



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 24, 2021 – 01:09 pm GMT

PDB ID : 7AZF  
Title : DNA polymerase sliding clamp from Escherichia coli with peptide 8 bound  
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Deposited on : 2020-11-16  
Resolution : 1.93 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4 (270009), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

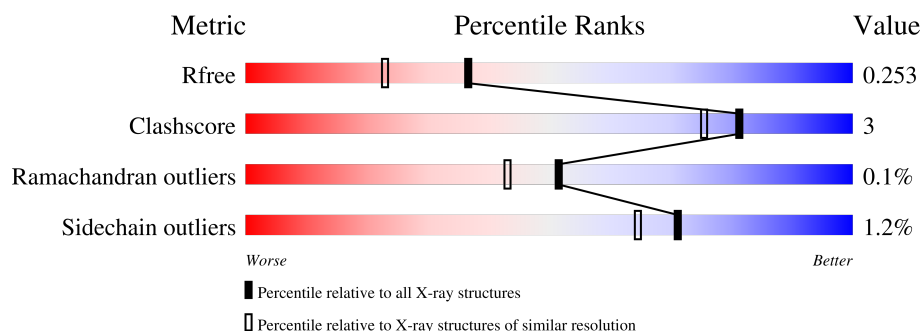
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.93 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	369	92% 7% .
1	B	369	95% 5%
1	C	369	91% 9%
1	D	369	93% 6%
2	H	4	100%
2	I	4	100%
2	J	4	100%

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Mol	Chain	Length	Quality of chain
2	K	4	 75% 25%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12840 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 Beta sliding clamp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	8	0
			2905	1825	509	550	21			
1	B	369	Total	C	N	O	S	0	7	0
			2900	1821	515	545	19			
1	C	368	Total	C	N	O	S	0	3	0
			2879	1807	506	547	19			
1	D	368	Total	C	N	O	S	0	1	0
			2828	1776	496	537	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A073FMV0
A	-1	SER	-	expression tag	UNP A0A073FMV0
A	0	HIS	-	expression tag	UNP A0A073FMV0
B	-2	GLY	-	expression tag	UNP A0A073FMV0
B	-1	SER	-	expression tag	UNP A0A073FMV0
B	0	HIS	-	expression tag	UNP A0A073FMV0
C	-2	GLY	-	expression tag	UNP A0A073FMV0
C	-1	SER	-	expression tag	UNP A0A073FMV0
C	0	HIS	-	expression tag	UNP A0A073FMV0
D	-2	GLY	-	expression tag	UNP A0A073FMV0
D	-1	SER	-	expression tag	UNP A0A073FMV0
D	0	HIS	-	expression tag	UNP A0A073FMV0

- Molecule 2 is a protein called Peptide 8.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	4	Total	C	N	O	0	0	0
			39	28	4	7			
2	I	4	Total	C	N	O	0	0	0
			39	28	4	7			

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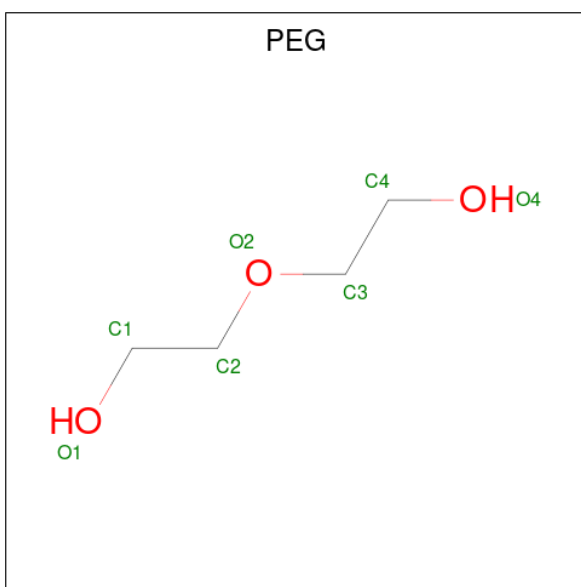
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	4	Total	C	N	O	0	0	0
			39	28	4	7			
2	K	4	Total	C	N	O	0	0	0
			39	28	4	7			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



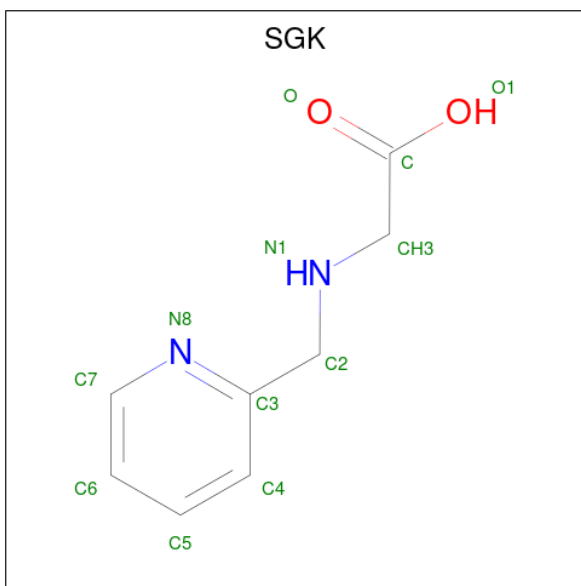
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is 2-(pyridin-2-ylmethylamino)ethanoic acid (three-letter code: SGK) (formula:  $C_8H_{10}N_2O_2$ ).



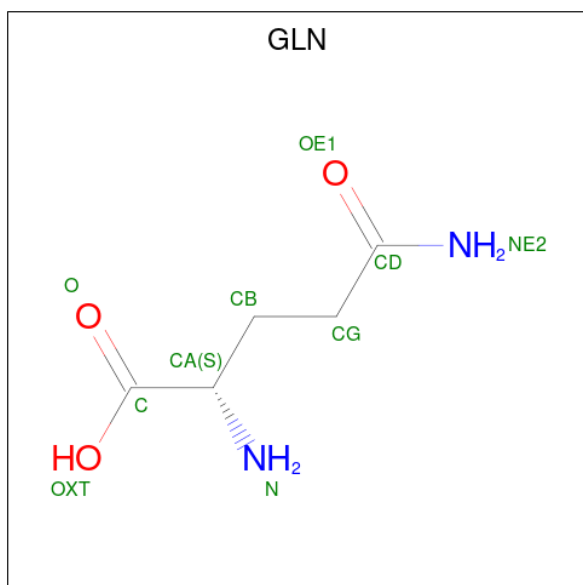
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			11	8	2	1		
5	B	1	Total	C	N	O	0	1
			22	16	4	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			3	2	1		
5	D	1	Total	C	O	0	0
			3	2	1		

- Molecule 6 is GLUTAMINE (three-letter code: GLN) (formula: C<sub>5</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	1	Total	C	N	O	0	0
			9	5	2	2		
6	I	1	Total	C	N	O	0	0
			9	5	2	2		
6	J	1	Total	C	N	O	0	0
			9	5	2	2		
6	K	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	312	Total	O	0	7
			315	315		
7	B	321	Total	O	0	10
			329	329		
7	C	193	Total	O	0	10
			203	203		

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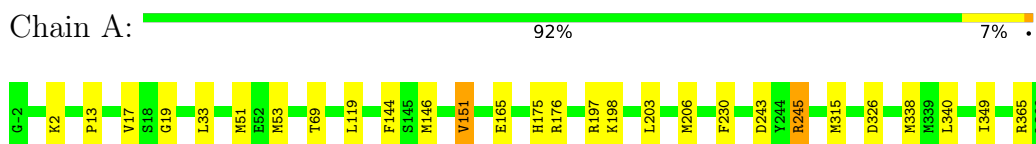
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	201	Total 203	O 203	0	3
7	H	7	Total 7	O 7	0	0
7	I	9	Total 9	O 9	0	0
7	J	9	Total 9	O 9	0	0
7	K	9	Total 9	O 9	0	0



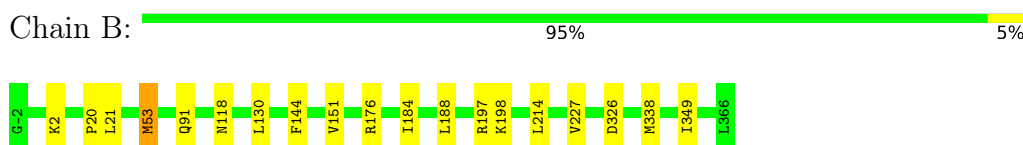
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

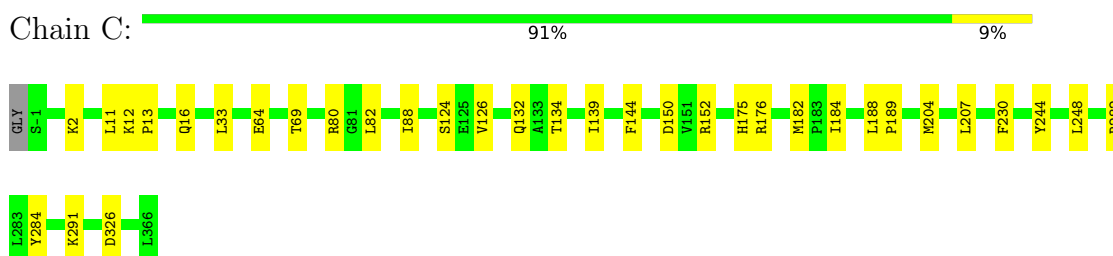
- Molecule 1: Beta sliding clamp



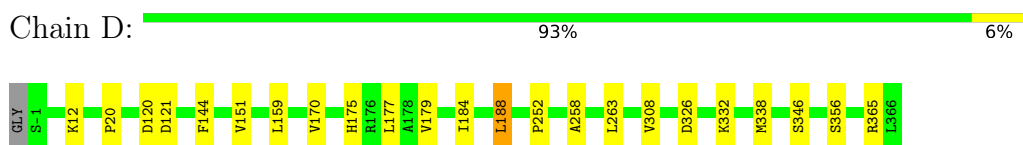
- Molecule 1: Beta sliding clamp



- Molecule 1: Beta sliding clamp



- Molecule 1: Beta sliding clamp



- Molecule 2: Peptide 8



There are no outlier residues recorded for this chain.

- Molecule 2: Peptide 8

Chain I:  100%


There are no outlier residues recorded for this chain.

- Molecule 2: Peptide 8

Chain J:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Peptide 8

Chain K:  75% 25%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.42Å 82.03Å 82.39Å 116.87° 100.26° 95.47°	Depositor
Resolution (Å)	37.75 – 1.93 71.69 – 1.92	Depositor EDS
% Data completeness (in resolution range)	70.8 (37.75-1.93) 70.7 (71.69-1.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 1.92Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.204 , 0.251 0.206 , 0.253	Depositor DCC
$R_{free}$ test set	4137 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.4	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12840	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: GOL, PEG, ALC, SGK

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	0.54	0/2973	0.58	0/4020
1	B	0.53	0/2969	0.56	0/4017
1	C	0.44	0/2938	0.55	0/3975
1	D	0.46	0/2880	0.56	0/3902
2	H	0.58	0/28	0.54	0/35
2	I	0.53	0/28	0.47	0/35
2	J	0.51	0/28	0.57	0/35
2	K	0.45	0/28	0.55	0/35
All	All	0.49	0/11872	0.56	0/16054

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2905	0	2929	20	0
1	B	2900	0	2918	13	0
1	C	2879	0	2898	20	0
1	D	2828	0	2824	13	0
2	H	39	0	38	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	39	0	38	0	0
2	J	39	0	38	0	0
2	K	39	0	38	1	0
3	A	6	0	8	0	0
4	A	7	0	10	0	0
5	A	11	0	0	1	0
5	B	22	0	0	0	0
5	C	3	0	0	0	0
5	D	3	0	0	0	0
6	H	9	0	7	0	0
6	I	9	0	7	0	0
6	J	9	0	7	0	0
6	K	9	0	7	0	0
7	A	315	0	0	3	0
7	B	329	0	0	1	0
7	C	203	0	0	0	0
7	D	203	0	0	2	0
7	H	7	0	0	0	0
7	I	9	0	0	0	0
7	J	9	0	0	0	0
7	K	9	0	0	0	0
All	All	12840	0	11767	62	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 3.

All (62) 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:214:LEU:HD12	1:B:227:VAL:CG2	2.11	0.79
1:B:184:ILE:HD11	1:B:188:LEU:HD11	1.67	0.76
1:B:184:ILE:HD11	1:B:188:LEU:CD1	2.16	0.75
1:B:214:LEU:HD12	1:B:227:VAL:HG22	1.73	0.71
1:D:177:LEU:HD21	1:D:179:VAL:HG23	1.81	0.62
1:A:151:VAL:HG13	1:D:175:HIS:CE1	2.38	0.58
1:C:184:ILE:HD11	1:C:188:LEU:HD11	1.84	0.58
1:C:16:GLN:HG3	1:C:230:PHE:CZ	2.39	0.58
1:A:144:PHE:CD2	1:A:326:ASP:HB3	2.39	0.58
1:A:17:VAL:HG12	1:A:33:LEU:HD22	1.87	0.56
1:D:159:LEU:HB3	1:D:170:VAL:CG1	2.35	0.56
1:D:258:ALA:HB2	1:D:308:VAL:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:GLN:HB2	1:C:207:LEU:HD22	1.87	0.56
1:C:150:ASP:OD1	1:C:152:ARG:HD3	2.05	0.55
1:B:2:LYS:NZ	1:B:91:GLN:OE1	2.39	0.54
1:A:151:VAL:HG13	1:D:175:HIS:NE2	2.21	0.53
1:C:134:THR:HG23	1:C:182:MET:HG2	1.90	0.52
1:C:139:ILE:HG21	1:C:204:MET:HG2	1.91	0.52
1:C:82:LEU:HD13	1:C:88:ILE:CD1	2.41	0.51
1:A:365:ARG:HD2	5:A:403:SGK:C7	2.41	0.51
1:D:159:LEU:HB3	1:D:170:VAL:HG13	1.92	0.50
1:B:144:PHE:CD2	1:B:326:ASP:HB3	2.47	0.49
1:B:184:ILE:CD1	1:B:188:LEU:HD11	2.41	0.48
1:C:144:PHE:CD2	1:C:326:ASP:HB3	2.48	0.48
1:A:2:LYS:NZ	7:A:502:HOH:O	2.47	0.48
1:A:19:GLY:HA2	7:A:515:HOH:O	2.13	0.47
1:A:146:MET:HE1	1:A:197:ARG:HA	1.97	0.47
1:A:13:PRO:HA	1:A:230:PHE:HE1	1.80	0.46
1:D:356:SER:HB3	7:D:599:HOH:O	2.14	0.46
1:B:338:MET:HG2	1:B:349:ILE:HG12	1.97	0.46
1:C:139:ILE:HG21	1:C:204:MET:CG	2.45	0.46
1:A:338:MET:HG2	1:A:349:ILE:HG12	1.98	0.46
1:A:175:HIS:CE1	1:D:151:VAL:HB	2.52	0.45
1:C:284:TYR:HB2	1:C:291:LYS:HB3	1.98	0.45
1:B:151:VAL:HB	1:C:175:HIS:CE1	2.51	0.45
1:C:126:VAL:HG22	1:C:189:PRO:HG2	1.99	0.45
1:D:144:PHE:CD2	1:D:326:ASP:HB3	2.52	0.45
1:D:365:ARG:HE	2:K:3:ALC:HZ3	1.82	0.45
1:C:11:LEU:HD11	1:C:80:ARG:HA	1.98	0.44
1:A:33:LEU:O	1:A:69:THR:HA	2.17	0.44
1:D:184:ILE:HD11	1:D:188:LEU:HD11	2.00	0.44
1:A:243:ASP:OD1	1:A:245:ARG:HG2	2.18	0.44
1:B:21:LEU:HD21	7:B:526:HOH:O	2.16	0.43
1:A:53:MET:HE1	1:A:230:PHE:HB3	2.00	0.43
1:C:33:LEU:O	1:C:69:THR:HA	2.18	0.43
1:C:282:ARG:HD2	1:C:284:TYR:OH	2.19	0.42
1:B:130:LEU:HD21	1:B:214:LEU:HD23	2.01	0.42
1:D:263:LEU:HD21	1:D:338:MET:CE	2.50	0.42
1:C:12:LYS:HB3	1:C:13:PRO:HD3	2.01	0.42
1:C:132:GLN:CB	1:C:207:LEU:HD22	2.50	0.42
1:A:17:VAL:CG1	1:A:33:LEU:HD22	2.50	0.42
1:A:165:GLU:HG3	7:A:748:HOH:O	2.20	0.41
1:A:51:MET:HE3	1:A:198:LYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:LYS:HG2	1:C:64:GLU:HG2	2.03	0.41
1:B:197[A]:ARG:HH22	1:B:198:LYS:HE3	1.84	0.41
1:C:13:PRO:HA	1:C:230:PHE:HE1	1.86	0.41
1:D:20:PRO:HG2	7:D:672:HOH:O	2.20	0.41
1:A:53:MET:CE	1:A:230:PHE:HB3	2.51	0.41
1:A:203:LEU:O	1:A:206[B]:MET:HG2	2.20	0.40
1:C:244:TYR:O	1:C:248:LEU:HG	2.22	0.40
1:B:20:PRO:HG2	1:B:53:MET:SD	2.62	0.40
1:A:315:MET:HE3	1:A:340:LEU:HD22	2.04	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	375/369 (102%)	364 (97%)	11 (3%)	0	100	100
1	B	374/369 (101%)	366 (98%)	8 (2%)	0	100	100
1	C	369/369 (100%)	361 (98%)	8 (2%)	0	100	100
1	D	367/369 (100%)	357 (97%)	9 (2%)	1 (0%)	41	32
2	H	2/4 (50%)	2 (100%)	0	0	100	100
2	I	2/4 (50%)	2 (100%)	0	0	100	100
2	J	2/4 (50%)	2 (100%)	0	0	100	100
2	K	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1493/1492 (100%)	1456 (98%)	36 (2%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	252	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	321/315 (102%)	317 (99%)	4 (1%)	71	64
1	B	318/315 (101%)	315 (99%)	3 (1%)	78	75
1	C	318/315 (101%)	316 (99%)	2 (1%)	86	85
1	D	308/315 (98%)	302 (98%)	6 (2%)	57	45
2	H	3/3 (100%)	3 (100%)	0	100	100
2	I	3/3 (100%)	3 (100%)	0	100	100
2	J	3/3 (100%)	3 (100%)	0	100	100
2	K	3/3 (100%)	3 (100%)	0	100	100
All	All	1277/1272 (100%)	1262 (99%)	15 (1%)	71	64

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	151	VAL
1	A	176	ARG
1	A	245	ARG
1	B	53	MET
1	B	118	ASN
1	B	176	ARG
1	C	124	SER
1	C	176	ARG
1	D	12	LYS
1	D	120	ASP
1	D	121	ASP
1	D	188	LEU
1	D	332	LYS
1	D	346	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	118	ASN
1	B	118	ASN
1	C	191	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

11 ligands are modelled in this entry.

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.

No monomer is involved in short contacts.

## 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 [i](#)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.