



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:36 am BST

PDB ID : 4N0O  
Title : Complex structure of Arterivirus nonstructural protein 10 (helicase) with DNA  
Authors : Deng, Z.; Chen, Z.  
Deposited on : 2013-10-02  
Resolution : 2.65 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

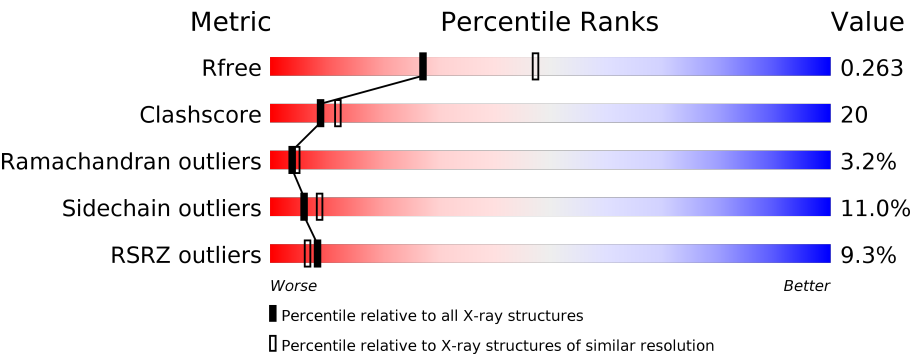
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 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	423	<div><div>8%</div><div><div></div><div>51%</div><div>36%</div><div>7%</div><div>7%</div></div></div>
1	C	423	<div><div>8%</div><div><div></div><div>55%</div><div>31%</div><div>8%</div><div>6%</div></div></div>
1	E	423	<div><div>9%</div><div><div></div><div>60%</div><div>27%</div><div>7%</div><div>6%</div></div></div>
1	G	423	<div><div>9%</div><div><div></div><div>58%</div><div>31%</div><div>•</div><div>7%</div></div></div>
2	B	7	<div><div>14%</div><div><div>14%</div><div>57%</div><div>29%</div></div></div>
2	D	7	<div><div>29%</div><div><div></div><div>57%</div><div>43%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	7	
2	H	7	

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
3	ZN	G	503	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12998 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 Replicase polypeptide 1ab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			2897	1850	508	519	20			
1	C	398	Total	C	N	O	S	0	0	0
			2916	1867	506	524	19			
1	E	396	Total	C	N	O	S	0	0	0
			2896	1850	505	523	18			
1	G	393	Total	C	N	O	S	0	0	0
			2889	1845	509	517	18			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP P19811
A	-19	GLY	-	EXPRESSION TAG	UNP P19811
A	-18	SER	-	EXPRESSION TAG	UNP P19811
A	-17	SER	-	EXPRESSION TAG	UNP P19811
A	-16	HIS	-	EXPRESSION TAG	UNP P19811
A	-15	HIS	-	EXPRESSION TAG	UNP P19811
A	-14	HIS	-	EXPRESSION TAG	UNP P19811
A	-13	HIS	-	EXPRESSION TAG	UNP P19811
A	-12	HIS	-	EXPRESSION TAG	UNP P19811
A	-11	SER	-	EXPRESSION TAG	UNP P19811
A	-10	SER	-	EXPRESSION TAG	UNP P19811
A	-9	GLY	-	EXPRESSION TAG	UNP P19811
A	-8	GLU	-	EXPRESSION TAG	UNP P19811
A	-7	ASN	-	EXPRESSION TAG	UNP P19811
A	-6	LEU	-	EXPRESSION TAG	UNP P19811
A	-5	TYR	-	EXPRESSION TAG	UNP P19811
A	-4	PHE	-	EXPRESSION TAG	UNP P19811
A	-3	GLN	-	EXPRESSION TAG	UNP P19811
A	-2	GLY	-	EXPRESSION TAG	UNP P19811
A	-1	HIS	-	EXPRESSION TAG	UNP P19811
A	0	MET	-	EXPRESSION TAG	UNP P19811

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	MET	-	EXPRESSION TAG	UNP P19811
C	-19	GLY	-	EXPRESSION TAG	UNP P19811
C	-18	SER	-	EXPRESSION TAG	UNP P19811
C	-17	SER	-	EXPRESSION TAG	UNP P19811
C	-16	HIS	-	EXPRESSION TAG	UNP P19811
C	-15	HIS	-	EXPRESSION TAG	UNP P19811
C	-14	HIS	-	EXPRESSION TAG	UNP P19811
C	-13	HIS	-	EXPRESSION TAG	UNP P19811
C	-12	HIS	-	EXPRESSION TAG	UNP P19811
C	-11	SER	-	EXPRESSION TAG	UNP P19811
C	-10	SER	-	EXPRESSION TAG	UNP P19811
C	-9	GLY	-	EXPRESSION TAG	UNP P19811
C	-8	GLU	-	EXPRESSION TAG	UNP P19811
C	-7	ASN	-	EXPRESSION TAG	UNP P19811
C	-6	LEU	-	EXPRESSION TAG	UNP P19811
C	-5	TYR	-	EXPRESSION TAG	UNP P19811
C	-4	PHE	-	EXPRESSION TAG	UNP P19811
C	-3	GLN	-	EXPRESSION TAG	UNP P19811
C	-2	GLY	-	EXPRESSION TAG	UNP P19811
C	-1	HIS	-	EXPRESSION TAG	UNP P19811
C	0	MET	-	EXPRESSION TAG	UNP P19811
E	-20	MET	-	EXPRESSION TAG	UNP P19811
E	-19	GLY	-	EXPRESSION TAG	UNP P19811
E	-18	SER	-	EXPRESSION TAG	UNP P19811
E	-17	SER	-	EXPRESSION TAG	UNP P19811
E	-16	HIS	-	EXPRESSION TAG	UNP P19811
E	-15	HIS	-	EXPRESSION TAG	UNP P19811
E	-14	HIS	-	EXPRESSION TAG	UNP P19811
E	-13	HIS	-	EXPRESSION TAG	UNP P19811
E	-12	HIS	-	EXPRESSION TAG	UNP P19811
E	-11	SER	-	EXPRESSION TAG	UNP P19811
E	-10	SER	-	EXPRESSION TAG	UNP P19811
E	-9	GLY	-	EXPRESSION TAG	UNP P19811
E	-8	GLU	-	EXPRESSION TAG	UNP P19811
E	-7	ASN	-	EXPRESSION TAG	UNP P19811
E	-6	LEU	-	EXPRESSION TAG	UNP P19811
E	-5	TYR	-	EXPRESSION TAG	UNP P19811
E	-4	PHE	-	EXPRESSION TAG	UNP P19811
E	-3	GLN	-	EXPRESSION TAG	UNP P19811
E	-2	GLY	-	EXPRESSION TAG	UNP P19811
E	-1	HIS	-	EXPRESSION TAG	UNP P19811
E	0	MET	-	EXPRESSION TAG	UNP P19811

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-20	MET	-	EXPRESSION TAG	UNP P19811
G	-19	GLY	-	EXPRESSION TAG	UNP P19811
G	-18	SER	-	EXPRESSION TAG	UNP P19811
G	-17	SER	-	EXPRESSION TAG	UNP P19811
G	-16	HIS	-	EXPRESSION TAG	UNP P19811
G	-15	HIS	-	EXPRESSION TAG	UNP P19811
G	-14	HIS	-	EXPRESSION TAG	UNP P19811
G	-13	HIS	-	EXPRESSION TAG	UNP P19811
G	-12	HIS	-	EXPRESSION TAG	UNP P19811
G	-11	SER	-	EXPRESSION TAG	UNP P19811
G	-10	SER	-	EXPRESSION TAG	UNP P19811
G	-9	GLY	-	EXPRESSION TAG	UNP P19811
G	-8	GLU	-	EXPRESSION TAG	UNP P19811
G	-7	ASN	-	EXPRESSION TAG	UNP P19811
G	-6	LEU	-	EXPRESSION TAG	UNP P19811
G	-5	TYR	-	EXPRESSION TAG	UNP P19811
G	-4	PHE	-	EXPRESSION TAG	UNP P19811
G	-3	GLN	-	EXPRESSION TAG	UNP P19811
G	-2	GLY	-	EXPRESSION TAG	UNP P19811
G	-1	HIS	-	EXPRESSION TAG	UNP P19811
G	0	MET	-	EXPRESSION TAG	UNP P19811

- Molecule 2 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	7	Total 137	C 70	N 14	O 47	P 6	0	0	0
2	D	7	Total 137	C 70	N 14	O 47	P 6	0	0	0
2	F	7	Total 137	C 70	N 14	O 47	P 6	0	0	0
2	H	7	Total 137	C 70	N 14	O 47	P 6	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	3	Total	Zn	0	0
			3	3		
3	A	3	Total	Zn	0	0
			3	3		
3	C	3	Total	Zn	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	3	Total 3	Zn 3	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Ca 1	0	0
4	A	2	Total 2	Ca 2	0	0
4	C	2	Total 2	Ca 2	0	0
4	E	2	Total 2	Ca 2	0	0

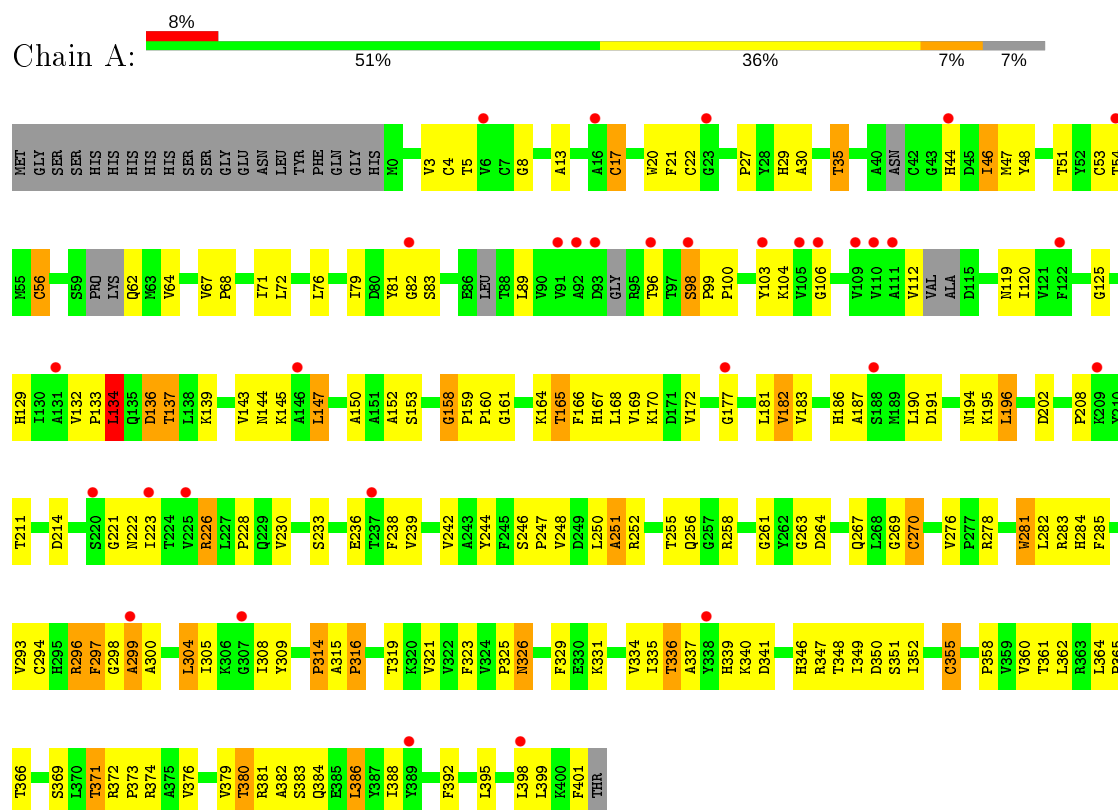
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	234	Total 234	O 234	0	0
5	C	169	Total 169	O 169	0	0
5	E	186	Total 186	O 186	0	0
5	G	216	Total 216	O 216	0	0
5	B	6	Total 6	O 6	0	0
5	D	4	Total 4	O 4	0	0
5	F	12	Total 12	O 12	0	0
5	H	6	Total 6	O 6	0	0

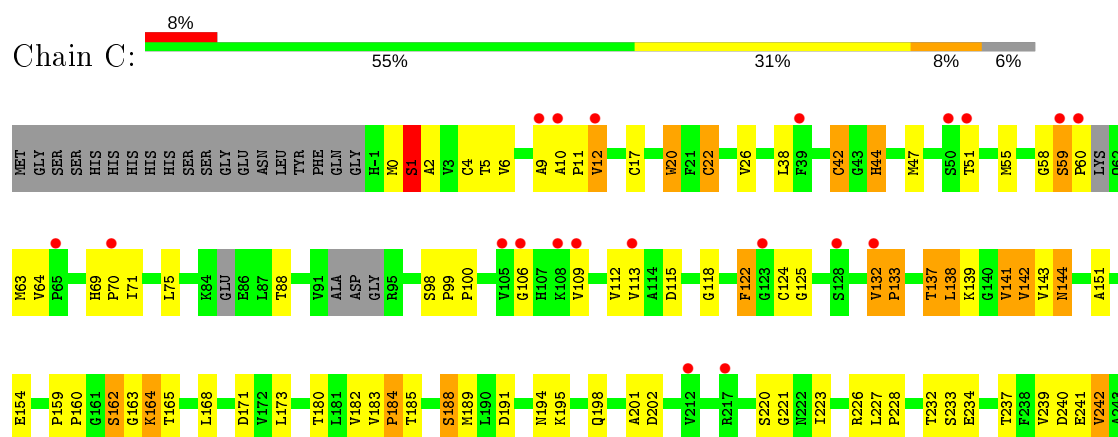
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

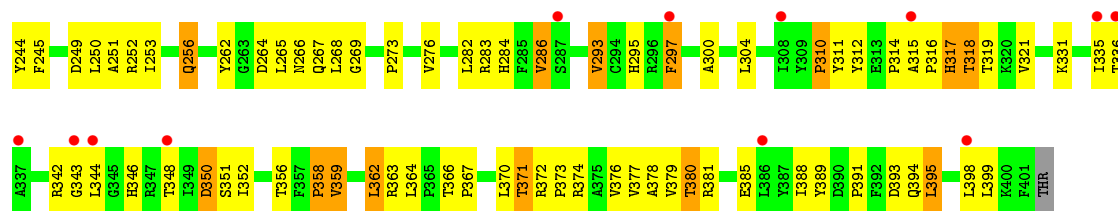
#### • Molecule 1: Replicase polyprotein 1ab



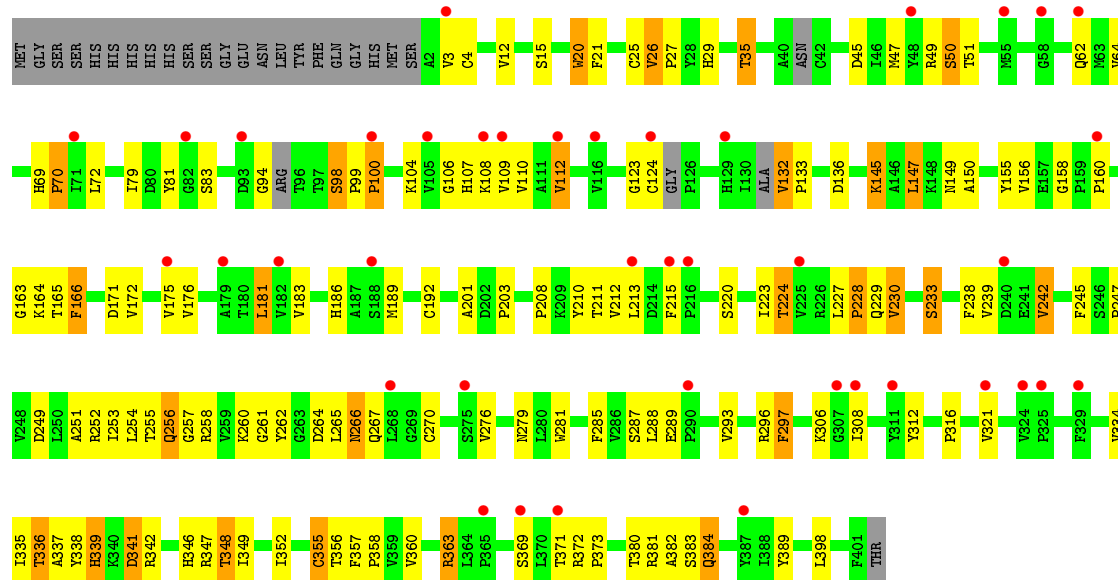
#### • Molecule 1: Replicase polyprotein 1ab



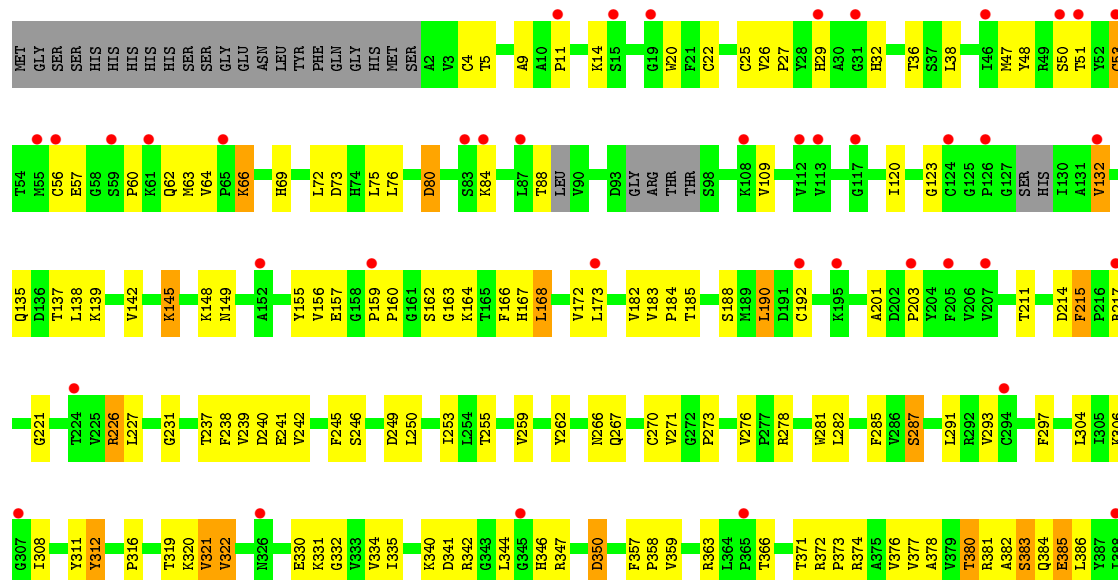




• Molecule 1: Replicase polyprotein 1ab

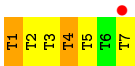
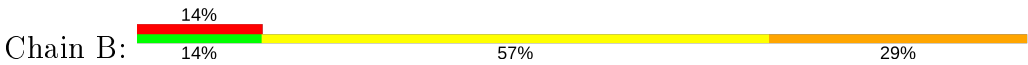


• Molecule 1: Replicase polyprotein 1ab

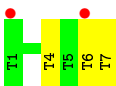




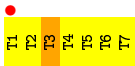
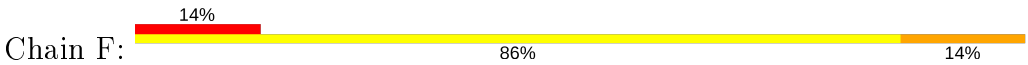
● Molecule 2: DNA



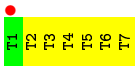
● Molecule 2: DNA



● Molecule 2: DNA



● Molecule 2: DNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.63Å 88.84Å 128.78Å 81.74° 90.01° 71.42°	Depositor
Resolution (Å)	50.00 – 2.65 42.43 – 2.63	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.00-2.65) 95.2 (42.43-2.63)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.246 , 0.264 0.246 , 0.263	Depositor DCC
$R_{free}$ test set	3375 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.0	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.457 for h,h-k,-l	Xtriage
Reported twinning fraction	0.532 for H, K, L 0.468 for H, H-K, -L	Depositor
Outliers	0 of 66828 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	12998	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4307e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: ZN, CA

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	0.51	2/2969 (0.1%)	0.70	2/4052 (0.0%)
1	C	0.50	1/2993 (0.0%)	0.65	0/4092
1	E	0.49	1/2970 (0.0%)	0.63	0/4057
1	G	0.49	1/2964 (0.0%)	0.64	1/4051 (0.0%)
2	B	0.31	0/150	1.04	2/230 (0.9%)
2	D	0.26	0/150	0.76	0/230
2	F	0.40	0/150	0.85	1/230 (0.4%)
2	H	0.32	0/150	0.79	0/230
All	All	0.49	5/12496 (0.0%)	0.67	6/17172 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	20	TRP	CD2-CE2	5.39	1.47	1.41
1	E	20	TRP	CD2-CE2	5.37	1.47	1.41
1	G	281	TRP	CD2-CE2	5.35	1.47	1.41
1	A	281	TRP	CD2-CE2	5.26	1.47	1.41
1	A	20	TRP	CD2-CE2	5.00	1.47	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	DT	P-O3'-C3'	9.78	131.44	119.70
2	B	4	DT	P-O3'-C3'	6.14	127.07	119.70
1	A	134	LEU	CA-CB-CG	5.37	127.66	115.30
1	G	190	LEU	CA-CB-CG	5.33	127.55	115.30
1	A	304	LEU	CA-CB-CG	5.27	127.43	115.30
2	F	3	DT	C1'-O4'-C4'	-5.14	104.96	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1	SER	Peptide

## 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	2897	0	2802	129	0
1	C	2916	0	2810	116	0
1	E	2896	0	2790	123	0
1	G	2889	0	2811	105	0
2	B	137	0	86	6	0
2	D	137	0	86	3	0
2	F	137	0	86	9	0
2	H	137	0	86	9	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	2	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
4	E	2	0	0	0	0
4	G	1	0	0	0	0
5	A	234	0	0	3	0
5	B	6	0	0	0	0
5	C	169	0	0	4	0
5	D	4	0	0	0	0
5	E	186	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	12	0	0	1	0
5	G	216	0	0	8	0
5	H	6	0	0	0	0
All	All	12998	0	11557	480	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 20.

All (480) 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)
2:F:1:DT:H2'	2:F:2:DT:H5'	1.15	1.12
2:H:4:DT:H2''	2:H:5:DT:H72	1.22	1.09
1:A:239:VAL:HG12	1:A:242:VAL:HG12	1.44	1.00
1:A:326:ASN:ND2	1:A:329:PHE:HB2	1.81	0.95
2:H:4:DT:H2''	2:H:5:DT:C7	1.96	0.95
1:E:172:VAL:HG21	1:E:181:LEU:HD13	1.49	0.93
1:E:358:PRO:HA	1:E:383:SER:HB2	1.52	0.91
1:E:242:VAL:HG11	1:E:261:GLY:HA3	1.52	0.90
2:F:1:DT:C2'	2:F:2:DT:H5'	2.00	0.90
1:G:25:CYS:HG	3:G:503:ZN:ZN	0.80	0.87
1:G:137:THR:HG22	1:G:139:LYS:H	1.40	0.86
1:C:154:GLU:HG2	1:C:286:VAL:HG22	1.56	0.85
1:E:21:PHE:HB3	1:E:25:CYS:O	1.76	0.85
1:A:242:VAL:HG11	1:A:261:GLY:CA	2.08	0.83
1:C:342:ARG:HG2	1:C:346:HIS:HB2	1.60	0.83
1:A:326:ASN:HD22	1:A:329:PHE:HB2	1.44	0.82
1:E:145:LYS:HE3	1:E:255:THR:O	1.80	0.82
1:A:239:VAL:CG1	1:A:242:VAL:HG12	2.10	0.81
1:E:266:ASN:HD22	1:E:308:ILE:HG23	1.44	0.81
1:G:237:THR:HB	1:G:259:VAL:HG12	1.63	0.80
1:G:173:LEU:HD21	1:G:201:ALA:HB2	1.62	0.80
1:E:372:ARG:HE	1:E:373:PRO:HD3	1.46	0.79
1:E:26:VAL:H	1:E:27:PRO:HD2	1.47	0.79
1:E:26:VAL:H	1:E:27:PRO:CD	1.96	0.78
1:E:293:VAL:HG11	1:G:293:VAL:HG11	1.64	0.78
1:E:239:VAL:HG12	1:E:242:VAL:HG12	1.64	0.77
1:A:358:PRO:HA	1:A:383:SER:HB3	1.66	0.76
1:A:242:VAL:HG11	1:A:261:GLY:HA2	1.65	0.75
1:G:267:GLN:O	1:G:278:ARG:NH2	2.20	0.75
1:A:71:ILE:CD1	1:A:147:LEU:HD21	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:GLU:HG2	1:C:286:VAL:CG2	2.17	0.75
1:C:159:PRO:O	1:C:162:SER:HB2	1.86	0.75
1:A:304:LEU:HD21	1:A:321:VAL:HG11	1.70	0.74
1:G:380:THR:HG23	1:G:381:ARG:HH21	1.51	0.74
2:B:1:DT:H1'	2:B:2:DT:O5'	1.88	0.74
1:G:72:LEU:O	1:G:76:LEU:HG	1.87	0.73
1:A:305:ILE:HD12	1:A:309:TYR:HD2	1.52	0.73
1:A:165:THR:HG22	1:A:195:LYS:HD2	1.69	0.73
1:G:357:PHE:O	1:G:383:SER:HB2	1.89	0.73
1:A:300:ALA:HB3	1:A:319:THR:O	1.89	0.73
1:C:165:THR:HG22	1:C:195:LYS:HD2	1.70	0.73
1:E:296:ARG:HD2	1:E:356:THR:HG21	1.71	0.72
1:E:227:LEU:HB2	1:E:230:VAL:HG23	1.72	0.72
1:E:242:VAL:HG11	1:E:261:GLY:CA	2.19	0.72
1:G:84:LYS:HG3	1:G:135:GLN:HE22	1.54	0.71
2:H:4:DT:C2'	2:H:5:DT:H72	2.10	0.71
1:G:331:LYS:HG3	1:G:332:GLY:H	1.55	0.71
1:A:278:ARG:NH1	5:A:693:HOH:O	2.23	0.70
1:G:358:PRO:HB3	1:G:384:GLN:HE21	1.56	0.70
1:A:181:LEU:CD1	1:A:238:PHE:HB2	2.21	0.69
1:A:247:PRO:HG3	1:A:276:VAL:HG11	1.74	0.69
1:E:335:ILE:HD12	1:E:349:ILE:HD13	1.75	0.68
1:E:335:ILE:HA	1:E:347:ARG:O	1.93	0.68
1:E:337:ALA:CB	1:E:369:SER:HB2	2.24	0.68
1:E:336:THR:HG21	1:E:341:ASP:HB2	1.75	0.68
1:E:212:VAL:HG23	1:E:213:LEU:HD12	1.75	0.67
1:G:372:ARG:O	1:G:376:VAL:HG23	1.94	0.67
1:C:300:ALA:HB1	1:C:321:VAL:HG12	1.75	0.67
1:C:364:LEU:HD21	1:C:370:LEU:HD11	1.75	0.67
1:E:352:ILE:HD13	1:E:381:ARG:HD2	1.77	0.67
1:A:137:THR:O	1:A:252:ARG:NH2	2.28	0.67
1:C:233:SER:H	1:C:256:GLN:NE2	1.93	0.67
1:G:168:LEU:HD21	1:G:238:PHE:HB3	1.77	0.67
1:G:160:PRO:O	1:G:312:TYR:OH	2.09	0.66
1:C:159:PRO:HA	1:C:264:ASP:OD2	1.94	0.66
1:G:145:LYS:NZ	1:G:255:THR:O	2.28	0.66
1:G:53:CYS:SG	1:G:56:CYS:HB3	2.36	0.65
1:A:233:SER:HB2	1:A:256:GLN:HB3	1.77	0.65
1:A:190:LEU:HG	1:A:194:ASN:HD21	1.59	0.65
1:E:293:VAL:CG1	1:G:293:VAL:HG11	2.26	0.65
1:E:108:LYS:HD3	1:E:109:VAL:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:VAL:HB	1:A:8:GLY:HA2	1.79	0.65
1:C:144:ASN:H	1:C:144:ASN:HD22	1.45	0.65
1:A:150:ALA:O	1:A:284:HIS:O	2.14	0.64
1:E:183:VAL:O	1:E:228:PRO:HD3	1.97	0.64
1:C:22:CYS:O	1:C:26:VAL:HG23	1.98	0.64
1:C:42:CYS:SG	1:C:44:HIS:HB2	2.37	0.64
1:A:334:VAL:HB	1:A:346:HIS:CD2	2.33	0.64
1:A:187:ALA:HB2	5:A:774:HOH:O	1.97	0.64
1:A:293:VAL:HG11	1:C:293:VAL:HG11	1.79	0.63
1:G:160:PRO:HD3	1:G:267:GLN:HE21	1.63	0.63
1:A:79:ILE:HG13	1:A:136:ASP:HB3	1.79	0.63
1:C:115:ASP:HB3	1:G:344:LEU:HD12	1.80	0.63
1:G:84:LYS:HG3	1:G:135:GLN:NE2	2.13	0.63
1:E:252:ARG:HG2	5:E:750:HOH:O	1.98	0.62
1:A:44:HIS:ND1	1:A:56:CYS:SG	2.72	0.62
1:G:382:ALA:HB2	1:G:386:LEU:HD13	1.80	0.62
1:E:238:PHE:HA	1:E:260:LYS:O	2.00	0.62
1:A:158:GLY:O	1:A:164:LYS:HE2	1.98	0.62
1:E:172:VAL:HG21	1:E:181:LEU:CD1	2.24	0.62
1:C:182:VAL:HB	1:C:239:VAL:HG22	1.82	0.62
1:E:297:PHE:HE2	1:E:380:THR:O	1.81	0.62
1:G:29:HIS:CD2	1:G:29:HIS:O	2.53	0.62
1:A:362:LEU:HD23	1:A:388:ILE:HG12	1.82	0.62
1:A:71:ILE:HD13	1:A:147:LEU:HD21	1.81	0.61
1:C:160:PRO:HG3	1:C:380:THR:HG21	1.81	0.61
1:A:355:CYS:O	1:A:381:ARG:NH1	2.30	0.61
1:A:339:HIS:CD2	2:B:3:DT:H5'	2.35	0.61
1:G:319:THR:HG23	1:G:384:GLN:HA	1.82	0.61
2:F:1:DT:H2'	2:F:2:DT:C5'	2.10	0.61
1:E:380:THR:HG22	1:E:381:ARG:NH2	2.16	0.61
1:C:160:PRO:HD3	1:C:267:GLN:NE2	2.16	0.60
1:E:158:GLY:O	1:E:164:LYS:HE2	2.02	0.60
1:G:159:PRO:O	1:G:162:SER:OG	2.11	0.60
1:G:359:VAL:HG13	1:G:385:GLU:HB3	1.83	0.60
1:G:25:CYS:SG	3:G:503:ZN:ZN	1.88	0.60
1:A:315:ALA:HB1	1:A:316:PRO:HD2	1.83	0.60
1:G:377:VAL:HA	1:G:380:THR:HG22	1.84	0.60
1:A:305:ILE:HD12	1:A:309:TYR:CD2	2.35	0.60
1:E:251:ALA:HB2	1:E:281:TRP:CE2	2.35	0.60
1:G:211:THR:HG21	1:G:215:PHE:HZ	1.67	0.60
1:A:21:PHE:CE2	1:A:29:HIS:HB2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:PHE:O	1:A:325:PRO:HD3	2.01	0.59
1:E:156:VAL:HG13	1:E:289:GLU:O	2.02	0.59
1:G:160:PRO:HD3	1:G:267:GLN:NE2	2.17	0.59
1:G:376:VAL:O	1:G:380:THR:HB	2.01	0.59
1:E:321:VAL:O	1:E:321:VAL:HG13	2.01	0.59
1:G:183:VAL:HG22	1:G:226:ARG:O	2.02	0.59
1:C:183:VAL:HG21	1:C:189:MET:HG3	1.84	0.59
1:C:173:LEU:HD21	1:C:201:ALA:HB2	1.85	0.59
1:G:330:GLU:HG2	1:G:334:VAL:HG21	1.84	0.59
1:A:242:VAL:HG11	1:A:261:GLY:HA3	1.85	0.59
1:C:348:THR:HG22	1:C:350:ASP:H	1.68	0.59
1:C:394:GLN:O	1:C:398:LEU:HD12	2.02	0.59
1:C:59:SER:H	1:C:60:PRO:CD	2.16	0.59
1:A:316:PRO:HG3	1:C:295:HIS:CE1	2.38	0.58
1:C:124:CYS:SG	1:C:125:GLY:N	2.73	0.58
1:A:244:TYR:O	1:A:270:CYS:HB3	2.03	0.58
1:A:96:THR:CB	1:A:119:ASN:O	2.51	0.58
2:B:4:DT:H2''	2:B:5:DT:OP2	2.02	0.58
1:C:362:LEU:HD23	1:C:388:ILE:HG12	1.85	0.58
1:A:371:THR:HB	1:A:373:PRO:HD2	1.84	0.58
1:E:296:ARG:CD	1:E:356:THR:HG21	2.32	0.58
1:E:338:TYR:OH	1:E:369:SER:HA	2.03	0.58
1:C:2:ALA:HB3	1:C:20:TRP:CD1	2.39	0.58
1:A:395:LEU:O	1:A:399:LEU:HB2	2.04	0.57
1:C:364:LEU:CD2	1:C:370:LEU:HD11	2.33	0.57
1:E:230:VAL:HG22	2:F:7:DT:H5'	1.86	0.57
1:G:342:ARG:HG2	1:G:346:HIS:HB2	1.84	0.57
1:E:227:LEU:O	1:E:229:GLN:N	2.36	0.57
1:G:14:LYS:HB2	1:G:38:LEU:HD21	1.86	0.57
1:E:100:PRO:HA	1:E:112:VAL:HG22	1.86	0.57
1:A:264:ASP:OD2	1:A:267:GLN:NE2	2.33	0.57
1:E:3:VAL:O	1:E:20:TRP:HB2	2.04	0.57
1:G:380:THR:CG2	1:G:381:ARG:HH21	2.16	0.57
1:E:160:PRO:HB2	1:E:380:THR:CG2	2.35	0.57
1:E:149:ASN:ND2	1:E:257:GLY:HA2	2.21	0.56
1:A:326:ASN:HD21	1:A:329:PHE:HB2	1.70	0.56
1:E:249:ASP:O	1:E:252:ARG:HB3	2.05	0.56
1:C:227:LEU:HD13	2:D:7:DT:OP1	2.06	0.56
1:C:163:GLY:O	1:C:164:LYS:C	2.42	0.56
1:E:251:ALA:HB2	1:E:281:TRP:NE1	2.20	0.56
1:A:186:HIS:CE1	2:B:7:DT:OP1	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:ASP:OD1	1:C:241:GLU:HG2	2.05	0.56
1:G:240:ASP:O	1:G:241:GLU:C	2.43	0.56
1:E:293:VAL:HG11	1:G:293:VAL:CG1	2.33	0.56
1:C:144:ASN:HD22	1:C:144:ASN:N	2.02	0.55
1:C:359:VAL:HG22	1:C:385:GLU:HB2	1.87	0.55
1:C:184:PRO:HD2	1:C:188:SER:OG	2.07	0.55
2:F:6:DT:H2"	2:F:7:DT:H71	1.88	0.55
1:C:297:PHE:HB2	1:C:319:THR:OG1	2.07	0.55
1:C:59:SER:H	1:C:60:PRO:HD2	1.71	0.55
1:E:156:VAL:HG22	1:E:288:LEU:HD12	1.89	0.55
1:A:300:ALA:O	1:A:304:LEU:HD23	2.07	0.55
1:C:249:ASP:HA	1:C:252:ARG:HH11	1.72	0.55
1:E:186:HIS:HA	1:E:189:MET:HB3	1.89	0.55
1:C:4:CYS:HB3	1:C:9:ALA:H	1.73	0.54
1:A:158:GLY:O	1:A:164:LYS:CE	2.55	0.54
1:A:282:LEU:O	1:A:285:PHE:HB2	2.07	0.54
1:A:172:VAL:HG11	1:A:223:ILE:HG21	1.90	0.54
1:A:47:MET:O	1:A:62:GLN:HA	2.08	0.54
1:E:26:VAL:N	1:E:27:PRO:CD	2.66	0.54
1:C:160:PRO:O	1:C:312:TYR:OH	2.18	0.54
1:C:297:PHE:HE2	1:C:380:THR:HG1	1.54	0.54
1:C:352:ILE:HD12	1:C:381:ARG:HG3	1.89	0.53
1:E:147:LEU:O	1:E:150:ALA:HB3	2.08	0.53
1:A:395:LEU:HB3	1:A:401:PHE:HE2	1.73	0.53
1:E:158:GLY:HA3	1:E:164:LYS:HG2	1.91	0.53
1:C:227:LEU:HB3	1:C:228:PRO:HD2	1.91	0.53
1:A:191:ASP:O	1:A:195:LYS:HG3	2.08	0.53
1:C:223:ILE:H	1:C:223:ILE:HD12	1.73	0.53
1:C:335:ILE:HG21	1:C:352:ILE:HD13	1.91	0.53
1:C:47:MET:O	1:C:63:MET:N	2.42	0.53
1:G:137:THR:HG22	1:G:138:LEU:N	2.24	0.53
1:A:321:VAL:HG23	1:A:386:LEU:HB3	1.89	0.53
1:E:29:HIS:CG	1:E:29:HIS:O	2.62	0.53
1:E:321:VAL:CG1	1:E:321:VAL:O	2.57	0.53
1:A:244:TYR:HA	1:A:269:GLY:HA2	1.90	0.53
1:G:331:LYS:HG3	1:G:332:GLY:N	2.24	0.53
1:E:233:SER:H	1:E:256:GLN:NE2	2.08	0.52
1:E:316:PRO:HB2	1:G:166:PHE:HB3	1.90	0.52
1:G:182:VAL:HB	1:G:239:VAL:HG22	1.91	0.52
1:C:12:VAL:H	1:C:22:CYS:HA	1.74	0.52
1:G:50:SER:HB3	1:G:63:MET:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4:CYS:HB3	1:G:9:ALA:H	1.74	0.52
1:C:283:ARG:HD2	1:C:284:HIS:NE2	2.23	0.52
1:E:342:ARG:HD3	1:E:348:THR:HG23	1.91	0.52
1:E:358:PRO:HA	1:E:383:SER:CB	2.31	0.52
1:G:4:CYS:HA	1:G:20:TRP:O	2.10	0.52
1:E:69:HIS:HB3	1:E:72:LEU:HB3	1.90	0.52
1:G:242:VAL:HG12	1:G:262:TYR:O	2.09	0.52
2:H:5:DT:H73	2:H:6:DT:H73	1.91	0.52
1:E:242:VAL:HG13	1:E:262:TYR:O	2.10	0.52
1:A:300:ALA:CB	1:A:319:THR:O	2.58	0.52
1:C:372:ARG:O	1:C:376:VAL:HG23	2.09	0.52
1:E:160:PRO:HB2	1:E:380:THR:HG23	1.92	0.52
1:E:81:TYR:OH	2:F:3:DT:O4	2.22	0.52
1:G:335:ILE:HG22	1:G:347:ARG:HB2	1.92	0.52
1:A:145:LYS:HE2	1:A:255:THR:O	2.10	0.51
1:C:194:ASN:O	1:C:198:GLN:HG3	2.10	0.51
1:E:223:ILE:HG22	1:E:224:THR:N	2.25	0.51
1:E:189:MET:HG2	1:E:215:PHE:HE2	1.75	0.51
1:A:233:SER:H	1:A:256:GLN:HE21	1.59	0.51
1:G:341:ASP:OD2	1:G:366:THR:OG1	2.28	0.51
1:G:266:ASN:O	1:G:373:PRO:HA	2.10	0.51
1:C:165:THR:CG2	1:C:195:LYS:HD2	2.39	0.51
1:E:208:PRO:HB2	1:E:211:THR:HB	1.92	0.51
1:A:137:THR:HG23	1:A:139:LYS:H	1.76	0.51
1:A:161:GLY:HA3	1:A:296:ARG:HB2	1.91	0.51
1:A:98:SER:CB	1:A:99:PRO:HD3	2.41	0.51
1:E:380:THR:CG2	1:E:381:ARG:NH2	2.73	0.51
1:A:190:LEU:HG	1:A:194:ASN:ND2	2.25	0.51
1:E:296:ARG:NE	1:E:356:THR:HG21	2.26	0.51
1:A:112:VAL:HA	1:A:120:ILE:O	2.11	0.51
1:A:160:PRO:HD3	1:A:267:GLN:NE2	2.26	0.51
1:A:82:GLY:O	1:A:83:SER:HB2	2.11	0.51
1:A:374:ARG:NH2	2:B:2:DT:O2	2.38	0.51
2:H:5:DT:C7	2:H:6:DT:H73	2.41	0.51
1:A:315:ALA:HB1	1:A:316:PRO:CD	2.41	0.50
1:C:376:VAL:O	1:C:380:THR:CG2	2.59	0.50
1:E:108:LYS:HD3	1:E:109:VAL:N	2.25	0.50
1:E:355:CYS:O	1:E:381:ARG:NH1	2.42	0.50
1:A:181:LEU:HD12	1:A:238:PHE:HB2	1.91	0.50
1:A:4:CYS:HB3	1:A:8:GLY:H	1.76	0.50
1:E:79:ILE:HD13	1:E:136:ASP:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LEU:HD12	1:A:379:VAL:HG11	1.93	0.50
1:A:360:VAL:HB	1:A:382:ALA:HB2	1.93	0.50
1:E:50:SER:OG	1:E:51:THR:N	2.45	0.50
1:C:98:SER:HB2	1:C:99:PRO:CD	2.42	0.50
1:C:98:SER:HB2	1:C:99:PRO:HD2	1.92	0.50
1:G:168:LEU:O	1:G:172:VAL:HG23	2.11	0.50
1:E:104:LYS:HG2	1:E:106:GLY:H	1.76	0.50
1:E:352:ILE:CD1	1:E:381:ARG:HD2	2.39	0.50
1:E:183:VAL:HG21	1:E:189:MET:HB2	1.94	0.49
1:E:251:ALA:HA	1:E:254:LEU:HD12	1.94	0.49
1:G:26:VAL:HG12	1:G:64:VAL:HG11	1.93	0.49
1:A:177:GLY:C	1:A:222:ASN:HD21	2.16	0.49
1:C:315:ALA:HB1	1:C:316:PRO:HD2	1.93	0.49
1:E:149:ASN:HD22	1:E:257:GLY:HA2	1.77	0.49
1:E:251:ALA:HB2	1:E:281:TRP:CZ2	2.46	0.49
1:C:38:LEU:HD23	5:C:620:HOH:O	2.11	0.49
1:C:377:VAL:O	1:C:381:ARG:HG2	2.13	0.49
1:A:79:ILE:HG13	1:A:136:ASP:CB	2.42	0.49
1:C:376:VAL:O	1:C:380:THR:HG22	2.13	0.49
1:E:83:SER:O	1:E:133:PRO:HG2	2.13	0.49
1:G:297:PHE:HE2	1:G:380:THR:O	1.96	0.49
1:A:299:ALA:N	1:A:314:PRO:HB3	2.28	0.49
1:A:183:VAL:O	1:A:228:PRO:HD3	2.13	0.48
1:A:169:VAL:HG22	1:A:196:LEU:HD13	1.95	0.48
2:F:2:DT:H2''	2:F:3:DT:O5'	2.14	0.48
1:G:377:VAL:O	1:G:381:ARG:HG2	2.13	0.48
1:A:294:CYS:SG	1:A:297:PHE:CE1	3.07	0.48
1:A:99:PRO:HB2	1:A:103:TYR:OH	2.13	0.48
1:E:372:ARG:N	1:E:373:PRO:HD2	2.29	0.48
1:A:104:LYS:HG2	1:A:106:GLY:H	1.77	0.48
1:C:6:VAL:O	1:C:144:ASN:ND2	2.46	0.48
1:C:226:ARG:HD3	1:C:232:THR:O	2.13	0.48
1:A:226:ARG:NH2	1:A:230:VAL:O	2.37	0.48
1:E:189:MET:HG2	1:E:215:PHE:CE2	2.49	0.48
1:A:134:LEU:HD12	1:A:134:LEU:O	2.12	0.48
1:G:358:PRO:HA	1:G:383:SER:HB3	1.94	0.48
1:G:62:GLN:NE2	1:G:64:VAL:O	2.47	0.48
1:C:122:PHE:C	1:C:124:CYS:H	2.17	0.48
1:E:316:PRO:HB3	1:G:167:HIS:CD2	2.49	0.48
1:E:110:VAL:HG12	1:E:123:GLY:HA3	1.95	0.48
1:A:167:HIS:HA	1:A:170:LYS:HE2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:245:PHE:HD2	1:G:249:ASP:HB3	1.79	0.48
1:A:366:THR:O	1:A:369:SER:HB3	2.14	0.48
1:A:5:THR:O	1:A:143:VAL:HG23	2.13	0.48
1:E:247:PRO:HG3	1:E:276:VAL:HG11	1.95	0.48
1:A:72:LEU:O	1:A:76:LEU:HG	2.13	0.47
1:C:168:LEU:CD1	1:C:240:ASP:HB2	2.44	0.47
1:E:181:LEU:HD23	1:E:192:CYS:HB3	1.95	0.47
1:G:26:VAL:N	1:G:27:PRO:CD	2.77	0.47
1:G:282:LEU:HA	1:G:285:PHE:CD1	2.49	0.47
1:E:227:LEU:C	1:E:229:GLN:H	2.16	0.47
1:E:363:ARG:NH2	5:E:654:HOH:O	2.46	0.47
1:E:339:HIS:HA	1:E:342:ARG:HB2	1.95	0.47
1:G:374:ARG:O	1:G:378:ALA:CB	2.62	0.47
1:C:336:THR:HG22	1:C:363:ARG:HB2	1.96	0.47
1:E:132:VAL:HG22	1:E:133:PRO:HD2	1.95	0.47
1:E:228:PRO:HB3	1:E:253:ILE:HD11	1.97	0.47
2:H:3:DT:H2''	2:H:4:DT:H5'	1.97	0.47
1:A:71:ILE:CD1	1:A:147:LEU:CD2	2.88	0.47
1:A:172:VAL:HG12	1:A:223:ILE:HG12	1.97	0.47
1:C:321:VAL:O	1:C:321:VAL:HG13	2.14	0.47
1:G:350:ASP:OD1	1:G:374:ARG:NE	2.46	0.47
1:A:352:ILE:HD13	1:A:381:ARG:HD2	1.97	0.47
1:A:365:PRO:O	1:A:392:PHE:HE1	1.98	0.47
1:A:380:THR:O	1:A:380:THR:HG23	2.15	0.47
1:C:250:LEU:HA	1:C:253:ILE:HD12	1.97	0.47
1:E:335:ILE:HD13	1:E:381:ARG:HG3	1.96	0.47
1:G:363:ARG:NE	1:G:389:TYR:CD2	2.80	0.47
1:A:242:VAL:HG22	1:A:263:GLY:HA3	1.95	0.47
1:C:362:LEU:HD13	1:C:378:ALA:HB1	1.96	0.46
1:G:138:LEU:O	1:G:139:LYS:C	2.51	0.46
1:A:208:PRO:O	1:A:211:THR:HG22	2.16	0.46
1:C:265:LEU:HD21	1:C:282:LEU:HD12	1.96	0.46
1:C:266:ASN:HD22	1:C:372:ARG:HH21	1.62	0.46
1:G:226:ARG:NH2	1:G:231:GLY:O	2.48	0.46
1:G:32:HIS:HE2	1:G:80:ASP:CG	2.18	0.46
1:C:141:VAL:HG12	1:C:142:VAL:N	2.31	0.46
1:E:334:VAL:HG11	1:E:346:HIS:CE1	2.50	0.46
1:G:163:GLY:O	1:G:166:PHE:HB2	2.16	0.46
1:C:371:THR:CG2	5:C:653:HOH:O	2.64	0.46
1:E:186:HIS:CE1	1:E:227:LEU:HD11	2.50	0.46
1:G:157:GLU:OE1	1:G:311:TYR:OH	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:ALA:HB3	1:C:319:THR:O	2.16	0.46
1:E:171:ASP:HB3	1:E:238:PHE:CE2	2.51	0.46
2:F:1:DT:H1'	5:F:106:HOH:O	2.15	0.46
1:G:190:LEU:HG	5:G:684:HOH:O	2.15	0.46
1:A:202:ASP:O	1:A:221:GLY:HA3	2.16	0.45
1:C:191:ASP:O	1:C:195:LYS:HG3	2.15	0.45
1:E:223:ILE:CG2	1:E:224:THR:N	2.79	0.45
1:E:337:ALA:HB3	1:E:369:SER:HB2	1.95	0.45
1:A:166:PHE:O	1:A:170:LYS:HB2	2.17	0.45
1:G:217:ARG:HG3	5:G:658:HOH:O	2.17	0.45
1:A:250:LEU:O	1:A:251:ALA:C	2.55	0.45
1:E:69:HIS:HA	1:E:70:PRO:HD2	1.70	0.45
1:A:182:VAL:HG13	1:A:226:ARG:HG3	1.97	0.45
1:C:185:THR:HB	2:D:6:DT:OP1	2.17	0.45
2:H:2:DT:H2''	2:H:3:DT:C6	2.52	0.45
1:A:351:SER:HB2	5:A:780:HOH:O	2.16	0.45
1:C:151:ALA:HA	1:C:284:HIS:O	2.16	0.45
1:G:363:ARG:HD2	1:G:389:TYR:HB3	1.98	0.45
1:G:69:HIS:O	1:G:73:ASP:HB2	2.15	0.45
1:G:66:LYS:HB3	5:G:737:HOH:O	2.15	0.45
1:A:297:PHE:HE2	1:A:380:THR:O	2.00	0.45
1:C:99:PRO:HA	1:C:100:PRO:HD3	1.90	0.45
1:A:35:THR:HB	1:A:46:ILE:HG22	1.98	0.45
1:E:360:VAL:HB	1:E:382:ALA:HB2	1.99	0.45
1:A:372:ARG:O	1:A:376:VAL:HG23	2.16	0.44
1:E:363:ARG:HG2	1:E:389:TYR:HB3	1.99	0.44
1:A:248:VAL:O	1:A:252:ARG:HB2	2.17	0.44
1:A:99:PRO:HA	1:A:100:PRO:HD3	1.73	0.44
1:E:163:GLY:O	1:E:164:LYS:C	2.54	0.44
1:G:215:PHE:CD1	1:G:215:PHE:N	2.84	0.44
1:A:376:VAL:O	1:A:380:THR:HB	2.18	0.44
1:E:26:VAL:HG12	1:E:64:VAL:HG11	1.98	0.44
1:E:297:PHE:HD2	1:E:382:ALA:O	2.01	0.44
1:E:384:GLN:HA	1:E:384:GLN:HE21	1.82	0.44
1:A:104:LYS:HG2	1:A:106:GLY:N	2.32	0.44
1:A:79:ILE:C	1:A:81:TYR:H	2.21	0.44
1:E:166:PHE:HB3	1:G:316:PRO:O	2.18	0.44
1:G:297:PHE:CE2	1:G:380:THR:O	2.70	0.44
1:G:159:PRO:HB2	1:G:312:TYR:CZ	2.53	0.44
1:G:331:LYS:HG2	5:G:696:HOH:O	2.17	0.44
1:A:336:THR:HG21	1:A:341:ASP:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:TYR:HB2	1:E:285:PHE:CD2	2.52	0.44
1:E:35:THR:O	1:E:45:ASP:HA	2.17	0.44
1:A:100:PRO:HA	1:A:112:VAL:HG21	1.99	0.43
1:C:286:VAL:CG2	1:C:286:VAL:O	2.65	0.43
1:A:340:LYS:HB2	1:E:94:GLY:HA2	1.99	0.43
1:G:183:VAL:HG23	1:G:227:LEU:HD23	1.98	0.43
1:G:273:PRO:HG2	1:G:276:VAL:HG23	2.00	0.43
1:C:266:ASN:O	1:C:373:PRO:HA	2.18	0.43
1:C:5:THR:O	1:C:142:VAL:HA	2.18	0.43
1:A:71:ILE:HD13	1:A:147:LEU:CD2	2.47	0.43
1:C:233:SER:N	1:C:256:GLN:NE2	2.64	0.43
1:E:265:LEU:C	1:E:267:GLN:H	2.21	0.43
1:E:266:ASN:ND2	1:E:308:ILE:HG23	2.23	0.43
1:A:337:ALA:O	1:A:348:THR:HG23	2.18	0.43
1:C:239:VAL:CG1	1:C:242:VAL:HG13	2.49	0.43
1:C:379:VAL:HG21	1:C:399:LEU:HD21	2.01	0.43
1:A:167:HIS:HE1	5:C:694:HOH:O	2.01	0.43
1:A:362:LEU:HD11	1:A:364:LEU:HD21	2.01	0.43
1:C:182:VAL:HG11	1:C:253:ILE:HG12	2.00	0.43
1:E:228:PRO:HG3	1:E:245:PHE:HE2	1.84	0.43
1:E:160:PRO:HB2	1:E:380:THR:HG21	2.00	0.43
1:A:13:ALA:HB1	1:A:35:THR:HG22	1.99	0.43
1:A:251:ALA:HB2	1:A:281:TRP:CZ2	2.53	0.43
1:G:308:ILE:HD12	1:G:372:ARG:HH21	1.83	0.43
1:C:17:CYS:SG	1:C:138:LEU:HD12	2.58	0.43
1:E:108:LYS:CD	1:E:109:VAL:H	2.29	0.43
1:G:168:LEU:CD2	1:G:238:PHE:HB3	2.46	0.43
1:A:172:VAL:HG11	1:A:223:ILE:CG2	2.48	0.43
1:A:186:HIS:CE1	1:A:208:PRO:HB3	2.54	0.43
1:C:202:ASP:O	1:C:221:GLY:HA3	2.18	0.43
1:E:110:VAL:HG12	1:E:124:CYS:H	1.83	0.43
1:E:349:ILE:HA	1:E:352:ILE:HD11	1.99	0.43
1:A:46:ILE:C	1:A:48:TYR:H	2.22	0.43
1:G:250:LEU:HA	1:G:253:ILE:HD12	2.00	0.43
1:G:372:ARG:HD3	5:G:638:HOH:O	2.19	0.43
2:H:7:DT:O4'	2:H:7:DT:O2	2.36	0.43
1:C:244:TYR:HA	1:C:269:GLY:HA2	2.01	0.42
2:F:4:DT:O3'	2:F:5:DT:O2	2.37	0.42
1:G:5:THR:O	1:G:142:VAL:HA	2.19	0.42
1:G:321:VAL:HB	1:G:386:LEU:HB3	2.00	0.42
1:E:166:PHE:HB3	1:G:316:PRO:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:60:PRO:HD3	5:G:757:HOH:O	2.19	0.42
1:A:17:CYS:SG	1:A:29:HIS:HE1	2.42	0.42
1:C:0:MET:O	1:C:1:SER:OG	2.20	0.42
1:G:330:GLU:HG2	1:G:334:VAL:CG2	2.49	0.42
1:C:164:LYS:HG2	1:C:165:THR:N	2.34	0.42
1:E:160:PRO:CB	1:E:380:THR:HG21	2.50	0.42
1:G:185:THR:HG1	1:G:188:SER:H	1.67	0.42
1:G:11:PRO:HA	1:G:22:CYS:HA	2.01	0.42
1:C:371:THR:HG21	5:C:653:HOH:O	2.19	0.42
1:C:70:PRO:HB2	1:C:71:ILE:HD12	2.01	0.42
1:C:137:THR:HG23	1:C:139:LYS:H	1.85	0.42
1:E:201:ALA:O	1:E:203:PRO:HD3	2.19	0.42
1:E:371:THR:HB	1:E:373:PRO:HD2	2.01	0.42
1:G:47:MET:HA	1:G:64:VAL:HB	2.02	0.42
1:E:47:MET:HA	1:E:64:VAL:HB	2.01	0.42
1:G:190:LEU:HD21	1:G:214:ASP:O	2.20	0.42
1:G:26:VAL:CG1	1:G:64:VAL:HG11	2.50	0.42
1:C:344:LEU:O	1:C:346:HIS:HD2	2.03	0.42
1:C:363:ARG:HD2	1:C:389:TYR:HD2	1.84	0.42
1:E:155:TYR:HB2	1:E:285:PHE:HD2	1.84	0.42
1:E:15:SER:HB3	1:E:35:THR:CG2	2.50	0.42
1:G:32:HIS:NE2	1:G:80:ASP:OD2	2.52	0.42
1:A:239:VAL:HG12	1:A:242:VAL:CG1	2.31	0.42
1:A:67:VAL:HA	1:A:68:PRO:HD3	1.92	0.42
1:C:366:THR:HA	1:C:367:PRO:HD3	1.89	0.42
1:C:188:SER:HA	1:C:191:ASP:HB2	2.02	0.42
1:C:317:HIS:HB2	1:C:318:THR:H	1.53	0.42
1:C:352:ILE:CD1	1:C:381:ARG:HG3	2.50	0.42
1:A:21:PHE:CZ	1:A:29:HIS:ND1	2.88	0.41
1:C:351:SER:OG	2:D:4:DT:OP1	2.36	0.41
1:A:323:PHE:HZ	1:A:401:PHE:CZ	2.38	0.41
1:E:363:ARG:HD2	1:E:389:TYR:CD2	2.55	0.41
2:H:4:DT:H2"	2:H:5:DT:C5	2.54	0.41
1:A:350:ASP:OD2	2:B:3:DT:H1'	2.20	0.41
1:C:389:TYR:CE1	1:C:391:PRO:HD3	2.55	0.41
1:G:282:LEU:O	1:G:285:PHE:HB2	2.20	0.41
1:G:357:PHE:C	1:G:383:SER:HB2	2.40	0.41
1:A:27:PRO:HB2	1:A:67:VAL:HG22	2.02	0.41
1:C:132:VAL:HG22	1:C:133:PRO:HD2	2.02	0.41
1:G:47:MET:HG2	1:G:48:TYR:N	2.35	0.41
1:G:84:LYS:HG2	1:G:132:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ALA:HB1	1:A:258:ARG:HD3	2.02	0.41
1:C:171:ASP:OD2	1:C:262:TYR:OH	2.33	0.41
1:E:98:SER:H	1:E:99:PRO:CD	2.33	0.41
1:A:297:PHE:O	1:A:315:ALA:HB3	2.20	0.41
1:C:286:VAL:HG23	1:C:286:VAL:O	2.20	0.41
1:C:372:ARG:N	1:C:373:PRO:CD	2.84	0.41
1:C:395:LEU:O	1:C:399:LEU:HB2	2.20	0.41
1:E:49:ARG:HG2	1:E:50:SER:N	2.35	0.41
1:G:148:LYS:NZ	1:G:149:ASN:OD1	2.53	0.41
1:G:278:ARG:HD2	5:G:706:HOH:O	2.19	0.41
1:G:320:LYS:HD2	1:G:322:VAL:HG23	2.03	0.41
1:A:147:LEU:HD22	1:A:281:TRP:CZ3	2.55	0.41
1:E:171:ASP:O	1:E:175:VAL:HG23	2.21	0.41
1:A:298:GLY:HA2	1:A:315:ALA:H	1.85	0.41
1:A:380:THR:O	1:A:380:THR:CG2	2.67	0.41
1:C:331:LYS:HD2	1:C:359:VAL:HG11	2.02	0.41
1:E:264:ASP:OD2	1:E:267:GLN:HG3	2.21	0.41
1:E:49:ARG:CG	1:E:50:SER:N	2.84	0.41
1:C:363:ARG:HD2	1:C:389:TYR:CD2	2.56	0.41
1:C:69:HIS:HA	1:C:70:PRO:HD3	1.93	0.41
1:A:335:ILE:HD12	1:A:349:ILE:HG12	2.03	0.41
1:G:172:VAL:HG22	1:G:238:PHE:CD1	2.56	0.41
1:C:228:PRO:HG3	1:C:245:PHE:HE2	1.86	0.40
1:C:310:PRO:O	1:C:312:TYR:N	2.54	0.40
1:G:155:TYR:HD2	1:G:287:SER:OG	2.03	0.40
1:A:132:VAL:HG22	1:A:133:PRO:HD2	2.04	0.40
1:C:268:LEU:HD23	1:C:373:PRO:HB2	2.03	0.40
1:E:47:MET:HG3	1:E:62:GLN:HG3	2.03	0.40
1:G:246:SER:HA	1:G:270:CYS:SG	2.61	0.40
1:C:109:VAL:O	1:C:109:VAL:HG23	2.22	0.40
1:C:10:ALA:HA	1:C:11:PRO:HD3	1.84	0.40
1:C:273:PRO:HG2	1:C:276:VAL:HG23	2.03	0.40
1:C:141:VAL:HG13	1:C:251:ALA:HB1	2.04	0.40
1:C:240:ASP:OD1	1:C:241:GLU:N	2.54	0.40
1:C:264:ASP:OD1	1:C:266:ASN:HB2	2.21	0.40
1:A:335:ILE:HA	1:A:347:ARG:O	2.22	0.40
1:C:180:THR:O	1:C:237:THR:HA	2.20	0.40
1:C:283:ARG:HD2	1:C:284:HIS:CE1	2.57	0.40
1:C:370:LEU:HD23	1:C:374:ARG:HD2	2.03	0.40
1:G:271:VAL:HG22	5:G:730:HOH:O	2.21	0.40

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	383/423 (90%)	316 (82%)	54 (14%)	13 (3%)	3	4
1	C	390/423 (92%)	324 (83%)	49 (13%)	17 (4%)	2	2
1	E	386/423 (91%)	332 (86%)	45 (12%)	9 (2%)	6	8
1	G	385/423 (91%)	326 (85%)	48 (12%)	11 (3%)	4	6
All	All	1544/1692 (91%)	1298 (84%)	196 (13%)	50 (3%)	4	5

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	THR
1	A	98	SER
1	A	159	PRO
1	A	165	THR
1	C	118	GLY
1	C	143	VAL
1	G	393	ASP
1	C	1	SER
1	C	59	SER
1	C	106	GLY
1	C	141	VAL
1	C	311	TYR
1	C	343	GLY
1	E	266	ASN
1	G	120	ILE
1	G	123	GLY
1	G	221	GLY
1	A	46	ILE
1	A	299	ALA
1	C	133	PRO
1	C	314	PRO
1	E	50	SER

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Mol	Chain	Res	Type
1	E	287	SER
1	G	53	CYS
1	G	109	VAL
1	G	184	PRO
1	G	350	ASP
1	A	17	CYS
1	A	30	ALA
1	A	314	PRO
1	C	184	PRO
1	G	203	PRO
1	C	138	LEU
1	E	26	VAL
1	G	80	ASP
1	A	251	ALA
1	C	58	GLY
1	E	70	PRO
1	E	100	PRO
1	E	279	ASN
1	G	57	GLU
1	C	113	VAL
1	C	310	PRO
1	E	98	SER
1	E	228	PRO
1	C	358	PRO
1	A	316	PRO
1	A	125	GLY
1	C	142	VAL
1	A	158	GLY

### 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	300/352 (85%)	264 (88%)	36 (12%)	5	7
1	C	301/352 (86%)	265 (88%)	36 (12%)	5	7
1	E	298/352 (85%)	265 (89%)	33 (11%)	6	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	300/352 (85%)	273 (91%)	27 (9%)	9 14
All	All	1199/1408 (85%)	1067 (89%)	132 (11%)	6 9

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	CYS
1	A	35	THR
1	A	51	THR
1	A	53	CYS
1	A	56	CYS
1	A	64	VAL
1	A	89	LEU
1	A	129	HIS
1	A	134	LEU
1	A	136	ASP
1	A	137	THR
1	A	144	ASN
1	A	147	LEU
1	A	153	SER
1	A	168	LEU
1	A	182	VAL
1	A	196	LEU
1	A	214	ASP
1	A	226	ARG
1	A	236	GLU
1	A	246	SER
1	A	270	CYS
1	A	283	ARG
1	A	296	ARG
1	A	297	PHE
1	A	308	ILE
1	A	326	ASN
1	A	331	LYS
1	A	336	THR
1	A	355	CYS
1	A	361	THR
1	A	371	THR
1	A	380	THR
1	A	384	GLN
1	A	386	LEU
1	A	398	LEU

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Mol	Chain	Res	Type
1	C	12	VAL
1	C	22	CYS
1	C	42	CYS
1	C	44	HIS
1	C	51	THR
1	C	55	MET
1	C	64	VAL
1	C	75	LEU
1	C	88	THR
1	C	112	VAL
1	C	122	PHE
1	C	132	VAL
1	C	137	THR
1	C	144	ASN
1	C	162	SER
1	C	164	LYS
1	C	188	SER
1	C	220	SER
1	C	234	GLU
1	C	242	VAL
1	C	256	GLN
1	C	286	VAL
1	C	293	VAL
1	C	297	PHE
1	C	304	LEU
1	C	317	HIS
1	C	318	THR
1	C	350	ASP
1	C	356	THR
1	C	358	PRO
1	C	359	VAL
1	C	362	LEU
1	C	371	THR
1	C	380	THR
1	C	393	ASP
1	C	395	LEU
1	E	4	CYS
1	E	12	VAL
1	E	35	THR
1	E	107	HIS
1	E	112	VAL
1	E	132	VAL

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Mol	Chain	Res	Type
1	E	145	LYS
1	E	147	LEU
1	E	165	THR
1	E	166	PHE
1	E	176	VAL
1	E	181	LEU
1	E	210	TYR
1	E	220	SER
1	E	224	THR
1	E	230	VAL
1	E	233	SER
1	E	242	VAL
1	E	256	GLN
1	E	258	ARG
1	E	270	CYS
1	E	297	PHE
1	E	306	LYS
1	E	312	TYR
1	E	336	THR
1	E	339	HIS
1	E	341	ASP
1	E	348	THR
1	E	355	CYS
1	E	357	PHE
1	E	363	ARG
1	E	384	GLN
1	E	398	LEU
1	G	36	THR
1	G	51	THR
1	G	66	LYS
1	G	75	LEU
1	G	88	THR
1	G	132	VAL
1	G	145	LYS
1	G	156	VAL
1	G	164	LYS
1	G	168	LEU
1	G	192	CYS
1	G	215	PHE
1	G	226	ARG
1	G	287	SER
1	G	291	LEU

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Mol	Chain	Res	Type
1	G	304	LEU
1	G	306	LYS
1	G	312	TYR
1	G	321	VAL
1	G	322	VAL
1	G	340	LYS
1	G	371	THR
1	G	380	THR
1	G	383	SER
1	G	385	GLU
1	G	395	LEU
1	G	399	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	74	HIS
1	A	144	ASN
1	A	186	HIS
1	A	194	ASN
1	A	222	ASN
1	A	256	GLN
1	A	266	ASN
1	A	326	ASN
1	A	384	GLN
1	C	74	HIS
1	C	144	ASN
1	C	256	GLN
1	C	266	ASN
1	C	267	GLN
1	C	346	HIS
1	E	149	ASN
1	E	186	HIS
1	E	222	ASN
1	E	256	GLN
1	E	266	ASN
1	E	384	GLN
1	G	62	GLN
1	G	69	HIS
1	G	135	GLN
1	G	144	ASN

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Mol	Chain	Res	Type
1	G	167	HIS
1	G	186	HIS
1	G	198	GLN
1	G	256	GLN
1	G	267	GLN
1	G	384	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 19 are monoatomic - leaving 0 for Mogul analysis.

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, 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	395/423 (93%)	0.76	32 (8%)	12   9	26, 48, 69, 83	0
1	C	398/423 (94%)	0.75	32 (8%)	12   9	27, 49, 67, 87	1 (0%)
1	E	396/423 (93%)	0.85	40 (10%)	7   4	30, 50, 72, 85	0
1	G	393/423 (92%)	0.81	40 (10%)	6   4	29, 50, 73, 94	0
2	B	7/7 (100%)	1.05	1 (14%)	2   1	54, 57, 67, 73	3 (42%)
2	D	7/7 (100%)	1.37	2 (28%)	0   0	60, 65, 67, 67	4 (57%)
2	F	7/7 (100%)	0.85	1 (14%)	2   1	54, 60, 63, 71	4 (57%)
2	H	7/7 (100%)	0.79	1 (14%)	2   1	49, 54, 62, 64	4 (57%)
All	All	1610/1720 (93%)	0.79	149 (9%)	8   7	26, 50, 70, 94	16 (0%)

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	335	ILE	6.7
1	E	62	GLN	5.4
1	C	297	PHE	4.9
1	A	177	GLY	4.9
1	C	344	LEU	4.8
1	G	55	MET	4.6
1	E	48	TYR	4.6
1	G	307	GLY	4.6
1	E	215	PHE	4.6
1	A	109	VAL	4.5
1	E	116	VAL	4.4
1	E	112	VAL	4.4
1	G	388	ILE	4.3
1	A	91	VAL	4.2
1	C	337	ALA	4.0
1	G	56	CYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	343	GLY	3.9
1	A	82	GLY	3.9
1	C	60	PRO	3.9
1	C	348	THR	3.9
1	E	179	ALA	3.8
1	C	128	SER	3.8
1	E	225	VAL	3.8
1	G	51	THR	3.8
1	G	132	VAL	3.8
1	G	112	VAL	3.7
1	A	307	GLY	3.7
1	E	307	GLY	3.7
2	D	1	DT	3.7
1	G	61	LYS	3.6
1	C	109	VAL	3.5
1	C	336	THR	3.5
1	C	108	LYS	3.4
1	E	55	MET	3.3
1	G	113	VAL	3.3
1	E	105	VAL	3.2
1	A	188	SER	3.2
1	E	124	CYS	3.2
1	E	93	ASP	3.2
1	G	108	LYS	3.2
1	G	15	SER	3.2
1	A	223	ILE	3.1
1	C	132	VAL	3.1
2	H	1	DT	3.1
1	E	321	VAL	3.1
1	A	111	ALA	3.1
1	G	31	GLY	3.1
1	E	371	THR	3.1
1	E	129	HIS	3.1
1	E	108	LYS	3.0
1	G	87	LEU	3.0
1	G	19	GLY	3.0
1	G	50	SER	3.0
1	A	220	SER	2.9
1	A	225	VAL	2.9
1	C	105	VAL	2.9
1	C	10	ALA	2.9
1	G	65	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	9	ALA	2.9
1	G	205	PHE	2.9
1	E	3	VAL	2.9
1	E	365	PRO	2.9
1	G	53	CYS	2.9
1	G	192	CYS	2.9
1	A	389	TYR	2.9
1	C	59	SER	2.8
1	C	287	SER	2.8
1	E	213	LEU	2.8
1	G	294	CYS	2.8
1	G	59	SER	2.8
1	E	325	PRO	2.8
1	A	122	PHE	2.8
1	E	109	VAL	2.8
1	E	160	PRO	2.8
1	G	152	ALA	2.7
1	E	82	GLY	2.7
1	G	29	HIS	2.7
1	E	71	ILE	2.7
1	G	195	LYS	2.7
1	C	217	ARG	2.6
1	C	50	SER	2.6
1	A	237	THR	2.6
1	A	16	ALA	2.6
1	A	92	ALA	2.6
1	E	324	VAL	2.6
1	A	131	ALA	2.5
1	C	12	VAL	2.5
1	E	188	SER	2.5
1	G	365	PRO	2.5
1	E	387	TYR	2.5
1	G	84	LYS	2.5
1	C	70	PRO	2.5
1	A	110	VAL	2.5
1	C	315	ALA	2.5
1	E	175	VAL	2.5
1	A	103	TYR	2.5
1	G	124	CYS	2.5
2	F	1	DT	2.4
1	C	308	ILE	2.4
1	G	217	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	216	PRO	2.4
1	A	398	LEU	2.4
1	A	105	VAL	2.4
1	C	51	THR	2.4
1	E	275	SER	2.4
1	G	345	GLY	2.4
1	G	207	VAL	2.3
1	E	369	SER	2.3
1	E	308	ILE	2.3
1	A	96	THR	2.3
1	A	98	SER	2.3
1	A	54	THR	2.3
1	G	126	PRO	2.3
1	C	65	PRO	2.3
1	C	386	LEU	2.3
1	A	6	VAL	2.3
1	C	398	LEU	2.2
1	A	209	LYS	2.2
1	G	117	GLY	2.2
2	D	6	DT	2.2
1	G	203	PRO	2.2
1	C	212	VAL	2.2
1	E	182	VAL	2.2
1	G	11	PRO	2.2
1	A	23	GLY	2.2
1	C	113	VAL	2.1
1	E	58	GLY	2.1
1	E	240	ASP	2.1
1	A	146	ALA	2.1
1	G	83	SER	2.1
1	A	44	HIS	2.1
1	E	311	TYR	2.1
2	B	7	DT	2.1
1	C	123	GLY	2.1
1	A	106	GLY	2.1
1	G	46	ILE	2.1
1	C	39	PHE	2.1
1	A	93	ASP	2.1
1	C	106	GLY	2.1
1	E	268	LEU	2.0
1	E	100	PRO	2.0
1	G	159	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	299	ALA	2.0
1	G	173	LEU	2.0
1	A	338	TYR	2.0
1	G	326	ASN	2.0
1	E	329	PHE	2.0
1	E	290	PRO	2.0
1	G	224	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	CA	E	504	1/1	0.75	0.14	65,65,65,65	0
4	CA	A	504	1/1	0.83	0.21	58,58,58,58	0
4	CA	A	505	1/1	0.88	0.16	77,77,77,77	0
4	CA	C	505	1/1	0.91	0.20	58,58,58,58	0
3	ZN	A	502	1/1	0.93	0.11	73,73,73,73	0
3	ZN	G	501	1/1	0.94	0.11	52,52,52,52	0
3	ZN	G	503	1/1	0.95	0.12	64,64,64,64	0
4	CA	G	504	1/1	0.95	0.15	38,38,38,38	0
3	ZN	G	502	1/1	0.95	0.13	78,78,78,78	0
3	ZN	E	502	1/1	0.95	0.09	69,69,69,69	0
3	ZN	C	502	1/1	0.97	0.10	83,83,83,83	0
3	ZN	E	503	1/1	0.98	0.18	62,62,62,62	0
3	ZN	A	501	1/1	0.98	0.18	53,53,53,53	0
4	CA	C	504	1/1	0.98	0.21	46,46,46,46	0
4	CA	E	505	1/1	0.98	0.22	61,61,61,61	0
3	ZN	E	501	1/1	0.99	0.11	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	A	503	1/1	0.99	0.12	46,46,46,46	0
3	ZN	C	503	1/1	0.99	0.12	41,41,41,41	0
3	ZN	C	501	1/1	0.99	0.15	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.