



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 24, 2021 – 02:08 pm GMT

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 ⓘ symbol.

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

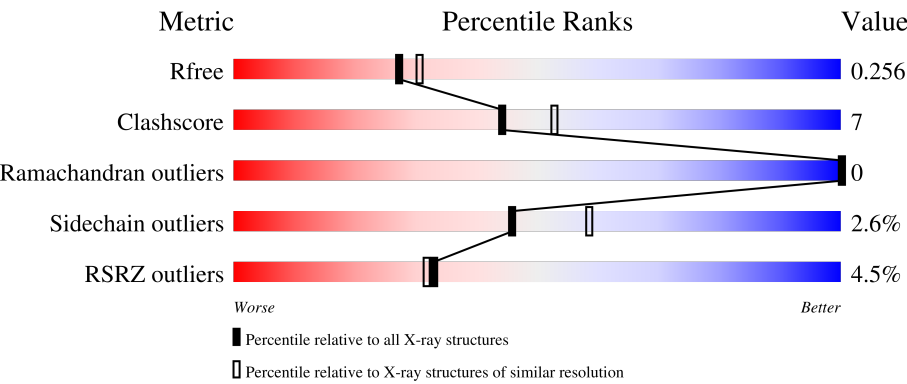
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-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.




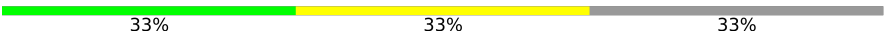

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 $\leq 5\%$. 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	386	<div><div>2%</div><div><div></div><div>79%</div><div>15%</div><div>• 5%</div></div></div>
1	B	386	<div><div>4%</div><div><div></div><div>77%</div><div>17%</div><div>• 5%</div></div></div>
1	C	386	<div><div>5%</div><div><div></div><div>83%</div><div>12%</div><div>• 5%</div></div></div>
1	D	386	<div><div>7%</div><div><div></div><div>80%</div><div>14%</div><div>• 6%</div></div></div>
2	H	6	<div><div></div><div><div></div><div>33%</div><div>33%</div><div>33%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	I	6	 67% 33%
2	J	6	 33% 33% 33%
2	K	6	 50% 17% 33%

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	B	501	-	-	X	-

2 Entry composition

There are 7 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.

- Molecule 1 is a protein called Beta sliding clamp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	4	0
			2872	1805	508	540	19			
1	B	365	Total	C	N	O	S	0	2	0
			2857	1796	503	539	19			
1	C	368	Total	C	N	O	S	0	1	0
			2841	1784	496	542	19			
1	D	363	Total	C	N	O	S	0	1	0
			2813	1770	490	534	19			

There are 80 discrepancies between the modelled and reference sequences:

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

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

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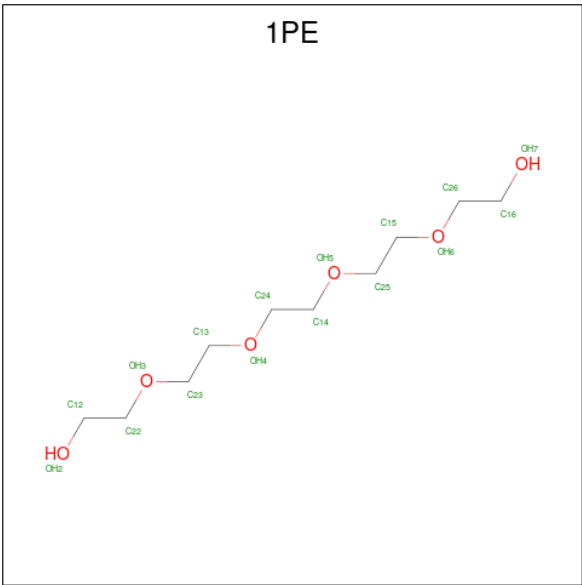
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A0A073FMV0
D	-15	HIS	-	expression tag	UNP A0A073FMV0
D	-14	HIS	-	expression tag	UNP A0A073FMV0
D	-13	HIS	-	expression tag	UNP A0A073FMV0
D	-12	HIS	-	expression tag	UNP A0A073FMV0
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.

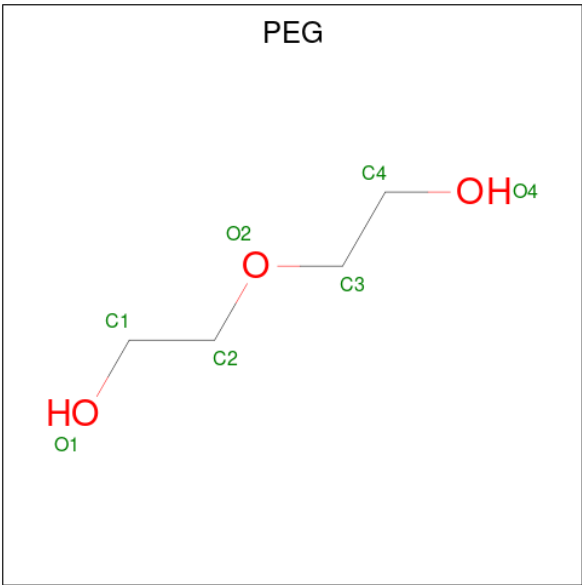
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	4	Total	C	N	O	0	0	0
			39	28	4	7			
2	I	4	Total	C	N	O	0	0	0
			39	28	4	7			
2	J	4	Total	C	N	O	0	0	0
			39	28	4	7			
2	K	4	Total	C	N	O	0	0	0
			39	28	4	7			

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



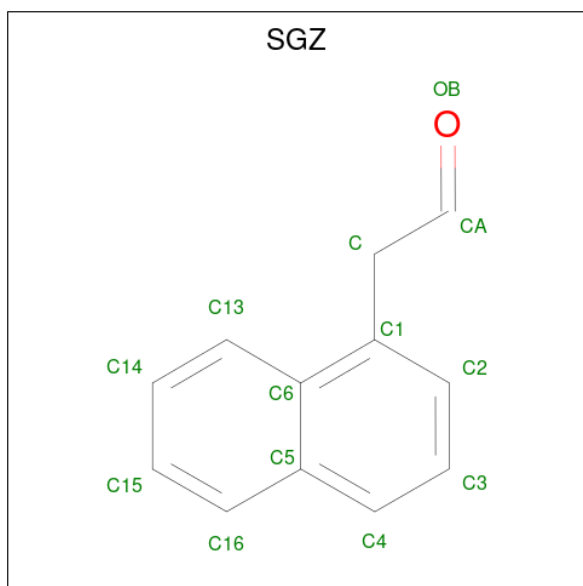
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

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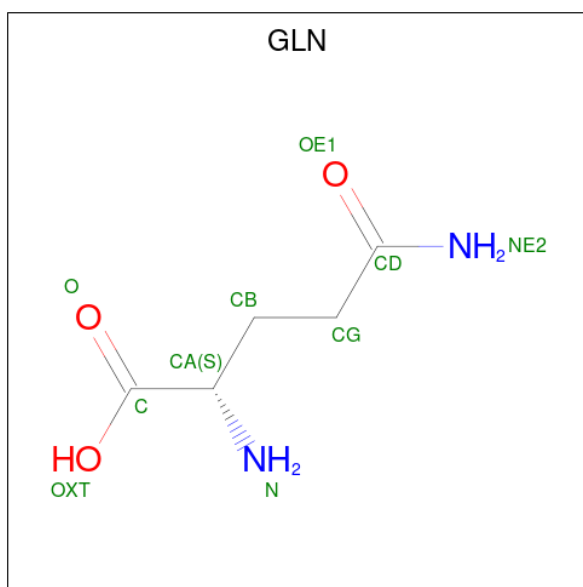
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is 2-naphthalen-1-ylethanal (three-letter code: SGZ) (formula: $C_{12}H_{10}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	12	1		
5	C	1	Total	C	O	0	0
			13	12	1		
5	D	1	Total	C	O	0	0
			13	12	1		
5	D	1	Total	C	O	0	0
			13	12	1		

- Molecule 6 is GLUTAMINE (three-letter code: GLN) (formula: $C_5H_{10}N_2O_3$).



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		

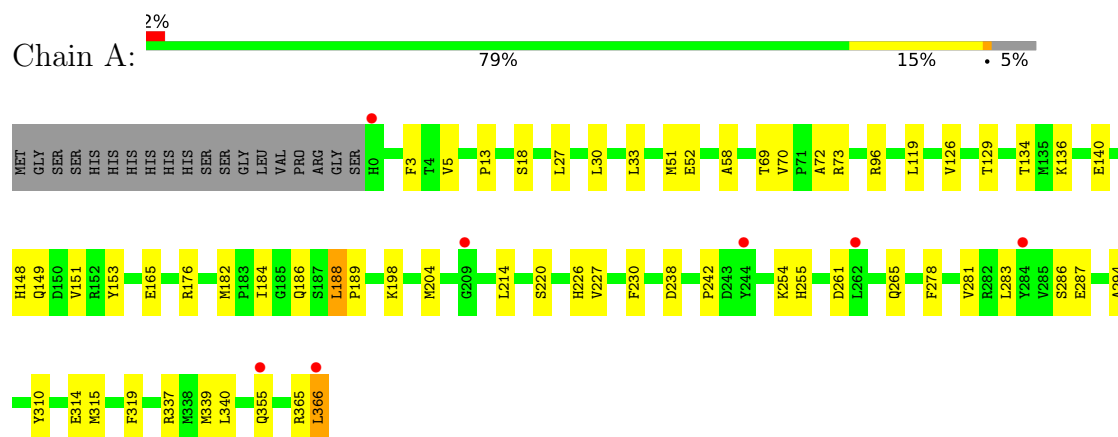
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	223	Total	O	0	0
			223	223		
7	B	185	Total	O	0	1
			186	186		
7	C	120	Total	O	0	1
			121	121		
7	D	131	Total	O	0	1
			131	131		
7	H	6	Total	O	0	0
			6	6		
7	I	2	Total	O	0	0
			2	2		
7	J	3	Total	O	0	0
			3	3		
7	K	5	Total	O	0	0
			5	5		

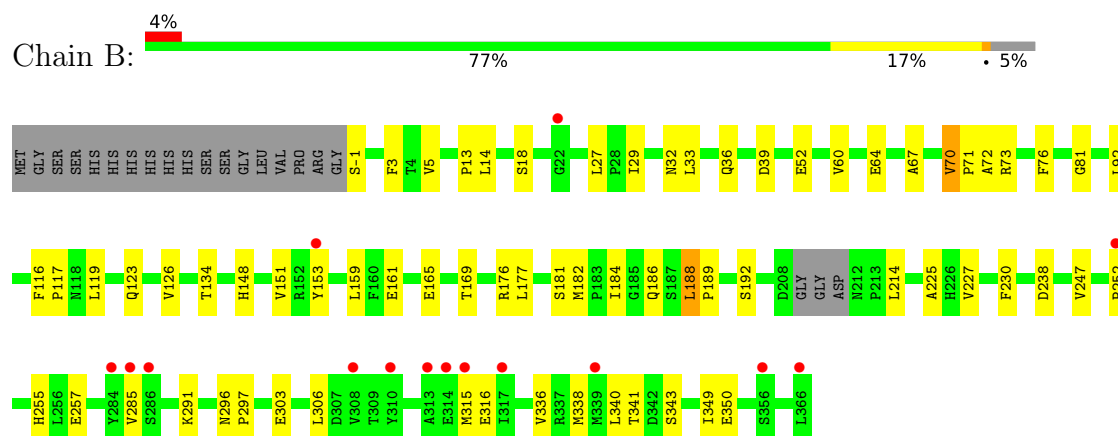
3 Residue-property plots [i](#)

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.

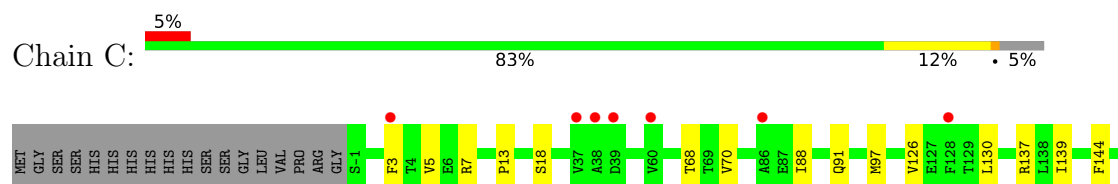
• Molecule 1: Beta sliding clamp

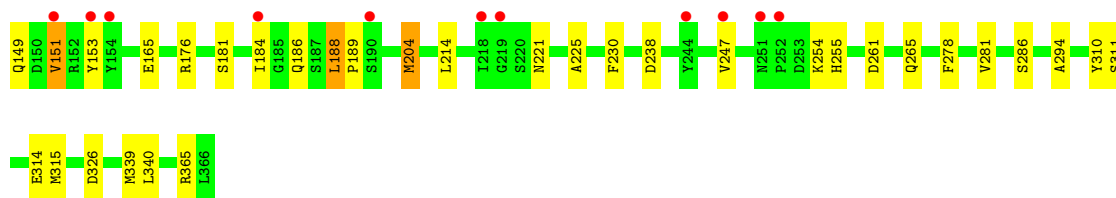


• Molecule 1: Beta sliding clamp

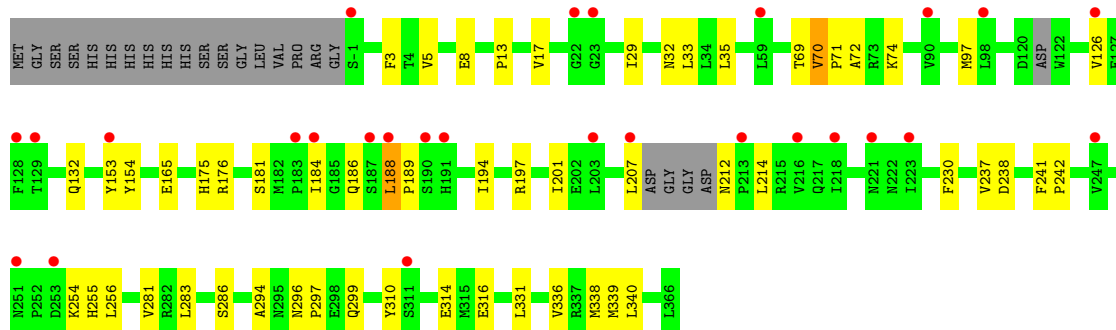
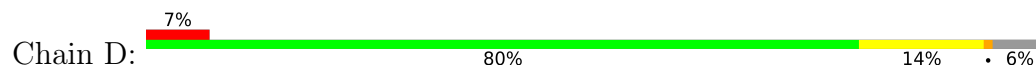


• Molecule 1: Beta sliding clamp

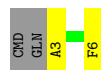




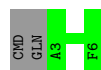
- Molecule 1: Beta sliding clamp



- Molecule 2: Peptide 20



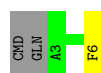
- Molecule 2: Peptide 20



- Molecule 2: Peptide 20



- Molecule 2: Peptide 20



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.68Å 81.76Å 141.93Å 90.00° 97.49° 90.00°	Depositor
Resolution (Å)	41.39 – 2.19 70.69 – 2.19	Depositor EDS
% Data completeness (in resolution range)	71.7 (41.39-2.19) 71.7 (70.69-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.189 , 0.242 0.195 , 0.256	Depositor 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)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

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.

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: PEG, ALC, SGZ, 1PE

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	0.59	0/2935	0.68	0/3972
1	B	0.54	0/2908	0.65	0/3935
1	C	0.51	0/2893	0.64	0/3918
1	D	0.48	0/2862	0.63	0/3875
2	H	0.77	0/28	0.77	0/35
2	I	0.62	0/28	0.60	0/35
2	J	0.70	0/28	0.68	0/35
2	K	0.65	0/28	0.66	0/35
All	All	0.53	0/11710	0.65	0/15840

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	2872	0	2890	47	0
1	B	2857	0	2864	42	0
1	C	2841	0	2837	37	0
1	D	2813	0	2806	37	0
2	H	39	0	38	3	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	5	0
2	K	39	0	38	1	0
3	A	10	0	13	3	0
3	B	13	0	17	1	0
4	A	7	0	10	1	0
4	B	7	0	10	4	0
4	C	7	0	10	2	0
5	A	13	0	0	0	0
5	C	13	0	0	0	0
5	D	26	0	0	2	0
6	H	9	0	7	0	0
6	I	9	0	7	1	0
6	J	9	0	7	0	0
6	K	9	0	7	0	0
7	A	223	0	0	3	0
7	B	186	0	0	5	0
7	C	121	0	0	1	0
7	D	131	0	0	1	0
7	H	6	0	0	0	0
7	I	2	0	0	0	0
7	J	3	0	0	1	0
7	K	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 distance (Å)	Clash 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:6:PHE:CE1	2.21	0.76
1:B:60:VAL:HG22	7: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	7:A:571:HOH:O	1.91	0.70
1:B:64:GLU:HG3	7: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3: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
1:D:70:VAL:HG22	1:D:71:PRO:HD2	1.79	0.64
2:J:6:PHE:HB3	7:J:202: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	7: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	6:I:101: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:6: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:6: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	7: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	5:D: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3: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
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	7:B:761:HOH:O	1.93	0.50
1:D:242:PRO:HG3	2:K:6: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	7: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	7:B:726:HOH:O	2.13	0.47
1:C:247:VAL:HG11	2:J:6: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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	7:A:503:HOH:O	2.50	0.44
1:C:7:ARG:HB2	1:C:88:ILE:HD11	2.00	0.44
5:D:401:SGZ:CA	5:D:401:SGZ:C13	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	7: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:3: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	Percentiles	
1	A	369/386 (96%)	358 (97%)	11 (3%)	0	100	100
1	B	363/386 (94%)	350 (96%)	13 (4%)	0	100	100
1	C	367/386 (95%)	355 (97%)	12 (3%)	0	100	100
1	D	358/386 (93%)	344 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	2/6 (33%)	2 (100%)	0	0	100	100
2	I	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 ⓘ

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	315/330 (96%)	306 (97%)	9 (3%)	42	54
1	B	314/330 (95%)	305 (97%)	9 (3%)	42	54
1	C	310/330 (94%)	300 (97%)	10 (3%)	39	50
1	D	308/330 (93%)	303 (98%)	5 (2%)	62	76
2	H	3/4 (75%)	3 (100%)	0	100	100
2	I	3/4 (75%)	3 (100%)	0	100	100
2	J	3/4 (75%)	3 (100%)	0	100	100
2	K	3/4 (75%)	3 (100%)	0	100	100
All	All	1259/1336 (94%)	1226 (97%)	33 (3%)	46	58

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

Mol	Chain	Res	Type
1	A	69	THR
1	A	70	VAL
1	A	176	ARG
1	A	188	LEU
1	A	220	SER
1	A	226	HIS

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Mol	Chain	Res	Type
1	A	287	GLU
1	A	340	LEU
1	A	366	LEU
1	B	27	LEU
1	B	70	VAL
1	B	176	ARG
1	B	181	SER
1	B	188	LEU
1	B	255	HIS
1	B	306	LEU
1	B	340	LEU
1	B	350	GLU
1	C	70	VAL
1	C	91	GLN
1	C	137	ARG
1	C	151	VAL
1	C	176	ARG
1	C	181	SER
1	C	188	LEU
1	C	204	MET
1	C	311	SER
1	C	340	LEU
1	D	70	VAL
1	D	176	ARG
1	D	181	SER
1	D	188	LEU
1	D	340	LEU

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

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

5.3.3 RNA ⓘ

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.

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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 [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, 95th 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 ²)	Q<0.9
1	A	367/386 (95%)	0.16	7 (1%) 66 65	17, 38, 73, 85	0
1	B	365/386 (94%)	0.38	15 (4%) 37 35	19, 47, 85, 108	0
1	C	368/386 (95%)	0.42	18 (4%) 29 28	26, 54, 83, 108	0
1	D	363/386 (94%)	0.50	27 (7%) 14 13	22, 55, 90, 111	0
2	H	3/6 (50%)	-0.13	0 100 100	37, 37, 39, 44	0
2	I	3/6 (50%)	1.02	0 100 100	47, 47, 51, 59	0
2	J	3/6 (50%)	0.82	0 100 100	48, 48, 49, 73	0
2	K	3/6 (50%)	0.41	0 100 100	39, 39, 39, 55	0
All	All	1475/1568 (94%)	0.36	67 (4%) 33 32	17, 50, 84, 111	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	22	GLY	6.4
1	D	126	VAL	5.1
1	B	284	TYR	4.7
1	B	366	LEU	4.7
1	D	128	PHE	4.5
1	C	184	ILE	3.8
1	D	207	LEU	3.8
1	B	317	ILE	3.7
1	D	188	LEU	3.5
1	C	219	GLY	3.5
1	D	253	ASP	3.4
1	C	252	PRO	3.4
1	A	262	LEU	3.3
1	B	285	VAL	3.3
1	C	244	TYR	3.3
1	B	339	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	153	TYR	3.2
1	C	60	VAL	3.2
1	D	203	LEU	3.1
1	D	311	SER	3.0
1	B	308	VAL	3.0
1	A	209	GLY	2.9
1	D	216	VAL	2.9
1	C	251	ASN	2.9
1	A	244	TYR	2.8
1	C	247	VAL	2.8
1	B	310	TYR	2.8
1	D	183	PRO	2.8
1	A	0	HIS	2.7
1	B	314	GLU	2.6
1	C	86	ALA	2.6
1	C	3	PHE	2.6
1	B	286	SER	2.5
1	D	223	ILE	2.5
1	C	153	TYR	2.5
1	D	221	ASN	2.5
1	B	153	TYR	2.5
1	C	39	ASP	2.5
1	C	38	ALA	2.5
1	B	313	ALA	2.4
1	D	184	ILE	2.4
1	A	355	GLN	2.4
1	D	90	VAL	2.4
1	C	190	SER	2.4
1	C	151	VAL	2.3
1	C	37	VAL	2.3
1	D	98	LEU	2.3
1	D	-1	SER	2.3
1	C	218	ILE	2.3
1	D	190	SER	2.3
1	C	128	PHE	2.2
1	B	356	SER	2.2
1	D	129	THR	2.2
1	D	218	ILE	2.1
1	D	23	GLY	2.1
1	D	251	ASN	2.1
1	C	154	TYR	2.1
1	D	59	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	187	SER	2.1
1	B	22	GLY	2.1
1	A	284	TYR	2.1
1	B	252	PRO	2.0
1	B	315	MET	2.0
1	A	366	LEU	2.0
1	D	247	VAL	2.0
1	D	213	PRO	2.0
1	D	191	HIS	2.0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ALC	J	3	11/12	0.94	0.14	37,40,42,45	0
2	ALC	I	3	11/12	0.96	0.12	43,45,49,49	0
2	ALC	H	3	11/12	0.96	0.14	40,42,49,49	0
2	ALC	K	3	11/12	0.96	0.10	28,34,46,46	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PEG	C	401	7/7	0.81	0.30	40,45,52,53	7
4	PEG	A	402	7/7	0.82	0.24	32,38,40,43	7
5	SGZ	D	402	13/13	0.83	0.21	29,32,39,42	0
3	1PE	B	502	13/16	0.85	0.25	26,38,46,50	13
4	PEG	B	501	7/7	0.87	0.25	17,20,30,32	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SGZ	D	401	13/13	0.93	0.17	43,59,65,65	0
5	SGZ	A	403	13/13	0.93	0.14	29,32,39,42	0
3	1PE	A	401	10/16	0.95	0.20	21,26,31,32	10
6	GLN	H	101	9/10	0.95	0.13	32,42,48,57	0
6	GLN	I	101	9/10	0.95	0.11	28,42,46,46	0
6	GLN	J	101	9/10	0.95	0.11	27,30,41,43	0
5	SGZ	C	402	13/13	0.97	0.14	30,33,35,36	0
6	GLN	K	101	9/10	0.97	0.14	23,30,35,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.