



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2016 – 05:47 PM EDT

PDB ID : 5K1C  
Title : Crystal structure of the UAF1/WDR20/USP12 complex  
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Deposited on : 2016-05-18  
Resolution : 3.00 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20027939

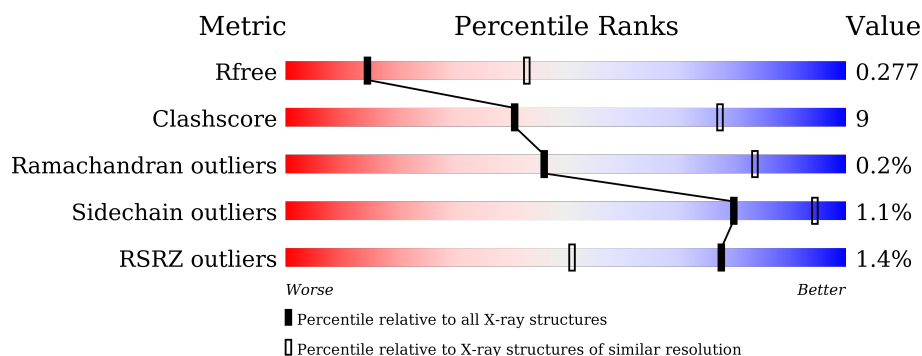
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	355	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>14%</div> <div>•</div> <div>15%</div> </div> </div>
2	B	563	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div>•</div> <div>9%</div> </div> </div>
3	C	569	<div> <div></div> <div> <div>58%</div> <div>13%</div> <div>28%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	TAM	C	601	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9633 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 Ubiquitin carboxyl-terminal hydrolase 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2374	1510	398	452	14			

- Molecule 2 is a protein called WD repeat-containing protein 48.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	515	Total	C	N	O	S	0	0	0
			4001	2521	698	761	21			

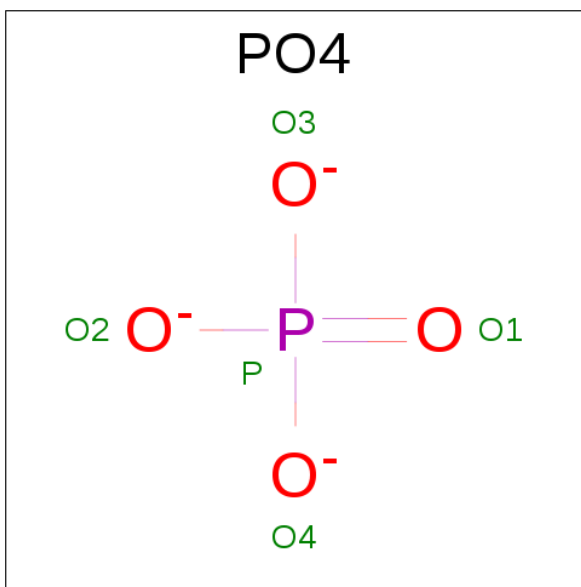
- Molecule 3 is a protein called WD repeat-containing protein 20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	407	Total	C	N	O	S	0	0	0
			3166	2019	540	589	18			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

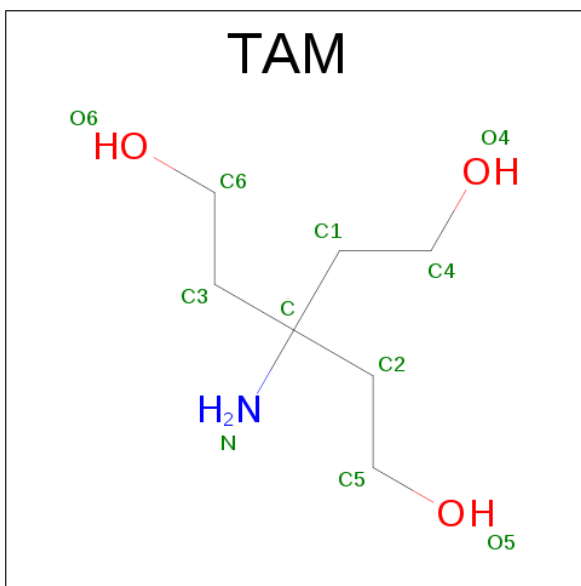
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 6 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: C<sub>7</sub>H<sub>17</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			11	7	1	3		

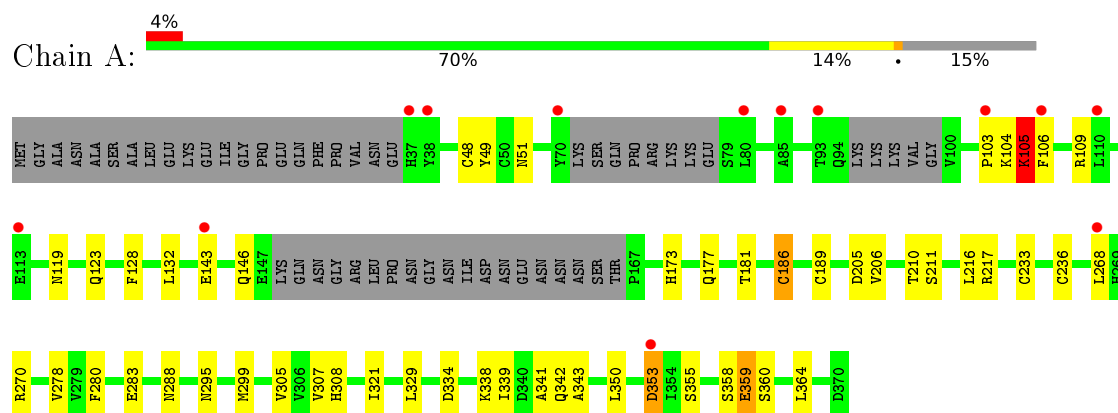
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	6	Total 6	O 6	0	0
7	B	42	Total 42	O 42	0	0
7	C	27	Total 27	O 27	0	0

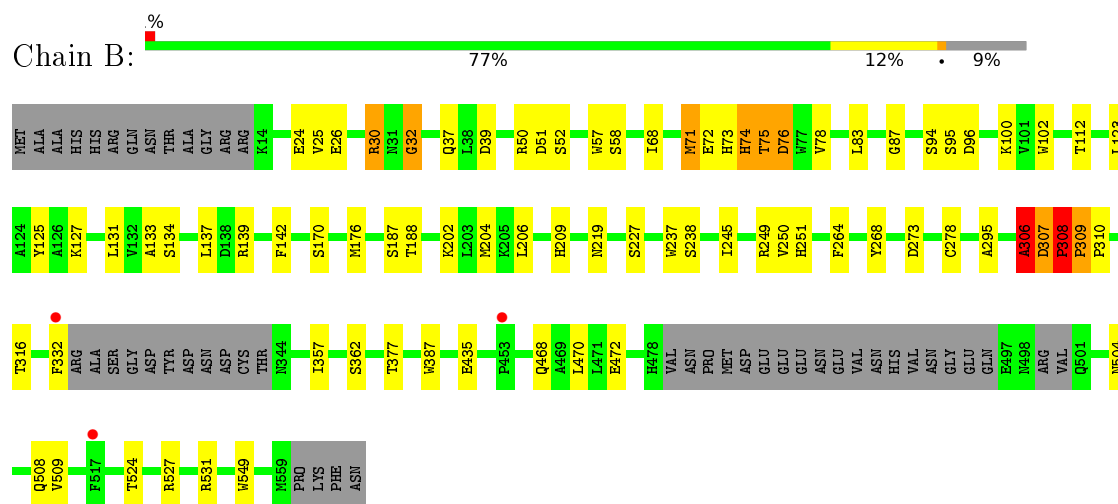
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

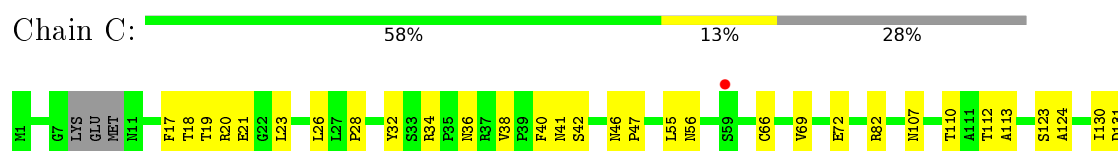
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 12



- Molecule 2: WD repeat-containing protein 48



- Molecule 3: WD repeat-containing protein 20



V564	HIS	ASN	GLY	R145
V565	GLU	ASN	SER	SER
V566	ASP	SER	GLU	ASP
PRU	HIS	VAL	PHE	S149
	LYS	THR	ASP	S150
	ARG	THR	GLN	R151
	ASN	PRO	ASP	W157
	HIS	GLY	LEU	S161
	SER	ASN	LEU	E162
	MET	SER	HIS	S163
	GLY	VAL	PHE	
	HIS	PRO	GLY	L166
	ILE	PRO	ARG	
	SER	PRO	ASP	M174
	SER	LEU	ARG	
	LYS	PRO	ALA	N178
	SER	ARG	ASN	
	SER	SER	SER	V201
	ASP	ASN	THR	
	LYS	SER	GLN	R211
	LEU	LEU	SER	P212
	ASN	PRO	ARG	L213
	LEU	HIS	LEU	L214
	VAL	THR	SER	
	THR	ALA	LYS	F226
	LYS	VAL	ARG	
	THR	SER	ASN	A236
	LYS	ASN	SER	
	THR	ALA	THR	D241
	ASP	GLY	ASP	S242
	PRO	SER	SER	
	ALA	LYS	ARG	R245
	LYS	SER	PRO	
	THR	SER	V363	V252
	L509	VAL		
G510	MET		R368	
T511	ASP	ASP		G264
P512	GLY	GLY	Q374	L265
L513	ALA	ALA		
G514	ILE	ILE	L394	T279
	ALA	ALA	SER	
L522	SER	SER	ARG	E282
	GLY	GLY	ALA	
L527	VAL	VAL	ARG	H301
	SER	SER	THR	
R535	LYS	LYS	HIS	S305
	PHE	PHE	THR	S306
V538	ALA	ALA	ASN	
L539	LEU	LEU	VAL	S318
L540	THR	THR	MET	VAL
F541	SER	LEU	ASN	GLU
L542	LEU	LEU	GLY	GLU
	HIS	HIS	THR	ASP
A549	ASP	ASP	PRO	PRO
	ARG	ARG	PRO	PRO
L555	LYS	LYS	PRO	MET
C556	GLU	GLU	ALA	GLU
T557	ARG	THR	GLY	PHE
H558	HIS	HIS	SER	



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	217.90Å 217.90Å 223.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.01 – 3.00 49.77 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.01-3.00) 97.7 (49.77-3.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, $R_{free}$	0.230 , 0.271 0.239 , 0.277	Depositor DCC
$R_{free}$ test set	3014 reflections (5.15%)	DCC
Wilson B-factor (Å <sup>2</sup> )	84.5	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 59.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9633	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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: TAM, ZN, PO4

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	0.62	2/2425 (0.1%)	0.89	10/3293 (0.3%)
2	B	0.67	5/4083 (0.1%)	0.92	8/5558 (0.1%)
3	C	0.60	0/3245	0.84	3/4406 (0.1%)
All	All	0.64	7/9753 (0.1%)	0.89	21/13257 (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	A	0	5
2	B	0	1
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	307	ASP	C-O	7.33	1.37	1.23
1	A	106	PHE	C-N	7.26	1.50	1.34
2	B	75	THR	C-N	7.11	1.50	1.34
1	A	105	LYS	C-O	6.94	1.36	1.23
2	B	71	MET	C-N	6.61	1.49	1.34
2	B	76	ASP	C-O	-6.48	1.11	1.23
2	B	332	PHE	C-O	5.84	1.34	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	307	ASP	C-N-CD	-9.71	99.23	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	LYS	O-C-N	8.44	136.20	122.70
2	B	74	HIS	CB-CA-C	-8.43	93.54	110.40
1	A	359	GLU	N-CA-C	-7.93	89.59	111.00
1	A	186	CYS	CA-CB-SG	7.87	128.16	114.00
2	B	306	ALA	C-N-CA	-7.84	102.09	121.70
3	C	162	GLU	CB-CA-C	7.71	125.83	110.40
2	B	72	GLU	O-C-N	-7.52	110.67	122.70
1	A	359	GLU	CB-CA-C	7.33	125.07	110.40
1	A	342	GLN	CB-CA-C	7.18	124.75	110.40
2	B	32	GLY	N-CA-C	6.43	129.19	113.10
2	B	75	THR	C-N-CA	-5.81	107.19	121.70
2	B	308	PRO	C-N-CD	-5.70	108.07	120.60
1	A	353	ASP	N-CA-C	5.68	126.33	111.00
1	A	105	LYS	CA-C-N	-5.58	104.92	117.20
3	C	82	ARG	NE-CZ-NH1	5.34	122.97	120.30
3	C	211	ASN	N-CA-C	5.22	125.09	111.00
1	A	353	ASP	CB-CG-OD2	5.20	122.98	118.30
2	B	307	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	359	GLU	N-CA-CB	-5.01	101.59	110.60
1	A	104	LYS	CA-C-N	-5.00	106.20	117.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	PRO	Mainchain
1	A	105	LYS	Mainchain
1	A	205	ASP	Peptide
1	A	295	ASN	Peptide
1	A	334	ASP	Peptide
2	B	306	ALA	Mainchain

## 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	2374	0	2188	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4001	0	3913	64	0
3	C	3166	0	3067	59	0
4	A	1	0	0	0	0
5	B	5	0	0	0	0
6	C	11	0	17	3	0
7	A	6	0	0	1	0
7	B	42	0	0	4	0
7	C	27	0	0	3	0
All	All	9633	0	9185	159	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 9.

All (159) 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:307:ASP:CB	2:B:308:PRO:HD3	1.52	1.21
2:B:307:ASP:HB3	2:B:308:PRO:CD	1.70	1.21
7:A:502:HOH:O	2:B:188:THR:HG21	1.60	1.01
2:B:307:ASP:CB	2:B:308:PRO:CD	2.35	0.96
3:C:110:THR:CG2	3:C:162:GLU:HG2	1.94	0.96
2:B:308:PRO:O	2:B:309:PRO:O	1.90	0.89
3:C:110:THR:HG21	3:C:162:GLU:HG2	1.53	0.86
3:C:110:THR:CG2	3:C:162:GLU:CG	2.57	0.82
1:A:105:LYS:O	1:A:109:ARG:CB	2.28	0.81
2:B:273:ASP:HB3	7:B:705:HOH:O	1.80	0.80
1:A:358:SER:O	1:A:359:GLU:C	2.21	0.79
3:C:211:ASN:O	3:C:213:LEU:N	2.20	0.73
3:C:55:LEU:O	3:C:56:ASN:HB2	1.87	0.73
2:B:306:ALA:O	2:B:307:ASP:C	2.23	0.72
2:B:468:GLN:HB3	2:B:504:ASN:ND2	2.03	0.72
2:B:74:HIS:HD2	2:B:78:VAL:HG22	1.55	0.71
1:A:233:CYS:HB3	1:A:236:CYS:HB2	1.71	0.71
1:A:268:LEU:HD22	1:A:270:ARG:HD3	1.72	0.70
2:B:308:PRO:O	2:B:309:PRO:C	2.29	0.70
1:A:173:HIS:O	1:A:177:GLN:HB3	1.91	0.70
2:B:26:GLU:OE1	2:B:30:ARG:NH1	2.24	0.70
3:C:542:LEU:HD23	6:C:601:TAM:H31	1.72	0.70
2:B:307:ASP:HB3	2:B:308:PRO:HD3	0.74	0.69
2:B:307:ASP:N	2:B:308:PRO:CD	2.55	0.67
2:B:307:ASP:N	2:B:308:PRO:HD2	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:ASP:O	2:B:309:PRO:HD3	1.95	0.67
3:C:511:THR:N	3:C:512:PRO:CD	2.60	0.65
3:C:69:VAL:O	3:C:69:VAL:HG23	1.96	0.65
2:B:307:ASP:O	2:B:309:PRO:CD	2.44	0.65
3:C:540:ILE:HG22	3:C:542:LEU:CD1	2.28	0.63
1:A:268:LEU:CD2	1:A:270:ARG:HD3	2.27	0.63
3:C:110:THR:HG23	3:C:162:GLU:CG	2.28	0.63
1:A:358:SER:O	1:A:360:SER:HB3	2.00	0.62
3:C:542:LEU:HD23	6:C:601:TAM:C3	2.30	0.61
3:C:265:LEU:HD22	3:C:279:THR:HG22	1.83	0.60
2:B:75:THR:HG21	2:B:524:THR:CB	2.31	0.60
2:B:209:HIS:HE2	2:B:227:SER:HG	1.48	0.59
2:B:32:GLY:O	2:B:50:ARG:HG3	2.02	0.59
1:A:189:CYS:N	1:A:236:CYS:SG	2.74	0.59
3:C:511:THR:H	3:C:512:PRO:HD3	1.68	0.58
3:C:212:PRO:O	3:C:213:LEU:C	2.36	0.57
2:B:73:HIS:CD2	2:B:100:LYS:HZ2	2.22	0.57
3:C:242:GLY:HA2	3:C:264:GLY:HA2	1.87	0.57
3:C:28:PRO:HD2	7:C:702:HOH:O	2.03	0.57
3:C:110:THR:HG23	3:C:162:GLU:HG3	1.88	0.56
3:C:166:LEU:HD21	3:C:174:MET:HE2	1.88	0.56
1:A:268:LEU:HB2	1:A:270:ARG:HG2	1.86	0.55
2:B:307:ASP:O	2:B:309:PRO:N	2.41	0.54
3:C:511:THR:O	3:C:514:CYS:O	2.24	0.54
2:B:435:GLU:HG3	2:B:549:TRP:CG	2.43	0.54
2:B:472:GLU:OE2	2:B:508:GLN:NE2	2.41	0.53
2:B:24:GLU:OE1	2:B:531:ARG:NH2	2.42	0.53
2:B:123:LEU:HD23	2:B:134:SER:HA	1.91	0.53
2:B:206:LEU:HB3	2:B:237:TRP:CZ3	2.44	0.53
3:C:151:ARG:HD2	7:C:724:HOH:O	2.09	0.53
2:B:306:ALA:HB3	2:B:310:PRO:HD3	1.92	0.52
1:A:353:ASP:C	1:A:353:ASP:OD1	2.47	0.51
1:A:305:VAL:HG12	1:A:321:ILE:HB	1.92	0.51
1:A:353:ASP:OD1	1:A:353:ASP:O	2.29	0.51
1:A:216:LEU:HB3	1:A:288:ASN:HD21	1.75	0.51
1:A:49:TYR:CG	1:A:123:GLN:HB3	2.45	0.51
2:B:75:THR:HG21	2:B:524:THR:HB	1.91	0.51
2:B:75:THR:OG1	2:B:96:ASP:HB2	2.10	0.51
3:C:242:GLY:CA	3:C:264:GLY:HA2	2.40	0.51
2:B:39:ASP:HB2	2:B:83:LEU:HD21	1.92	0.51
3:C:301:HIS:HB3	3:C:522:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:SER:O	1:A:360:SER:N	2.44	0.50
1:A:49:TYR:CZ	1:A:123:GLN:HG2	2.47	0.50
1:A:48:CYS:HA	1:A:51:ASN:HB2	1.93	0.50
1:A:329:LEU:HD23	1:A:338:LYS:HA	1.94	0.50
3:C:241:ASP:OD2	3:C:245:ARG:NH2	2.44	0.49
3:C:511:THR:N	3:C:512:PRO:HD3	2.25	0.49
3:C:17:PHE:CD1	3:C:527:ILE:HD13	2.47	0.49
1:A:307:VAL:HG12	1:A:308:HIS:N	2.28	0.49
3:C:374:GLN:HA	3:C:535:ARG:HB2	1.94	0.48
1:A:353:ASP:C	1:A:355:SER:H	2.16	0.48
2:B:307:ASP:H	2:B:308:PRO:HD2	1.75	0.48
1:A:339:ILE:CG1	1:A:343:ALA:CB	2.91	0.48
2:B:74:HIS:CD2	2:B:94:SER:HB2	2.48	0.48
3:C:564:VAL:HG12	3:C:565:VAL:HG23	1.94	0.48
1:A:233:CYS:CB	1:A:236:CYS:HB2	2.43	0.48
1:A:283:GLU:HG2	1:A:299:MET:SD	2.54	0.48
1:A:280:PHE:CG	1:A:364:LEU:HD21	2.49	0.48
3:C:32:TYR:HB2	3:C:555:ILE:HB	1.94	0.48
1:A:143:GLU:HG3	1:A:146:GLN:NE2	2.29	0.47
2:B:25:VAL:HG23	2:B:26:GLU:N	2.29	0.47
2:B:142:PHE:HB3	7:B:722:HOH:O	2.13	0.47
2:B:131:LEU:HD23	2:B:176:MET:SD	2.55	0.47
2:B:100:LYS:NZ	2:B:112:THR:OG1	2.48	0.47
3:C:539:LEU:O	3:C:540:ILE:HD13	2.14	0.47
3:C:130:ILE:HG22	3:C:131:ASP:N	2.30	0.47
3:C:282:GLU:HA	3:C:306:TRP:CD1	2.49	0.47
1:A:339:ILE:HG13	1:A:343:ALA:HB3	1.96	0.46
1:A:217:ARG:NH2	3:C:301:HIS:CE1	2.83	0.46
2:B:295:ALA:HB3	2:B:316:THR:HB	1.97	0.46
3:C:538:VAL:HB	3:C:549:ALA:HB3	1.98	0.46
2:B:73:HIS:HD2	2:B:100:LYS:NZ	2.14	0.46
1:A:210:THR:HG22	1:A:211:SER:N	2.31	0.46
2:B:273:ASP:HB2	7:B:714:HOH:O	2.16	0.46
3:C:211:ASN:O	3:C:213:LEU:HD12	2.15	0.46
2:B:32:GLY:O	2:B:50:ARG:CG	2.63	0.46
2:B:71:MET:HB3	2:B:102:TRP:CZ3	2.51	0.46
3:C:212:PRO:O	3:C:214:LEU:N	2.49	0.46
2:B:206:LEU:HB3	2:B:237:TRP:CE3	2.50	0.46
3:C:556:CYS:HA	7:C:708:HOH:O	2.16	0.46
3:C:145:ARG:NH1	3:C:149:LYS:O	2.48	0.46
3:C:34:ARG:NH2	3:C:40:PHE:HA	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:ASN:O	3:C:42:SER:C	2.53	0.46
2:B:73:HIS:CD2	2:B:100:LYS:NZ	2.84	0.45
2:B:125:TYR:CZ	2:B:127:LYS:HA	2.52	0.45
2:B:76:ASP:HB3	2:B:95:SER:HB2	1.99	0.45
1:A:353:ASP:CG	1:A:353:ASP:O	2.53	0.45
3:C:19:THR:HG22	3:C:20:ARG:N	2.32	0.45
1:A:339:ILE:HG13	1:A:343:ALA:CB	2.47	0.45
3:C:21:GLU:CD	3:C:368:ARG:HH12	2.21	0.45
3:C:201:VAL:HG21	3:C:252:VAL:CG1	2.47	0.45
3:C:46:ASN:HB2	3:C:47:PRO:HD2	1.99	0.45
1:A:49:TYR:CD1	1:A:123:GLN:HB3	2.52	0.45
2:B:133:ALA:HA	2:B:142:PHE:O	2.17	0.45
1:A:128:PHE:CZ	1:A:132:LEU:HD22	2.53	0.44
1:A:206:VAL:HG13	1:A:278:VAL:HG21	1.99	0.44
1:A:350:LEU:HD13	1:A:358:SER:HA	1.99	0.44
2:B:37:GLN:NE2	2:B:37:GLN:HA	2.32	0.44
3:C:34:ARG:HH22	3:C:40:PHE:HA	1.83	0.44
2:B:83:LEU:HD11	2:B:87:GLY:HA2	1.99	0.44
2:B:30:ARG:O	2:B:362:SER:OG	2.22	0.44
3:C:36:ASN:OD1	3:C:38:VAL:HG12	2.16	0.44
2:B:202:LYS:HE3	7:B:724:HOH:O	2.18	0.44
3:C:112:THR:OG1	3:C:113:ALA:N	2.51	0.44
3:C:26:LEU:HB2	3:C:558:TRP:CZ3	2.52	0.43
3:C:161:SER:OG	3:C:162:GLU:N	2.52	0.43
2:B:268:TYR:CE1	2:B:278:CYS:SG	3.11	0.43
3:C:178:ASN:O	3:C:211:ASN:OD1	2.36	0.43
2:B:238:SER:HB2	2:B:245:ILE:HD11	1.99	0.43
2:B:187:SER:OG	2:B:188:THR:N	2.51	0.43
2:B:57:TRP:CZ3	2:B:357:ILE:HG23	2.54	0.43
3:C:211:ASN:C	3:C:213:LEU:N	2.73	0.42
2:B:73:HIS:O	2:B:527:ARG:NE	2.53	0.42
3:C:107:ASN:HB2	3:C:157:TRP:CE2	2.55	0.42
3:C:34:ARG:HH21	3:C:38:VAL:HG13	1.85	0.42
2:B:204:MET:SD	2:B:206:LEU:HD21	2.60	0.42
3:C:124:ALA:HB1	3:C:145:ARG:HD3	2.02	0.42
1:A:173:HIS:HA	1:A:177:GLN:HB2	2.00	0.41
2:B:137:LEU:HA	2:B:170:SER:HB3	2.03	0.41
1:A:341:ALA:C	1:A:343:ALA:H	2.23	0.41
2:B:51:ASP:O	2:B:51:ASP:OD1	2.37	0.41
3:C:123:SER:HA	3:C:151:ARG:HB2	2.02	0.41
2:B:307:ASP:C	2:B:309:PRO:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:SER:HB2	2:B:68:ILE:HD11	2.02	0.41
2:B:470:LEU:HD12	2:B:509:VAL:HG21	2.03	0.40
3:C:542:LEU:HG	6:C:601:TAM:H32	2.04	0.40
3:C:69:VAL:CG2	3:C:72:GLU:HB2	2.51	0.40
2:B:377:THR:HG23	2:B:387:TRP:CD1	2.56	0.40
2:B:250:VAL:HG23	2:B:251:HIS:CD2	2.56	0.40
3:C:18:THR:HG22	3:C:23:LEU:HD13	2.02	0.40
3:C:265:LEU:HD22	3:C:279:THR:CG2	2.49	0.40
1:A:339:ILE:CG1	1:A:343:ALA:HB3	2.50	0.40
2:B:219:ASN:HB3	2:B:264:PHE:CD2	2.57	0.40
3:C:226:PHE:HA	3:C:236:ALA:O	2.21	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	294/355 (83%)	259 (88%)	35 (12%)	0	100	100
2	B	507/563 (90%)	457 (90%)	49 (10%)	1 (0%)	52	88
3	C	399/569 (70%)	363 (91%)	34 (8%)	2 (0%)	34	76
All	All	1200/1487 (81%)	1079 (90%)	118 (10%)	3 (0%)	46	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	309	PRO
3	C	211	ASN
3	C	212	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	248/324 (76%)	245 (99%)	3 (1%)	78	94
2	B	438/492 (89%)	433 (99%)	5 (1%)	80	94
3	C	348/499 (70%)	345 (99%)	3 (1%)	84	95
All	All	1034/1315 (79%)	1023 (99%)	11 (1%)	80	94

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	181	THR
1	A	186	CYS
2	B	30	ARG
2	B	52	SER
2	B	139	ARG
2	B	249	ARG
2	B	308	PRO
3	C	66	CYS
3	C	163	SER
3	C	305	SER

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	46	ASN
1	A	51	ASN
1	A	119	ASN
1	A	141	GLN
1	A	288	ASN
2	B	73	HIS
2	B	74	HIS
2	B	367	HIS
2	B	381	ASN
3	C	104	HIS

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Mol	Chain	Res	Type
3	C	126	GLN
3	C	224	ASN
3	C	301	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
5	PO4	B	601	-	4,4,4	0.44	0	6,6,6	0.34	0
6	TAM	C	601	-	7,10,10	0.74	0	9,12,12	2.08	2 (22%)

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
5	PO4	B	601	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TAM	C	601	-	-	0/12/12/12	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	601	TAM	C1-C-N	-3.66	100.88	108.28
6	C	601	TAM	C2-C-N	3.87	116.11	108.28

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
6	C	601	TAM	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	302/355 (85%)	0.07	13 (4%)	39 16	59, 129, 186, 207	0
2	B	515/563 (91%)	-0.33	3 (0%)	90 73	49, 87, 140, 217	0
3	C	407/569 (71%)	-0.33	1 (0%)	95 87	47, 85, 138, 177	0
All	All	1224/1487 (82%)	-0.23	17 (1%)	78 51	47, 93, 168, 217	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	TYR	4.5
2	B	453	PRO	3.4
1	A	80	LEU	3.1
3	C	59	SER	3.0
1	A	93	THR	2.7
2	B	332	PHE	2.6
1	A	268	LEU	2.5
1	A	106	PHE	2.4
1	A	113	GLU	2.3
1	A	110	LEU	2.2
1	A	143	GLU	2.2
1	A	85	ALA	2.2
1	A	103	PRO	2.2
1	A	353	ASP	2.2
1	A	37	HIS	2.2
2	B	517	PHE	2.0
1	A	38	TYR	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	TAM	C	601	11/11	0.77	0.61	9.25	90,108,133,148	0
4	ZN	A	401	1/1	0.92	0.11	-1.69	60,60,60,60	0
5	PO4	B	601	5/5	0.94	0.22	-	68,69,84,85	0

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

There are no such residues in this entry.