



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 02:51 AM GMT

PDB ID : 3A9C  
Title : Crystal structure of ribose-1,5-bisphosphate isomerase from *Thermococcus kodakaraensis* KOD1 in complex with ribulose-1,5-bisphosphate  
Authors : Nakamura, A.; Fujihashi, M.; Nishiba, Y.; Yoshida, S.; Yano, A.; Atomi, H.; Imanaka, T.; Miki, K.  
Deposited on : 2009-10-22  
Resolution : 2.60 Å (reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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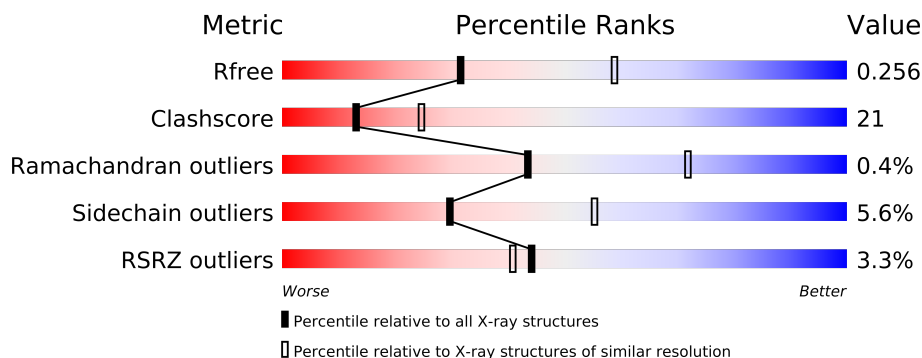
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.60 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))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	339	
1	B	339	
1	C	339	
1	D	339	
1	E	339	
1	F	339	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15788 atoms, of which 0 are hydrogen and 0 are deuterium.

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, delta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	1	0
			2549	1634	429	473	13			
1	B	325	Total	C	N	O	S	0	1	0
			2593	1660	440	479	14			
1	C	321	Total	C	N	O	S	0	1	0
			2554	1637	430	474	13			
1	D	322	Total	C	N	O	S	0	1	0
			2559	1640	431	475	13			
1	E	321	Total	C	N	O	S	0	1	0
			2554	1637	430	474	13			
1	F	322	Total	C	N	O	S	0	1	0
			2559	1640	431	475	13			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	EXPRESSION TAG	UNP Q5JFM9
A	-14	ASN	-	EXPRESSION TAG	UNP Q5JFM9
A	-13	HIS	-	EXPRESSION TAG	UNP Q5JFM9
A	-12	LYS	-	EXPRESSION TAG	UNP Q5JFM9
A	-11	VAL	-	EXPRESSION TAG	UNP Q5JFM9
A	-10	HIS	-	EXPRESSION TAG	UNP Q5JFM9
A	-9	HIS	-	EXPRESSION TAG	UNP Q5JFM9
A	-8	HIS	-	EXPRESSION TAG	UNP Q5JFM9
A	-7	HIS	-	EXPRESSION TAG	UNP Q5JFM9
A	-6	HIS	-	EXPRESSION TAG	UNP Q5JFM9
A	-5	HIS	-	EXPRESSION TAG	UNP Q5JFM9
A	-4	ILE	-	EXPRESSION TAG	UNP Q5JFM9
A	-3	GLU	-	EXPRESSION TAG	UNP Q5JFM9
A	-2	GLY	-	EXPRESSION TAG	UNP Q5JFM9
A	-1	ARG	-	EXPRESSION TAG	UNP Q5JFM9
A	0	HIS	-	EXPRESSION TAG	UNP Q5JFM9
A	133	CSD	CYS	MICROHETEROGENEITY	UNP Q5JFM9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	EXPRESSION TAG	UNP Q5JFM9
B	-14	ASN	-	EXPRESSION TAG	UNP Q5JFM9
B	-13	HIS	-	EXPRESSION TAG	UNP Q5JFM9
B	-12	LYS	-	EXPRESSION TAG	UNP Q5JFM9
B	-11	VAL	-	EXPRESSION TAG	UNP Q5JFM9
B	-10	HIS	-	EXPRESSION TAG	UNP Q5JFM9
B	-9	HIS	-	EXPRESSION TAG	UNP Q5JFM9
B	-8	HIS	-	EXPRESSION TAG	UNP Q5JFM9
B	-7	HIS	-	EXPRESSION TAG	UNP Q5JFM9
B	-6	HIS	-	EXPRESSION TAG	UNP Q5JFM9
B	-5	HIS	-	EXPRESSION TAG	UNP Q5JFM9
B	-4	ILE	-	EXPRESSION TAG	UNP Q5JFM9
B	-3	GLU	-	EXPRESSION TAG	UNP Q5JFM9
B	-2	GLY	-	EXPRESSION TAG	UNP Q5JFM9
B	-1	ARG	-	EXPRESSION TAG	UNP Q5JFM9
B	0	HIS	-	EXPRESSION TAG	UNP Q5JFM9
B	133	CSD	CYS	MICROHETEROGENEITY	UNP Q5JFM9
C	-15	MET	-	EXPRESSION TAG	UNP Q5JFM9
C	-14	ASN	-	EXPRESSION TAG	UNP Q5JFM9
C	-13	HIS	-	EXPRESSION TAG	UNP Q5JFM9
C	-12	LYS	-	EXPRESSION TAG	UNP Q5JFM9
C	-11	VAL	-	EXPRESSION TAG	UNP Q5JFM9
C	-10	HIS	-	EXPRESSION TAG	UNP Q5JFM9
C	-9	HIS	-	EXPRESSION TAG	UNP Q5JFM9
C	-8	HIS	-	EXPRESSION TAG	UNP Q5JFM9
C	-7	HIS	-	EXPRESSION TAG	UNP Q5JFM9
C	-6	HIS	-	EXPRESSION TAG	UNP Q5JFM9
C	-5	HIS	-	EXPRESSION TAG	UNP Q5JFM9
C	-4	ILE	-	EXPRESSION TAG	UNP Q5JFM9
C	-3	GLU	-	EXPRESSION TAG	UNP Q5JFM9
C	-2	GLY	-	EXPRESSION TAG	UNP Q5JFM9
C	-1	ARG	-	EXPRESSION TAG	UNP Q5JFM9
C	0	HIS	-	EXPRESSION TAG	UNP Q5JFM9
C	133	CSD	CYS	MICROHETEROGENEITY	UNP Q5JFM9
D	-15	MET	-	EXPRESSION TAG	UNP Q5JFM9
D	-14	ASN	-	EXPRESSION TAG	UNP Q5JFM9
D	-13	HIS	-	EXPRESSION TAG	UNP Q5JFM9
D	-12	LYS	-	EXPRESSION TAG	UNP Q5JFM9
D	-11	VAL	-	EXPRESSION TAG	UNP Q5JFM9
D	-10	HIS	-	EXPRESSION TAG	UNP Q5JFM9
D	-9	HIS	-	EXPRESSION TAG	UNP Q5JFM9
D	-8	HIS	-	EXPRESSION TAG	UNP Q5JFM9

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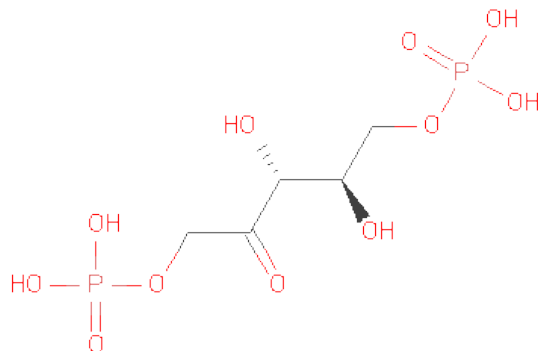
Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	HIS	-	EXPRESSION TAG	UNP Q5JFM9
D	-6	HIS	-	EXPRESSION TAG	UNP Q5JFM9
D	-5	HIS	-	EXPRESSION TAG	UNP Q5JFM9
D	-4	ILE	-	EXPRESSION TAG	UNP Q5JFM9
D	-3	GLU	-	EXPRESSION TAG	UNP Q5JFM9
D	-2	GLY	-	EXPRESSION TAG	UNP Q5JFM9
D	-1	ARG	-	EXPRESSION TAG	UNP Q5JFM9
D	0	HIS	-	EXPRESSION TAG	UNP Q5JFM9
D	133	CSD	CYS	MICROHETEROGENEITY	UNP Q5JFM9
E	-15	MET	-	EXPRESSION TAG	UNP Q5JFM9
E	-14	ASN	-	EXPRESSION TAG	UNP Q5JFM9
E	-13	HIS	-	EXPRESSION TAG	UNP Q5JFM9
E	-12	LYS	-	EXPRESSION TAG	UNP Q5JFM9
E	-11	VAL	-	EXPRESSION TAG	UNP Q5JFM9
E	-10	HIS	-	EXPRESSION TAG	UNP Q5JFM9
E	-9	HIS	-	EXPRESSION TAG	UNP Q5JFM9
E	-8	HIS	-	EXPRESSION TAG	UNP Q5JFM9
E	-7	HIS	-	EXPRESSION TAG	UNP Q5JFM9
E	-6	HIS	-	EXPRESSION TAG	UNP Q5JFM9
E	-5	HIS	-	EXPRESSION TAG	UNP Q5JFM9
E	-4	ILE	-	EXPRESSION TAG	UNP Q5JFM9
E	-3	GLU	-	EXPRESSION TAG	UNP Q5JFM9
E	-2	GLY	-	EXPRESSION TAG	UNP Q5JFM9
E	-1	ARG	-	EXPRESSION TAG	UNP Q5JFM9
E	0	HIS	-	EXPRESSION TAG	UNP Q5JFM9
E	133	CSD	CYS	MICROHETEROGENEITY	UNP Q5JFM9
F	-15	MET	-	EXPRESSION TAG	UNP Q5JFM9
F	-14	ASN	-	EXPRESSION TAG	UNP Q5JFM9
F	-13	HIS	-	EXPRESSION TAG	UNP Q5JFM9
F	-12	LYS	-	EXPRESSION TAG	UNP Q5JFM9
F	-11	VAL	-	EXPRESSION TAG	UNP Q5JFM9
F	-10	HIS	-	EXPRESSION TAG	UNP Q5JFM9
F	-9	HIS	-	EXPRESSION TAG	UNP Q5JFM9
F	-8	HIS	-	EXPRESSION TAG	UNP Q5JFM9
F	-7	HIS	-	EXPRESSION TAG	UNP Q5JFM9
F	-6	HIS	-	EXPRESSION TAG	UNP Q5JFM9
F	-5	HIS	-	EXPRESSION TAG	UNP Q5JFM9
F	-4	ILE	-	EXPRESSION TAG	UNP Q5JFM9
F	-3	GLU	-	EXPRESSION TAG	UNP Q5JFM9
F	-2	GLY	-	EXPRESSION TAG	UNP Q5JFM9
F	-1	ARG	-	EXPRESSION TAG	UNP Q5JFM9
F	0	HIS	-	EXPRESSION TAG	UNP Q5JFM9

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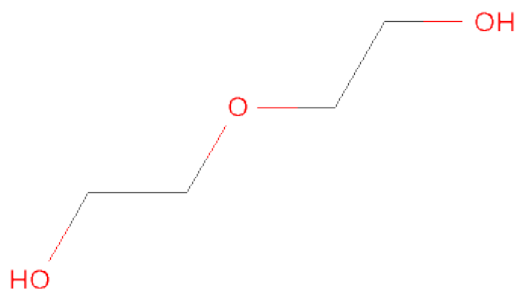
Chain	Residue	Modelled	Actual	Comment	Reference
F	133	CSD	CYS	MICROHETEROGENEITY	UNP Q5JFM9

- Molecule 2 is SUGAR (RIBULOSE-1,5-DIPHOSPHATE) (three-letter code: RUB) (formula:  $C_5H_{12}O_{11}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			18	5	11	2		
2	B	1	Total	C	O	P	0	0
			18	5	11	2		
2	C	1	Total	C	O	P	0	0
			18	5	11	2		
2	D	1	Total	C	O	P	0	0
			18	5	11	2		
2	E	1	Total	C	O	P	0	0
			18	5	11	2		
2	F	1	Total	C	O	P	0	0
			18	5	11	2		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	E	1	Total	C	O	0	0
			7	4	3		
3	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	60	Total	O	0	0
			60	60		

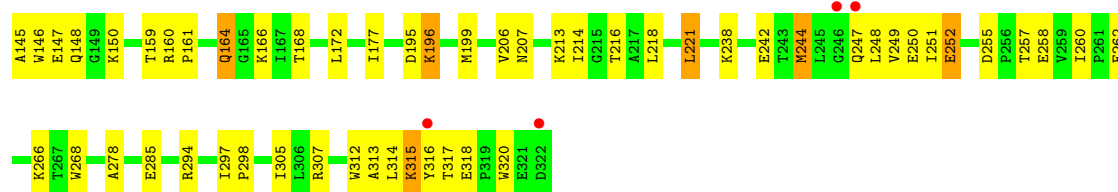
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	64	Total 64	O 64	0	0
5	C	23	Total 23	O 23	0	0
5	D	39	Total 39	O 39	0	0
5	E	48	Total 48	O 48	0	0
5	F	34	Total 34	O 34	0	0

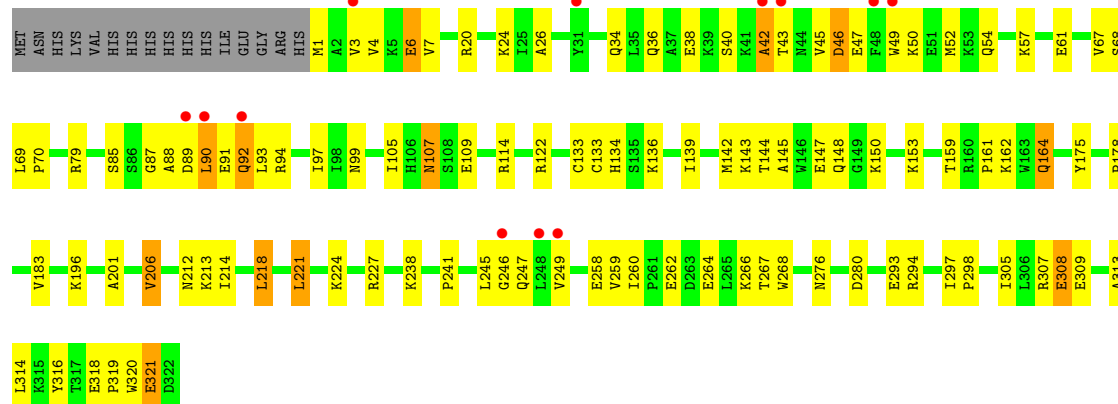






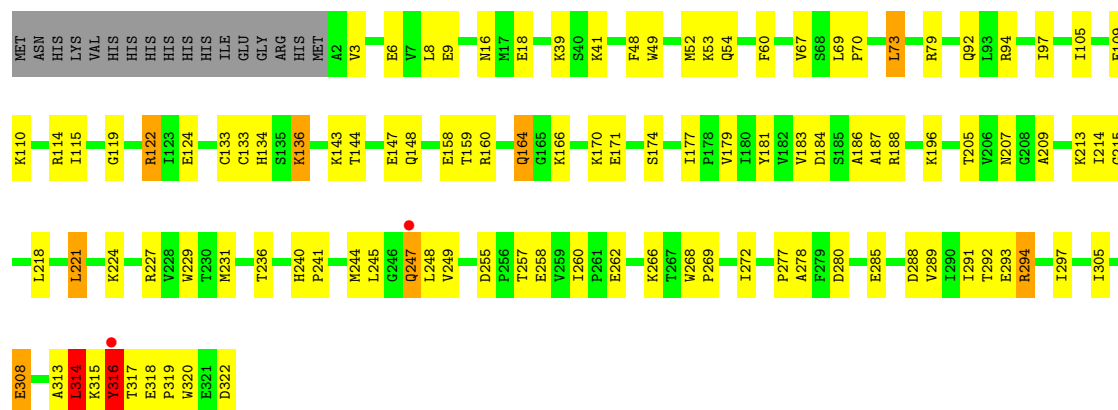
• Molecule 1: Translation initiation factor eIF-2B, delta subunit

Chain D:



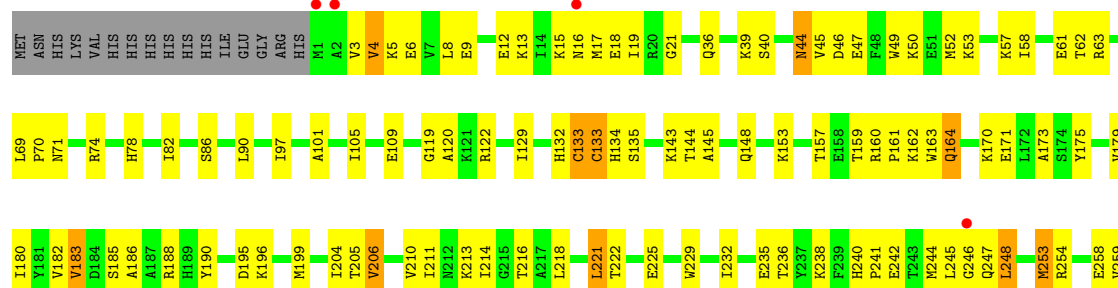
• Molecule 1: Translation initiation factor eIF-2B, delta subunit

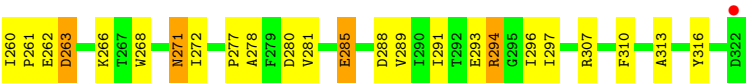
Chain E:



• Molecule 1: Translation initiation factor eIF-2B, delta subunit

Chain F:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.31Å 130.62Å 132.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.64 – 2.60 43.64 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.64-2.60) 99.8 (43.64-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.68 (at 2.61Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.201 , 0.255 0.202 , 0.256	Depositor DCC
$R_{free}$ test set	3202 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 32.7	EDS
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 63078 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15788	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RUB, CSD, MG, PEG

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	0.37	0/2594	0.61	0/3511
1	B	0.39	0/2639	0.63	1/3569 (0.0%)
1	C	0.33	0/2599	0.58	0/3518
1	D	0.36	0/2604	0.60	0/3525
1	E	0.34	0/2599	0.58	0/3518
1	F	0.34	0/2604	0.58	1/3525 (0.0%)
All	All	0.36	0/15639	0.60	2/21166 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	246	GLY	N-CA-C	5.40	126.59	113.10
1	B	221	LEU	CA-CB-CG	5.33	127.55	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2549	0	2585	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2593	0	2626	118	0
1	C	2554	0	2590	128	0
1	D	2559	0	2595	99	0
1	E	2554	0	2590	107	0
1	F	2559	0	2595	143	0
2	A	18	0	8	0	0
2	B	18	0	8	0	0
2	C	18	0	8	0	0
2	D	18	0	8	0	0
2	E	18	0	8	1	0
2	F	18	0	8	1	0
3	A	7	0	10	4	0
3	B	7	0	10	3	0
3	C	7	0	10	0	0
3	D	7	0	10	1	0
3	E	7	0	10	6	0
3	F	7	0	10	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	60	0	0	5	0
5	B	64	0	0	2	0
5	C	23	0	0	1	0
5	D	39	0	0	3	0
5	E	48	0	0	1	0
5	F	34	0	0	3	0
All	All	15788	0	15689	637	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

The worst 5 of 637 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:292:THR:HG22	1:E:294:ARG:H	1.14	1.09
1:D:164:GLN:HE21	1:D:164:GLN:H	1.07	1.01
1:C:164:GLN:HE21	1:C:164:GLN:H	1.01	1.00
1:C:218:LEU:HD22	1:D:218:LEU:HD22	1.40	0.97
1:A:52:MET:HE1	1:A:97:ILE:HG21	1.46	0.97

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	317/339 (94%)	302 (95%)	15 (5%)	0	100	100
1	B	320/339 (94%)	309 (97%)	10 (3%)	1 (0%)	50	77
1	C	318/339 (94%)	295 (93%)	22 (7%)	1 (0%)	50	77
1	D	319/339 (94%)	303 (95%)	15 (5%)	1 (0%)	50	77
1	E	318/339 (94%)	297 (93%)	18 (6%)	3 (1%)	25	49
1	F	319/339 (94%)	298 (93%)	19 (6%)	2 (1%)	33	63
All	All	1911/2034 (94%)	1804 (94%)	99 (5%)	8 (0%)	43	72

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	249	VAL
1	E	316	TYR
1	B	314	LEU
1	D	42	ALA
1	C	252	GLU

### 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	268/284 (94%)	256 (96%)	12 (4%)	38	67
1	B	272/284 (96%)	256 (94%)	16 (6%)	28	52
1	C	268/284 (94%)	249 (93%)	19 (7%)	21	40
1	D	268/284 (94%)	253 (94%)	15 (6%)	30	55
1	E	268/284 (94%)	255 (95%)	13 (5%)	35	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	268/284 (94%)	253 (94%)	15 (6%)	30	55
All	All	1612/1704 (95%)	1522 (94%)	90 (6%)	30	55

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	242	GLU
1	D	92	GLN
1	F	248	LEU
1	C	244	MET
1	C	315	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	164	GLN
1	D	164	GLN
1	F	207	ASN
1	C	207	ASN
1	D	107	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	CSD	A	133[A]	1	7,7,8	6.72	2 (28%)	6,8,10	1.87	2 (33%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CSD	B	133[A]	1	7,7,8	6.79	2 (28%)	6,8,10	1.86	2 (33%)
1	CSD	C	133[A]	1	7,7,8	6.78	2 (28%)	6,8,10	1.98	2 (33%)
1	CSD	D	133[A]	1	7,7,8	6.76	2 (28%)	6,8,10	1.73	2 (33%)
1	CSD	E	133[A]	1	7,7,8	6.89	2 (28%)	6,8,10	1.97	2 (33%)
1	CSD	F	133[A]	1	7,7,8	6.69	2 (28%)	6,8,10	2.03	2 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	A	133[A]	1	-	0/3/6/8	0/0/0/0
1	CSD	B	133[A]	1	-	0/3/6/8	0/0/0/0
1	CSD	C	133[A]	1	-	0/3/6/8	0/0/0/0
1	CSD	D	133[A]	1	-	0/3/6/8	0/0/0/0
1	CSD	E	133[A]	1	-	0/3/6/8	0/0/0/0
1	CSD	F	133[A]	1	-	0/3/6/8	0/0/0/0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	133[A]	CSD	O-C	17.86	1.23	1.11
1	C	133[A]	CSD	O-C	17.58	1.23	1.11
1	B	133[A]	CSD	O-C	17.57	1.23	1.11
1	D	133[A]	CSD	O-C	17.47	1.23	1.11
1	A	133[A]	CSD	O-C	17.36	1.23	1.11

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	133[A]	CSD	CA-CB-SG	3.20	115.39	110.82
1	B	133[A]	CSD	OD2-SG-CB	3.19	110.27	97.42
1	E	133[A]	CSD	OD2-SG-CB	3.19	110.26	97.42
1	F	133[A]	CSD	OD2-SG-CB	3.18	110.22	97.42
1	A	133[A]	CSD	OD2-SG-CB	3.17	110.19	97.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	$\# Z  > 2$
2	RUB	A	401	-	17,17,17	1.09	0	25,25,25	0.84	1 (4%)
3	PEG	A	402	-	6,6,6	0.53	0	5,5,5	0.41	0
2	RUB	B	401	-	17,17,17	1.10	0	25,25,25	0.79	1 (4%)
3	PEG	B	402	-	6,6,6	0.53	0	5,5,5	0.33	0
2	RUB	C	401	-	17,17,17	1.09	0	25,25,25	0.85	1 (4%)
3	PEG	C	402	-	6,6,6	0.51	0	5,5,5	0.47	0
2	RUB	D	401	-	17,17,17	1.09	0	25,25,25	0.82	1 (4%)
3	PEG	D	402	-	6,6,6	0.52	0	5,5,5	0.44	0
2	RUB	E	401	-	17,17,17	1.07	0	25,25,25	0.83	1 (4%)
3	PEG	E	402	-	6,6,6	0.53	0	5,5,5	0.32	0
2	RUB	F	401	-	17,17,17	1.08	0	25,25,25	0.86	0
3	PEG	F	402	-	6,6,6	0.53	0	5,5,5	0.44	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
2	RUB	A	401	-	-	0/20/20/20	0/0/0/0
3	PEG	A	402	-	-	0/4/4/4	0/0/0/0
2	RUB	B	401	-	-	0/20/20/20	0/0/0/0
3	PEG	B	402	-	-	0/4/4/4	0/0/0/0
2	RUB	C	401	-	-	0/20/20/20	0/0/0/0
3	PEG	C	402	-	-	0/4/4/4	0/0/0/0
2	RUB	D	401	-	-	0/20/20/20	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	D	402	-	-	0/4/4/4	0/0/0/0
2	RUB	E	401	-	-	0/20/20/20	0/0/0/0
3	PEG	E	402	-	-	0/4/4/4	0/0/0/0
2	RUB	F	401	-	-	0/20/20/20	0/0/0/0
3	PEG	F	402	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	RUB	O5-P2-O4P	2.37	113.65	106.71
2	D	401	RUB	O5-P2-O4P	2.20	113.17	106.71
2	A	401	RUB	O5-P2-O4P	2.19	113.12	106.71
2	E	401	RUB	O5-P2-O4P	2.17	113.07	106.71
2	B	401	RUB	O5-P2-O4P	2.08	112.81	106.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	321/339 (94%)	-0.15	7 (2%) 59 56	12, 35, 75, 88	2 (0%)
1	B	326/339 (96%)	-0.31	7 (2%) 60 58	11, 28, 55, 90	2 (0%)
1	C	322/339 (94%)	0.31	29 (9%) 10 7	23, 49, 104, 112	2 (0%)
1	D	323/339 (95%)	-0.13	12 (3%) 39 35	17, 36, 76, 84	2 (0%)
1	E	322/339 (94%)	-0.23	2 (0%) 86 89	25, 40, 64, 87	2 (0%)
1	F	323/339 (95%)	-0.05	5 (1%) 70 71	23, 44, 69, 87	2 (0%)
All	All	1937/2034 (95%)	-0.09	62 (3%) 44 42	11, 39, 81, 112	12 (0%)

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	VAL	5.9
1	C	93	LEU	5.5
1	C	33	LEU	4.5
1	B	-4	ILE	4.3
1	C	48	PHE	4.2

### 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. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSD	E	133[A]	8/9	0.13	-	28,32,34,34	8
1	CSD	C	133[A]	8/9	0.14	-	30,30,32,33	8

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CSD	B	133[A]	8/9	0.11	-	12,17,18,19	8
1	CSD	F	133[A]	8/9	0.11	-	26,30,33,33	8
1	CSD	D	133[A]	8/9	0.12	-	21,25,25,25	8
1	CSD	A	133[A]	8/9	0.13	-	14,17,18,18	8

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PEG	A	402	7/7	0.35	-	43,45,47,47	0
4	MG	A	411	1/1	0.42	-	49,49,49,49	0
3	PEG	D	402	7/7	0.32	-	46,47,49,49	0
3	PEG	E	402	7/7	0.42	-	87,88,88,89	0
3	PEG	B	402	7/7	0.22	-	45,47,48,49	0
2	RUB	E	401	18/18	0.16	-	33,43,56,56	18
2	RUB	B	401	18/18	0.15	-	26,32,43,43	18
2	RUB	C	401	18/18	0.14	-	37,42,48,49	18
2	RUB	A	401	18/18	0.17	-	23,30,33,34	18
2	RUB	F	401	18/18	0.18	-	31,38,41,42	18
2	RUB	D	401	18/18	0.18	-	27,34,45,46	18
3	PEG	F	402	7/7	0.22	-	57,58,58,59	0
3	PEG	C	402	7/7	0.30	-	49,49,53,53	0
4	MG	B	411	1/1	0.45	-	47,47,47,47	0

### 6.5 Other polymers

There are no such residues in this entry.