

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	7AZD
Title	:	DNA polymerase sliding clamp from Escherichia coli with peptide 20 bound
Authors	:	Monsarrat, C.; Compain, G.; Andre, C.; Martiel, I.; Engilberge, S.; Olieric, V.;
		Wolff, P.; Brillet, K.; Landolfo, M.; Silva da Veiga, C.; Wagner, J.; Guichard,
		G.; Burnouf, D.Y.
Deposited on	:	2020-11-16
Resolution	:	2.19 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.19 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))		
	130704	<u>(7)</u> <u>1808</u> (2 20 2 20)		
Infree	130704	4090 (2.20-2.20)		
Clashscore	141614	$5594 \ (2.20-2.20)$		
Ramachandran outliers	138981	5503 (2.20-2.20)		
Sidechain outliers	138945	5504 (2.20-2.20)		
RSRZ outliers	127900	4800 (2.20-2.20)		

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 >=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 <=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	А	386	% • 79%	15%	• 5%
1	В	386	4%	17%	• 5%
1	С	386	83%	12%	• 5%
1	D	386	5% 80%	14%	• 6%
2	Н	6	67%	33%	



Mol	Chain	Length	Quality of chain					
2	Ι	6	67%	33%				
2	J	6	67%	33%				
2	K	6	83%	17%				

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
4	PEG	В	501	-	-	Х	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12348 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	267	Total	С	Ν	Ο	\mathbf{S}	0	4	0
1	A	307	2872	1805	508	540	19	0		
1	В	365	Total	С	Ν	0	S	0	2	0
1	I D		2857	1796	503	539	19			U
1	C	368	Total	С	Ν	0	S	0	1	0
			2841	1784	496	542	19	0		
1 D	363	Total	С	Ν	Ο	S	0	1	0	
	303	2813	1770	490	534	19			0	

• Molecule 1 is a protein called Beta sliding clamp.

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-19	MET	-	initiating methionine	UNP A0A073FMV0
А	-18	GLY	-	expression tag	UNP A0A073FMV0
А	-17	SER	-	expression tag	UNP A0A073FMV0
А	-16	SER	-	expression tag	UNP A0A073FMV0
А	-15	HIS	-	expression tag	UNP A0A073FMV0
А	-14	HIS	-	expression tag	UNP A0A073FMV0
А	-13	HIS	-	expression tag	UNP A0A073FMV0
А	-12	HIS	-	expression tag	UNP A0A073FMV0
А	-11	HIS	-	expression tag	UNP A0A073FMV0
А	-10	HIS	-	expression tag	UNP A0A073FMV0
А	-9	SER	-	expression tag	UNP A0A073FMV0
А	-8	SER	-	expression tag	UNP A0A073FMV0
А	-7	GLY	-	expression tag	UNP A0A073FMV0
А	-6	LEU	-	expression tag	UNP A0A073FMV0
А	-5	VAL	-	expression tag	UNP A0A073FMV0
А	-4	PRO	-	expression tag	UNP A0A073FMV0
А	-3	ARG	-	expression tag	UNP A0A073FMV0
A	-2	GLY	-	expression tag	UNP A0A073FMV0
A	-1	SER	-	expression tag	UNP A0A073FMV0
А	0	HIS	-	expression tag	UNP A0A073FMV0
В	-19	MET	-	initiating methionine	UNP A0A073FMV0



Chain	Residue	Modelled	Actual	Comment	Reference
В	-18	GLY	_	expression tag	UNP A0A073FMV0
В	-17	SER	_	expression tag	UNP A0A073FMV0
В	-16	SER	_	expression tag	UNP A0A073FMV0
В	-15	HIS	_	expression tag	UNP A0A073FMV0
В	-14	HIS	-	expression tag	UNP A0A073FMV0
В	-13	HIS	_	expression tag	UNP A0A073FMV0
В	-12	HIS	-	expression tag	UNP A0A073FMV0
В	-11	HIS	-	expression tag	UNP A0A073FMV0
В	-10	HIS	-	expression tag	UNP A0A073FMV0
В	-9	SER	_	expression tag	UNP A0A073FMV0
В	-8	SER	-	expression tag	UNP A0A073FMV0
В	-7	GLY	-	expression tag	UNP A0A073FMV0
В	-6	LEU	-	expression tag	UNP A0A073FMV0
В	-5	VAL	_	expression tag	UNP A0A073FMV0
В	-4	PRO	-	expression tag	UNP A0A073FMV0
В	-3	ARG	-	expression tag	UNP A0A073FMV0
В	-2	GLY	-	expression tag	UNP A0A073FMV0
В	-1	SER	-	expression tag	UNP A0A073FMV0
В	0	HIS	-	expression tag	UNP A0A073FMV0
С	-19	MET	-	initiating methionine	UNP A0A073FMV0
С	-18	GLY	-	expression tag	UNP A0A073FMV0
С	-17	SER	-	expression tag	UNP A0A073FMV0
С	-16	SER	-	expression tag	UNP A0A073FMV0
С	-15	HIS	-	expression tag	UNP A0A073FMV0
С	-14	HIS	-	expression tag	UNP A0A073FMV0
С	-13	HIS	-	expression tag	UNP A0A073FMV0
С	-12	HIS	-	expression tag	UNP A0A073FMV0
С	-11	HIS	-	expression tag	UNP A0A073FMV0
C	-10	HIS	-	expression tag	UNP A0A073FMV0
C	-9	SER	-	expression tag	UNP A0A073FMV0
С	-8	SER	-	expression tag	UNP A0A073FMV0
С	-7	GLY	-	expression tag	UNP A0A073FMV0
С	-6	LEU	-	expression tag	UNP A0A073FMV0
С	-5	VAL	-	expression tag	UNP A0A073FMV0
С	-4	PRO	-	expression tag	UNP A0A073FMV0
С	-3	ARG	-	expression tag	UNP A0A073FMV0
С	-2	GLY	-	expression tag	UNP A0A073FMV0
C	-1	SER	-	expression tag	UNP A0A073FMV0
C	0	HIS	-	expression tag	UNP A0A073FMV0
D	-19	MET	-	initiating methionine	UNP A0A073FMV0
D	-18	GLY	-	expression tag	UNP A0A073FMV0
D	-17	SER	_	expression tag	UNP A0A073FMV0



Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A0A073FMV0
D	-15	HIS	-	expression tag	UNP A0A073FMV0
D	-14	HIS	-	expression tag	UNP A0A073FMV0
D	-13	HIS	-	expression tag	UNP A0A073FMV0
D	-12	HIS	-	expression tag	UNP A0A073FMV0
D	-11	HIS	-	expression tag	UNP A0A073FMV0
D	-10	HIS	-	expression tag	UNP A0A073FMV0
D	-9	SER	-	expression tag	UNP A0A073FMV0
D	-8	SER	-	expression tag	UNP A0A073FMV0
D	-7	GLY	-	expression tag	UNP A0A073FMV0
D	-6	LEU	-	expression tag	UNP A0A073FMV0
D	-5	VAL	-	expression tag	UNP A0A073FMV0
D	-4	PRO	-	expression tag	UNP A0A073FMV0
D	-3	ARG	-	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 20.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	Н	6	Total C N O	0	0	0
	11	0	61 45 6 10	0	0	U
9	T	6	Total C N O	0	0	0
		0	61 45 6 10	0	0	0
0	т	6	Total C N O	0	0	0
	J	1 0	61 45 6 10	0	0	U
0	V	6	Total C N O	0	0	0
	ſΛ	n 0	61 45 6 10	0	0	0

• Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total C O 10 6 4	0	0
3	В	1	Total C O 13 8 5	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	223	Total O 223 223	0	0
5	В	185	Total O 186 186	0	1
5	С	120	Total O 121 121	0	1
5	D	131	Total O 131 131	0	1
5	Н	6	Total O 6 6	0	0
5	Ι	2	Total O 2 2	0	0
5	J	3	Total O 3 3	0	0
5	К	5	Total O 5 5	0	0



3 Residue-property plots (i)

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 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: Beta sliding clamp

M315 D326 M339 L340 L340 R365 L366

 \bullet Molecule 1: Beta sliding clamp

Chain D:	80%	14% • 6%
MET SER SER SER SER HIS HIS HIS HIS SER RIS SER VIL VAL VAL CLY CLY CLY	F3 14 14 15 18 13 13 13 13 13 13 13 13 13 13 13 13 13	L35 169 770 771 771 773 773 773 773 773 773 772 7120 7120 7120 7120 7120 7120
L1 30 P1 31 P1 31 P1 32 P1 32 P1 32 P1 32 P1 55 P1 85 P1 85	P189 1194 1194 1194 1201 1201 1203 6202 1203 61.Y 61.Y 61.Y 61.Y 61.Y 61.Y 61.Y 61.Y	V215 V216 M221 N223 N223 F230 F231 F231 F233 K254 H255 H255 H256 H256 H256 H256 H258 R282
L283 2286 2286 2295 8295 8295 8295 8295 8295 8295 8295	V 336 M337 M338 M338 M338 M338 M338 L340 L340	
• Molecule 2: Peptide 20		
Chain H:	67%	33%
502403 0404 1405 1405 1408		
• Molecule 2: Peptide 20		
Chain I:	67%	33%
SC2401 Q402 F406		
• Molecule 2: Peptide 20		
Chain J:	67%	33%
SGZ402 0403 1404 1407 1407		
• Molecule 2: Peptide 20		
Chain K:	83%	17%
802402 		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	69.68Å 81.76Å 141.93Å	Depositor
a, b, c, α , β , γ	90.00° 97.49° 90.00°	Depositor
Bosolution (Å)	41.39 - 2.19	Depositor
Resolution (A)	70.69 - 2.19	EDS
% Data completeness	71.7 (41.39-2.19)	Depositor
(in resolution range)	71.7(70.69-2.19)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.78 (at 2.20 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
B B.	0.189 , 0.242	Depositor
n, n_{free}	0.195 , 0.256	DCC
R_{free} test set	2847 reflections $(4.88%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	40.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 69.3	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12348	wwPDB-VP
Average B, all atoms $(Å^2)$	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: SGZ, PEG, 1PE, ALC

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).

Mal	Chain	Bond lengths		Bond angles	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.59	0/2935	0.68	0/3972
1	В	0.54	0/2908	0.65	0/3935
1	С	0.51	0/2893	0.64	0/3918
1	D	0.48	0/2862	0.63	0/3875
2	Н	0.70	0/36	0.74	0/44
2	Ι	0.60	0/36	0.62	0/44
2	J	0.66	0/36	0.70	0/44
2	Κ	0.63	0/36	0.71	0/44
All	All	0.53	0/11742	0.65	0/15876

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	А	2872	0	2890	47	0
1	В	2857	0	2864	42	0
1	С	2841	0	2837	37	0
1	D	2813	0	2806	37	0
2	Н	61	0	45	3	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Ι	61	0	45	3	0
2	J	61	0	45	5	0
2	K	61	0	45	1	0
3	А	10	0	13	3	0
3	В	13	0	17	1	0
4	А	7	0	10	1	0
4	В	7	0	10	4	0
4	С	7	0	10	2	0
5	А	223	0	0	3	0
5	В	186	0	0	5	0
5	С	121	0	0	1	0
5	D	131	0	0	1	0
5	Н	6	0	0	0	0
5	Ι	2	0	0	0	0
5	J	3	0	0	1	0
5	Κ	5	0	0	0	0
All	All	12348	0	11637	154	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 7.

All (154) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:139:ILE:HG21	1:C:204:MET:HG2	1.62	0.80
1:A:278:PHE:CG	1:C:151:VAL:HG13	2.17	0.80
1:C:247:VAL:HG11	2:J:407:PHE:CE1	2.21	0.76
1:B:60:VAL:HG22	5:B:746:HOH:O	1.87	0.73
1:A:149:GLN:O	1:C:278:PHE:CZ	2.43	0.72
1:A:52:GLU:HG2	1:A:119:LEU:HD12	1.74	0.70
1:A:366:LEU:HD22	5:A:571:HOH:O	1.91	0.70
1:B:64:GLU:HG3	5:B:718:HOH:O	1.91	0.69
1:C:254:LYS:HD3	1:C:315:MET:HE3	1.73	0.69
1:A:73[A]:ARG:HD2	3:A:401:1PE:H152	1.73	0.69
1:C:18:SER:HB3	4:C:401:PEG:H21	1.73	0.68
1:D:13:PRO:O	1:D:17:VAL:HG22	1.93	0.67
1:B:73:ARG:HA	4:B:501:PEG:H21	1.75	0.67
1:A:151:VAL:HG23	1:C:278:PHE:CD1	2.30	0.66
1:A:365:ARG:HB2	2:H:405:ALC:HZ3	1.76	0.66
1:C:254:LYS:HD3	1:C:315:MET:CE	2.26	0.65
1:D:154:TYR:HA	1:D:237:VAL:HG11	1.79	0.65



A 4 1	A t and D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:70:VAL:HG22	1:D:71:PRO:HD2	1.79	0.64
2:J:407:PHE:HB3	5:J:502:HOH:O	1.97	0.64
1:A:149:GLN:O	1:C:278:PHE:CE2	2.51	0.64
1:C:221:ASN:HB3	5:C:567:HOH:O	1.96	0.63
1:B:252:PRO:HA	1:B:341:THR:HG22	1.82	0.62
1:C:18:SER:HB3	4:C:401:PEG:C2	2.29	0.62
1:C:254:LYS:HG2	1:C:310:TYR:OH	2.00	0.62
1:D:153:TYR:HH	2:I:402:GLN:N	2.00	0.60
1:A:165:GLU:HG2	1:A:165:GLU:O	2.02	0.59
1:A:254:LYS:HG2	1:A:310:TYR:OH	2.04	0.58
1:A:242:PRO:HB2	2:H:408:PHE:CE1	2.39	0.57
1:A:184:ILE:HD11	1:A:188:LEU:HD11	1.86	0.56
1:C:184:ILE:HD11	1:C:188:LEU:HD11	1.88	0.56
1:B:177:LEU:HD13	1:B:247:VAL:HG21	1.87	0.56
1:A:149:GLN:O	1:C:278:PHE:HZ	1.87	0.56
1:A:18:SER:HB3	3:A:401:1PE:H251	1.89	0.55
1:C:184:ILE:HD11	1:C:188:LEU:HD21	1.88	0.55
1:D:184:ILE:HD11	1:D:188:LEU:HD21	1.89	0.55
1:B:285:VAL:CG1	1:B:315:MET:HG2	2.37	0.55
1:C:247:VAL:CG1	2:J:407:PHE:CE1	2.89	0.55
1:B:296:ASN:HB2	1:B:297:PRO:CD	2.37	0.55
1:B:52:GLU:HG2	1:B:119:LEU:HD12	1.89	0.54
1:B:81:GLY:HA2	3:B:502:1PE:H252	1.88	0.54
1:A:254:LYS:HD3	1:A:315:MET:CE	2.37	0.54
1:A:278:PHE:CB	1:C:151:VAL:HG13	2.38	0.54
1:B:184:ILE:HD11	1:B:188:LEU:HD21	1.90	0.54
1:A:3:PHE:HD1	1:A:5:VAL:HG23	1.73	0.54
1:B:39:ASP:HB2	5:B:619:HOH:O	2.07	0.53
1:D:331:LEU:HD13	1:D:336:VAL:HG12	1.90	0.53
1:A:278:PHE:CD2	1:C:151:VAL:HG13	2.43	0.53
1:D:153:TYR:HE2	1:D:238:ASP:O	1.92	0.53
1:D:238:ASP:HB3	2:I:401:SGZ:C2	2.39	0.53
1:A:165:GLU:HA	1:A:186:GLN:O	2.09	0.53
1:D:254:LYS:HG2	1:D:310:TYR:OH	2.09	0.53
1:B:151:VAL:HB	1:D:175:HIS:CE1	2.44	0.53
1:D:184:ILE:HD11	1:D:188:LEU:HD11	1.90	0.53
1:C:365:ARG:HB2	2:J:404:ALC:HZ3	1.92	0.52
1:B:214:LEU:HD11	1:B:225:ALA:HB1	1.90	0.52
1:C:3:PHE:HD1	1:C:5:VAL:HG23	1.74	0.52
1:B:184:ILE:HD11	1:B:188:LEU:HD11	1.91	0.52
1:A:184:ILE:HD11	1:A:188:LEU:HD21	1.93	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:296:ASN:HB2	1:B:297:PRO:HD2	1.93	0.51
1:B:29:ILE:O	1:B:32:ASN:HB2	2.12	0.50
1:B:73:ARG:CA	4:B:501:PEG:H21	2.41	0.50
1:B:148[B]:HIS:HD2	5:B:761:HOH:O	1.93	0.50
1:D:242:PRO:HG3	2:K:407:PHE:CZ	2.47	0.50
1:A:151:VAL:CG2	1:C:278:PHE:CD1	2.95	0.50
1:D:194:ILE:HD11	1:D:241:PHE:HB2	1.94	0.49
1:D:8:GLU:HB2	5:D:508:HOH:O	2.11	0.49
1:D:207:LEU:CD2	1:D:214:LEU:HD12	2.41	0.49
1:B:-1:SER:HB3	1:B:92:LEU:CD1	2.43	0.49
1:B:33:LEU:HG	1:B:72:ALA:HB2	1.95	0.49
1:B:3:PHE:HD1	1:B:5:VAL:HG23	1.76	0.49
1:A:58:ALA:HB2	4:A:402:PEG:H22	1.94	0.49
1:D:13:PRO:HA	1:D:230:PHE:HE1	1.78	0.49
1:B:316:GLU:O	1:B:343:SER:HB3	2.13	0.49
1:B:285:VAL:HG12	1:B:315:MET:HG2	1.95	0.49
1:C:281:VAL:HG12	1:C:294:ALA:HB2	1.95	0.48
1:D:29:ILE:O	1:D:32:ASN:HB2	2.14	0.48
1:A:134:THR:HG23	1:A:182:MET:HE2	1.96	0.48
1:D:132:GLN:HG3	1:D:212:ASN:O	2.13	0.48
1:A:153:TYR:HE2	1:A:238:ASP:O	1.97	0.47
1:B:76:PHE:CD2	4:B:501:PEG:H31	2.48	0.47
1:D:286:SER:HA	1:D:314:GLU:HG2	1.97	0.47
1:B:13:PRO:HA	1:B:230:PHE:HE1	1.79	0.47
1:B:123:GLN:HG2	5:B:726:HOH:O	2.13	0.47
1:C:247:VAL:HG11	2:J:407:PHE:CD1	2.49	0.47
1:B:153:TYR:HE2	1:B:238:ASP:O	1.97	0.47
1:D:3:PHE:HD1	1:D:5:VAL:HG23	1.80	0.47
1:C:13:PRO:HA	1:C:230:PHE:HE1	1.80	0.47
1:B:291:LYS:HD2	1:B:303:GLU:OE2	2.14	0.47
1:C:126:VAL:HG22	1:C:189:PRO:HG2	1.97	0.46
1:D:207:LEU:HD21	1:D:214:LEU:CD1	2.45	0.46
1:A:73[B]:ARG:HD3	3:A:401:1PE:H152	1.98	0.46
1:A:96:ARG:HH11	1:D:299:GLN:HB2	1.80	0.46
1:A:129:THR:HA	1:A:214:LEU:O	2.16	0.46
1:D:165:GLU:HA	1:D:186:GLN:O	2.16	0.46
1:D:283:LEU:O	1:D:316:GLU:HA	2.15	0.46
1:D:207:LEU:HD21	1:D:214:LEU:HD12	1.97	0.46
1:D:255:HIS:ND1	1:D:339:MET:HG2	2.31	0.46
1:A:281:VAL:HG12	1:A:294:ALA:HB2	1.97	0.46
1:D:71:PRO:HB2	1:D:74:LYS:HB2	1.98	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:165:GLU:HA	1:B:186:GLN:O	2.17	0.45
1:B:214:LEU:HD13	1:B:227:VAL:CG2	2.47	0.45
1:A:261:ASP:O	1:A:265:GLN:HG2	2.17	0.45
1:B:36:GLN:HG3	1:B:67:ALA:HB2	1.98	0.45
1:B:14:LEU:HD23	1:B:14:LEU:HA	1.85	0.45
1:A:278:PHE:CE2	1:C:149:GLN:O	2.70	0.44
1:C:153:TYR:HE2	1:C:238:ASP:O	1.98	0.44
1:D:281:VAL:HG12	1:D:294:ALA:HB2	1.99	0.44
1:A:337:ARG:NH1	5:A:503:HOH:O	2.50	0.44
1:C:7:ARG:HB2	1:C:88:ILE:HD11	2.00	0.44
2:I:401:SGZ:C13	2:I:401:SGZ:CA	2.96	0.44
1:A:126:VAL:HG22	1:A:189:PRO:HG2	2.00	0.44
1:B:338:MET:HG2	1:B:349:ILE:HG12	2.00	0.44
1:A:33:LEU:HG	1:A:72:ALA:HB2	2.00	0.43
1:D:296:ASN:HB2	1:D:297:PRO:CD	2.47	0.43
1:A:13:PRO:HA	1:A:230:PHE:HE1	1.84	0.43
1:A:355:GLN:O	1:A:355:GLN:HG3	2.18	0.43
1:C:261:ASP:O	1:C:265:GLN:HG2	2.18	0.43
1:D:35:LEU:HD12	1:D:97:MET:CE	2.49	0.43
1:D:296:ASN:HB2	1:D:297:PRO:HD2	2.01	0.43
1:A:27:LEU:O	1:A:30:LEU:HB2	2.18	0.43
1:B:257:GLU:HA	1:B:336:VAL:O	2.18	0.43
1:C:255:HIS:ND1	1:C:339:MET:HG2	2.34	0.43
1:C:139:ILE:CG2	1:C:204:MET:HG2	2.42	0.43
1:A:51:MET:CE	1:A:198:LYS:HE2	2.48	0.43
1:B:70:VAL:HG22	1:B:71:PRO:HD2	2.01	0.42
1:A:148[B]:HIS:HE1	5:A:662:HOH:O	2.01	0.42
1:C:68:THR:HG21	1:C:97:MET:CE	2.49	0.42
1:B:18:SER:HB3	4:B:501:PEG:H11	2.01	0.42
1:A:182:MET:HE3	1:A:182:MET:HB3	1.91	0.42
1:B:134:THR:HG23	1:B:182:MET:HE2	2.01	0.42
1:C:165:GLU:HA	1:C:186:GLN:O	2.19	0.42
1:B:126:VAL:HG22	1:B:189:PRO:HG2	2.02	0.42
1:D:32:ASN:HB3	1:D:69:THR:HB	2.02	0.42
1:A:255:HIS:ND1	1:A:339:MET:HG2	2.34	0.42
1:D:126:VAL:HG22	1:D:189:PRO:HG2	2.01	0.42
1:B:116:PHE:HA	1:B:117:PRO:HD3	1.89	0.41
1:A:283:LEU:HD13	1:A:319:PHE:HD2	1.84	0.41
1:B:159:LEU:O	1:B:169:THR:HA	2.20	0.41
1:C:144:PHE:CD2	1:C:326:ASP:HB3	2.56	0.41
1:A:140:GLU:HG3	1:A:204:MET:HE1	2.03	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:214:LEU:HD11	1:C:225:ALA:HB1	2.02	0.41
1:A:136:LYS:HG3	1:A:204:MET:HE1	2.01	0.41
1:A:365:ARG:HB2	2:H:405:ALC:CZ	2.48	0.41
1:D:13:PRO:HA	1:D:230:PHE:CE1	2.55	0.41
1:D:33:LEU:HG	1:D:72:ALA:HB2	2.03	0.41
1:A:214:LEU:HD13	1:A:227:VAL:CG2	2.50	0.41
1:B:161:GLU:HG3	1:B:192:SER:HB3	2.03	0.41
1:D:197:ARG:O	1:D:201:ILE:HG12	2.21	0.40
1:A:286:SER:HA	1:A:314:GLU:HG2	2.03	0.40
1:B:3:PHE:CD1	1:B:5:VAL:HG23	2.56	0.40
1:C:130:LEU:HD21	1:C:214:LEU:HD23	2.03	0.40
1:A:254:LYS:HD3	1:A:315:MET:HE3	2.04	0.40
1:C:286:SER:HA	1:C:314:GLU:HG2	2.02	0.40
1:D:256:LEU:HB3	1:D:338:MET:HB2	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	Perce	entiles
1	А	369/386~(96%)	358~(97%)	11 (3%)	0	100	100
1	В	363/386~(94%)	350 (96%)	13 (4%)	0	100	100
1	С	367/386~(95%)	355~(97%)	12 (3%)	0	100	100
1	D	358/386~(93%)	344 (96%)	14 (4%)	0	100	100
2	Н	2/6~(33%)	2 (100%)	0	0	100	100
2	Ι	2/6~(33%)	2 (100%)	0	0	100	100
2	J	2/6~(33%)	2 (100%)	0	0	100	100
2	K	2/6~(33%)	2 (100%)	0	0	100	100
All	All	1465/1568~(93%)	1415 (97%)	50 (3%)	0	100	100





There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	ntiles
1	А	315/330~(96%)	306~(97%)	9~(3%)	42	54
1	В	314/330~(95%)	305~(97%)	9~(3%)	42	54
1	\mathbf{C}	310/330~(94%)	300~(97%)	10 (3%)	39	50
1	D	308/330~(93%)	303~(98%)	5(2%)	62	76
2	Η	4/4~(100%)	4 (100%)	0	100	100
2	Ι	4/4~(100%)	4 (100%)	0	100	100
2	J	4/4~(100%)	4 (100%)	0	100	100
2	К	4/4~(100%)	4 (100%)	0	100	100
All	All	1263/1336~(94%)	1230 (97%)	33 (3%)	46	58

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	69	THR
1	А	70	VAL
1	А	176	ARG
1	А	188	LEU
1	А	220	SER
1	А	226	HIS
1	А	287	GLU
1	А	340	LEU
1	А	366	LEU
1	В	27	LEU
1	В	70	VAL
1	В	176	ARG
1	В	181	SER
1	В	188	LEU
1	В	255	HIS
1	В	306	LEU



Mol	Chain	\mathbf{Res}	Type
1	В	340	LEU
1	В	350	GLU
1	С	70	VAL
1	С	91	GLN
1	С	137	ARG
1	С	151	VAL
1	С	176	ARG
1	С	181	SER
1	С	188	LEU
1	С	204	MET
1	С	311	SER
1	С	340	LEU
1	D	70	VAL
1	D	176	ARG
1	D	181	SER
1	D	188	LEU
1	D	340	LEU

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

Mol	Chain	Res	Type
1	С	148	HIS
1	С	226	HIS
1	С	295	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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).



Mal	Туре	Chain	Dec	Tink	B	ond leng	$_{ m gths}$	В	ond ang	les
WIOI			nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ALC	Н	405	2	9,11,12	0.55	0	$10,\!13,\!15$	0.63	0
2	ALC	Ι	403	2	9,11,12	0.51	0	$10,\!13,\!15$	0.67	0
2	ALC	K	404	2	9,11,12	0.47	0	$10,\!13,\!15$	0.70	0
2	ALC	J	404	2	9,11,12	0.42	0	10,13,15	0.66	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	ALC	Н	405	2	-	2/5/14/16	0/1/1/1
2	ALC	Ι	403	2	-	2/5/14/16	0/1/1/1
2	ALC	K	404	2	-	2/5/14/16	0/1/1/1
2	ALC	J	404	2	-	2/5/14/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Н	405	ALC	CA-CB-CG-CD2
2	Ι	403	ALC	CA-CB-CG-CD2
2	J	404	ALC	CA-CB-CG-CD2
2	Κ	404	ALC	CA-CB-CG-CD2
2	Н	405	ALC	CA-CB-CG-CD1
2	Ι	403	ALC	CA-CB-CG-CD1
2	J	404	ALC	CA-CB-CG-CD1
2	Κ	404	ALC	CA-CB-CG-CD1

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Ν	/lol	Chain	Res	Type	Clashes	Symm-Clashes
	2	Н	405	ALC	2	0
	2	J	404	ALC	1	0



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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).

Mal	Turne	Chain	Dec	Tink	Bond le		$_{\rm ths}$	Bond angles		
Moi Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
4	PEG	A	402	-	6,6,6	0.22	0	5,5,5	0.15	0
3	1PE	В	502	-	12,12,15	0.58	0	11,11,14	0.41	0
3	1PE	А	401	-	9,9,15	0.47	0	8,8,14	0.42	0
4	PEG	В	501	-	6,6,6	0.21	0	5,5,5	0.30	0
4	PEG	С	401	-	6,6,6	0.26	0	$5,\!5,\!5$	0.21	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
4	PEG	А	402	-	-	2/4/4/4	-
3	1PE	В	502	-	-	5/10/10/13	-
3	1PE	А	401	-	-	4/7/7/13	-
4	PEG	В	501	-	-	1/4/4/4	-
4	PEG	С	401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
3	В	502	1PE	OH6-C15-C25-OH5
3	В	502	1PE	OH7-C16-C26-OH6
4	А	402	PEG	O2-C3-C4-O4
3	А	401	1PE	OH5-C14-C24-OH4
3	А	401	1PE	OH7-C16-C26-OH6
3	В	502	1PE	OH5-C14-C24-OH4
3	А	401	1PE	OH6-C15-C25-OH5
3	В	502	1PE	C24-C14-OH5-C25
3	А	401	1PE	С16-С26-ОН6-С15
4	С	401	PEG	O1-C1-C2-O2
4	А	402	PEG	C4-C3-O2-C2
4	В	501	PEG	C1-C2-O2-C3
3	В	502	1PE	OH4-C13-C23-OH3
4	С	401	PEG	C4-C3-O2-C2

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	402	PEG	1	0
3	В	502	1PE	1	0
3	А	401	1PE	3	0
4	В	501	PEG	4	0
4	С	401	PEG	2	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^{th} 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	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	367/386~(95%)	0.01	5 (1%) 75 73	17, 38, 73, 85	0
1	В	365/386~(94%)	0.26	15 (4%) 37 35	19, 47, 85, 108	0
1	С	368/386~(95%)	0.31	17 (4%) 32 31	26, 54, 83, 108	0
1	D	363/386~(94%)	0.40	20 (5%) 25 24	22, 55, 90, 111	0
2	Н	4/6~(66%)	-0.23	0 100 100	37, 39, 44, 44	0
2	Ι	4/6~(66%)	0.48	0 100 100	41, 47, 51, 59	0
2	J	4/6~(66%)	0.32	0 100 100	35, 48, 49, 73	0
2	K	4/6~(66%)	0.11	0 100 100	33, 39, 39, 55	0
All	All	1479/1568~(94%)	0.24	57 (3%) 39 37	17, 50, 84, 111	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	22	GLY	6.5
1	D	126	VAL	4.9
1	В	366	LEU	4.4
1	В	284	TYR	4.4
1	D	188	LEU	4.3
1	С	184	ILE	4.0
1	D	207	LEU	3.7
1	D	128	PHE	3.7
1	С	219	GLY	3.6
1	В	317	ILE	3.4
1	В	339	MET	3.3
1	А	209	GLY	3.3
1	А	262	LEU	3.3
1	В	285	VAL	3.2
1	D	253	ASP	3.2
1	С	60	VAL	3.1



Mol	Chain	Res	Type	RSRZ
1	С	244	TYR	3.1
1	С	39	ASP	3.0
1	D	-1	SER	3.0
1	С	252	PRO	2.9
1	С	247	VAL	2.8
1	D	203	LEU	2.8
1	D	153	TYR	2.8
1	С	38	ALA	2.7
1	D	216	VAL	2.7
1	D	187	SER	2.7
1	С	153	TYR	2.7
1	В	308	VAL	2.7
1	В	310	TYR	2.6
1	D	311	SER	2.6
1	D	183	PRO	2.5
1	D	90	VAL	2.5
1	В	315	MET	2.4
1	С	251	ASN	2.4
1	D	184	ILE	2.4
1	В	153	TYR	2.4
1	D	98	LEU	2.3
1	В	286	SER	2.3
1	В	313	ALA	2.3
1	А	0	HIS	2.3
1	D	130	LEU	2.3
1	А	244	TYR	2.2
1	С	37	VAL	2.2
1	В	314	GLU	2.1
1	D	221	ASN	2.1
1	В	283	LEU	2.1
1	D	23	GLY	2.1
1	С	218	ILE	2.1
1	D	223	ILE	2.1
1	С	151	VAL	2.1
1	С	3	PHE	2.1
1	С	190	SER	2.0
1	В	290	LEU	2.0
1	С	9	HIS	2.0
1	В	22	GLY	2.0
1	С	154	TYR	2.0
1	А	255	HIS	2.0

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6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	ALC	J	404	11/12	0.96	0.12	37,40,42,45	0
2	ALC	K	404	11/12	0.96	0.10	$28,\!34,\!46,\!46$	0
2	ALC	Н	405	11/12	0.97	0.13	40,42,49,49	0
2	ALC	Ι	403	11/12	0.97	0.10	43,45,49,49	0

6.3 Carbohydrates (i)

There are no monosaccharides 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^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
4	PEG	А	402	7/7	0.83	0.22	32,38,40,43	7
3	1PE	В	502	13/16	0.86	0.23	$26,\!38,\!46,\!50$	13
4	PEG	С	401	7/7	0.86	0.26	40,45,52,53	7
4	PEG	В	501	7/7	0.89	0.22	17,20,30,32	7
3	1PE	А	401	10/16	0.95	0.17	21,26,31,32	10

6.5 Other polymers (i)

There are no such residues in this entry.

