



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:11 AM UTC

PDB ID : 2C4K / pdb\_00002c4k  
Title : Crystal structure of human phosphoribosylpyrophosphate synthetase- associated protein 39 (PAP39)  
Authors : Kursula, P.; Stenmark, P.; Arrowsmith, C.; Berglund, H.; Edwards, A.; Ehn, M.; Flodin, S.; Graslund, S.; Hammarstrom, M.; Hallberg, B.M.; Holmberg Schiavone, L.; Kotenyova, T.; Nilsson-Ehle, P.; Ogg, D.; Persson, C.; Sage- mark, J.; Schuler, H.; Sundstrom, M.; Thorsell, A.G.; Van Den Berg, S.; Weigelt, J.; Nordlund, P.  
Deposited on : 2005-10-20  
Resolution : 2.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)

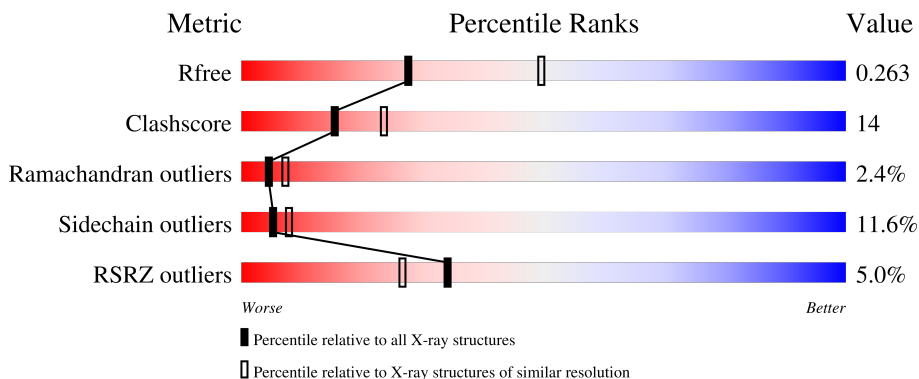
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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 of 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	370	 4% 53% 24% 5% 18%
1	B	370	 4% 54% 23% 5% 18%
1	C	370	 6% 54% 24% 5% 18%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	370	<p>4% 55% 22% 5% 18%</p>
1	E	370	<p>3% 53% 23% 6% 18%</p>
1	F	370	<p>5% 55% 23% 5% 18%</p>

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
3	TAM	B	1353	-	-	X	-

## 2 Entry composition [i](#)

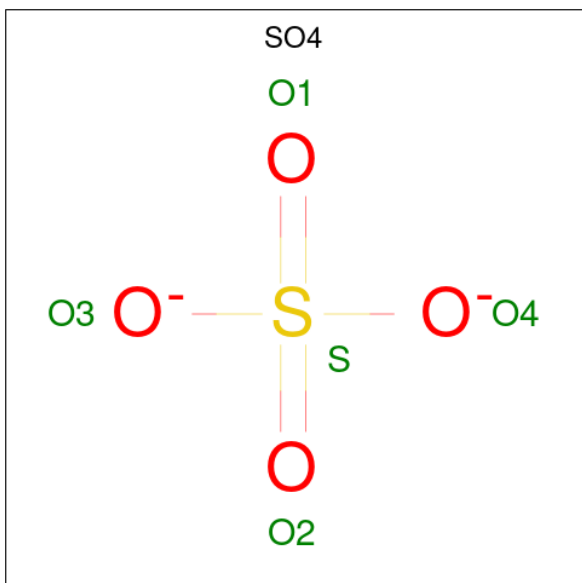
There are 4 unique types of molecules in this entry. The entry contains 14378 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHORIBOSYL PYROPHOSPHATE SYNTHETASE-ASSOCIATED PROTEIN 1.

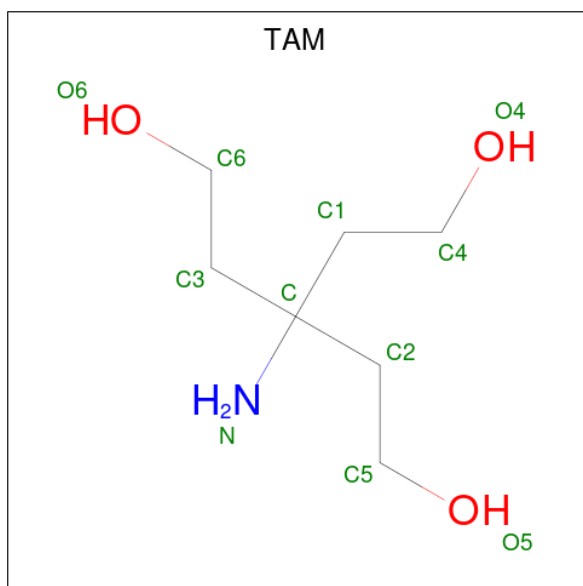
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	305	Total 2376	C 1513	N 414	O 438	S 11	0	0	0
1	B	305	Total 2376	C 1513	N 414	O 438	S 11	0	0	0
1	C	305	Total 2376	C 1513	N 414	O 438	S 11	0	0	0
1	D	305	Total 2376	C 1513	N 414	O 438	S 11	0	0	0
1	E	305	Total 2376	C 1513	N 414	O 438	S 11	0	0	0
1	F	305	Total 2376	C 1513	N 414	O 438	S 11	0	0	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

- Molecule 3 is TRIS(HYDROXYETHYL)AMINOMETHANE (CCD ID: TAM) (formula:  $C_7H_{17}NO_3$ ).



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

- Molecule 4 is water.

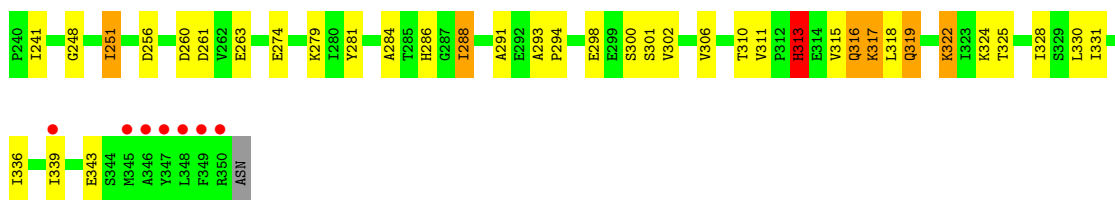
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0

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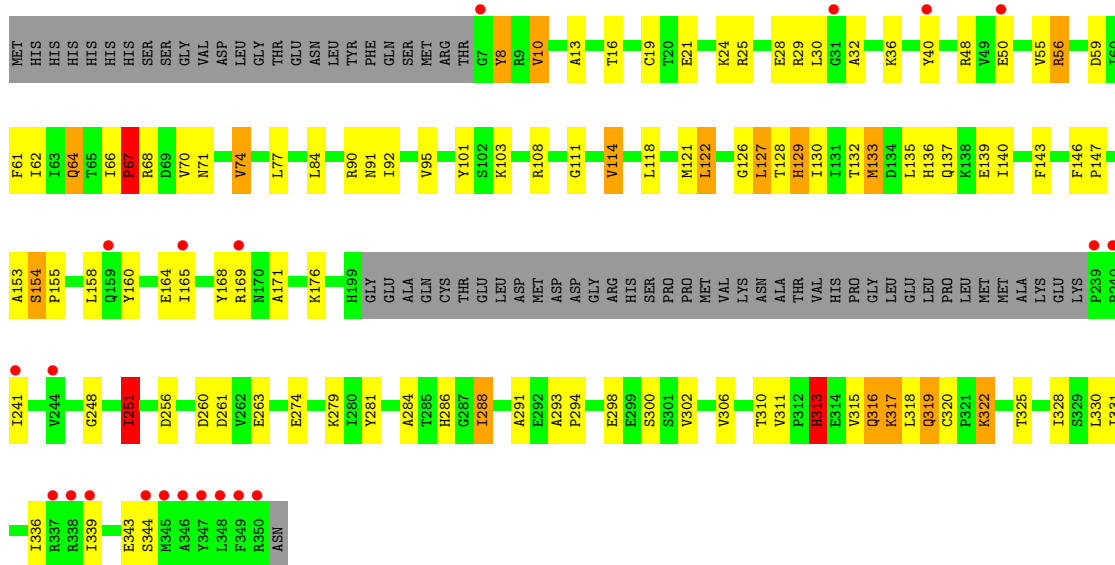
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	B	22	Total O 22 22	0	0
4	C	10	Total O 10 10	0	0
4	D	11	Total O 11 11	0	0
4	E	17	Total O 17 17	0	0
4	F	7	Total O 7 7	0	0

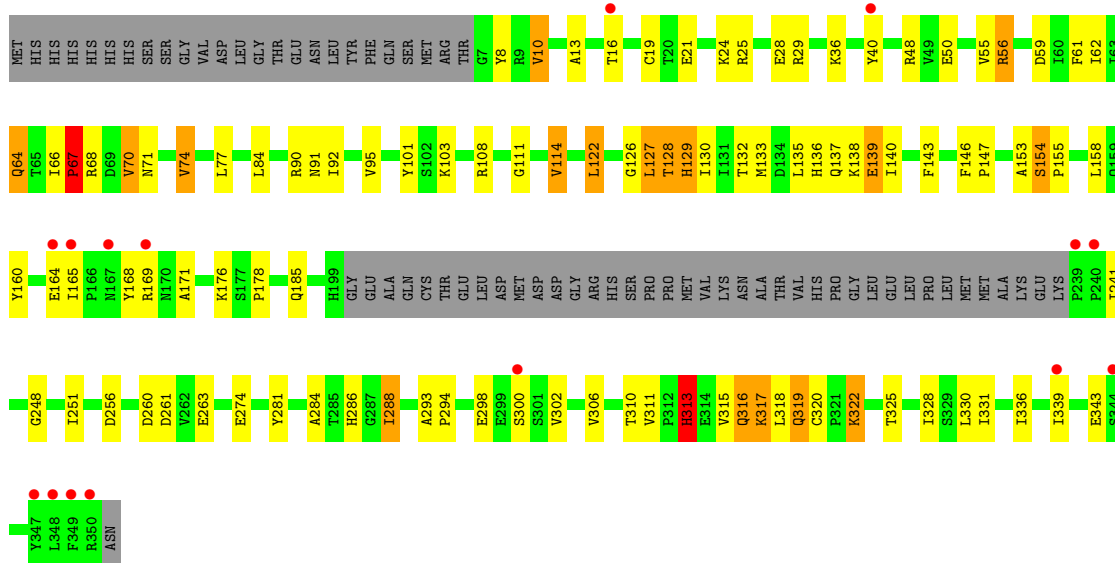




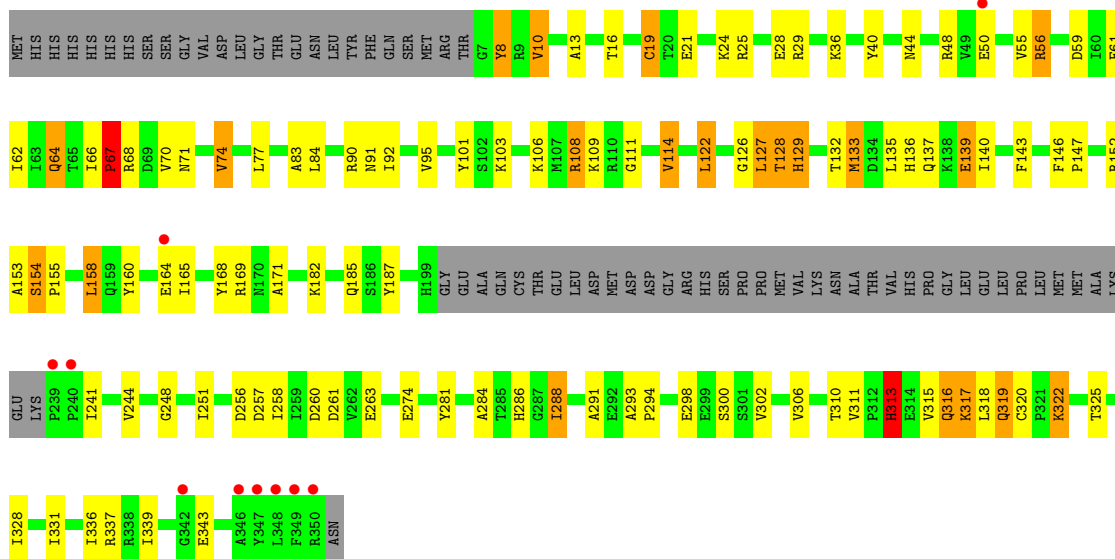
● Molecule 1: PHOSPHORIBOSYL PYROPHOSPHATE SYNTHETASE-ASSOCIATED PROTEIN 1



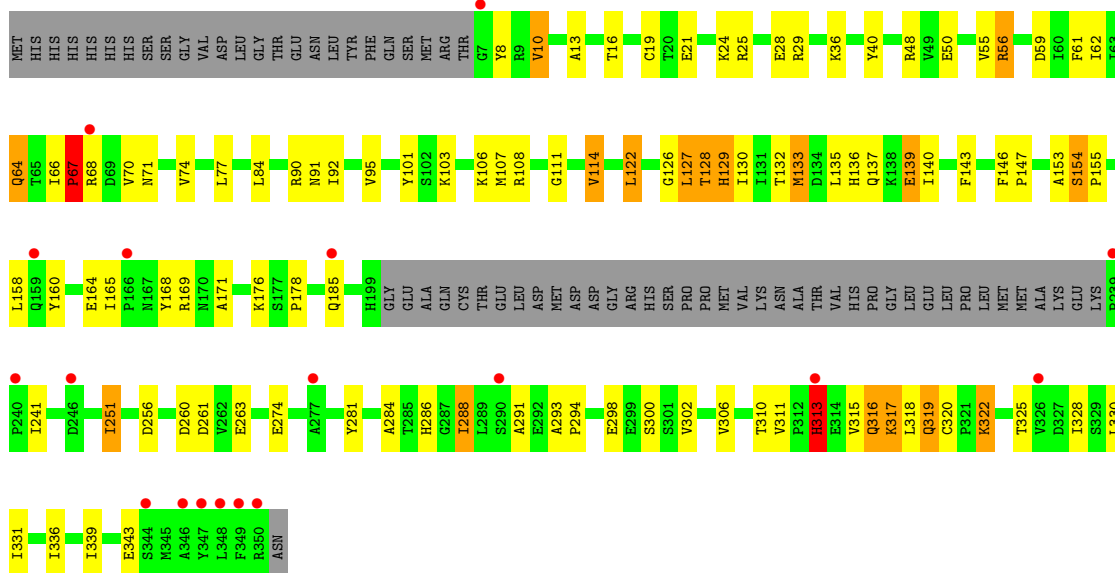
● Molecule 1: PHOSPHORIBOSYL PYROPHOSPHATE SYNTHETASE-ASSOCIATED PROTEIN 1



● Molecule 1: PHOSPHORIBOSYL PYROPHOSPHATE SYNTHETASE-ASSOCIATED PROTEIN 1



● Molecule 1: PHOSPHORIBOSYL PYROPHOSPHATE SYNTHETASE-ASSOCIATED PROTEIN 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	180.06Å 103.88Å 127.16Å 90.00° 97.63° 90.00°	Depositor
Resolution (Å)	20.00 – 2.65 20.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.65) 99.7 (20.00-2.65)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.67Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.269 , 0.299 (Not available) , 0.263	Depositor DCC
$R_{free}$ test set	3370 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtrriage
Anisotropy	0.791	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 57.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	14378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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: SO4, TAM

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	0.76	0/2412	1.00	2/3261 (0.1%)
1	B	0.77	0/2412	1.00	3/3261 (0.1%)
1	C	0.76	1/2412 (0.0%)	0.99	2/3261 (0.1%)
1	D	0.76	0/2412	0.99	2/3261 (0.1%)
1	E	0.76	0/2412	1.00	2/3261 (0.1%)
1	F	0.76	1/2412 (0.0%)	1.00	3/3261 (0.1%)
All	All	0.76	2/14472 (0.0%)	1.00	14/19566 (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
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
All	All	0	12

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	251	ILE	CA-CB	5.22	1.60	1.53
1	C	251	ILE	CA-CB	5.00	1.59	1.53

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	313	HIS	CB-CA-C	-7.20	96.34	109.15
1	B	313	HIS	CB-CA-C	-7.06	96.59	109.15
1	F	313	HIS	CB-CA-C	-6.66	97.29	109.15
1	A	313	HIS	CB-CA-C	-6.63	97.35	109.15
1	D	313	HIS	CB-CA-C	-6.54	97.50	109.15

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	GLU	Peptide
1	A	313	HIS	Peptide
1	B	164	GLU	Peptide
1	B	313	HIS	Peptide
1	C	164	GLU	Peptide

## 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	2376	0	2464	69	0
1	B	2376	0	2464	77	0
1	C	2376	0	2464	63	0
1	D	2376	0	2464	63	0
1	E	2376	0	2464	70	0
1	F	2376	0	2464	62	0
2	B	10	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
2	E	10	0	0	0	0
2	F	5	0	0	0	0
3	B	11	0	17	10	0
4	A	9	0	0	0	0
4	B	22	0	0	6	0
4	C	10	0	0	1	0
4	D	11	0	0	0	0
4	E	17	0	0	3	0
4	F	7	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14378	0	14801	394	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 14.

The worst 5 of 394 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:136:HIS:CD2	1:B:137:GLN:HE21	2.02	0.78
1:A:8:TYR:OH	1:A:337:ARG:HG3	1.85	0.77
1:B:324:LYS:NZ	3:B:1353:TAM:H32	2.00	0.76
1:C:315:VAL:O	1:C:319:GLN:NE2	2.21	0.74
1:D:129:HIS:HA	1:D:146:PHE:CD1	2.23	0.73

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	301/370 (81%)	270 (90%)	24 (8%)	7 (2%)	5 8
1	B	301/370 (81%)	270 (90%)	23 (8%)	8 (3%)	4 6
1	C	301/370 (81%)	271 (90%)	22 (7%)	8 (3%)	4 6
1	D	301/370 (81%)	272 (90%)	22 (7%)	7 (2%)	5 8
1	E	301/370 (81%)	272 (90%)	21 (7%)	8 (3%)	4 6
1	F	301/370 (81%)	271 (90%)	24 (8%)	6 (2%)	6 10
All	All	1806/2220 (81%)	1626 (90%)	136 (8%)	44 (2%)	4 7

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	ILE
1	B	241	ILE
1	C	241	ILE
1	D	241	ILE
1	E	241	ILE

### 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	258/315 (82%)	228 (88%)	30 (12%)	5	8
1	B	258/315 (82%)	229 (89%)	29 (11%)	6	8
1	C	258/315 (82%)	228 (88%)	30 (12%)	5	8
1	D	258/315 (82%)	228 (88%)	30 (12%)	5	8
1	E	258/315 (82%)	228 (88%)	30 (12%)	5	8
1	F	258/315 (82%)	227 (88%)	31 (12%)	5	7
All	All	1548/1890 (82%)	1368 (88%)	180 (12%)	5	8

5 of 180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	318	LEU
1	E	316	GLN
1	E	10	VAL
1	E	122	LEU
1	F	10	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	91	ASN
1	F	137	GLN
1	E	137	GLN
1	F	14	ASN

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Mol	Chain	Res	Type
1	F	316	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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	SO4	B	1352	-	4,4,4	0.31	0	6,6,6	0.42	0
2	SO4	E	1351	-	4,4,4	0.32	0	6,6,6	0.25	0
2	SO4	B	1351	-	4,4,4	0.40	0	6,6,6	0.29	0
2	SO4	F	1351	-	4,4,4	0.35	0	6,6,6	0.23	0
3	TAM	B	1353	-	10,10,10	0.59	0	12,12,12	1.71	2 (16%)
2	SO4	E	1352	-	4,4,4	0.24	0	6,6,6	0.26	0
2	SO4	C	1351	-	4,4,4	0.30	0	6,6,6	0.25	0
2	SO4	D	1351	-	4,4,4	0.31	0	6,6,6	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TAM	B	1353	-	-	6/12/12/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1353	TAM	C6-C3-C	4.88	121.72	115.97
3	B	1353	TAM	C3-C-C2	-2.13	106.75	110.50

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1353	TAM	C1-C-C3-C6
3	B	1353	TAM	C2-C-C3-C6
3	B	1353	TAM	N-C-C3-C6
3	B	1353	TAM	C-C1-C4-O4
3	B	1353	TAM	C-C2-C5-O5

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1353	TAM	10	0
2	C	1351	SO4	1	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	305/370 (82%)	0.54	13 (4%) 40 32	6, 36, 55, 82	0
1	B	305/370 (82%)	0.48	15 (4%) 35 27	7, 33, 52, 81	0
1	C	305/370 (82%)	0.57	21 (6%) 23 17	7, 35, 53, 83	0
1	D	305/370 (82%)	0.59	15 (4%) 35 27	4, 37, 56, 86	0
1	E	305/370 (82%)	0.54	10 (3%) 49 40	5, 36, 57, 84	0
1	F	305/370 (82%)	0.53	18 (5%) 28 21	9, 36, 54, 81	0
All	All	1830/2220 (82%)	0.54	92 (5%) 34 26	4, 36, 55, 86	0

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	239	PRO	4.8
1	C	347	TYR	4.4
1	A	347	TYR	4.3
1	D	40	TYR	4.0
1	D	347	TYR	4.0

### 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 oligosaccharides 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. 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( $\text{\AA}^2$ )	Q<0.9
3	TAM	B	1353	11/11	0.85	0.12	30,31,32,32	0
2	SO4	E	1352	5/5	0.87	0.12	65,65,66,66	0
2	SO4	C	1351	5/5	0.87	0.12	69,69,70,70	0
2	SO4	F	1351	5/5	0.91	0.11	49,50,51,51	0
2	SO4	B	1351	5/5	0.91	0.12	40,42,42,42	0
2	SO4	E	1351	5/5	0.92	0.10	55,55,56,57	0
2	SO4	B	1352	5/5	0.94	0.08	46,47,48,48	0
2	SO4	D	1351	5/5	0.96	0.08	38,38,39,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.