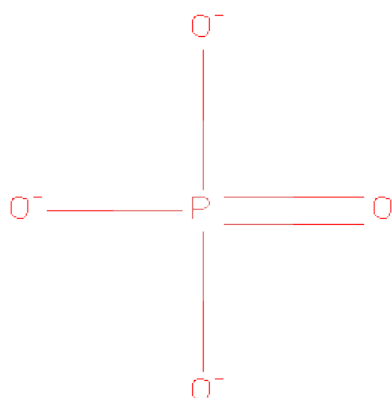
- Molecule 1 is a protein called 3'(2'),5'-bisphosphatenucleotidase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2278	1468	362	435	13			
1	B	289	Total	C	N	O	S	0	0	0
			2288	1474	365	436	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	LEU	-	EXPRESSION TAG	UNP C4M633
A	287	GLN	-	EXPRESSION TAG	UNP C4M633
A	288	HIS	-	EXPRESSION TAG	UNP C4M633
A	289	HIS	-	EXPRESSION TAG	UNP C4M633
A	290	HIS	-	EXPRESSION TAG	UNP C4M633
A	291	HIS	-	EXPRESSION TAG	UNP C4M633
A	292	HIS	-	EXPRESSION TAG	UNP C4M633
A	293	HIS	-	EXPRESSION TAG	UNP C4M633
B	286	LEU	-	EXPRESSION TAG	UNP C4M633
B	287	GLN	-	EXPRESSION TAG	UNP C4M633
B	288	HIS	-	EXPRESSION TAG	UNP C4M633
B	289	HIS	-	EXPRESSION TAG	UNP C4M633
B	290	HIS	-	EXPRESSION TAG	UNP C4M633
B	291	HIS	-	EXPRESSION TAG	UNP C4M633
B	292	HIS	-	EXPRESSION TAG	UNP C4M633
B	293	HIS	-	EXPRESSION TAG	UNP C4M633

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Mg	0	0
			3	3		
3	A	3	Total	Mg	0	0
			3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	B	13	Total	O	0	0
			13	13		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.74Å 76.29Å 101.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.23 – 2.55 31.22 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (31.23-2.55) 99.9 (31.22-2.55)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.24 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.226 , 0.256 0.239 , 0.292	Depositor DCC
$R_{free}$ test set	975 reflections (5.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.5	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 23.1	EDS
Estimated twinning fraction	0.980 for h,k,l 0.020 for k,h,-l 0.026 for k,h,-l	Xtriage
Reported twinning fraction	0.980 for h,k,l 0.020 for k,h,-l	Depositor
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 19010 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4619	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG

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	1.15	4/2325 (0.2%)	0.94	5/3149 (0.2%)
1	B	1.21	3/2336 (0.1%)	0.91	6/3164 (0.2%)
All	All	1.18	7/4661 (0.2%)	0.92	11/6313 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	CYS	CB-SG	-5.89	1.72	1.81
1	B	44	VAL	CB-CG2	-5.44	1.41	1.52
1	A	150	PHE	CD1-CE1	-5.39	1.28	1.39
1	B	248	TYR	CD1-CE1	-5.39	1.31	1.39
1	A	114	TYR	CD2-CE2	-5.26	1.31	1.39
1	B	248	TYR	CE2-CZ	-5.26	1.31	1.38
1	A	128	VAL	CB-CG2	-5.04	1.42	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	153	GLU	N-CA-C	-8.33	88.52	111.00
1	B	28	GLU	N-CA-C	-7.41	90.99	111.00
1	B	36	SER	N-CA-CB	6.70	120.55	110.50
1	A	28	GLU	CB-CA-C	-6.17	98.05	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	SER	N-CA-C	-5.99	94.82	111.00
1	A	181	LEU	N-CA-CB	-5.92	98.55	110.40
1	A	29	GLU	N-CA-CB	-5.76	100.24	110.60
1	B	20	SER	CB-CA-C	-5.59	99.48	110.10
1	A	96	ILE	CB-CA-C	-5.48	100.64	111.60
1	B	12	LEU	CB-CG-CD1	-5.12	102.29	111.00
1	A	70	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	72	GLU	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2278	0	2313	108	0
1	B	2288	0	2320	87	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	24	0	0	3	0
4	B	13	0	0	0	0
All	All	4619	0	4633	195	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (195) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:251:SER:OG	1:B:253:LYS:HG2	1.35	1.19
1:B:213:TYR:OH	1:B:280:SER:HB3	1.41	1.16

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:27:LYS:N	1:B:27:LYS:HD2	1.51	1.11
1:B:27:LYS:HD2	1:B:27:LYS:H	1.05	1.08
1:B:43:GLN:O	1:B:47:GLN:HG2	1.51	1.08
1:A:18:GLU:HG3	1:A:81:PRO:HG3	1.36	1.08
1:A:98:ILE:HD13	1:A:98:ILE:H	1.02	1.08
1:A:62:THR:HG22	4:A:424:HOH:O	1.52	1.07
1:A:98:ILE:HD13	1:A:98:ILE:N	1.55	1.04
1:A:168:ILE:HD13	1:A:272:TYR:CE2	1.97	0.99
1:A:175:LYS:HG2	1:A:176:ASN:OD1	1.66	0.96
1:A:168:ILE:CD1	1:A:272:TYR:CE2	2.49	0.96
1:B:181:LEU:HD23	1:B:279:ILE:HD13	1.48	0.94
1:B:181:LEU:HD21	1:B:279:ILE:HG23	1.50	0.92
1:B:18:GLU:HG3	1:B:81:PRO:HG3	1.53	0.90
1:B:213:TYR:HH	1:B:280:SER:HB3	1.30	0.90
1:A:98:ILE:CD1	1:A:98:ILE:N	2.31	0.88
1:B:181:LEU:CD2	1:B:279:ILE:HD13	2.03	0.88
1:A:175:LYS:O	1:A:176:ASN:OD1	1.95	0.84
1:A:43:GLN:O	1:A:47:GLN:HG2	1.78	0.83
1:B:181:LEU:HD22	1:B:279:ILE:HG21	1.60	0.82
1:B:251:SER:HG	1:B:253:LYS:HG2	1.44	0.81
1:A:168:ILE:CD1	1:A:272:TYR:HE2	1.91	0.81
1:A:37:ASP:OD1	1:A:37:ASP:N	2.12	0.81
1:B:181:LEU:CD2	1:B:279:ILE:CG2	2.59	0.80
1:B:25:LYS:O	1:B:25:LYS:CD	2.30	0.80
1:A:175:LYS:C	1:A:176:ASN:OD1	2.20	0.79
1:B:148:ILE:CG2	1:B:148:ILE:O	2.30	0.79
1:A:25:LYS:HG3	1:A:25:LYS:O	1.82	0.79
1:A:116:HIS:O	1:A:117:LYS:HB2	1.84	0.78
1:B:52:ILE:O	1:B:56:ILE:HG12	1.84	0.78
1:B:149:THR:HG21	1:B:159:ILE:CD1	2.14	0.78
1:B:27:LYS:CD	1:B:27:LYS:N	2.40	0.77
1:B:25:LYS:CG	1:B:25:LYS:O	2.30	0.76
1:B:181:LEU:HD21	1:B:279:ILE:CG2	2.16	0.76
1:A:25:LYS:O	1:A:25:LYS:CG	2.30	0.76
1:B:186:PRO:HB2	1:B:187:ASP:OD2	1.84	0.76
1:A:168:ILE:HD11	1:A:272:TYR:HE2	1.50	0.75
1:B:181:LEU:CD2	1:B:279:ILE:HG23	2.18	0.74
1:B:111:THR:O	1:B:115:THR:HG23	1.87	0.73
1:B:181:LEU:HD23	1:B:279:ILE:CD1	2.19	0.71
1:B:213:TYR:OH	1:B:280:SER:CB	2.30	0.71
1:B:181:LEU:CD2	1:B:279:ILE:HG21	2.20	0.70
1:B:211:ILE:HG12	1:B:265:LEU:HD23	1.71	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:115:THR:HG22	1:A:116:HIS:HD2	1.56	0.69
1:A:68:GLU:HG3	1:A:222:TRP:CZ2	2.27	0.69
1:A:18:GLU:CG	1:A:81:PRO:HG3	2.19	0.69
1:A:189:TYR:HD1	1:A:190:GLU:N	1.91	0.69
1:B:181:LEU:CD2	1:B:279:ILE:CD1	2.71	0.69
1:B:160:SER:O	1:B:206:HIS:HD2	1.75	0.69
1:A:2:GLN:HE21	1:A:97:ASN:ND2	1.90	0.69
1:B:148:ILE:HG22	1:B:148:ILE:O	1.92	0.68
1:A:189:TYR:C	1:A:189:TYR:CD1	2.66	0.68
1:B:211:ILE:HG12	1:B:265:LEU:CD2	2.24	0.67
1:B:25:LYS:HG2	1:B:25:LYS:O	1.95	0.67
1:B:149:THR:HG21	1:B:159:ILE:HD13	1.77	0.66
1:B:181:LEU:HD23	1:B:181:LEU:O	1.96	0.66
1:B:149:THR:CG2	1:B:159:ILE:CD1	2.73	0.66
1:A:32:ILE:HG21	1:A:34:TYR:CZ	2.31	0.65
1:A:175:LYS:O	1:A:175:LYS:CG	2.45	0.65
1:B:149:THR:CG2	1:B:159:ILE:HD11	2.27	0.64
1:B:237:ILE:HD12	1:B:270:LYS:HG2	1.78	0.64
1:A:196:GLY:O	1:A:200:LYS:HE2	1.98	0.64
1:B:37:ASP:OD1	1:B:37:ASP:N	2.30	0.63
1:A:115:THR:HG22	1:A:116:HIS:CD2	2.33	0.63
1:A:172:CYS:O	1:A:193:TYR:HA	1.98	0.63
1:A:169:ILE:HB	1:A:209:ALA:HA	1.81	0.63
1:A:175:LYS:O	1:A:175:LYS:HG2	1.98	0.63
1:B:287:GLN:HG2	1:B:288:HIS:N	2.14	0.62
1:B:287:GLN:HG2	1:B:288:HIS:H	1.65	0.62
1:A:77:ASP:N	1:A:77:ASP:OD2	2.29	0.61
1:A:189:TYR:CD1	1:A:190:GLU:N	2.68	0.60
1:A:196:GLY:HA3	1:A:199:ALA:HB3	1.84	0.60
1:B:251:SER:OG	1:B:253:LYS:CG	2.30	0.60
1:A:219:SER:HB2	4:A:408:HOH:O	2.02	0.60
1:A:202:MET:HA	1:A:202:MET:HE2	1.82	0.60
1:B:149:THR:HG21	1:B:159:ILE:HD11	1.81	0.60
1:A:194:LYS:HD3	1:A:195:GLY:H	1.67	0.59
1:B:252:LYS:HA	1:B:256:MET:HE2	1.83	0.59
1:B:6:PHE:HE2	1:B:91:LEU:HD23	1.67	0.59
1:A:168:ILE:HD11	1:A:272:TYR:CE2	2.31	0.59
1:B:6:PHE:CE2	1:B:91:LEU:HD23	2.38	0.59
1:B:25:LYS:O	1:B:25:LYS:CE	2.52	0.58
1:B:115:THR:OG1	1:B:116:HIS:CD2	2.55	0.58
1:B:139:VAL:HG21	1:B:202:MET:HE3	1.85	0.58
1:A:182:ILE:HD12	1:A:182:ILE:O	2.03	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:20:SER:OG	1:A:146:ASN:ND2	2.35	0.57
1:B:148:ILE:O	1:B:148:ILE:HG23	2.04	0.57
1:A:96:ILE:CG2	1:A:130:TYR:CE1	2.87	0.57
1:B:66:ILE:HD13	1:B:256:MET:HE1	1.86	0.56
1:B:25:LYS:HD3	1:B:25:LYS:O	2.04	0.56
1:B:115:THR:OG1	1:B:116:HIS:HD2	1.88	0.56
1:A:32:ILE:CG2	1:A:34:TYR:CE2	2.89	0.56
1:B:77:ASP:HA	1:B:80:LEU:HD12	1.87	0.56
1:A:135:MET:HE3	1:A:136:ILE:HG13	1.88	0.55
1:A:2:GLN:HE21	1:A:97:ASN:HD21	1.54	0.55
1:B:149:THR:CG2	1:B:159:ILE:HD13	2.35	0.55
1:A:62:THR:HG23	1:A:98:ILE:HG21	1.88	0.55
1:A:16:VAL:HG12	1:A:148:ILE:CD1	2.36	0.55
1:A:160:SER:O	1:A:206:HIS:HD2	1.91	0.54
1:A:16:VAL:HG12	1:A:148:ILE:HD11	1.90	0.54
1:B:27:LYS:CD	1:B:27:LYS:H	1.98	0.54
1:B:18:GLU:CG	1:B:81:PRO:HG3	2.34	0.54
1:A:43:GLN:OE1	1:A:43:GLN:N	2.41	0.54
1:A:32:ILE:HG22	1:A:34:TYR:CE2	2.42	0.54
1:A:18:GLU:HG3	1:A:81:PRO:CG	2.25	0.54
1:B:2:GLN:HG2	1:B:97:ASN:ND2	2.24	0.52
1:A:73:ASN:O	1:A:74:GLY:C	2.47	0.52
1:A:217:ILE:O	1:A:217:ILE:HG22	2.10	0.52
1:A:194:LYS:CE	1:A:194:LYS:HA	2.39	0.52
1:A:102:ILE:HB	1:A:129:THR:HG22	1.91	0.52
1:B:25:LYS:HE2	1:B:25:LYS:O	2.10	0.51
1:A:96:ILE:HG23	1:A:130:TYR:CE1	2.45	0.51
1:B:181:LEU:O	1:B:279:ILE:CD1	2.59	0.51
1:A:25:LYS:CD	1:A:25:LYS:O	2.58	0.51
1:A:165:ASN:O	1:A:166:ASP:OD1	2.29	0.51
1:A:97:ASN:O	1:A:98:ILE:C	2.47	0.51
1:A:266:SER:HB2	1:A:267:PRO:HD2	1.92	0.50
1:A:180:HIS:HD2	1:A:183:LYS:NZ	2.09	0.50
1:B:73:ASN:O	1:B:73:ASN:OD1	2.30	0.50
1:B:217:ILE:HG22	1:B:257:ARG:HD3	1.94	0.50
1:A:202:MET:CE	1:A:205:ILE:HD13	2.43	0.49
1:B:26:PHE:CZ	1:B:28:GLU:HG3	2.47	0.49
1:A:282:THR:OG1	1:A:282:THR:O	2.30	0.49
1:B:152:ILE:O	1:B:153:GLU:C	2.48	0.48
1:B:41:VAL:HG13	1:B:41:VAL:O	2.13	0.48
1:B:216:LEU:HD22	1:B:218:GLN:HG3	1.96	0.48
1:B:12:LEU:HD23	1:B:56:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:228:GLN:HA	1:A:238:VAL:HG21	1.95	0.48
1:A:251:SER:OG	1:A:253:LYS:HG2	2.14	0.48
1:B:202:MET:HE2	1:B:205:ILE:HD12	1.95	0.48
1:A:139:VAL:O	1:A:148:ILE:HA	2.13	0.48
1:A:58:ASN:OD1	1:A:77:ASP:OD1	2.31	0.48
1:A:115:THR:C	1:A:116:HIS:HD2	2.17	0.47
1:B:26:PHE:CE2	1:B:28:GLU:HG3	2.49	0.47
1:A:75:ILE:HG23	1:A:76:PRO:HD2	1.96	0.47
1:A:174:LYS:HE2	1:A:193:TYR:CE2	2.49	0.47
1:A:66:ILE:HG21	1:A:256:MET:HE3	1.96	0.47
1:B:252:LYS:HA	1:B:256:MET:CE	2.45	0.47
1:A:2:GLN:NE2	1:A:97:ASN:ND2	2.62	0.47
1:B:30:VAL:HA	1:B:43:GLN:HE22	1.80	0.46
1:B:221:THR:HG22	1:B:248:TYR:CD1	2.51	0.46
1:A:150:PHE:H	1:A:157:SER:HB3	1.81	0.46
1:A:27:LYS:HG2	1:A:27:LYS:O	2.15	0.46
1:A:133:LYS:HB3	1:A:133:LYS:HE2	1.53	0.46
1:A:194:LYS:HD3	1:A:195:GLY:N	2.30	0.46
1:A:32:ILE:HG21	1:A:34:TYR:CE2	2.51	0.46
1:A:116:HIS:N	1:A:116:HIS:CD2	2.84	0.45
1:B:231:LEU:HD23	1:B:238:VAL:HG23	1.97	0.45
1:A:149:THR:CG2	1:A:159:ILE:CD1	2.95	0.45
1:A:56:ILE:HD13	1:A:56:ILE:N	2.31	0.45
1:B:27:LYS:HD2	1:B:28:GLU:N	2.32	0.45
1:A:178:ILE:HG13	1:A:178:ILE:H	1.42	0.45
1:A:52:ILE:O	1:A:56:ILE:HG12	2.16	0.45
1:A:201:MET:CE	1:A:227:ALA:HB3	2.46	0.45
1:A:11:VAL:HG12	1:A:56:ILE:HD12	1.98	0.44
1:B:43:GLN:H	1:B:43:GLN:HG3	1.51	0.44
1:B:24:SER:HA	1:B:143:PHE:CE1	2.52	0.44
1:A:288:HIS:N	1:A:288:HIS:ND1	2.65	0.44
1:A:59:LYS:HD3	1:A:59:LYS:HA	1.73	0.43
1:A:185:PHE:HD1	1:A:275:TYR:CE2	2.36	0.43
1:A:183:LYS:N	4:A:410:HOH:O	2.50	0.43
1:B:27:LYS:CD	1:B:28:GLU:N	2.82	0.43
1:B:152:ILE:O	1:B:153:GLU:HB2	2.17	0.43
1:A:186:PRO:HB2	1:A:187:ASP:OD2	2.18	0.43
1:B:169:ILE:HB	1:B:209:ALA:HA	1.99	0.43
1:B:148:ILE:HG23	1:B:148:ILE:HD13	1.71	0.43
1:A:149:THR:HG21	1:A:159:ILE:CD1	2.49	0.42
1:A:168:ILE:O	1:A:189:TYR:HA	2.19	0.42
1:B:150:PHE:O	1:B:150:PHE:CD1	2.72	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:135:MET:HE3	1:A:135:MET:HB3	1.87	0.42
1:B:158:SER:C	1:B:159:ILE:HG12	2.40	0.42
1:A:169:ILE:CG2	1:A:192:LYS:HG3	2.50	0.42
1:B:130:TYR:HB2	1:B:135:MET:HE2	2.01	0.42
1:A:102:ILE:HG22	1:A:104:TYR:CE2	2.55	0.42
1:B:187:ASP:HB3	1:B:188:PRO:CD	2.50	0.42
1:A:202:MET:HE2	1:A:205:ILE:CD1	2.50	0.41
1:A:102:ILE:HB	1:A:129:THR:CG2	2.51	0.41
1:A:196:GLY:O	1:A:200:LYS:CE	2.68	0.41
1:A:202:MET:HE1	1:A:205:ILE:HD13	2.02	0.41
1:A:96:ILE:HG23	1:A:130:TYR:CZ	2.55	0.41
1:A:60:TYR:O	1:A:63:ILE:HG22	2.21	0.41
1:A:69:GLU:OE1	1:A:69:GLU:HA	2.20	0.41
1:B:15:ALA:HB1	1:B:52:ILE:HA	2.01	0.41
1:A:273:LEU:HB3	1:A:274:PRO:HD3	2.02	0.41
1:B:287:GLN:CG	1:B:288:HIS:N	2.81	0.41
1:A:164:LEU:HD12	1:A:207:GLN:NE2	2.35	0.41
1:B:273:LEU:HB3	1:B:274:PRO:HD3	2.03	0.41
1:B:284:LEU:HA	1:B:284:LEU:HD23	1.54	0.41
1:A:176:ASN:O	1:A:178:ILE:HG23	2.21	0.40
1:A:240:ASP:HB2	1:A:244:ASN:H	1.86	0.40
1:A:151:ALA:HB3	1:A:229:VAL:HG12	2.03	0.40
1:A:2:GLN:CG	1:A:97:ASN:HD22	2.34	0.40
1:A:171:VAL:HG13	1:A:209:ALA:HB2	2.04	0.40
1:A:116:HIS:O	1:A:117:LYS:CB	2.57	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	286/293 (98%)	260 (91%)	26 (9%)	0	100	100
1	B	287/293 (98%)	260 (91%)	25 (9%)	2 (1%)	30	49
All	All	573/586 (98%)	520 (91%)	51 (9%)	2 (0%)	50	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	84	THR
1	B	41	VAL

### 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	262/267 (98%)	237 (90%)	25 (10%)	12	21
1	B	263/267 (98%)	228 (87%)	35 (13%)	6	9
All	All	525/534 (98%)	465 (89%)	60 (11%)	8	14

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	18	GLU
1	A	25	LYS
1	A	28	GLU
1	A	29	GLU
1	A	31	GLU
1	A	33	LYS
1	A	36	SER
1	A	37	ASP
1	A	71	VAL
1	A	72	GLU
1	A	77	ASP
1	A	94	LYS
1	A	97	ASN
1	A	98	ILE
1	A	129	THR
1	A	135	MET
1	A	175	LYS
1	A	178	ILE
1	A	183	LYS
1	A	194	LYS
1	A	219	SER

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Mol	Chain	Res	Type
1	A	251	SER
1	A	253	LYS
1	A	282	THR
1	B	20	SER
1	B	27	LYS
1	B	28	GLU
1	B	36	SER
1	B	37	ASP
1	B	39	SER
1	B	40	GLU
1	B	42	THR
1	B	43	GLN
1	B	47	GLN
1	B	62	THR
1	B	65	ILE
1	B	77	ASP
1	B	82	THR
1	B	91	LEU
1	B	99	ASN
1	B	133	LYS
1	B	135	MET
1	B	146	ASN
1	B	147	GLU
1	B	148	ILE
1	B	149	THR
1	B	159	ILE
1	B	167	LYS
1	B	168	ILE
1	B	169	ILE
1	B	171	VAL
1	B	174	LYS
1	B	175	LYS
1	B	181	LEU
1	B	187	ASP
1	B	216	LEU
1	B	250	SER
1	B	279	ILE
1	B	282	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	97	ASN
1	A	116	HIS
1	A	118	GLN
1	A	146	ASN
1	A	180	HIS
1	A	228	GLN
1	B	43	GLN
1	B	73	ASN
1	B	97	ASN
1	B	116	HIS
1	B	118	GLN
1	B	206	HIS
1	B	207	GLN
1	B	228	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	$\# Z  > 2$
2	PO4	A	301	3	4,4,4	0.21	0	6,6,6	0.31	0
2	PO4	B	303	3	4,4,4	0.28	0	6,6,6	0.31	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	PO4	A	301	3	-	0/0/0/0	0/0/0/0
2	PO4	B	303	3	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	288/293 (98%)	0.47	21 (7%) 15 15	21, 35, 58, 73	0
1	B	289/293 (98%)	0.50	21 (7%) 15 15	23, 37, 62, 73	0
All	All	577/586 (98%)	0.49	42 (7%) 15 15	21, 36, 60, 73	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	36	SER	7.1
1	B	28	GLU	4.0
1	B	29	GLU	3.7
1	A	32	ILE	3.5
1	A	31	GLU	3.5
1	B	27	LYS	3.5
1	A	180	HIS	3.3
1	B	40	GLU	3.2
1	B	193	TYR	3.2
1	B	37	ASP	3.2
1	A	27	LYS	3.1
1	A	30	VAL	3.0
1	A	36	SER	3.0
1	B	180	HIS	2.9
1	B	150	PHE	2.8
1	B	253	LYS	2.8
1	A	38	GLY	2.8
1	B	30	VAL	2.8
1	A	26	PHE	2.7
1	A	288	HIS	2.6
1	A	29	GLU	2.6
1	A	164	LEU	2.6
1	B	126	VAL	2.6
1	A	34	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	38	GLY	2.5
1	A	28	GLU	2.5
1	B	166	ASP	2.4
1	A	139	VAL	2.4
1	A	125	LEU	2.4
1	B	32	ILE	2.4
1	A	166	ASP	2.4
1	B	33	LYS	2.3
1	B	31	GLU	2.3
1	A	21	TYR	2.3
1	B	35	LYS	2.2
1	B	175	LYS	2.2
1	A	123	CYS	2.1
1	A	105	VAL	2.1
1	A	182	ILE	2.1
1	A	115	THR	2.1
1	B	189	TYR	2.1
1	B	289	HIS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	B	302	1/1	0.29	2.15	23,23,23,23	0
3	MG	A	302	1/1	0.29	2.08	23,23,23,23	0
2	PO4	A	301	5/5	0.22	0.53	35,36,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	B	301	1/1	0.19	0.35	19,19,19,19	0
3	MG	A	303	1/1	0.24	0.27	27,27,27,27	0
3	MG	A	304	1/1	0.19	-0.26	23,23,23,23	0
3	MG	B	304	1/1	0.20	-0.44	34,34,34,34	0
2	PO4	B	303	5/5	0.16	-0.51	35,36,37,37	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.