



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:42 am BST

PDB ID : 5X3F  
Title : Crystal structure of the YgjG-Protein A-Zpa963-PKA catalytic domain  
Authors : Youn, S.J.; Kwon, N.Y.; Lee, J.H.; Kim, J.H.; Lee, H.; Lee, J.O.  
Deposited on : 2017-02-05  
Resolution : 3.38 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

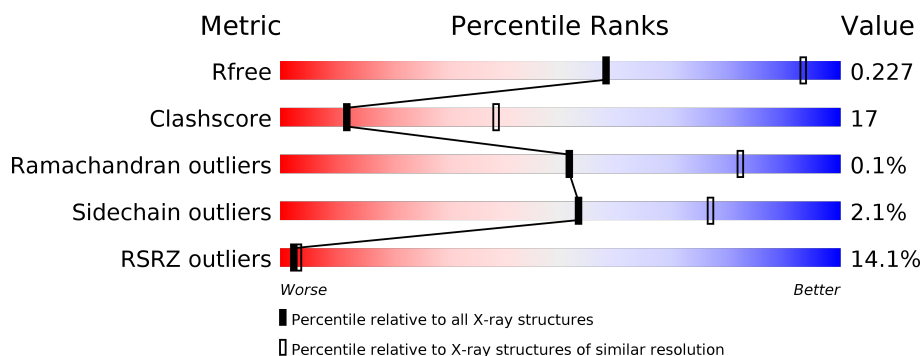
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.38 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))
$R_{free}$	130704	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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 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	501	<div> <div>5%</div> <div>76%</div> <div>21%</div> <div>••</div> </div>
2	B	393	<div> <div>24%</div> <div>61%</div> <div>27%</div> <div>• 11%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6616 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 Putrescine aminotransferase,Immunoglobulin G-binding protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3764	2390	649	703	22			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	-	expression tag	UNP P42588
A	4	SER	-	expression tag	UNP P42588
A	5	HIS	-	expression tag	UNP P42588
A	6	MET	-	expression tag	UNP P42588
A	456	VAL	ASN	engineered mutation	UNP P38507
A	474	ALA	GLY	engineered mutation	UNP P38507

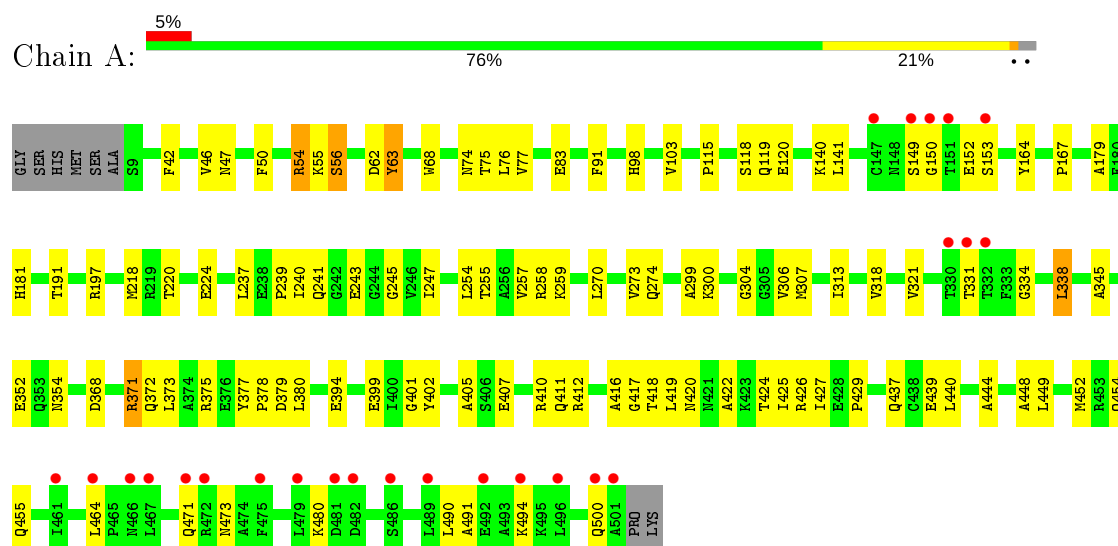
- Molecule 2 is a protein called Zpa963,cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	349	Total	C	N	O	P S	0	0	0
			2852	1850	483	511	1 7			

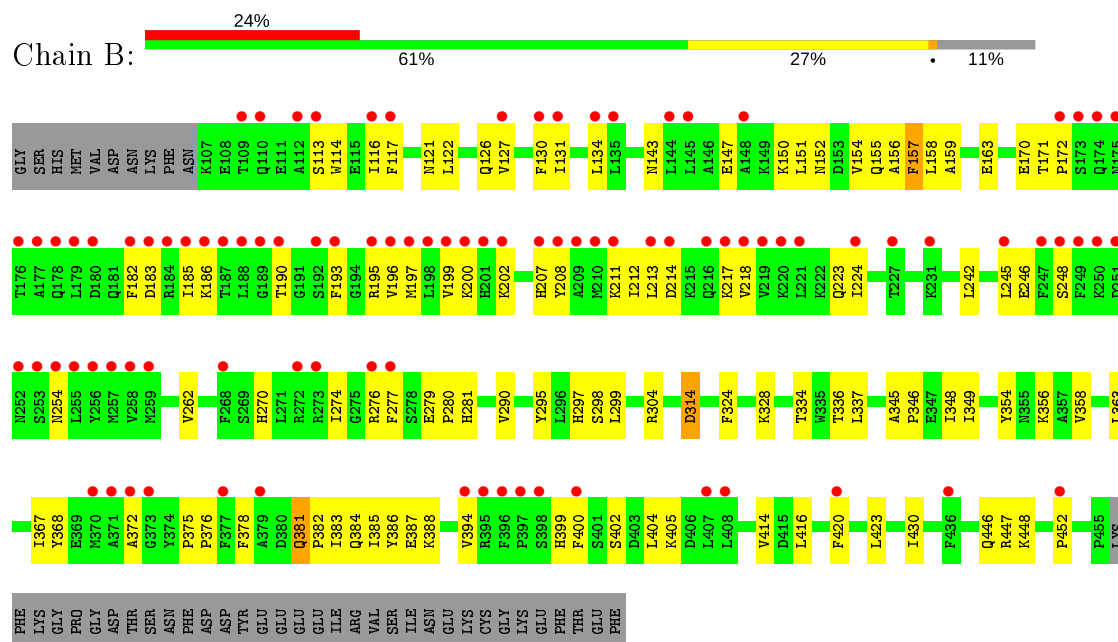
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Putrescine aminotransferase,Immunoglobulin G-binding protein A



- Molecule 2: Zpa963,cAMP-dependent protein kinase catalytic subunit alpha



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.52Å 153.50Å 205.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.38 48.08 – 3.38	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.00-3.38) 99.0 (48.08-3.38)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.190 , 0.227 0.192 , 0.227	Depositor DCC
$R_{free}$ test set	1493 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	102.7	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 85.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6616	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.54	0/3834	0.77	2/5188 (0.0%)
2	B	0.50	0/2911	0.72	2/3932 (0.1%)
All	All	0.53	0/6745	0.75	4/9120 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	LEU	CA-CB-CG	6.85	131.05	115.30
1	A	464	LEU	N-CA-C	-6.68	92.96	111.00
2	B	423	LEU	N-CA-C	-5.91	95.06	111.00
2	B	423	LEU	CB-CA-C	5.04	119.78	110.20

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3764	0	3789	82	5
2	B	2852	0	2864	151	3
All	All	6616	0	6653	230	5

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 17.

All (230) 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)
2:B:185:ILE:HD11	2:B:200:LYS:CG	1.56	1.33
2:B:183:ASP:HB2	2:B:202:LYS:CE	1.64	1.28
2:B:349:ILE:HD11	2:B:386:TYR:CD2	1.69	1.27
2:B:185:ILE:CD1	2:B:200:LYS:HG3	1.65	1.25
2:B:151:LEU:O	2:B:154:VAL:HG13	1.49	1.12
2:B:193:PHE:HB3	2:B:213:LEU:HG	1.27	1.11
2:B:183:ASP:HB2	2:B:202:LYS:HE2	1.11	1.09
2:B:151:LEU:O	2:B:154:VAL:CG1	2.03	1.06
1:A:368:ASP:OD1	1:A:371:ARG:NH2	1.88	1.06
2:B:182:PHE:HB3	2:B:199:VAL:CG1	1.86	1.05
2:B:182:PHE:HB3	2:B:199:VAL:HG11	1.38	1.05
2:B:349:ILE:CD1	2:B:386:TYR:CD2	2.40	1.03
2:B:183:ASP:HB2	2:B:202:LYS:NZ	1.73	1.03
1:A:490:LEU:HG	1:A:494:LYS:HE2	1.41	1.00
2:B:150:LYS:O	2:B:154:VAL:HG12	1.62	0.99
1:A:402:TYR:CD2	1:A:419:LEU:HA	2.00	0.97
2:B:193:PHE:CB	2:B:213:LEU:HG	1.95	0.97
1:A:91:PHE:O	1:A:300:LYS:NZ	1.98	0.95
2:B:197:MET:CE	2:B:212:ILE:HD12	1.95	0.95
2:B:383:ILE:HG23	2:B:384:GLN:N	1.81	0.94
1:A:448:ALA:O	1:A:452:MET:HG3	1.69	0.92
2:B:151:LEU:HA	2:B:154:VAL:HG11	1.50	0.90
2:B:200:LYS:HE2	2:B:207:HIS:NE2	1.87	0.89
2:B:183:ASP:CB	2:B:202:LYS:HE2	2.02	0.88
2:B:183:ASP:CB	2:B:202:LYS:NZ	2.37	0.87
2:B:383:ILE:CG2	2:B:384:GLN:N	2.36	0.86
2:B:151:LEU:HA	2:B:154:VAL:CG1	2.04	0.86
2:B:349:ILE:HD11	2:B:386:TYR:HD2	1.35	0.86
1:A:402:TYR:CE2	1:A:419:LEU:HA	2.10	0.85
2:B:383:ILE:CG2	2:B:384:GLN:H	1.88	0.85
2:B:126:GLN:HE22	2:B:155:GLN:HE22	1.24	0.85
2:B:200:LYS:CE	2:B:207:HIS:NE2	2.41	0.84
2:B:126:GLN:HE22	2:B:155:GLN:NE2	1.76	0.83
2:B:121:ASN:ND2	2:B:156:ALA:HB2	1.92	0.83
1:A:419:LEU:CD2	1:A:420:ASN:ND2	2.43	0.81
2:B:363:LEU:CD2	2:B:367:ILE:HD11	2.11	0.80
2:B:193:PHE:HB3	2:B:213:LEU:CG	2.08	0.80
2:B:197:MET:HE1	2:B:212:ILE:HD12	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:LEU:C	2:B:154:VAL:HG12	2.02	0.80
2:B:382:PRO:O	2:B:383:ILE:C	2.18	0.79
2:B:185:ILE:CD1	2:B:200:LYS:HE3	2.13	0.79
2:B:151:LEU:C	2:B:154:VAL:CG1	2.52	0.79
2:B:157:PHE:O	2:B:157:PHE:CD1	2.37	0.77
2:B:183:ASP:OD2	2:B:202:LYS:NZ	2.16	0.76
2:B:274:ILE:HD12	2:B:277:PHE:HE1	1.51	0.76
2:B:151:LEU:CA	2:B:154:VAL:CG1	2.63	0.76
2:B:336:TPO:N	2:B:336:TPO:O3P	2.17	0.75
2:B:381:GLN:O	2:B:384:GLN:HB2	1.87	0.74
2:B:200:LYS:HG2	2:B:207:HIS:NE2	2.02	0.74
1:A:419:LEU:HD22	1:A:420:ASN:HD21	1.53	0.74
2:B:185:ILE:HD13	2:B:200:LYS:HE3	1.69	0.74
1:A:394:GLU:HG3	1:A:424:THR:HG22	1.70	0.73
1:A:419:LEU:HD22	1:A:420:ASN:ND2	2.04	0.73
1:A:419:LEU:HD23	1:A:420:ASN:ND2	2.03	0.73
1:A:405:ALA:HB2	1:A:425:ILE:CD1	2.19	0.72
2:B:381:GLN:OE1	2:B:381:GLN:HA	1.88	0.72
1:A:405:ALA:HB2	1:A:425:ILE:HD12	1.71	0.72
1:A:380:LEU:HD23	1:A:452:MET:CE	2.20	0.72
2:B:349:ILE:HD13	2:B:386:TYR:CG	2.24	0.72
2:B:200:LYS:HE2	2:B:207:HIS:CE1	2.25	0.71
1:A:448:ALA:O	1:A:452:MET:CG	2.39	0.70
1:A:402:TYR:HD2	1:A:418:THR:O	1.75	0.70
2:B:185:ILE:HD11	2:B:200:LYS:HG3	0.76	0.70
2:B:182:PHE:CB	2:B:199:VAL:HG11	2.17	0.70
2:B:151:LEU:O	2:B:154:VAL:HG12	1.91	0.69
2:B:183:ASP:CB	2:B:202:LYS:HZ3	2.04	0.69
1:A:380:LEU:HD23	1:A:452:MET:HE2	1.75	0.69
2:B:363:LEU:CD2	2:B:367:ILE:CD1	2.71	0.69
2:B:446:GLN:HE21	2:B:448:LYS:NZ	1.89	0.69
2:B:446:GLN:HE21	2:B:448:LYS:HZ3	1.40	0.69
1:A:274:GLN:OE1	1:A:426:ARG:NH2	2.26	0.69
2:B:157:PHE:C	2:B:157:PHE:CD1	2.66	0.68
2:B:197:MET:CE	2:B:212:ILE:CD1	2.72	0.68
2:B:126:GLN:NE2	2:B:155:GLN:HE22	1.91	0.68
2:B:394:VAL:HG13	2:B:394:VAL:O	1.92	0.68
2:B:185:ILE:HD11	2:B:200:LYS:CD	2.24	0.68
2:B:349:ILE:CD1	2:B:386:TYR:CG	2.76	0.68
2:B:383:ILE:HG23	2:B:384:GLN:H	1.54	0.67
1:A:118:SER:O	1:A:119:GLN:HB2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:HIS:CE1	2:B:274:ILE:CD1	2.79	0.66
1:A:55:LYS:NZ	1:A:416:ALA:O	2.29	0.65
2:B:151:LEU:CA	2:B:154:VAL:HG12	2.25	0.65
2:B:197:MET:HE1	2:B:212:ILE:CD1	2.26	0.65
1:A:419:LEU:CD2	1:A:420:ASN:HD21	2.10	0.63
2:B:183:ASP:CG	2:B:202:LYS:HZ1	2.01	0.63
2:B:183:ASP:CG	2:B:202:LYS:NZ	2.52	0.63
2:B:281:HIS:CD2	2:B:452:PRO:HB2	2.33	0.63
1:A:115:PRO:HA	1:A:338:LEU:HD23	1.80	0.63
2:B:122:LEU:HD11	2:B:151:LEU:HG	1.81	0.63
2:B:270:HIS:CE1	2:B:274:ILE:HD12	2.33	0.63
2:B:346:PRO:HG3	2:B:414:VAL:HG12	1.80	0.62
1:A:454:GLN:NE2	2:B:117:PHE:HE1	1.98	0.62
1:A:407:GLU:OE1	1:A:407:GLU:HA	1.98	0.62
2:B:190:THR:HG22	2:B:195:ARG:HB3	1.81	0.61
2:B:200:LYS:CG	2:B:207:HIS:NE2	2.63	0.61
2:B:363:LEU:HD21	2:B:367:ILE:HD11	1.79	0.61
2:B:383:ILE:HG22	2:B:384:GLN:H	1.63	0.61
2:B:185:ILE:CD1	2:B:207:HIS:CD2	2.83	0.60
2:B:150:LYS:O	2:B:154:VAL:CG1	2.46	0.60
1:A:55:LYS:HE2	1:A:417:GLY:O	2.02	0.60
2:B:336:TPO:O	2:B:354:TYR:OH	2.17	0.59
1:A:255:THR:O	1:A:259:LYS:HD2	2.03	0.59
1:A:372:GLN:HA	1:A:375:ARG:NH1	2.18	0.59
2:B:328:LYS:HD3	2:B:334:THR:HG21	1.86	0.58
2:B:262:VAL:HG11	2:B:314:ASP:HA	1.85	0.58
1:A:218:MET:HE1	1:A:257:VAL:HG13	1.85	0.57
1:A:377:TYR:N	1:A:378:PRO:HD3	2.19	0.57
2:B:113:SER:OG	2:B:134:LEU:HD23	2.04	0.57
2:B:382:PRO:O	2:B:385:ILE:N	2.37	0.57
1:A:62:ASP:HB3	1:A:63:TYR:CE1	2.40	0.57
1:A:373:LEU:HD13	1:A:449:LEU:HD12	1.85	0.57
2:B:156:ALA:O	2:B:159:ALA:HB3	2.05	0.56
2:B:276:ARG:NH1	2:B:399:HIS:NE2	2.54	0.56
1:A:220:THR:O	1:A:224:GLU:HG2	2.05	0.56
1:A:42:PHE:O	1:A:47:ASN:O	2.24	0.56
1:A:237:LEU:HD21	1:A:257:VAL:HG11	1.87	0.56
2:B:270:HIS:CE1	2:B:274:ILE:HD11	2.41	0.55
2:B:381:GLN:OE1	2:B:382:PRO:CD	2.54	0.55
1:A:490:LEU:HG	1:A:494:LYS:CE	2.28	0.54
1:A:402:TYR:CE2	1:A:419:LEU:CA	2.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:LEU:HD23	1:A:419:LEU:C	2.28	0.54
2:B:157:PHE:HD1	2:B:157:PHE:O	1.88	0.53
2:B:297:HIS:CD2	2:B:356:LYS:HB2	2.43	0.53
1:A:240:ILE:HG23	1:A:247:ILE:O	2.09	0.53
1:A:455:GLN:HB2	2:B:114:TRP:CH2	2.44	0.53
2:B:197:MET:HE3	2:B:212:ILE:HD12	1.88	0.53
2:B:274:ILE:HD12	2:B:277:PHE:CE1	2.38	0.52
2:B:381:GLN:OE1	2:B:382:PRO:HD2	2.09	0.52
1:A:254:LEU:HD11	1:A:270:LEU:HD21	1.91	0.52
1:A:239:PRO:HG3	1:A:270:LEU:HD22	1.90	0.52
1:A:307:MET:SD	1:A:338:LEU:HD12	2.49	0.52
1:A:50:PHE:O	1:A:54:ARG:HB2	2.09	0.52
2:B:185:ILE:HD11	2:B:200:LYS:HE3	1.90	0.51
1:A:74:ASN:ND2	1:A:437:GLN:OE1	2.43	0.51
2:B:276:ARG:NH1	2:B:399:HIS:CD2	2.78	0.51
2:B:394:VAL:O	2:B:394:VAL:CG1	2.58	0.51
2:B:276:ARG:HH12	2:B:399:HIS:CD2	2.29	0.51
2:B:200:LYS:HG2	2:B:207:HIS:CD2	2.44	0.51
2:B:337:LEU:C	2:B:337:LEU:HD23	2.31	0.51
1:A:427:ILE:HG22	1:A:429:PRO:HD3	1.93	0.50
2:B:196:VAL:HG22	2:B:211:LYS:HG2	1.93	0.50
2:B:290:VAL:HG22	2:B:363:LEU:HD11	1.93	0.50
2:B:121:ASN:HD21	2:B:156:ALA:HB2	1.72	0.50
1:A:115:PRO:CA	1:A:338:LEU:HD23	2.42	0.49
2:B:290:VAL:CG1	2:B:430:ILE:HD11	2.42	0.49
1:A:63:TYR:N	1:A:63:TYR:CD1	2.76	0.49
2:B:348:ILE:HD11	2:B:358:VAL:HG11	1.92	0.49
1:A:419:LEU:HD23	1:A:419:LEU:O	2.11	0.49
2:B:214:ASP:HB3	2:B:217:LYS:HB2	1.94	0.49
2:B:242:LEU:HD22	2:B:324:PHE:HZ	1.77	0.49
2:B:116:ILE:HG21	2:B:130:PHE:HB2	1.93	0.49
2:B:163:GLU:OE2	2:B:163:GLU:HA	2.12	0.49
1:A:62:ASP:C	1:A:63:TYR:CD1	2.86	0.49
2:B:218:VAL:HG13	2:B:223:GLN:HB2	1.95	0.49
1:A:439:GLU:O	1:A:440:LEU:C	2.50	0.49
2:B:381:GLN:OE1	2:B:382:PRO:HD3	2.13	0.48
2:B:200:LYS:HG2	2:B:207:HIS:CE1	2.48	0.48
1:A:379:ASP:OD1	1:A:379:ASP:N	2.40	0.48
1:A:68:TRP:HB3	1:A:77:VAL:O	2.14	0.48
1:A:318:VAL:O	1:A:321:VAL:HG22	2.13	0.48
2:B:185:ILE:HD11	2:B:200:LYS:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200:LYS:HE3	2:B:207:HIS:NE2	2.27	0.48
1:A:164:TYR:O	1:A:167:PRO:HD2	2.14	0.48
2:B:363:LEU:HD23	2:B:367:ILE:CD1	2.44	0.48
2:B:193:PHE:HB2	2:B:213:LEU:HG	1.91	0.47
2:B:372:ALA:HB2	2:B:400:PHE:CZ	2.50	0.47
1:A:241:GLN:HB2	1:A:247:ILE:HB	1.97	0.47
2:B:208:TYR:HE2	2:B:246:GLU:HG3	1.80	0.47
1:A:255:THR:HG22	1:A:259:LYS:NZ	2.29	0.47
1:A:191:THR:O	1:A:197:ARG:HD2	2.14	0.47
2:B:126:GLN:NE2	2:B:151:LEU:HD21	2.30	0.47
1:A:380:LEU:CD2	1:A:452:MET:HE2	2.44	0.47
1:A:405:ALA:HB2	1:A:425:ILE:HD11	1.92	0.47
2:B:122:LEU:HD13	2:B:152:ASN:HA	1.97	0.47
2:B:183:ASP:CB	2:B:202:LYS:CE	2.60	0.47
2:B:378:PHE:C	2:B:378:PHE:CD2	2.88	0.47
2:B:199:VAL:HG12	2:B:200:LYS:N	2.31	0.46
2:B:143:ASN:O	2:B:147:GLU:HG2	2.16	0.46
2:B:446:GLN:O	2:B:447:ARG:HB2	2.17	0.45
1:A:411:GLN:OE1	1:A:444:ALA:O	2.34	0.45
1:A:75:THR:HB	1:A:83:GLU:HG2	1.99	0.45
2:B:378:PHE:O	2:B:388:LYS:NZ	2.49	0.45
1:A:410:ARG:C	1:A:412:ARG:H	2.19	0.45
1:A:480:LYS:HE2	2:B:117:PHE:O	2.16	0.45
2:B:375:PRO:HG2	2:B:378:PHE:HB2	1.99	0.45
2:B:416:LEU:H	2:B:416:LEU:HD23	1.80	0.45
2:B:337:LEU:O	2:B:337:LEU:HD23	2.16	0.45
2:B:155:GLN:O	2:B:158:LEU:HB2	2.17	0.45
2:B:197:MET:HE3	2:B:212:ILE:CD1	2.46	0.45
2:B:214:ASP:HB3	2:B:217:LYS:HD2	1.99	0.45
2:B:208:TYR:CE2	2:B:246:GLU:HG3	2.51	0.45
2:B:420:PHE:HD1	2:B:430:ILE:HG22	1.82	0.45
2:B:224:ILE:H	2:B:224:ILE:HD12	1.81	0.45
2:B:290:VAL:HG11	2:B:430:ILE:HD11	1.98	0.44
2:B:345:ALA:HB3	2:B:358:VAL:HG22	1.99	0.44
2:B:185:ILE:HG22	2:B:186:LYS:HG3	1.99	0.44
1:A:255:THR:O	1:A:258:ARG:HB3	2.18	0.44
1:A:411:GLN:OE1	1:A:444:ALA:HB1	2.18	0.44
1:A:141:LEU:HB3	1:A:313:ILE:HG22	1.99	0.44
1:A:179:ALA:HB1	1:A:181:HIS:NE2	2.33	0.44
2:B:382:PRO:O	2:B:383:ILE:O	2.35	0.44
2:B:113:SER:OG	2:B:134:LEU:CD2	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:GLU:C	1:A:354:ASN:H	2.21	0.43
2:B:171:THR:HA	2:B:172:PRO:HD3	1.65	0.43
1:A:150:GLY:O	1:A:153:SER:HB3	2.18	0.43
2:B:262:VAL:CG1	2:B:314:ASP:HA	2.48	0.43
1:A:115:PRO:CB	1:A:338:LEU:HD23	2.48	0.43
2:B:430:ILE:C	2:B:430:ILE:HD12	2.39	0.43
1:A:304:GLY:O	1:A:306:VAL:HG23	2.19	0.43
1:A:77:VAL:HG22	1:A:83:GLU:HG3	2.00	0.43
2:B:295:TYR:O	2:B:298:SER:HB3	2.19	0.42
2:B:127:VAL:O	2:B:131:ILE:HG12	2.19	0.42
1:A:76:LEU:HD21	1:A:98:HIS:CE1	2.55	0.42
1:A:373:LEU:HA	1:A:373:LEU:HD23	1.88	0.42
1:A:471:GLN:HE22	1:A:500:GLN:NE2	2.18	0.42
2:B:245:LEU:HD21	2:B:248:SER:HB2	2.02	0.41
2:B:304:ARG:NH2	2:B:328:LYS:HB2	2.35	0.41
1:A:331:THR:HG23	1:A:334:GLY:H	1.85	0.41
2:B:185:ILE:CD1	2:B:200:LYS:CE	2.92	0.41
1:A:103:VAL:HA	1:A:345:ALA:HB1	2.03	0.41
2:B:402:SER:HA	2:B:405:LYS:HD2	2.03	0.41
1:A:425:ILE:HG22	1:A:426:ARG:N	2.34	0.41
2:B:363:LEU:HD23	2:B:367:ILE:HG13	2.03	0.41
2:B:368:TYR:CD2	2:B:376:PRO:HD3	2.55	0.41
1:A:42:PHE:HA	1:A:46:VAL:HB	2.03	0.41
1:A:243:GLU:C	1:A:245:GLY:H	2.25	0.41
2:B:279:GLU:N	2:B:280:PRO:HD2	2.36	0.40
1:A:401:GLY:HA3	1:A:422:ALA:O	2.21	0.40
1:A:491:ALA:HA	1:A:494:LYS:HE3	2.03	0.40
2:B:199:VAL:CG1	2:B:200:LYS:N	2.85	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:GLU:OE2	2:B:387:GLU:OE1[8_544]	1.60	0.60
1:A:56:SER:OG	1:A:120:GLU:O[2_545]	1.77	0.43
1:A:439:GLU:OE2	2:B:387:GLU:CD[8_544]	1.91	0.29
1:A:439:GLU:OE2	2:B:387:GLU:OE2[8_544]	1.92	0.28
1:A:149:SER:OG	1:A:152:GLU:OE2[2_545]	2.16	0.04

## 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	491/501 (98%)	445 (91%)	45 (9%)	1 (0%)	47	78
2	B	346/393 (88%)	328 (95%)	18 (5%)	0	100	100
All	All	837/894 (94%)	773 (92%)	63 (8%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	ALA

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	395/401 (98%)	387 (98%)	8 (2%)	55	77
2	B	304/344 (88%)	297 (98%)	7 (2%)	50	75
All	All	699/745 (94%)	684 (98%)	15 (2%)	53	77

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

Mol	Chain	Res	Type
1	A	54	ARG
1	A	56	SER
1	A	63	TYR
1	A	140	LYS
1	A	273	VAL

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Mol	Chain	Res	Type
1	A	371	ARG
1	A	399	GLU
1	A	473	ASN
2	B	157	PHE
2	B	170	GLU
2	B	254	ASN
2	B	299	LEU
2	B	314	ASP
2	B	381	GLN
2	B	404	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	288	HIS
1	A	420	ASN
1	A	437	GLN
1	A	471	GLN
1	A	473	ASN
1	A	500	GLN
2	B	121	ASN
2	B	143	ASN
2	B	152	ASN
2	B	155	GLN
2	B	223	GLN
2	B	446	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	TPO	B	336	2	8,10,11	0.93	0	10,14,16	2.52	1 (10%)

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	TPO	B	336	2	-	0/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	336	TPO	P-OG1-CB	-7.48	100.63	123.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	336	TPO	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

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	493/501 (98%)	0.37	25 (5%)	28 31	72, 100, 163, 199	0
2	B	348/393 (88%)	1.21	94 (27%)	0 0	120, 168, 247, 281	0
All	All	841/894 (94%)	0.72	119 (14%)	2 3	72, 124, 216, 281	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	187	THR	7.8
2	B	208	TYR	7.2
2	B	209	ALA	6.7
2	B	257	MET	6.4
2	B	198	LEU	6.2
2	B	253	SER	6.0
2	B	179	LEU	5.8
2	B	188	LEU	5.7
2	B	394	VAL	5.7
2	B	210	MET	5.7
2	B	182	PHE	5.6
2	B	177	ALA	5.3
1	A	467	LEU	5.3
2	B	185	ILE	5.3
2	B	216	GLN	5.3
2	B	199	VAL	5.1
2	B	254	ASN	5.0
2	B	197	MET	4.8
2	B	251	ASP	4.8
2	B	255	LEU	4.7
2	B	145	LEU	4.6
2	B	252	ASN	4.6
2	B	218	VAL	4.4
2	B	371	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	268	PHE	4.2
2	B	372	ALA	4.2
2	B	396	PHE	4.2
2	B	183	ASP	4.1
2	B	192	SER	4.1
2	B	186	LYS	4.1
1	A	331	THR	4.1
2	B	134	LEU	4.0
2	B	256	TYR	4.0
2	B	227	THR	4.0
2	B	395	ARG	3.9
2	B	420	PHE	3.9
2	B	116	ILE	3.9
2	B	373	GLY	3.8
2	B	112	ALA	3.7
2	B	213	LEU	3.7
2	B	272	ARG	3.6
2	B	189	GLY	3.6
2	B	131	ILE	3.6
2	B	190	THR	3.6
2	B	175	ASN	3.6
2	B	214	ASP	3.5
1	A	464	LEU	3.5
1	A	332	THR	3.5
2	B	201	HIS	3.5
2	B	220	LYS	3.4
1	A	501	ALA	3.4
2	B	178	GLN	3.3
2	B	258	VAL	3.2
2	B	176	THR	3.2
2	B	249	PHE	3.2
2	B	259	MET	3.2
2	B	195	ARG	3.2
1	A	472	ARG	3.1
2	B	202	LYS	3.1
2	B	113	SER	3.1
1	A	471	GLN	3.1
2	B	109	THR	3.0
2	B	245	LEU	3.0
1	A	486	SER	3.0
2	B	250	LYS	3.0
2	B	193	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	231	LYS	2.9
2	B	247	PHE	2.9
2	B	217	LYS	2.9
2	B	180	ASP	2.9
2	B	174	GLN	2.9
2	B	110	GLN	2.8
2	B	370	MET	2.8
2	B	400	PHE	2.8
2	B	196	VAL	2.8
2	B	144	LEU	2.7
1	A	489	LEU	2.7
2	B	219	VAL	2.7
2	B	377	PHE	2.7
2	B	277	PHE	2.6
1	A	494	LYS	2.6
1	A	149	SER	2.6
1	A	475	PHE	2.5
1	A	147	CYS	2.5
2	B	407	LEU	2.5
2	B	211	LYS	2.5
1	A	466	ASN	2.5
1	A	151	THR	2.5
2	B	184	ARG	2.5
1	A	461	ILE	2.4
1	A	482	ASP	2.4
2	B	173	SER	2.4
2	B	276	ARG	2.4
1	A	496	LEU	2.4
2	B	172	PRO	2.4
2	B	248	SER	2.3
2	B	397	PRO	2.3
1	A	500	GLN	2.3
2	B	452	PRO	2.3
2	B	224	ILE	2.3
1	A	492	GLU	2.2
1	A	153	SER	2.2
2	B	200	LYS	2.2
1	A	481	ASP	2.2
2	B	148	ALA	2.2
2	B	127	VAL	2.2
2	B	273	ARG	2.2
2	B	221	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	207	HIS	2.1
2	B	408	LEU	2.1
1	A	150	GLY	2.1
1	A	479	LEU	2.1
1	A	330	THR	2.1
2	B	130	PHE	2.1
2	B	117	PHE	2.0
2	B	436	PHE	2.0
2	B	135	LEU	2.0
2	B	398	SER	2.0
2	B	379	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
2	TPO	B	336	11/12	0.95	0.19	126,136,143,150	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.