



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:19 pm BST

PDB ID : 5WXN  
Title : Structure of the LKB1 and 14-3-3 complex  
Authors : Ding, S.; Shi, Z.B.  
Deposited on : 2017-01-08  
Resolution : 2.93 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

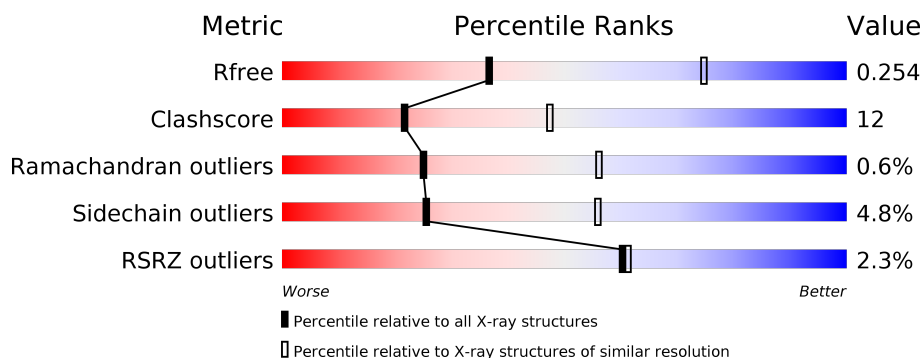
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.93 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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	267	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>20%</div> <div>••</div> <div>13%</div> </div> </div>
1	B	267	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>20%</div> <div>•</div> <div>14%</div> </div> </div>
2	C	13	<div> <div></div> <div> <div>31%</div> <div>31%</div> <div>15%</div> <div>23%</div> </div> </div>
2	D	13	<div> <div>8%</div> <div> <div></div> <div>38%</div> <div>31%</div> <div>8%</div> <div>23%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3670 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 14-3-3 protein zeta/delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	2	0
			1766	1110	297	349	10			
1	B	230	Total	C	N	O	S	0	1	0
			1725	1083	291	342	9			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP P63104
A	-20	SER	-	expression tag	UNP P63104
A	-19	TYR	-	expression tag	UNP P63104
A	-18	TYR	-	expression tag	UNP P63104
A	-17	HIS	-	expression tag	UNP P63104
A	-16	HIS	-	expression tag	UNP P63104
A	-15	HIS	-	expression tag	UNP P63104
A	-14	HIS	-	expression tag	UNP P63104
A	-13	HIS	-	expression tag	UNP P63104
A	-12	HIS	-	expression tag	UNP P63104
A	-11	LEU	-	expression tag	UNP P63104
A	-10	GLU	-	expression tag	UNP P63104
A	-9	SER	-	expression tag	UNP P63104
A	-8	THR	-	expression tag	UNP P63104
A	-7	SER	-	expression tag	UNP P63104
A	-6	LEU	-	expression tag	UNP P63104
A	-5	TYR	-	expression tag	UNP P63104
A	-4	LYS	-	expression tag	UNP P63104
A	-3	LYS	-	expression tag	UNP P63104
A	-2	ALA	-	expression tag	UNP P63104
A	-1	GLY	-	expression tag	UNP P63104
A	0	LEU	-	expression tag	UNP P63104
B	-21	MET	-	expression tag	UNP P63104
B	-20	SER	-	expression tag	UNP P63104
B	-19	TYR	-	expression tag	UNP P63104

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	TYR	-	expression tag	UNP P63104
B	-17	HIS	-	expression tag	UNP P63104
B	-16	HIS	-	expression tag	UNP P63104
B	-15	HIS	-	expression tag	UNP P63104
B	-14	HIS	-	expression tag	UNP P63104
B	-13	HIS	-	expression tag	UNP P63104
B	-12	HIS	-	expression tag	UNP P63104
B	-11	LEU	-	expression tag	UNP P63104
B	-10	GLU	-	expression tag	UNP P63104
B	-9	SER	-	expression tag	UNP P63104
B	-8	THR	-	expression tag	UNP P63104
B	-7	SER	-	expression tag	UNP P63104
B	-6	LEU	-	expression tag	UNP P63104
B	-5	TYR	-	expression tag	UNP P63104
B	-4	LYS	-	expression tag	UNP P63104
B	-3	LYS	-	expression tag	UNP P63104
B	-2	ALA	-	expression tag	UNP P63104
B	-1	GLY	-	expression tag	UNP P63104
B	0	LEU	-	expression tag	UNP P63104

- Molecule 2 is a protein called Serine/threonine-protein kinase STK11.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	S	0	0	0
			82	51	13	16	1	1			
2	D	10	Total	C	N	O	P	S	0	0	0
			79	48	13	16	1	1			

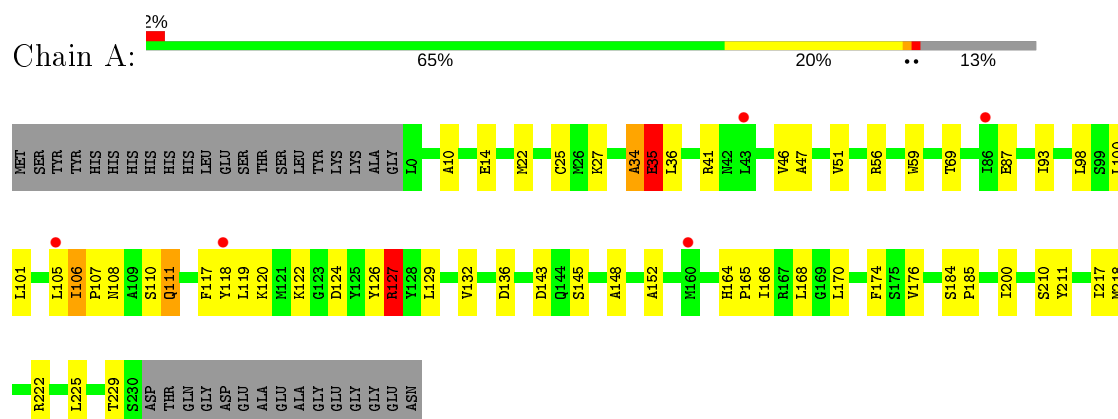
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	9	Total	O	0	0
			9	9		
3	C	1	Total	O	0	0
			1	1		
3	D	2	Total	O	0	0
			2	2		

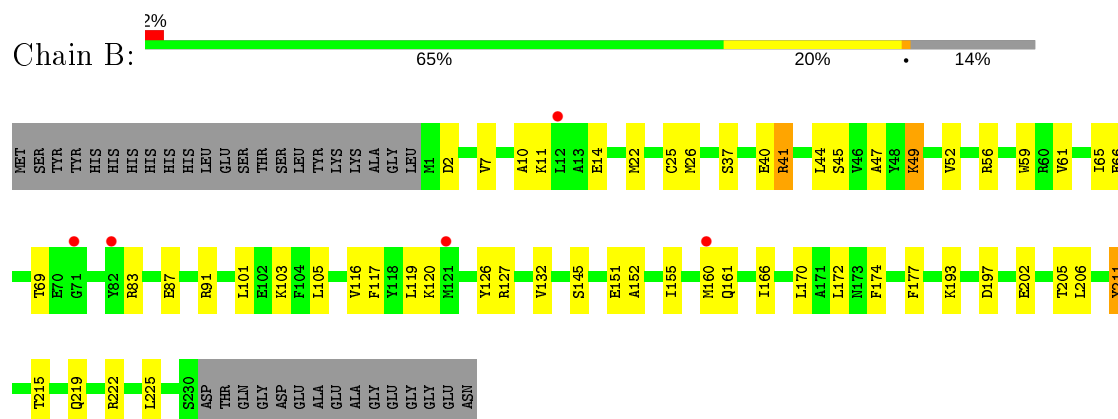
### 3 Residue-property plots [i](#)

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

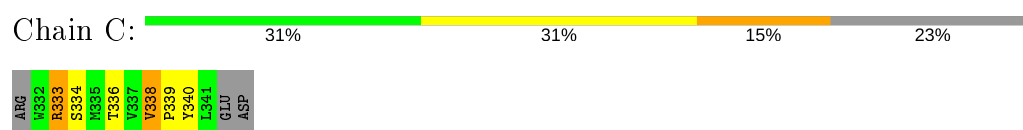
- Molecule 1: 14-3-3 protein zeta/delta



- Molecule 1: 14-3-3 protein zeta/delta



- Molecule 2: Serine/threonine-protein kinase STK11



- Molecule 2: Serine/threonine-protein kinase STK11





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.77Å 85.38Å 112.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.56 – 2.93 44.56 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.56-2.93) 90.0 (44.56-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.193 , 0.254 0.195 , 0.254	Depositor DCC
$R_{free}$ test set	1591 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.7	Xtriage
Anisotropy	0.716	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 61.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3670	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.72% 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

### 5.1 Standard geometry

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	0.73	2/1791 (0.1%)	0.78	5/2426 (0.2%)
1	B	0.44	0/1749	0.69	1/2375 (0.0%)
2	C	0.81	0/71	0.86	0/94
2	D	0.46	0/68	0.88	0/90
All	All	0.61	2/3679 (0.1%)	0.74	6/4985 (0.1%)

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
2	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	PRO	CA-C	-5.78	1.41	1.52
1	A	127	ARG	CZ-NH1	-5.14	1.26	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	ILE	C-N-CD	-8.38	102.16	120.60
1	B	49	LYS	CD-CE-NZ	-6.09	97.68	111.70
1	A	34	ALA	C-N-CA	5.93	136.53	121.70
1	A	35	GLU	N-CA-C	-5.55	96.02	111.00
1	A	35	GLU	N-CA-CB	5.21	119.99	110.60
1	A	168	LEU	CA-CB-CG	5.04	126.89	115.30



There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	338	VAL	Peptide

## 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	1766	0	1662	44	0
1	B	1725	0	1605	34	0
2	C	82	0	78	13	0
2	D	79	0	69	7	0
3	A	6	0	0	0	0
3	B	9	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
All	All	3670	0	3414	84	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 12.

All (84) 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:56:ARG:NH1	2:C:336:TPO:O2P	2.24	0.71
1:A:46:VAL:HG12	2:C:340:TYR:CE1	2.27	0.69
1:B:22:MET:HG2	1:B:47:ALA:HB2	1.74	0.69
2:C:333:ARG:CB	2:C:333:ARG:HH11	2.07	0.68
2:D:338:VAL:O	2:D:340:TYR:N	2.27	0.68
2:C:333:ARG:HB2	2:C:333:ARG:NH1	2.12	0.64
1:B:56:ARG:NH2	2:D:336:TPO:O2P	2.34	0.61
1:A:124:ASP:O	1:A:127:ARG:HB3	2.01	0.61
1:A:106:ILE:HG22	1:A:107:PRO:HD3	1.83	0.60
1:A:120:LYS:HZ1	2:C:338:VAL:HA	1.67	0.59
1:A:35:GLU:OE1	1:A:108:ASN:HB3	2.03	0.59
1:A:106:ILE:CB	1:A:107:PRO:CD	2.81	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:SER:HB2	1:B:40:GLU:H	1.68	0.58
1:B:59:TRP:CE2	1:B:132:VAL:HG23	2.38	0.57
2:C:333:ARG:HB2	2:C:333:ARG:HH11	1.68	0.57
1:B:61:VAL:O	1:B:65:ILE:HD13	2.04	0.57
1:B:101:LEU:HA	1:B:105:LEU:HB2	1.87	0.55
1:A:14:GLU:HB2	1:A:22:MET:SD	2.47	0.55
1:A:22:MET:HG2	1:A:47:ALA:HB2	1.89	0.54
1:A:98:LEU:HA	1:A:101:LEU:HD12	1.90	0.53
1:A:106:ILE:HB	1:A:107:PRO:CD	2.39	0.53
1:A:122:LYS:HD3	1:A:148:ALA:HB2	1.91	0.53
1:B:10:ALA:HB2	1:B:25:CYS:HB2	1.91	0.53
1:A:106:ILE:N	1:A:107:PRO:HD2	2.23	0.52
1:B:206:LEU:HD13	1:B:211:TYR:HB2	1.90	0.51
1:A:225:LEU:O	1:A:229:THR:HG23	2.10	0.51
1:A:106:ILE:CB	1:A:107:PRO:HD3	2.41	0.51
2:C:333:ARG:CB	2:C:333:ARG:NH1	2.72	0.51
1:A:10:ALA:HB2	1:A:25:CYS:HB2	1.93	0.50
1:A:69:THR:O	1:A:69:THR:HG22	2.11	0.50
1:A:127:ARG:NH2	2:C:336:TPO:HG21	2.27	0.50
1:A:164:HIS:HD2	1:A:165:PRO:HD2	1.77	0.50
1:B:215:THR:O	1:B:219:GLN:HG3	2.11	0.49
1:B:7:VAL:O	1:B:11:LYS:HB2	2.12	0.49
1:B:151:GLU:O	1:B:155:ILE:HD12	2.12	0.49
1:B:126:TYR:CB	1:B:145:SER:HB2	2.42	0.49
1:A:51:VAL:HG12	1:A:93:ILE:HD13	1.94	0.49
1:A:59:TRP:CD1	1:A:87:GLU:HG3	2.48	0.49
1:B:41:ARG:HD3	1:B:117:PHE:CD1	2.48	0.49
1:B:172:LEU:HD23	2:D:337:VAL:HG22	1.94	0.49
1:B:49:LYS:NZ	2:D:336:TPO:O2P	2.44	0.48
1:A:101:LEU:HA	1:A:105:LEU:HB2	1.94	0.48
1:A:127:ARG:NH2	2:C:336:TPO:O3P	2.46	0.48
1:A:106:ILE:CG2	1:A:107:PRO:HD3	2.44	0.47
1:B:14:GLU:HB2	1:B:22:MET:SD	2.54	0.47
1:B:69:THR:HG22	1:B:69:THR:O	2.15	0.46
1:B:193:LYS:NZ	1:B:197:ASP:OD2	2.48	0.46
1:A:106:ILE:HB	1:A:107:PRO:HD2	1.98	0.46
1:A:46:VAL:HG12	2:C:340:TYR:CD1	2.51	0.46
1:A:164:HIS:HD2	1:A:165:PRO:CD	2.28	0.45
1:B:126:TYR:HB3	1:B:145:SER:HB2	1.99	0.45
1:B:119:LEU:HB2	1:B:152:ALA:HB2	1.97	0.45
2:D:337:VAL:HB	2:D:338:VAL:H	1.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:VAL:HG21	1:B:160:MET:HE3	1.98	0.45
1:A:117:PHE:HD2	1:A:166:ILE:CD1	2.30	0.44
1:B:202:GLU:O	1:B:205:THR:HG22	2.17	0.44
1:B:222:ARG:HA	1:B:225:LEU:HB2	1.99	0.44
1:A:41:ARG:HD2	1:A:117:PHE:CD1	2.52	0.44
1:B:166:ILE:HA	2:D:339:PRO:HG3	1.99	0.43
1:B:45:SER:HB3	2:D:338:VAL:HG21	1.98	0.43
1:B:120:LYS:HB2	1:B:170:LEU:HD13	2.00	0.43
1:A:119:LEU:HB2	1:A:152:ALA:HB2	2.01	0.43
1:A:217:ILE:HD11	2:C:339:PRO:HB3	2.00	0.43
1:B:206:LEU:HD22	1:B:211:TYR:HA	1.99	0.43
1:A:129:LEU:HA	1:A:129:LEU:HD23	1.78	0.42
1:A:176:VAL:HG22	2:C:334:SER:HB3	2.01	0.42
1:A:105:LEU:HD13	1:A:118:TYR:CE1	2.55	0.42
1:A:126:TYR:CB	1:A:145:SER:HB2	2.50	0.42
1:A:126:TYR:HB3	1:A:145:SER:HB2	2.01	0.42
1:B:49:LYS:HA	1:B:52:VAL:HG12	2.01	0.42
1:A:120:LYS:NZ	2:C:338:VAL:HA	2.34	0.41
1:A:200:ILE:HG23	1:A:218:MET:CE	2.50	0.41
1:B:105:LEU:HD23	1:B:105:LEU:HA	1.83	0.41
1:A:222:ARG:HD2	1:A:222:ARG:HH21	1.71	0.41
1:B:87:GLU:OE2	1:B:91:ARG:NH2	2.43	0.41
1:A:106:ILE:N	1:A:107:PRO:CD	2.82	0.41
1:A:164:HIS:CD2	1:A:165:PRO:HD2	2.55	0.41
1:A:110:SER:OG	1:A:111:GLN:N	2.53	0.41
1:B:26:MET:HB3	1:B:44:LEU:HB2	2.03	0.41
1:B:127:ARG:HD3	1:B:177:PHE:HD1	1.86	0.41
1:B:66:GLU:OE2	1:B:83:ARG:NH1	2.54	0.40
1:A:87:GLU:HG2	1:A:132:VAL:HG13	2.02	0.40
1:B:161:GLN:OE1	1:B:205:THR:OG1	2.37	0.40
1:A:27:LYS:HG3	1:A:100:LEU:HD11	2.03	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	231/267 (86%)	217 (94%)	12 (5%)	2 (1%)	17	46
1	B	229/267 (86%)	221 (96%)	8 (4%)	0	100	100
2	C	7/13 (54%)	5 (71%)	2 (29%)	0	100	100
2	D	7/13 (54%)	3 (43%)	3 (43%)	1 (14%)	0	0
All	All	474/560 (85%)	446 (94%)	25 (5%)	3 (1%)	25	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ALA
1	A	35	GLU
2	D	339	PRO

### 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	174/229 (76%)	162 (93%)	12 (7%)	15	40
1	B	169/229 (74%)	164 (97%)	5 (3%)	41	72
2	C	8/12 (67%)	7 (88%)	1 (12%)	4	13
2	D	7/12 (58%)	7 (100%)	0	100	100
All	All	358/482 (74%)	340 (95%)	18 (5%)	25	54

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	36	LEU
1	A	111	GLN
1	A	127	ARG
1	A	136	ASP

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Mol	Chain	Res	Type
1	A	143	ASP
1	A	170	LEU
1	A	174	PHE
1	A	184	SER
1	A	210[A]	SER
1	A	210[B]	SER
1	A	211	TYR
1	B	2	ASP
1	B	41	ARG
1	B	103	LYS
1	B	174	PHE
1	B	211	TYR
2	C	333	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z  > 2$
2	TPO	C	336	2	8,10,11	1.43	1 (12%)	10,14,16	1.61	2 (20%)
2	TPO	D	336	2	8,10,11	1.14	0	10,14,16	1.39	2 (20%)

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	C	336	2	-	2/9/11/13	-
2	TPO	D	336	2	-	3/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	336	TPO	P-O1P	2.84	1.59	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	336	TPO	P-OG1-CB	-3.50	112.64	123.21
2	C	336	TPO	CG2-CB-CA	-2.89	107.45	113.16
2	D	336	TPO	P-OG1-CB	-2.71	115.02	123.21
2	D	336	TPO	O3P-P-OG1	2.45	116.98	105.99

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	336	TPO	CB-OG1-P-O2P
2	C	336	TPO	CB-OG1-P-O1P
2	D	336	TPO	CB-OG1-P-O1P
2	C	336	TPO	O-C-CA-CB
2	D	336	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	336	TPO	3	0
2	D	336	TPO	2	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 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	231/267 (86%)	0.28	5 (2%) 62 63	47, 81, 117, 192	0
1	B	230/267 (86%)	0.29	5 (2%) 62 63	57, 90, 132, 155	0
2	C	9/13 (69%)	0.63	0 100 100	75, 93, 116, 118	0
2	D	9/13 (69%)	0.49	1 (11%) 5 5	85, 110, 152, 153	0
All	All	479/560 (85%)	0.29	11 (2%) 60 61	47, 85, 128, 192	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	GLY	3.9
1	B	160	MET	3.4
2	D	339	PRO	2.7
1	A	160	MET	2.6
1	A	105	LEU	2.6
1	B	82	TYR	2.6
1	B	12	LEU	2.4
1	B	121	MET	2.3
1	A	118	TYR	2.1
1	A	43	LEU	2.1
1	A	86	ILE	2.1

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

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	C	336	11/12	0.97	0.21	53,59,79,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	TPO	D	336	11/12	0.97	0.21	70,77,87,97	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.