



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 21, 2016 – 06:05 PM EDT

PDB ID : 5B04  
Title : Crystal structure of the eukaryotic translation initiation factor 2B from Schizosaccharomyces pombe  
Authors : Kashiwagi, K.; Ito, T.; Yokoyama, S.  
Deposited on : 2015-10-27  
Resolution : 2.99 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  
<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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

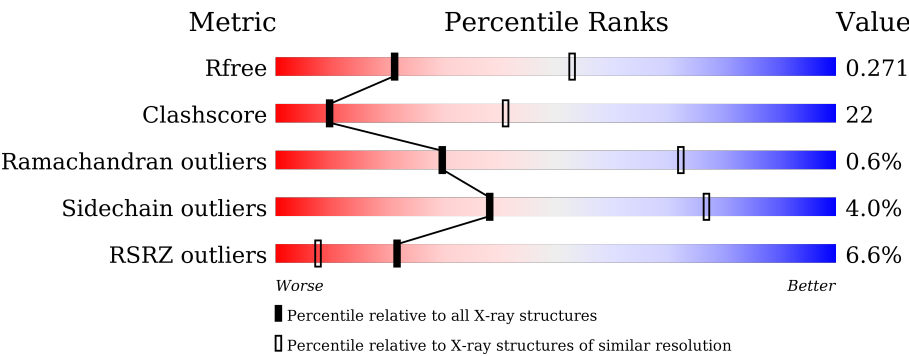
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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	341	<div><div>9%</div><div><div></div><div></div><div></div><div></div></div><div>59%29%•7%</div></div>
1	B	341	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>75%17%•6%</div></div>
2	C	399	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>66%19%•13%</div></div>
2	D	399	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>69%17%•13%</div></div>
3	E	458	<div><div>9%</div><div><div></div><div></div><div></div><div></div></div><div>45%30%7%•16%</div></div>
3	F	458	<div><div>12%</div><div><div></div><div></div><div></div><div></div></div><div>38%36%9%•16%</div></div>

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Mol	Chain	Length	Quality of chain
4	G	467	<div><div><div></div><div></div><div></div></div><div><div>4%</div><div>58%</div><div>15%</div><div>•</div><div>25%</div></div></div>
4	H	467	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>62%</div><div>12%</div><div>•</div><div>25%</div></div></div>
5	I	678	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>47%</div><div>13%</div><div>••</div><div>37%</div></div></div>
5	J	678	<div><div><div></div><div></div><div></div></div><div><div>4%</div><div>44%</div><div>17%</div><div>•</div><div>37%</div></div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28584 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 Translation initiation factor eIF-2B subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2472	1571	430	458	13			
1	B	319	Total	C	N	O	S	0	0	0
			2489	1582	434	460	13			

- Molecule 2 is a protein called Probable translation initiation factor eIF-2B subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	349	Total	C	N	O	S	0	0	0
			2702	1714	459	515	14			
2	D	346	Total	C	N	O	S	0	0	0
			2674	1697	453	511	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	expression tag	UNP Q9UT76
C	-4	PRO	-	expression tag	UNP Q9UT76
C	-3	ILE	-	expression tag	UNP Q9UT76
C	-2	SER	-	expression tag	UNP Q9UT76
C	-1	GLU	-	expression tag	UNP Q9UT76
C	0	PHE	-	expression tag	UNP Q9UT76
D	-5	GLY	-	expression tag	UNP Q9UT76
D	-4	PRO	-	expression tag	UNP Q9UT76
D	-3	ILE	-	expression tag	UNP Q9UT76
D	-2	SER	-	expression tag	UNP Q9UT76
D	-1	GLU	-	expression tag	UNP Q9UT76
D	0	PHE	-	expression tag	UNP Q9UT76

- Molecule 3 is a protein called Probable translation initiation factor eIF-2B subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	384	Total	C	N	O	S	0	0	0
			2976	1895	511	553	17			
3	F	383	Total	C	N	O	S	0	0	0
			2967	1890	509	551	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	157	TYR	ILE	engineered mutation	UNP P56288
E	158	THR	TYR	engineered mutation	UNP P56288
E	159	VAL	GLY	engineered mutation	UNP P56288
F	157	TYR	ILE	engineered mutation	UNP P56288
F	158	THR	TYR	engineered mutation	UNP P56288
F	159	VAL	GLY	engineered mutation	UNP P56288

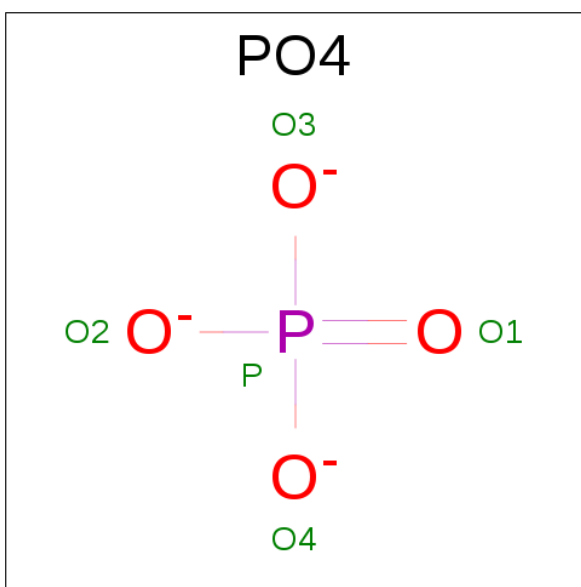
- Molecule 4 is a protein called Probable translation initiation factor eIF-2B subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	349	Total	C	N	O	S	0	0	0
			2755	1763	466	513	13			
4	H	349	Total	C	N	O	S	0	0	0
			2755	1763	466	513	13			

- Molecule 5 is a protein called Probable translation initiation factor eIF-2B subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	428	Total	C	N	O	S	0	0	0
			3377	2123	592	647	15			
5	J	428	Total	C	N	O	S	0	0	0
			3372	2119	591	647	15			

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

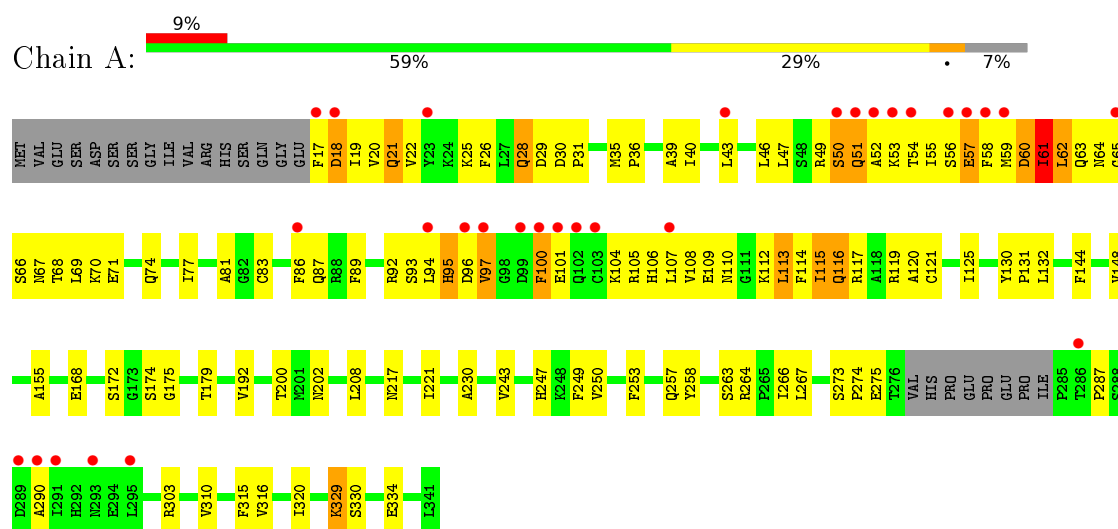


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	D	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		
6	H	1	Total	O	P	0	0
			5	4	1		
6	H	1	Total	O	P	0	0
			5	4	1		
6	I	1	Total	O	P	0	0
			5	4	1		

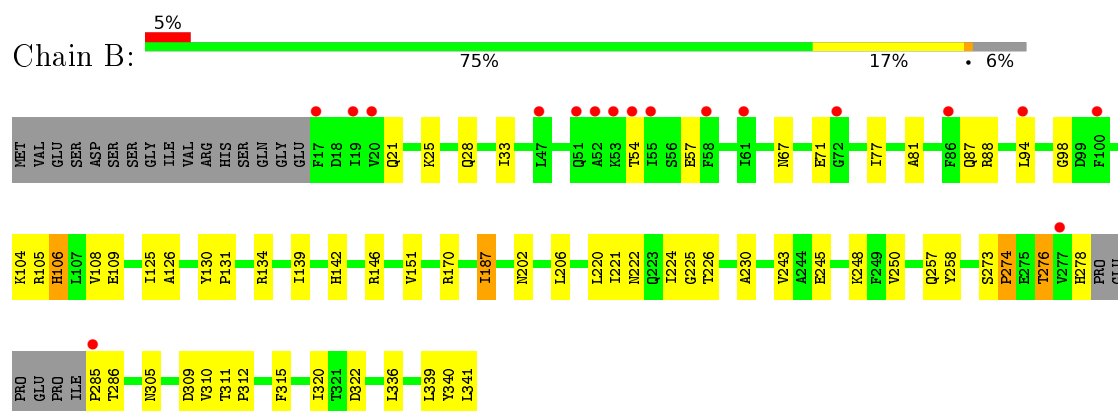
### 3 Residue-property plots

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.

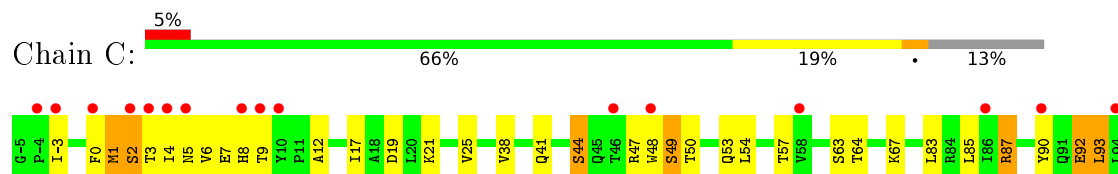
- Molecule 1: Translation initiation factor eIF-2B subunit alpha

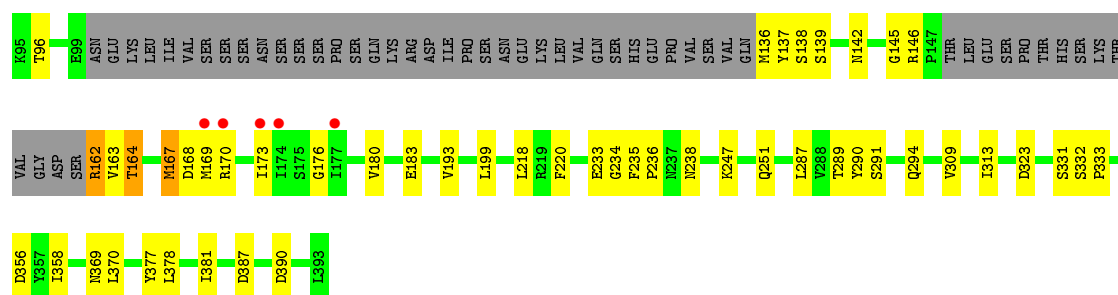


- Molecule 1: Translation initiation factor eIF-2B subunit alpha

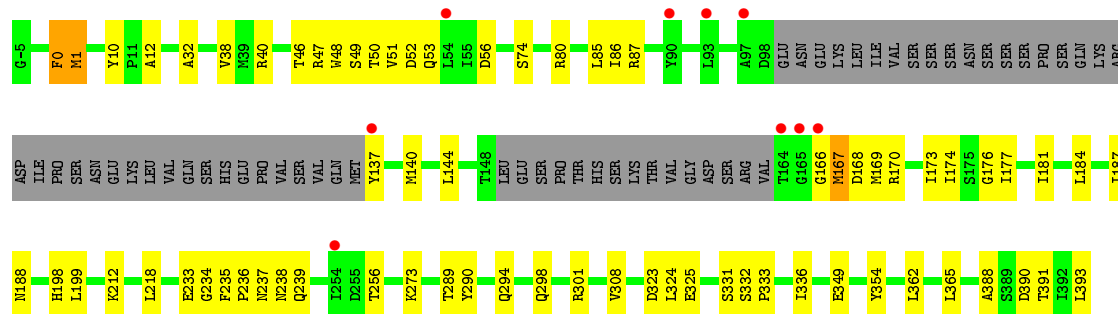


- Molecule 2: Probable translation initiation factor eIF-2B subunit beta

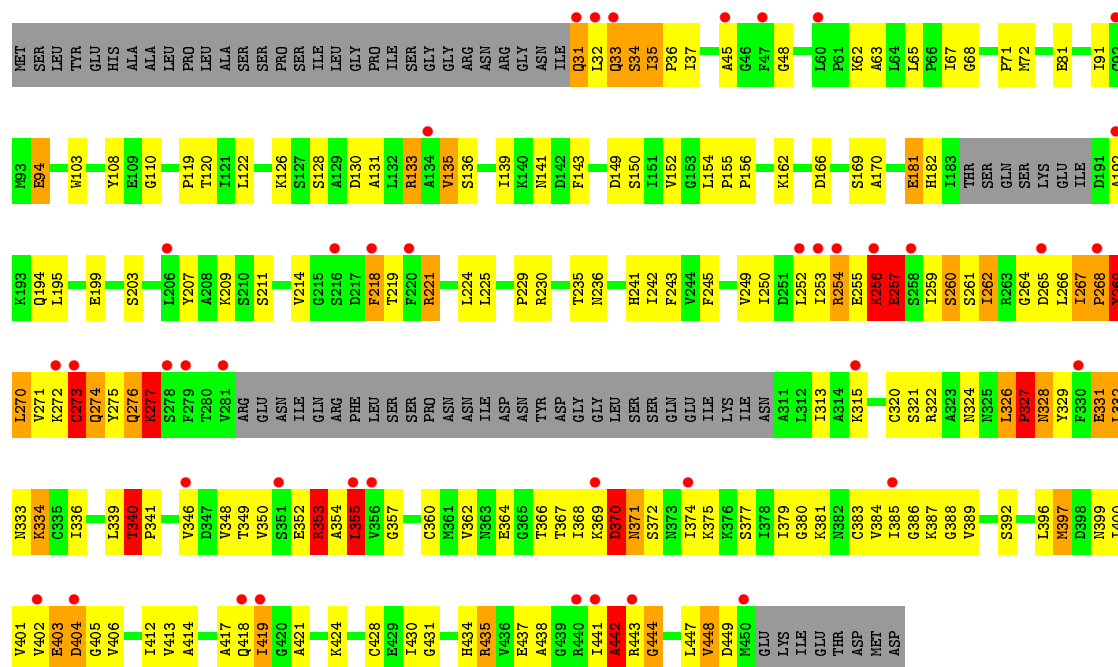
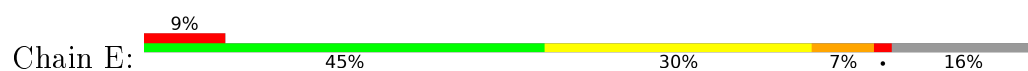




• Molecule 2: Probable translation initiation factor eIF-2B subunit beta



• Molecule 3: Probable translation initiation factor eIF-2B subunit gamma

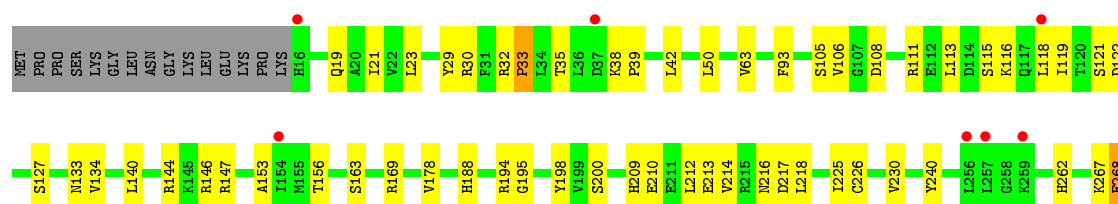


• Molecule 3: Probable translation initiation factor eIF-2B subunit gamma









GLU	ASP	PRO	GLY	SER	V388	N269
ASN	LYS	LYS	ASP	ASP	GLU	Y270
ALA	GLU	ALA	PHE	ASP	G391	R273
ILE	ILE	ALA	ASN	GLU	N392	V274
GLN	LEU	LEU	LYS	GLY	N393	
TRP	GLU	ALA	ALA	GLU	G394	K285
TYR	VAL	LYS	ALA	PHE	S395	
SER	MET	VAL	GLN	MET	I396	R290
ASP	THR	THR	GLN	GLU	E397	
PRO	ARG	PRO	SER	ALA	D398	Y293
ARG	TRP	TRP	LEU	SER	G399	P294
SER	GLY	GLY	GLU	GLY	A400	
SER	PRO	PRO	ALA	LEU	I401	D298
GLU	LEU	LEU	PHE	ILE	V402	
GLU	LEU	LEU	GLU	GLU	A403	
GLU	ALA	ALA	GLU	THR	V406	Q304
LEU	LYS	LYS	ASN	ASN	V407	T305
ALA	LEU	LEU	HIS	GLU	I408	Q309
THR	THR	THR	GLN	LEU	G409	R310
ALA	PHE	ALA	ILE	LEU	D410	H311
LEU	SER	SER	ASP	SER	N411	Q312
ARG	HIS	HIS	ILE	LEU	I414	I313
ASP	ASP	ASP	ALA	ASP	E415	
ALA	GLU	GLU	ALA	SER	K416	E317
GLY	GLN	GLN	LEU	GLU	N417	
GLY	VAL	VAL	GLU	SER	K418	
LYS	VAL	ASP	LEU	SER	R419	V320
GLN	ASN	ASN	ASN	GLU	I420	L321
PHE	VAL	VAL	THR	THR		A322
ASP	LEU	LEU	LEU	SER		R323
TRP	THR	THR	ARG	SER	F423	S324
LEU	LEU	LEU	MET	SER	E424	C325
LEU	LEU	LEU	ARG	SER	S425	I326
ASN	GLN	GLN	ALA	SER	N426	I327
THR	THR	THR	LYS	GLU	G427	K328
ALA	ALA	ALA	ASN	GLU	S428	A329
GLU	TYR	TYR	ALA	ASP	Q428	R330
SER	VAL	VAL	ASN	MET	G429	
GLU	ARG	ARG	TYR	GLU	T430	V339
SER	LEU	LEU	HIS	PHE	I431	
SER	GLU	GLU	GLU	ILE	N432	A346
GLU	SER	SER	VAL	PRO	D433	
GLU	THR	THR	ARG	PHE	P434	I356
GLY	ARG	ARG	SER	SER	S435	
SER	HIS	HIS	ALA	ALA	L436	
SER	PHE	PHE	ILE	ARG	V437	F366
SER	LEU	LEU	VAL	ARG	G438	L367
SER	LEU	LEU	LEU	ASP	I439	G374
SER	GLN	GLN	ALA	SER	G440	
SER	LEU	LEU	LEU	ALA	G441	
SER	GLY	GLY	LEU	ASN	R442	I379
SER	TYR	TYR	ARG	THR	G443	
SER	PHE	PHE	ARG	ILE	G380	G380
SER	TYR	TYR	ILE	ASN	K381	A382
SER	GLN	GLN	MET	SER	TYR	I383
SER	LEU	LEU	HIS	GLU	HIS	L384
SER	GLU	GLU	LEU	ASP	ALA	A385
SER	ILE	ILE	ASP	PHE	GLU	N386
SER	ALA	ALA	VAL	ASP	ASP	S387
SER	GLU	GLU	SER	GLU		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.50Å 209.23Å 223.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 2.99 49.29 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.29-2.99) 99.6 (49.29-2.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.222 , 0.271 0.224 , 0.271	Depositor DCC
$R_{free}$ test set	6802 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	80.9	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 136110 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	28584	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.32	0/2519	0.63	5/3409 (0.1%)
1	B	0.29	0/2537	0.48	2/3434 (0.1%)
2	C	0.31	0/2747	0.49	1/3726 (0.0%)
2	D	0.26	0/2719	0.46	2/3690 (0.1%)
3	E	0.57	2/3029 (0.1%)	0.91	21/4100 (0.5%)
3	F	0.51	3/3020 (0.1%)	1.08	30/4088 (0.7%)
4	G	0.38	1/2802 (0.0%)	0.58	3/3797 (0.1%)
4	H	0.27	0/2802	0.43	0/3797
5	I	0.46	1/3437 (0.0%)	0.77	14/4658 (0.3%)
5	J	0.45	2/3432 (0.1%)	0.63	5/4652 (0.1%)
All	All	0.40	9/29044 (0.0%)	0.69	83/39351 (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	2
3	E	0	5
3	F	0	6
4	H	0	1
5	I	0	1
5	J	0	1
All	All	0	16

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	268	PRO	N-CD	-13.76	1.28	1.47
5	J	434	PRO	N-CD	-9.39	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	33	PRO	N-CD	8.86	1.60	1.47
5	I	434	PRO	N-CD	7.20	1.57	1.47
3	E	257	GLU	CG-CD	-6.17	1.42	1.51

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	429	GLY	N-CA-C	16.66	154.74	113.10
3	F	370	ASP	N-CA-C	16.40	155.28	111.00
3	F	370	ASP	CB-CA-C	-15.86	78.69	110.40
5	I	432	ASN	CB-CA-C	-14.98	80.44	110.40
3	F	212	ALA	CB-CA-C	13.37	130.15	110.10

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	329	LYS	Peptide
1	A	60	ASP	Peptide
3	E	257	GLU	Peptide
3	E	260	SER	Peptide
3	E	269	TYR	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	2472	0	2492	150	0
1	B	2489	0	2512	52	0
2	C	2702	0	2744	95	0
2	D	2674	0	2714	52	1
3	E	2976	0	3032	265	0
3	F	2967	0	3022	325	7
4	G	2755	0	2841	91	0
4	H	2755	0	2841	45	0
5	I	3377	0	3361	140	1
5	J	3372	0	3351	134	7

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	1	0
6	G	10	0	0	1	0
6	H	10	0	0	0	0
6	I	5	0	0	1	0
All	All	28584	0	28910	1287	8

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 22.

The worst 5 of 1287 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)
3:F:218:PHE:CE2	5:I:203:PRO:HB3	1.37	1.58
3:F:368:ILE:HA	3:F:385:ILE:O	1.17	1.24
3:E:355:LEU:HD21	3:E:369:LYS:O	1.05	1.23
3:F:218:PHE:HE2	5:I:203:PRO:CB	1.54	1.21
3:F:265:ASP:O	3:F:268:PRO:HD2	1.35	1.21

The worst 5 of 8 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:113:ARG:NH2	5:J:443:GLY:C[2_555]	0.64	1.56
3:F:113:ARG:CZ	5:J:443:GLY:O[2_555]	0.66	1.54
3:F:113:ARG:NH2	5:J:443:GLY:O[2_555]	0.96	1.24
3:F:113:ARG:NH1	5:J:443:GLY:O[2_555]	1.51	0.69
3:F:113:ARG:CZ	5:J:443:GLY:C[2_555]	1.76	0.44

## 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	313/341 (92%)	293 (94%)	17 (5%)	3 (1%)	19	61
1	B	315/341 (92%)	302 (96%)	12 (4%)	1 (0%)	46	84
2	C	343/399 (86%)	330 (96%)	13 (4%)	0	100	100
2	D	340/399 (85%)	327 (96%)	13 (4%)	0	100	100
3	E	378/458 (82%)	334 (88%)	36 (10%)	8 (2%)	9	40
3	F	377/458 (82%)	334 (89%)	40 (11%)	3 (1%)	24	66
4	G	347/467 (74%)	331 (95%)	15 (4%)	1 (0%)	46	84
4	H	347/467 (74%)	339 (98%)	8 (2%)	0	100	100
5	I	426/678 (63%)	400 (94%)	24 (6%)	2 (0%)	34	76
5	J	426/678 (63%)	385 (90%)	37 (9%)	4 (1%)	21	64
All	All	3612/4686 (77%)	3375 (93%)	215 (6%)	22 (1%)	30	72

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	262	ILE
3	E	442	ALA
3	E	270	LEU
3	E	277	LYS
5	J	432	ASN

### 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	276/298 (93%)	264 (96%)	12 (4%)	35	75
1	B	278/298 (93%)	274 (99%)	4 (1%)	74	93
2	C	301/350 (86%)	290 (96%)	11 (4%)	41	79
2	D	298/350 (85%)	295 (99%)	3 (1%)	82	95
3	E	330/395 (84%)	299 (91%)	31 (9%)	11	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	329/395 (83%)	306 (93%)	23 (7%)	19	55
4	G	314/408 (77%)	307 (98%)	7 (2%)	60	88
4	H	314/408 (77%)	307 (98%)	7 (2%)	60	88
5	I	379/596 (64%)	363 (96%)	16 (4%)	36	76
5	J	378/596 (63%)	365 (97%)	13 (3%)	44	81
All	All	3197/4094 (78%)	3070 (96%)	127 (4%)	38	77

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	370	ASP
3	F	315	LYS
5	J	398	ASP
3	E	424	LYS
3	F	200	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
4	G	403	ASN
4	G	460	ASN
5	J	386	ASN
3	F	325	ASN
3	F	343	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

9 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	$\# Z  > 2$
6	PO4	A	401	-	4,4,4	0.69	0	6,6,6	0.23	0
6	PO4	B	401	-	4,4,4	0.70	0	6,6,6	0.23	0
6	PO4	C	401	-	4,4,4	0.66	0	6,6,6	0.23	0
6	PO4	D	401	-	4,4,4	0.68	0	6,6,6	0.23	0
6	PO4	G	501	-	4,4,4	0.68	0	6,6,6	0.23	0
6	PO4	G	502	-	4,4,4	0.68	0	6,6,6	0.23	0
6	PO4	H	501	-	4,4,4	0.67	0	6,6,6	0.23	0
6	PO4	H	502	-	4,4,4	0.69	0	6,6,6	0.23	0
6	PO4	I	701	-	4,4,4	0.66	0	6,6,6	0.23	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
6	PO4	A	401	-	-	0/0/0/0	0/0/0/0
6	PO4	B	401	-	-	0/0/0/0	0/0/0/0
6	PO4	C	401	-	-	0/0/0/0	0/0/0/0
6	PO4	D	401	-	-	0/0/0/0	0/0/0/0
6	PO4	G	501	-	-	0/0/0/0	0/0/0/0
6	PO4	G	502	-	-	0/0/0/0	0/0/0/0
6	PO4	H	501	-	-	0/0/0/0	0/0/0/0
6	PO4	H	502	-	-	0/0/0/0	0/0/0/0
6	PO4	I	701	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	401	PO4	1	0
6	G	501	PO4	1	0
6	I	701	PO4	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 ⓘ

### 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	317/341 (92%)	0.58	30 (9%) 10 4	55, 86, 150, 173	0
1	B	319/341 (93%)	0.47	17 (5%) 30 12	49, 80, 123, 180	0
2	C	349/399 (87%)	0.44	21 (6%) 25 9	42, 68, 138, 165	0
2	D	346/399 (86%)	0.17	9 (2%) 59 29	41, 66, 111, 161	0
3	E	384/458 (83%)	0.66	42 (10%) 7 3	61, 99, 142, 163	0
3	F	383/458 (83%)	0.78	56 (14%) 3 1	66, 108, 153, 168	0
4	G	349/467 (74%)	0.44	20 (5%) 27 10	44, 75, 136, 167	0
4	H	349/467 (74%)	0.17	11 (3%) 51 23	44, 65, 116, 153	0
5	I	428/678 (63%)	0.22	10 (2%) 64 33	42, 73, 115, 148	0
5	J	428/678 (63%)	0.38	25 (5%) 26 10	50, 87, 122, 153	0
All	All	3652/4686 (77%)	0.43	241 (6%) 22 7	41, 80, 137, 180	0

The worst 5 of 241 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	423	SER	7.6
2	C	8	HIS	7.5
3	E	450	MET	6.5
4	G	226	ASP	5.9
2	C	4	ILE	5.7

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

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	PO4	D	401	5/5	0.98	0.21	1.08	50,53,72,73	0
6	PO4	H	502	5/5	0.95	0.20	-0.27	71,82,90,98	0
6	PO4	H	501	5/5	0.89	0.17	-0.28	81,85,101,134	0
6	PO4	G	501	5/5	0.88	0.17	-0.34	91,94,118,136	0
6	PO4	B	401	5/5	0.98	0.19	-0.49	63,67,86,93	0
6	PO4	G	502	5/5	0.90	0.17	-0.58	62,67,102,104	0
6	PO4	C	401	5/5	0.99	0.18	-0.68	51,53,68,70	0
6	PO4	I	701	5/5	0.90	0.15	-0.97	101,102,127,141	0
6	PO4	A	401	5/5	0.98	0.15	-2.39	70,71,84,89	0

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

There are no such residues in this entry.