



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2018 – 01:34 PM EST

PDB ID : 6B2Q  
Title : Dual Inhibition of the Essential Protein Kinases A and B in Mycobacterium tuberculosis  
Authors : Zuccola, H.J.  
Deposited on : 2017-09-20  
Resolution : 2.88 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030736

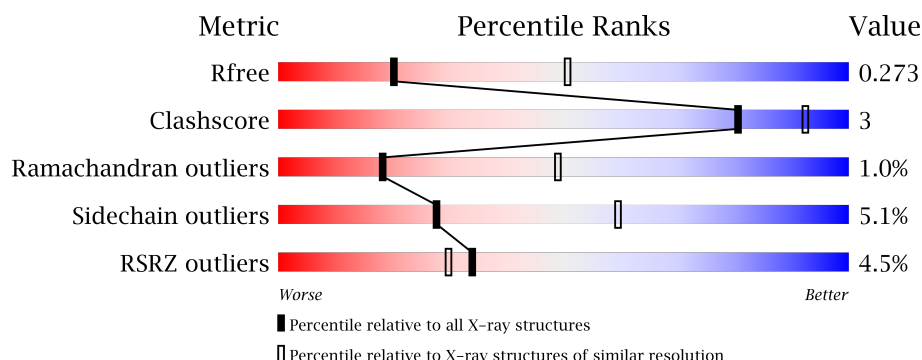
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.88 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))
$R_{free}$	100719	2135 (2.90-2.86)
Clashscore	112137	2400 (2.90-2.86)
Ramachandran outliers	110173	2346 (2.90-2.86)
Sidechain outliers	110143	2349 (2.90-2.86)
RSRZ outliers	101464	2149 (2.90-2.86)

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	317	<div> <div>0.1%</div> <div>70% 12% 17%</div> </div>
1	B	317	<div> <div>2%</div> <div>75% 8% 16%</div> </div>
1	C	317	<div> <div>6%</div> <div>74% 10% 16%</div> </div>
1	D	317	<div> <div>7%</div> <div>71% 11% 18%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	0BD	A	302	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8162 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 Serine/threonine-protein kinase PknA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	P	S	0	0	0
			1990	1250	370	363	1	6			
1	B	267	Total	C	N	O	P	S	0	0	0
			2024	1272	375	368	1	8			
1	C	265	Total	C	N	O	P	S	0	1	0
			2023	1269	380	367	1	6			
1	D	260	Total	C	N	O	P	S	0	1	0
			1993	1253	373	359	1	7			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP A5TY85
A	-19	GLY	-	expression tag	UNP A5TY85
A	-18	SER	-	expression tag	UNP A5TY85
A	-17	SER	-	expression tag	UNP A5TY85
A	-16	HIS	-	expression tag	UNP A5TY85
A	-15	HIS	-	expression tag	UNP A5TY85
A	-14	HIS	-	expression tag	UNP A5TY85
A	-13	HIS	-	expression tag	UNP A5TY85
A	-12	HIS	-	expression tag	UNP A5TY85
A	-11	HIS	-	expression tag	UNP A5TY85
A	-10	SER	-	expression tag	UNP A5TY85
A	-9	SER	-	expression tag	UNP A5TY85
A	-8	GLY	-	expression tag	UNP A5TY85
A	-7	LEU	-	expression tag	UNP A5TY85
A	-6	VAL	-	expression tag	UNP A5TY85
A	-5	PRO	-	expression tag	UNP A5TY85
A	-4	ARG	-	expression tag	UNP A5TY85
A	-3	GLY	-	expression tag	UNP A5TY85
A	-2	SER	-	expression tag	UNP A5TY85
A	-1	LEU	-	expression tag	UNP A5TY85
A	0	HIS	-	expression tag	UNP A5TY85

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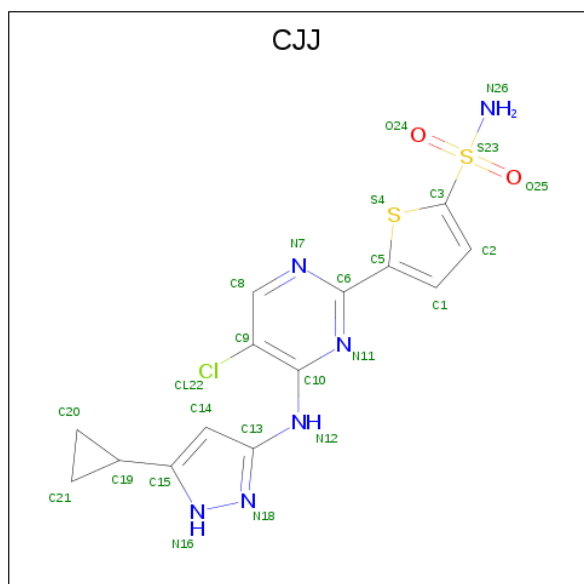
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	expression tag	UNP A5TY85
B	-19	GLY	-	expression tag	UNP A5TY85
B	-18	SER	-	expression tag	UNP A5TY85
B	-17	SER	-	expression tag	UNP A5TY85
B	-16	HIS	-	expression tag	UNP A5TY85
B	-15	HIS	-	expression tag	UNP A5TY85
B	-14	HIS	-	expression tag	UNP A5TY85
B	-13	HIS	-	expression tag	UNP A5TY85
B	-12	HIS	-	expression tag	UNP A5TY85
B	-11	HIS	-	expression tag	UNP A5TY85
B	-10	SER	-	expression tag	UNP A5TY85
B	-9	SER	-	expression tag	UNP A5TY85
B	-8	GLY	-	expression tag	UNP A5TY85
B	-7	LEU	-	expression tag	UNP A5TY85
B	-6	VAL	-	expression tag	UNP A5TY85
B	-5	PRO	-	expression tag	UNP A5TY85
B	-4	ARG	-	expression tag	UNP A5TY85
B	-3	GLY	-	expression tag	UNP A5TY85
B	-2	SER	-	expression tag	UNP A5TY85
B	-1	LEU	-	expression tag	UNP A5TY85
B	0	HIS	-	expression tag	UNP A5TY85
C	-20	MET	-	expression tag	UNP A5TY85
C	-19	GLY	-	expression tag	UNP A5TY85
C	-18	SER	-	expression tag	UNP A5TY85
C	-17	SER	-	expression tag	UNP A5TY85
C	-16	HIS	-	expression tag	UNP A5TY85
C	-15	HIS	-	expression tag	UNP A5TY85
C	-14	HIS	-	expression tag	UNP A5TY85
C	-13	HIS	-	expression tag	UNP A5TY85
C	-12	HIS	-	expression tag	UNP A5TY85
C	-11	HIS	-	expression tag	UNP A5TY85
C	-10	SER	-	expression tag	UNP A5TY85
C	-9	SER	-	expression tag	UNP A5TY85
C	-8	GLY	-	expression tag	UNP A5TY85
C	-7	LEU	-	expression tag	UNP A5TY85
C	-6	VAL	-	expression tag	UNP A5TY85
C	-5	PRO	-	expression tag	UNP A5TY85
C	-4	ARG	-	expression tag	UNP A5TY85
C	-3	GLY	-	expression tag	UNP A5TY85
C	-2	SER	-	expression tag	UNP A5TY85
C	-1	LEU	-	expression tag	UNP A5TY85
C	0	HIS	-	expression tag	UNP A5TY85

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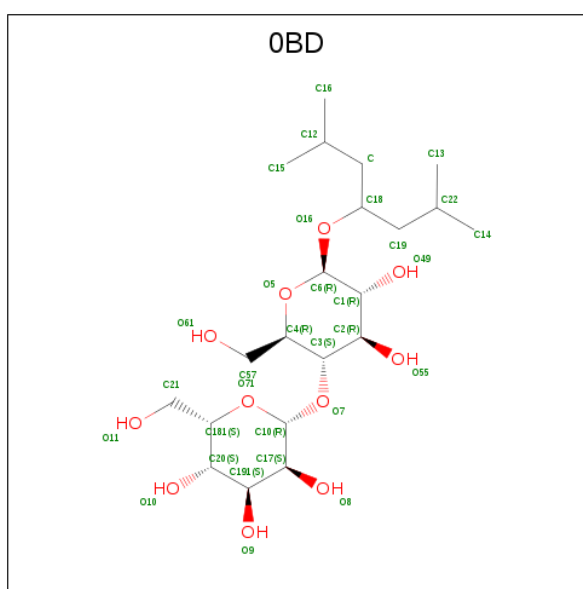
Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	expression tag	UNP A5TY85
D	-19	GLY	-	expression tag	UNP A5TY85
D	-18	SER	-	expression tag	UNP A5TY85
D	-17	SER	-	expression tag	UNP A5TY85
D	-16	HIS	-	expression tag	UNP A5TY85
D	-15	HIS	-	expression tag	UNP A5TY85
D	-14	HIS	-	expression tag	UNP A5TY85
D	-13	HIS	-	expression tag	UNP A5TY85
D	-12	HIS	-	expression tag	UNP A5TY85
D	-11	HIS	-	expression tag	UNP A5TY85
D	-10	SER	-	expression tag	UNP A5TY85
D	-9	SER	-	expression tag	UNP A5TY85
D	-8	GLY	-	expression tag	UNP A5TY85
D	-7	LEU	-	expression tag	UNP A5TY85
D	-6	VAL	-	expression tag	UNP A5TY85
D	-5	PRO	-	expression tag	UNP A5TY85
D	-4	ARG	-	expression tag	UNP A5TY85
D	-3	GLY	-	expression tag	UNP A5TY85
D	-2	SER	-	expression tag	UNP A5TY85
D	-1	LEU	-	expression tag	UNP A5TY85
D	0	HIS	-	expression tag	UNP A5TY85

- Molecule 2 is 5-{5-chloro-4-[(5-cyclopropyl-1H-pyrazol-3-yl)amino]pyrimidin-2-yl}thiophene-2-sulfonamide (three-letter code: CJJ) (formula: C<sub>14</sub>H<sub>13</sub>ClN<sub>6</sub>O<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	
			25	14	1	6	2	2	
2	B	1	Total	C	Cl	N	O	S	
			25	14	1	6	2	2	
2	C	1	Total	C	Cl	N	O	S	
			25	14	1	6	2	2	
2	D	1	Total	C	Cl	N	O	S	
			25	14	1	6	2	2	

- Molecule 3 is 3-methyl-1-(2-methylpropyl)butyl 4-O-beta-L-gulopyranosyl-beta-D-glucopyranoside (three-letter code: 0BD) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>11</sub>).

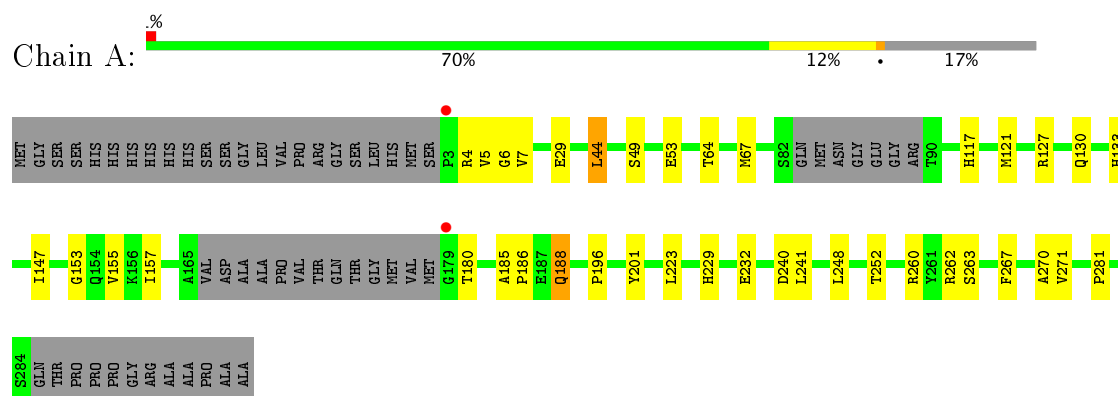


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O		
			32	21	11	0	0

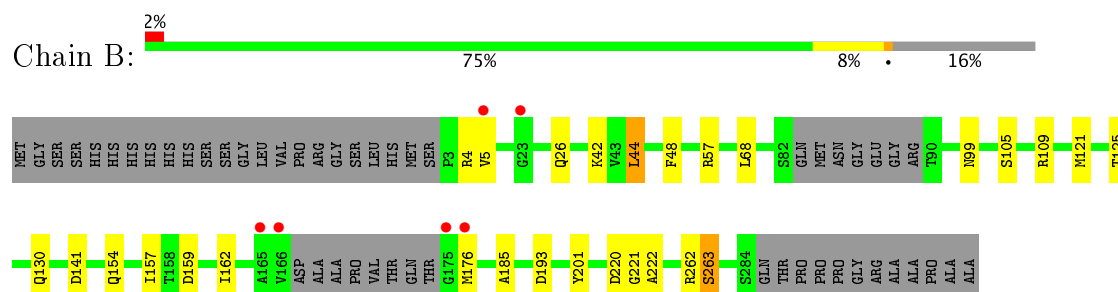
### 3 Residue-property plots [i](#)

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

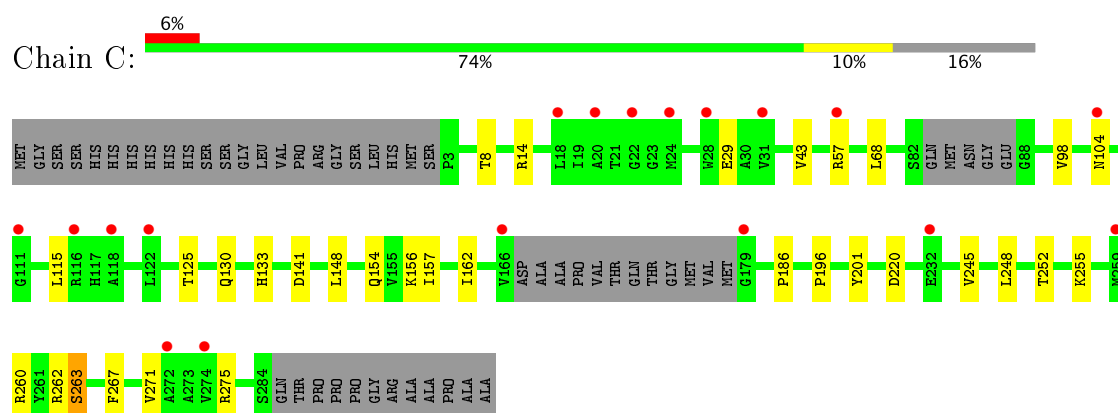
- Molecule 1: Serine/threonine-protein kinase PknA



- Molecule 1: Serine/threonine-protein kinase PknA

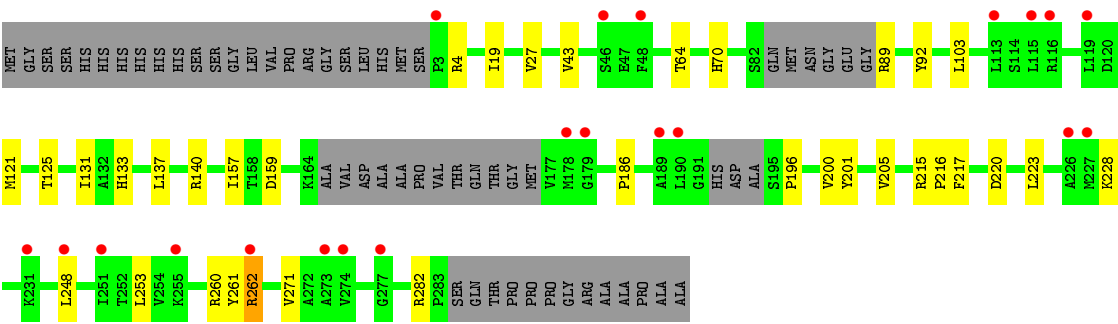


- Molecule 1: Serine/threonine-protein kinase PknA



- Molecule 1: Serine/threonine-protein kinase PknA





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.06Å 227.43Å 158.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.72 – 2.88 113.72 – 2.55	Depositor EDS
% Data completeness (in resolution range)	94.7 (113.72-2.88) 81.9 (113.72-2.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 2.55Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, $R_{free}$	0.230 , 0.263 0.231 , 0.273	Depositor DCC
$R_{free}$ test set	1600 reflections (5.43%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.0	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 63.4	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	0.93	EDS
Total number of atoms	8162	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: CJJ, TPO, 0BD

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	0.44	0/2019	0.66	0/2736
1	B	0.43	0/2053	0.64	0/2781
1	C	0.42	0/2052	0.60	0/2779
1	D	0.43	0/2020	0.62	0/2733
All	All	0.43	0/8144	0.63	0/11029

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 [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	1990	0	2025	15	0
1	B	2024	0	2064	8	0
1	C	2023	0	2062	15	0
1	D	1993	0	2041	13	0
2	A	25	0	0	0	0
2	B	25	0	0	0	0
2	C	25	0	0	0	0
2	D	25	0	0	0	0
3	A	32	0	40	3	0
All	All	8162	0	8232	51	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 3.

All (51) 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:125:THR:HG23	1:B:157:ILE:HD11	1.62	0.80
1:D:125:THR:HG23	1:D:157:ILE:HD11	1.70	0.72
1:C:125:THR:HG23	1:C:157:ILE:HD11	1.76	0.67
1:C:98:VAL:HG11	1:C:156:LYS:HG3	1.86	0.57
1:A:201:TYR:HD2	1:A:260:ARG:NH1	2.03	0.55
1:A:153:GLY:CA	3:A:302:0BD:H13B	2.38	0.53
1:A:130:GLN:OE1	1:A:263:SER:HB3	2.08	0.52
1:C:248:LEU:HD21	1:C:271:VAL:HG22	1.91	0.52
1:A:153:GLY:HA2	3:A:302:0BD:H13B	1.91	0.52
1:B:105:SER:O	1:B:109:ARG:HG3	2.10	0.51
1:D:103:LEU:HD22	1:D:121:MET:HE1	1.93	0.51
1:B:26:GLN:O	1:B:42:LYS:HA	2.11	0.50
1:C:133:HIS:CG	1:C:196:PRO:HB3	2.47	0.50
1:D:200:VAL:HG11	1:D:261:TYR:HB2	1.95	0.49
1:A:270:ALA:HA	1:A:281:PRO:HD2	1.95	0.48
1:B:57:ARG:HE	1:B:162:ILE:HG22	1.78	0.48
1:D:43:VAL:HG12	1:D:92:TYR:HB3	1.94	0.48
1:B:130:GLN:OE1	1:B:263:SER:HB3	2.13	0.48
1:D:205:VAL:HG22	1:D:253:LEU:HD21	1.96	0.48
1:A:252:THR:HG21	1:A:267:PHE:CE1	2.49	0.47
1:C:8:THR:HA	1:C:14[B]:ARG:HA	1.97	0.47
1:D:248:LEU:HD21	1:D:271:VAL:HG22	1.96	0.47
1:D:64:THR:HG23	1:D:137:LEU:HD22	1.95	0.47
1:A:147:ILE:HG23	1:A:155:VAL:HG13	1.97	0.47
1:B:141:ASP:HB2	1:B:162:ILE:HD11	1.97	0.47
1:A:201:TYR:CD2	1:A:260:ARG:NH1	2.83	0.46
1:D:186:PRO:HD3	1:D:201:TYR:CZ	2.51	0.46
1:D:70:HIS:HB2	1:D:131:ILE:HG13	1.98	0.45
1:A:133:HIS:CG	1:A:196:PRO:HB3	2.52	0.45
1:C:201:TYR:HB2	1:C:260:ARG:HE	1.82	0.45
1:C:130:GLN:OE1	1:C:263:SER:HB3	2.16	0.44
1:A:248:LEU:HD21	1:A:271:VAL:HG22	1.99	0.44
1:C:141:ASP:HB2	1:C:162:ILE:HD11	1.98	0.44
1:A:44:LEU:HD13	1:A:49:SER:HA	2.00	0.44
1:B:44:LEU:HD22	1:B:48:PHE:HB2	2.00	0.43
1:A:117:HIS:CE1	3:A:302:0BD:H15A	2.54	0.43
1:C:57:ARG:HH21	1:C:162:ILE:HG22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:PHE:CD1	1:D:228:LYS:HB3	2.53	0.43
1:C:201:TYR:HB2	1:C:260:ARG:NE	2.33	0.43
1:C:148:LEU:HB2	1:C:156:LYS:HB2	1.99	0.43
1:C:252:THR:HG21	1:C:267:PHE:CE1	2.54	0.43
1:C:8:THR:HA	1:C:14[A]:ARG:HA	2.01	0.42
1:A:186:PRO:HG3	1:A:229:HIS:O	2.20	0.42
1:D:196:PRO:HB2	1:D:262:ARG:O	2.20	0.42
1:A:64:THR:O	1:A:67:MET:HB3	2.20	0.42
1:C:186:PRO:HG2	1:C:255:LYS:HA	2.01	0.42
1:B:185:ALA:HA	1:B:201:TYR:CD1	2.55	0.42
1:C:115:LEU:HD22	1:C:245:VAL:HG21	2.02	0.41
1:D:19:ILE:HD12	1:D:27:VAL:HG12	2.03	0.41
1:A:185:ALA:HB3	1:A:188:GLN:HB2	2.03	0.40
1:D:133:HIS:CD2	1:D:196:PRO:HB3	2.57	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	255/317 (80%)	243 (95%)	9 (4%)	3 (1%)	15	44
1	B	260/317 (82%)	247 (95%)	9 (4%)	4 (2%)	12	37
1	C	259/317 (82%)	246 (95%)	12 (5%)	1 (0%)	38	70
1	D	252/317 (80%)	241 (96%)	9 (4%)	2 (1%)	22	55
All	All	1026/1268 (81%)	977 (95%)	39 (4%)	10 (1%)	18	49

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	VAL

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Mol	Chain	Res	Type
1	B	222	ALA
1	B	263	SER
1	C	263	SER
1	A	6	GLY
1	A	7	VAL
1	B	159	ASP
1	D	159	ASP
1	D	216	PRO
1	B	221	GLY

### 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	206/248 (83%)	192 (93%)	14 (7%)	18	45
1	B	210/248 (85%)	199 (95%)	11 (5%)	27	58
1	C	209/248 (84%)	201 (96%)	8 (4%)	38	71
1	D	207/248 (84%)	198 (96%)	9 (4%)	33	66
All	All	832/992 (84%)	790 (95%)	42 (5%)	28	60

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	29	GLU
1	A	44	LEU
1	A	53	GLU
1	A	121	MET
1	A	127	ARG
1	A	157	ILE
1	A	180	THR
1	A	188	GLN
1	A	223	LEU
1	A	232	GLU
1	A	240	ASP

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Mol	Chain	Res	Type
1	A	241	LEU
1	A	262	ARG
1	B	4	ARG
1	B	5	VAL
1	B	44	LEU
1	B	68	LEU
1	B	99	ASN
1	B	121	MET
1	B	154	GLN
1	B	176	MET
1	B	193	ASP
1	B	220	ASP
1	B	262	ARG
1	C	29	GLU
1	C	43	VAL
1	C	68	LEU
1	C	104	ASN
1	C	154	GLN
1	C	220	ASP
1	C	262	ARG
1	C	275	ARG
1	D	4	ARG
1	D	89	ARG
1	D	140	ARG
1	D	215	ARG
1	D	220	ASP
1	D	223	LEU
1	D	260	ARG
1	D	262	ARG
1	D	282	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	B	146	ASN
1	C	146	ASN
1	D	146	ASN
1	D	188	GLN
1	D	244	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	TPO	A	224	1	9,10,11	1.90	2 (22%)	10,14,16	1.06	1 (10%)
1	TPO	B	224	1	9,10,11	1.41	2 (22%)	10,14,16	0.89	1 (10%)
1	TPO	C	224	1	9,10,11	1.57	1 (11%)	10,14,16	1.05	1 (10%)
1	TPO	D	224	1	9,10,11	1.55	2 (22%)	10,14,16	1.01	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
1	TPO	A	224	1	-	0/8/11/13	0/0/0/0
1	TPO	B	224	1	-	0/8/11/13	0/0/0/0
1	TPO	C	224	1	-	0/8/11/13	0/0/0/0
1	TPO	D	224	1	-	0/8/11/13	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	TPO	P-OG1	-4.74	1.51	1.59
1	C	224	TPO	P-OG1	-4.00	1.52	1.59
1	D	224	TPO	P-OG1	-3.19	1.54	1.59
1	B	224	TPO	P-OG1	-2.50	1.55	1.59
1	A	224	TPO	CA-C	2.13	1.53	1.50
1	D	224	TPO	CA-C	2.26	1.53	1.50
1	B	224	TPO	CA-C	2.59	1.53	1.50



All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	TPO	O-C-CA	-2.52	119.26	125.15
1	D	224	TPO	O-C-CA	-2.48	119.38	125.15
1	C	224	TPO	O-C-CA	-2.41	119.52	125.15
1	B	224	TPO	O-C-CA	-2.29	119.81	125.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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	CJJ	A	301	-	25,28,28	1.17	3 (12%)	28,42,42	2.41	11 (39%)
3	0BD	A	302	-	33,33,33	0.32	0	45,47,47	1.12	2 (4%)
2	CJJ	B	300	-	25,28,28	1.17	2 (8%)	28,42,42	2.27	13 (46%)
2	CJJ	C	300	-	25,28,28	1.13	3 (12%)	28,42,42	2.26	11 (39%)
2	CJJ	D	300	-	25,28,28	1.21	3 (12%)	28,42,42	2.29	11 (39%)

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	CJJ	A	301	-	-	0/6/20/20	0/3/4/4
3	0BD	A	302	-	-	0/20/60/60	0/2/2/2
2	CJJ	B	300	-	-	0/6/20/20	0/3/4/4
2	CJJ	C	300	-	-	0/6/20/20	0/3/4/4
2	CJJ	D	300	-	-	0/6/20/20	0/3/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CJJ	C14-C15	-2.16	1.35	1.39
2	C	300	CJJ	C14-C15	-2.10	1.35	1.39
2	D	300	CJJ	C10-N12	2.02	1.40	1.36
2	A	301	CJJ	C3-S4	2.11	1.76	1.72
2	D	300	CJJ	C3-S4	2.14	1.76	1.72
2	C	300	CJJ	C3-S4	2.15	1.76	1.72
2	B	300	CJJ	C3-S4	2.16	1.76	1.72
2	C	300	CJJ	S23-N26	2.68	1.66	1.60
2	B	300	CJJ	S23-N26	2.75	1.66	1.60
2	D	300	CJJ	S23-N26	2.84	1.66	1.60
2	A	301	CJJ	S23-N26	3.00	1.66	1.60

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	CJJ	C21-C19-C15	-5.19	114.97	120.20
2	C	300	CJJ	C21-C19-C15	-4.96	115.19	120.20
2	A	301	CJJ	N7-C6-N11	-4.15	121.07	125.27
2	C	300	CJJ	N7-C6-N11	-4.07	121.14	125.27
2	D	300	CJJ	N7-C6-N11	-3.86	121.36	125.27
2	D	300	CJJ	C8-C9-C10	-3.63	118.17	120.16
2	C	300	CJJ	C8-C9-C10	-3.44	118.27	120.16
2	D	300	CJJ	C20-C19-C15	-3.44	116.73	120.20
2	B	300	CJJ	N7-C6-N11	-3.41	121.81	125.27
2	A	301	CJJ	C9-C8-N7	-3.36	119.46	122.84
2	B	300	CJJ	C9-C8-N7	-3.07	119.75	122.84
2	B	300	CJJ	C14-C13-N18	-2.87	106.29	110.45
2	B	300	CJJ	C21-C19-C15	-2.82	117.36	120.20
2	C	300	CJJ	C9-C8-N7	-2.78	120.04	122.84
2	D	300	CJJ	C14-C13-N18	-2.74	106.47	110.45
2	C	300	CJJ	C13-N12-C10	-2.70	120.51	128.83
2	D	300	CJJ	C9-C8-N7	-2.70	120.12	122.84
2	A	301	CJJ	C8-C9-C10	-2.63	118.71	120.16
2	A	301	CJJ	C14-C13-N18	-2.40	106.97	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300	CJJ	C8-C9-C10	-2.31	118.89	120.16
2	D	300	CJJ	C14-C15-N16	-2.22	107.25	110.26
2	B	300	CJJ	C5-C6-N11	-2.19	114.72	117.41
3	A	302	0BD	C-C18-C19	-2.13	108.27	112.50
2	C	300	CJJ	C14-C13-N18	-2.04	107.49	110.45
2	B	300	CJJ	C14-C15-N16	-2.01	107.54	110.26
2	B	300	CJJ	C8-C9-CL22	2.01	121.31	118.47
2	C	300	CJJ	O24-S23-O25	2.37	123.05	118.70
2	A	301	CJJ	O24-S23-O25	2.38	123.07	118.70
2	D	300	CJJ	O24-S23-O25	2.39	123.09	118.70
2	C	300	CJJ	C13-C14-C15	2.43	108.26	106.09
2	A	301	CJJ	C13-C14-C15	2.43	108.26	106.09
2	A	301	CJJ	C8-C9-CL22	2.49	121.98	118.47
2	B	300	CJJ	O24-S23-O25	2.53	123.34	118.70
2	B	300	CJJ	C8-N7-C6	2.57	119.56	116.19
2	D	300	CJJ	C8-N7-C6	2.86	119.94	116.19
2	D	300	CJJ	C19-C15-N16	2.91	124.53	120.21
2	A	301	CJJ	C19-C15-N16	2.98	124.64	120.21
2	D	300	CJJ	C13-C14-C15	3.05	108.81	106.09
2	B	300	CJJ	C13-C14-C15	3.06	108.83	106.09
2	C	300	CJJ	C8-N7-C6	3.17	120.34	116.19
2	A	301	CJJ	C8-N7-C6	3.22	120.41	116.19
2	B	300	CJJ	C19-C15-N16	3.33	125.16	120.21
2	C	300	CJJ	C19-C15-N16	3.69	125.69	120.21
2	C	300	CJJ	C5-C6-N7	4.16	121.58	117.07
3	A	302	0BD	O16-C18-C19	4.56	116.50	108.18
2	A	301	CJJ	C5-C6-N7	5.74	123.29	117.07
2	B	300	CJJ	C5-C6-N7	5.90	123.46	117.07
2	D	300	CJJ	C5-C6-N7	6.06	123.64	117.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	0BD	3	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	261/317 (82%)	-0.00	2 (0%) 86 85	41, 64, 91, 121	0
1	B	266/317 (83%)	0.25	6 (2%) 61 58	49, 80, 133, 168	0
1	C	264/317 (83%)	0.56	18 (6%) 18 14	65, 102, 135, 165	0
1	D	259/317 (81%)	0.64	21 (8%) 13 9	55, 101, 146, 175	0
All	All	1050/1268 (82%)	0.36	47 (4%) 34 30	41, 85, 136, 175	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	46	SER	4.4
1	D	251	ILE	4.0
1	B	175	GLY	3.9
1	C	179	GLY	3.8
1	D	115	LEU	3.7
1	C	274	VAL	3.7
1	D	231	LYS	3.7
1	D	113	LEU	3.6
1	D	178	MET	3.6
1	B	23	GLY	3.6
1	B	165	ALA	3.4
1	C	20	ALA	3.4
1	D	119	LEU	3.3
1	D	190	LEU	3.3
1	C	116	ARG	3.2
1	C	166	VAL	3.1
1	C	272	ALA	2.9
1	C	31	VAL	2.8
1	C	111	GLY	2.8
1	B	176	MET	2.8
1	D	3	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	48	PHE	2.6
1	D	262	ARG	2.6
1	D	248	LEU	2.6
1	D	255	LYS	2.6
1	D	179	GLY	2.6
1	C	22	GLY	2.5
1	A	3	PRO	2.5
1	D	116	ARG	2.5
1	D	274	VAL	2.5
1	C	18	LEU	2.5
1	D	189	ALA	2.4
1	D	277	GLY	2.4
1	A	179	GLY	2.4
1	B	5	VAL	2.4
1	D	227	MET	2.4
1	C	232	GLU	2.4
1	C	24	MET	2.3
1	C	28	TRP	2.3
1	C	57	ARG	2.3
1	B	166	VAL	2.3
1	C	104	ASN	2.3
1	C	118	ALA	2.2
1	D	226	ALA	2.1
1	D	273	ALA	2.1
1	C	259	MET	2.0
1	C	122	LEU	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. 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
1	TPO	A	224	11/12	0.98	0.18	-	65,68,75,76	0
1	TPO	B	224	11/12	0.98	0.17	-	63,65,72,74	0
1	TPO	C	224	11/12	0.96	0.19	-	100,106,117,118	0
1	TPO	D	224	11/12	0.95	0.18	-	108,109,113,119	0

### 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	0BD	A	302	32/32	0.76	0.28	3.02	76,89,98,99	0
2	CJJ	D	300	25/25	0.92	0.22	0.93	65,91,100,102	0
2	CJJ	A	301	25/25	0.92	0.21	0.84	50,69,87,87	0
2	CJJ	C	300	25/25	0.83	0.31	0.69	116,143,146,148	0
2	CJJ	B	300	25/25	0.92	0.18	-0.56	59,77,100,101	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.