



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:14 AM GMT

PDB ID : 3HM7  
Title : Crystal structure of allantoinase from *Bacillus halodurans* C-125  
Authors : Patskovsky, Y.; Romero, R.; Rutter, M.; Miller, S.; Wasserman, S.R.; Sauder, J.M.; Raushel, F.M.; Burley, S.K.; Almo, S.C.; New York Structural Genomix Research Consortium (Nysgxrc); New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2009-05-28  
Resolution : 2.60 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

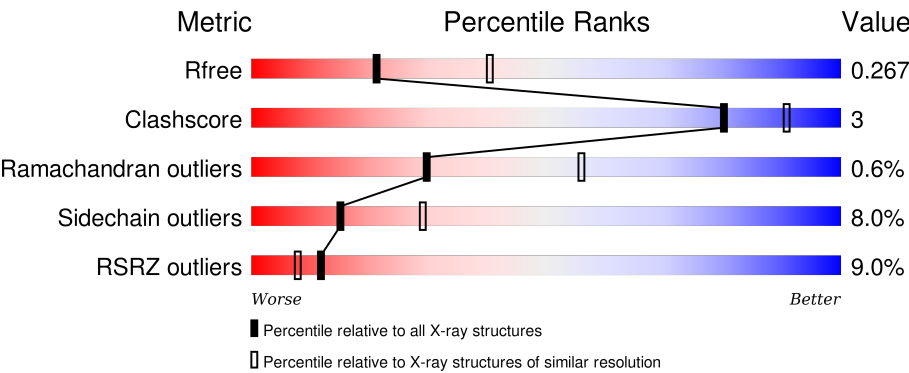
MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

# 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 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	448	<div><div>7%</div><div>82%14% . .</div></div>
1	B	448	<div><div>6%</div><div>82%15% . .</div></div>
1	C	448	<div><div>28%</div><div>78%18% . .</div></div>
1	D	448	<div><div>7%</div><div>81%15% . .</div></div>
1	E	448	<div><div>3%</div><div>87%10% . .</div></div>

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Mol	Chain	Length	Quality of chain
1	F	448	<div><div></div><div>2%</div><div>84%</div><div>13%</div><div>••</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20901 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 Allantoinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	4	0
			3425	2166	593	649	17			
1	B	437	Total	C	N	O	S	0	5	0
			3437	2173	594	653	17			
1	C	435	Total	C	N	O	S	0	3	0
			3410	2154	588	651	17			
1	D	436	Total	C	N	O	S	0	2	0
			3415	2157	591	650	17			
1	E	436	Total	C	N	O	S	0	2	0
			3412	2156	590	649	17			
1	F	436	Total	C	N	O	S	0	4	0
			3425	2165	592	651	17			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP Q9KAH8
A	0	SER	-	EXPRESSION TAG	UNP Q9KAH8
A	1	LEU	-	EXPRESSION TAG	UNP Q9KAH8
A	439	GLU	-	EXPRESSION TAG	UNP Q9KAH8
A	440	GLY	-	EXPRESSION TAG	UNP Q9KAH8
A	441	HIS	-	EXPRESSION TAG	UNP Q9KAH8
A	442	HIS	-	EXPRESSION TAG	UNP Q9KAH8
A	443	HIS	-	EXPRESSION TAG	UNP Q9KAH8
A	444	HIS	-	EXPRESSION TAG	UNP Q9KAH8
A	445	HIS	-	EXPRESSION TAG	UNP Q9KAH8
A	446	HIS	-	EXPRESSION TAG	UNP Q9KAH8
B	-1	MET	-	EXPRESSION TAG	UNP Q9KAH8
B	0	SER	-	EXPRESSION TAG	UNP Q9KAH8
B	1	LEU	-	EXPRESSION TAG	UNP Q9KAH8
B	439	GLU	-	EXPRESSION TAG	UNP Q9KAH8
B	440	GLY	-	EXPRESSION TAG	UNP Q9KAH8
B	441	HIS	-	EXPRESSION TAG	UNP Q9KAH8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	442	HIS	-	EXPRESSION TAG	UNP Q9KAH8
B	443	HIS	-	EXPRESSION TAG	UNP Q9KAH8
B	444	HIS	-	EXPRESSION TAG	UNP Q9KAH8
B	445	HIS	-	EXPRESSION TAG	UNP Q9KAH8
B	446	HIS	-	EXPRESSION TAG	UNP Q9KAH8
C	-1	MET	-	EXPRESSION TAG	UNP Q9KAH8
C	0	SER	-	EXPRESSION TAG	UNP Q9KAH8
C	1	LEU	-	EXPRESSION TAG	UNP Q9KAH8
C	439	GLU	-	EXPRESSION TAG	UNP Q9KAH8
C	440	GLY	-	EXPRESSION TAG	UNP Q9KAH8
C	441	HIS	-	EXPRESSION TAG	UNP Q9KAH8
C	442	HIS	-	EXPRESSION TAG	UNP Q9KAH8
C	443	HIS	-	EXPRESSION TAG	UNP Q9KAH8
C	444	HIS	-	EXPRESSION TAG	UNP Q9KAH8
C	445	HIS	-	EXPRESSION TAG	UNP Q9KAH8
C	446	HIS	-	EXPRESSION TAG	UNP Q9KAH8
D	-1	MET	-	EXPRESSION TAG	UNP Q9KAH8
D	0	SER	-	EXPRESSION TAG	UNP Q9KAH8
D	1	LEU	-	EXPRESSION TAG	UNP Q9KAH8
D	439	GLU	-	EXPRESSION TAG	UNP Q9KAH8
D	440	GLY	-	EXPRESSION TAG	UNP Q9KAH8
D	441	HIS	-	EXPRESSION TAG	UNP Q9KAH8
D	442	HIS	-	EXPRESSION TAG	UNP Q9KAH8
D	443	HIS	-	EXPRESSION TAG	UNP Q9KAH8
D	444	HIS	-	EXPRESSION TAG	UNP Q9KAH8
D	445	HIS	-	EXPRESSION TAG	UNP Q9KAH8
D	446	HIS	-	EXPRESSION TAG	UNP Q9KAH8
E	-1	MET	-	EXPRESSION TAG	UNP Q9KAH8
E	0	SER	-	EXPRESSION TAG	UNP Q9KAH8
E	1	LEU	-	EXPRESSION TAG	UNP Q9KAH8
E	439	GLU	-	EXPRESSION TAG	UNP Q9KAH8
E	440	GLY	-	EXPRESSION TAG	UNP Q9KAH8
E	441	HIS	-	EXPRESSION TAG	UNP Q9KAH8
E	442	HIS	-	EXPRESSION TAG	UNP Q9KAH8
E	443	HIS	-	EXPRESSION TAG	UNP Q9KAH8
E	444	HIS	-	EXPRESSION TAG	UNP Q9KAH8
E	445	HIS	-	EXPRESSION TAG	UNP Q9KAH8
E	446	HIS	-	EXPRESSION TAG	UNP Q9KAH8
F	-1	MET	-	EXPRESSION TAG	UNP Q9KAH8
F	0	SER	-	EXPRESSION TAG	UNP Q9KAH8
F	1	LEU	-	EXPRESSION TAG	UNP Q9KAH8
F	439	GLU	-	EXPRESSION TAG	UNP Q9KAH8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	440	GLY	-	EXPRESSION TAG	UNP Q9KAH8
F	441	HIS	-	EXPRESSION TAG	UNP Q9KAH8
F	442	HIS	-	EXPRESSION TAG	UNP Q9KAH8
F	443	HIS	-	EXPRESSION TAG	UNP Q9KAH8
F	444	HIS	-	EXPRESSION TAG	UNP Q9KAH8
F	445	HIS	-	EXPRESSION TAG	UNP Q9KAH8
F	446	HIS	-	EXPRESSION TAG	UNP Q9KAH8

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total 1	Zn 1	0	0
2	E	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	A	1	Total 1	Zn 1	0	0
2	F	1	Total 1	Zn 1	0	0

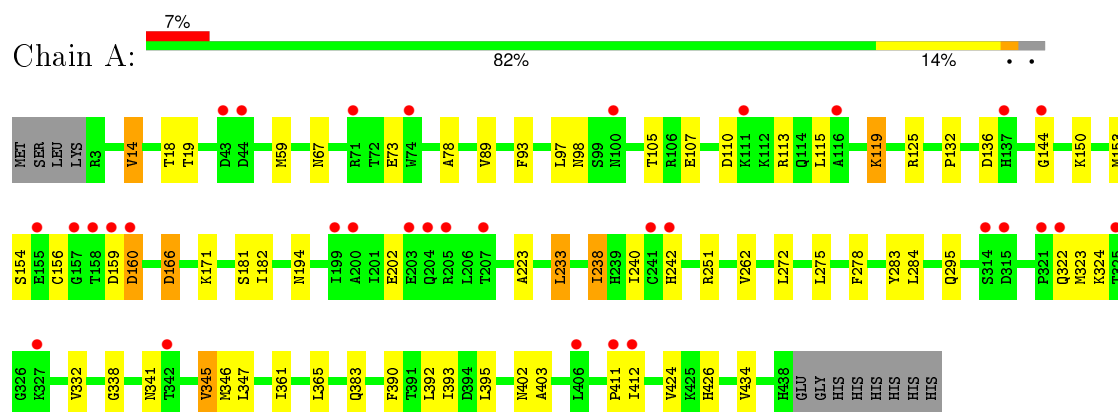
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	53	Total 53	O 53	0	0
3	B	69	Total 69	O 69	0	0
3	C	39	Total 39	O 39	0	0
3	D	47	Total 47	O 47	0	0
3	E	74	Total 74	O 74	0	0
3	F	89	Total 89	O 89	0	0

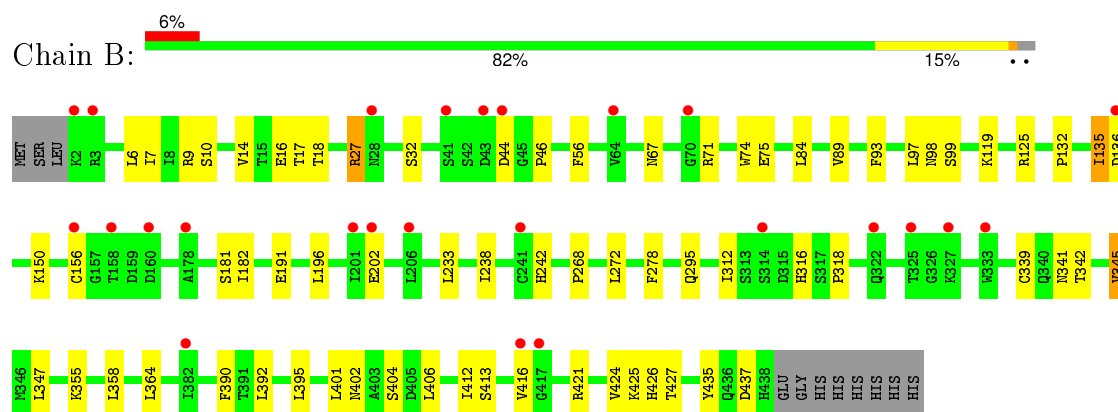
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

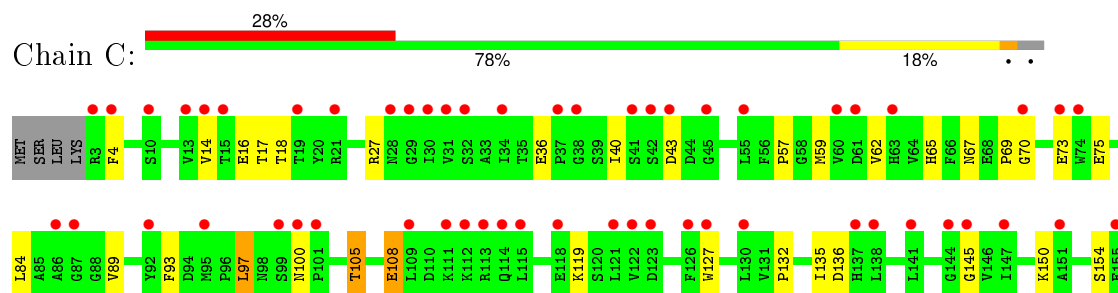
#### • Molecule 1: Allantoinase

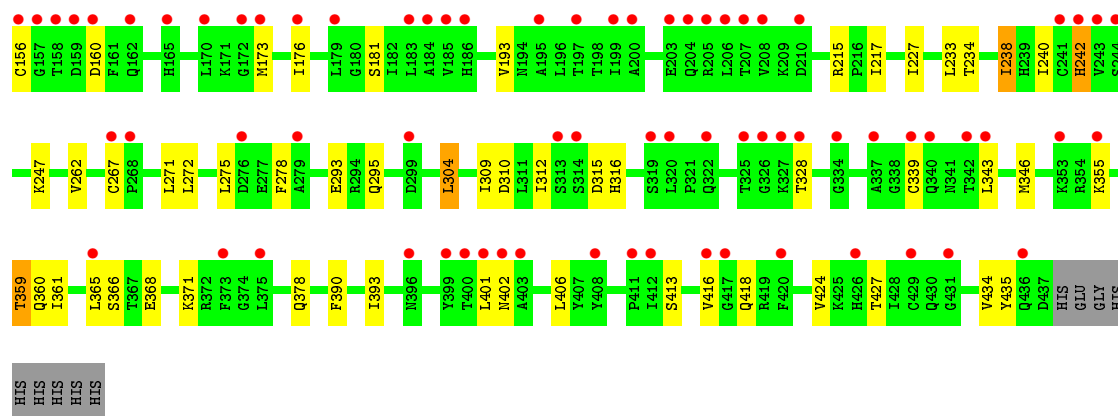


#### • Molecule 1: Allantoinase

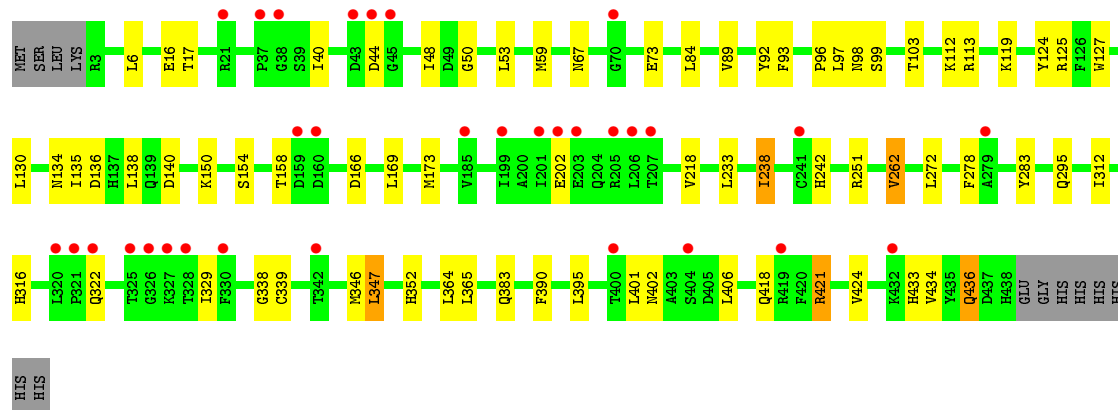
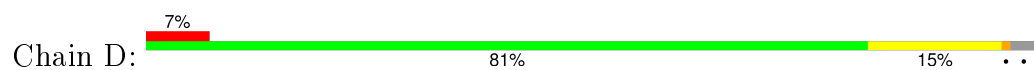


#### • Molecule 1: Allantoinase

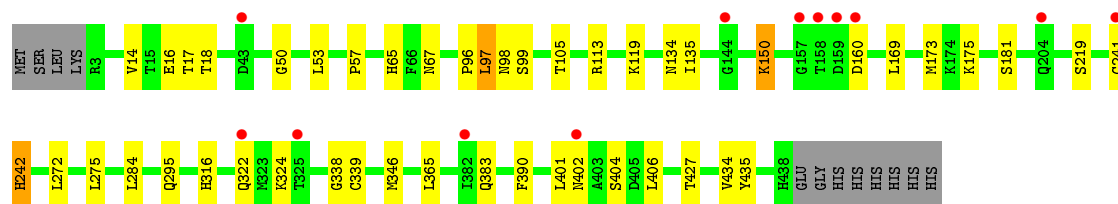
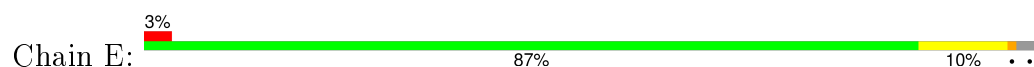




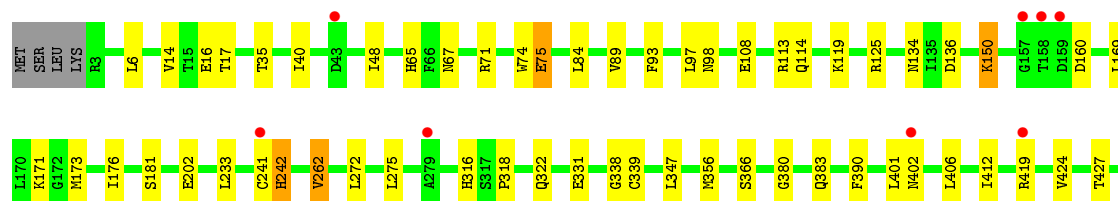
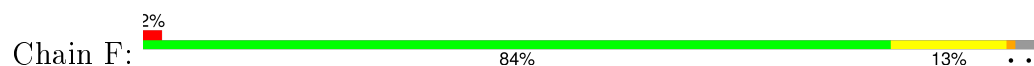
• Molecule 1: Allantoinase



• Molecule 1: Allantoinase



• Molecule 1: Allantoinase





H433	GLU
Y434	GLY
Y435	HIS
Q436	HIS
D437	HIS
H438	HIS
	HIS
	HIS
	HIS
	HIS
	HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.66Å 157.66Å 418.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.60 27.39 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.60) 100.0 (27.39-2.60)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.94 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, $R_{free}$	0.240 , 0.267 0.240 , 0.267	Depositor DCC
$R_{free}$ test set	2847 reflections (3.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.8	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	37 of 94701 reflections (0.039%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20901	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	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 69.84 % 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 3.4571e-06. 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.41	0/3507	0.60	0/4749
1	B	0.44	0/3523	0.61	1/4770 (0.0%)
1	C	0.43	0/3485	0.62	0/4720
1	D	0.42	0/3488	0.59	0/4724
1	E	0.43	0/3488	0.59	0/4724
1	F	0.41	0/3508	0.61	1/4752 (0.0%)
All	All	0.42	0/20999	0.60	2/28439 (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	A	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	395	LEU	CA-CB-CG	6.19	129.54	115.30
1	F	262	VAL	CB-CA-C	-5.13	101.65	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	ASP	Peptide
1	A	160	ASP	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	3425	0	3404	27	0
1	B	3437	0	3411	25	0
1	C	3410	0	3376	32	0
1	D	3415	0	3379	29	0
1	E	3412	0	3380	16	0
1	F	3425	0	3393	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	53	0	0	0	0
3	B	69	0	0	0	0
3	C	39	0	0	0	0
3	D	47	0	0	0	0
3	E	74	0	0	0	0
3	F	89	0	0	0	0
All	All	20901	0	20343	138	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (138) 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:D:67:ASN:ND2	1:D:98:ASN:HB2	1.96	0.80
1:F:75:GLU:HG2	1:F:318:PRO:HG3	1.69	0.73
1:B:75:GLU:HG2	1:B:318:PRO:HG3	1.76	0.68
1:F:67:ASN:ND2	1:F:98:ASN:HB2	2.09	0.67
1:E:67:ASN:ND2	1:E:98:ASN:HB2	2.09	0.67
1:B:67:ASN:ND2	1:B:98:ASN:HB2	2.10	0.67
1:D:96:PRO:HD3	1:D:127:TRP:HB2	1.76	0.67
1:D:97:LEU:O	1:D:98:ASN:HB2	1.94	0.66
1:A:393:ILE:HG22	1:A:395:LEU:HD23	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:TYR:HE1	1:D:329:ILE:HA	1.63	0.62
1:C:70:GLY:HA3	1:C:100:ASN:H	1.64	0.62
1:F:16[B]:GLU:HG3	1:F:17:THR:HG23	1.83	0.61
1:C:359:THR:HG22	1:C:360:GLN:N	2.16	0.60
1:A:18:THR:HG21	1:E:383:GLN:HE22	1.67	0.60
1:B:18:THR:HG21	1:F:383:GLN:HE22	1.67	0.60
1:D:67:ASN:ND2	1:D:98:ASN:CB	2.64	0.59
1:B:316:HIS:HB2	1:B:339:CYS:HB3	1.85	0.58
1:A:14:VAL:HG12	1:A:19:THR:HG22	1.86	0.58
1:E:16[B]:GLU:HG3	1:E:17:THR:HG23	1.86	0.57
1:C:359:THR:CG2	1:C:360:GLN:N	2.67	0.57
1:E:65:HIS:HB3	1:E:67:ASN:HD21	1.69	0.57
1:C:18:THR:HG21	1:D:383:GLN:HE22	1.68	0.57
1:D:346:MET:HG3	1:D:365:LEU:HD11	1.88	0.55
1:D:283:TYR:CE1	1:D:329:ILE:HA	2.40	0.55
1:B:84:LEU:HB3	1:B:89:VAL:HB	1.87	0.55
1:B:9:ARG:O	1:B:10:SER:HB2	2.07	0.55
1:C:62:VAL:HA	1:C:93:PHE:HB2	1.89	0.54
1:B:392:LEU:HB2	1:B:426:HIS:HB2	1.90	0.54
1:D:97:LEU:C	1:D:99:SER:H	2.12	0.53
1:F:427:THR:HB	1:F:435:TYR:HB3	1.91	0.53
1:A:18:THR:HG21	1:E:383:GLN:NE2	2.23	0.53
1:B:56:PHE:HZ	1:B:358:LEU:HD22	1.73	0.53
1:B:268:PRO:HG3	1:B:342:THR:HG23	1.91	0.53
1:C:238:ILE:HD11	1:C:240:ILE:HD11	1.91	0.53
1:F:433:HIS:HE1	1:F:436:GLN:HB2	1.73	0.52
1:D:316:HIS:HB2	1:D:339:CYS:HB3	1.91	0.52
1:C:4:PHE:HE2	1:C:40:ILE:HG12	1.75	0.52
1:D:84:LEU:HB3	1:D:89:VAL:HB	1.90	0.52
1:F:65:HIS:HB3	1:F:67:ASN:HD21	1.75	0.52
1:C:346:MET:HG3	1:C:365:LEU:HD11	1.91	0.52
1:D:50:GLY:HA2	1:D:53:LEU:HD12	1.91	0.51
1:C:368:GLU:HA	1:C:371:LYS:HB2	1.92	0.51
1:A:166:ASP:HB2	1:B:191:GLU:HG3	1.93	0.51
1:D:59:MET:HB2	1:D:89:VAL:HG22	1.93	0.51
1:A:403:ALA:HB1	1:A:411:PRO:HB2	1.93	0.51
1:D:96:PRO:HD3	1:D:127:TRP:CB	2.41	0.50
1:C:65:HIS:HB3	1:C:67:ASN:HD21	1.77	0.50
1:C:401:LEU:HD21	1:C:406:LEU:HD21	1.94	0.50
1:D:401:LEU:HD21	1:D:406:LEU:HD21	1.92	0.50
1:C:16[A]:GLU:HG2	1:C:17:THR:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:PHE:CD1	1:F:125:ARG:HB2	2.47	0.49
1:D:16[B]:GLU:HG3	1:D:17:THR:HG23	1.94	0.49
1:A:383:GLN:NE2	1:E:18:THR:HG21	2.28	0.49
1:A:78:ALA:HB2	1:A:119:LYS:HG3	1.95	0.48
1:A:341:ASN:O	1:A:345:VAL:HG12	2.13	0.48
1:E:346:MET:HG3	1:E:365:LEU:HD11	1.96	0.48
1:B:16[B]:GLU:HG3	1:B:17:THR:HG23	1.95	0.47
1:C:173:MET:HB3	1:C:234:THR:HG21	1.96	0.47
1:F:176:ILE:HG23	1:F:181:SER:HB3	1.97	0.47
1:C:271:LEU:HD11	1:C:304:LEU:HD13	1.97	0.47
1:C:217:ILE:HG21	1:C:247:LYS:HD2	1.96	0.47
1:A:110:ASP:HA	1:A:113:ARG:HB3	1.97	0.47
1:A:153:MET:CE	1:A:223:ALA:HB1	2.45	0.47
1:C:267:CYS:SG	1:C:315:ASP:HB2	2.54	0.47
1:E:316:HIS:HB2	1:E:339:CYS:HB3	1.97	0.46
1:C:427:THR:HB	1:C:435:TYR:HB3	1.98	0.46
1:A:233:LEU:HD21	1:B:196:LEU:HD11	1.96	0.46
1:F:316:HIS:HB2	1:F:339:CYS:HB3	1.97	0.46
1:A:383:GLN:HE22	1:E:18:THR:HG21	1.81	0.46
1:F:401:LEU:HD21	1:F:406:LEU:HD21	1.96	0.46
1:C:59:MET:HA	1:C:366:SER:HB2	1.98	0.46
1:A:93:PHE:CD1	1:A:125:ARG:HB2	2.51	0.46
1:A:181:SER:OG	1:A:182:ILE:N	2.49	0.46
1:F:169:LEU:HB3	1:F:173:MET:HE3	1.98	0.46
1:D:130:LEU:HD13	1:D:138:LEU:HD11	1.98	0.46
1:F:150:LYS:NZ	1:F:241:CYS:SG	2.89	0.45
1:E:169:LEU:HB3	1:E:173:MET:HE2	1.98	0.45
1:C:304:LEU:HD12	1:C:309:ILE:HD12	1.99	0.45
1:D:6:LEU:HD11	1:D:48:ILE:HG12	1.99	0.45
1:E:401:LEU:HD21	1:E:406:LEU:HD21	1.98	0.45
1:D:352:HIS:CD2	1:D:421:ARG:HB3	2.52	0.45
1:C:84:LEU:HB3	1:C:89:VAL:HB	1.99	0.45
1:B:135:ILE:H	1:B:135:ILE:HG13	1.56	0.45
1:A:238:ILE:HD11	1:A:240:ILE:HD11	1.99	0.45
1:B:312:ILE:HG12	1:B:364:LEU:HB3	1.99	0.44
1:A:392:LEU:HB2	1:A:426:HIS:HB2	2.00	0.44
1:B:427:THR:HB	1:B:435:TYR:HB3	2.00	0.44
1:D:84:LEU:HD22	1:D:89:VAL:HG11	1.99	0.44
1:E:284:LEU:HD23	1:E:324:LYS:HG2	2.00	0.44
1:F:84:LEU:HB3	1:F:89:VAL:HB	1.99	0.44
1:B:27:ARG:HB2	1:B:32:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:LYS:NZ	1:E:241:CYS:SG	2.89	0.43
1:C:105:THR:HG23	1:C:108:GLU:HB2	2.00	0.43
1:B:18:THR:HG21	1:F:383:GLN:NE2	2.32	0.43
1:D:312:ILE:HG12	1:D:364:LEU:HB3	1.99	0.43
1:C:93:PHE:HB3	1:C:127:TRP:NE1	2.34	0.43
1:B:401:LEU:HD21	1:B:406:LEU:HD21	1.99	0.43
1:A:346:MET:HG3	1:A:365:LEU:HD11	1.99	0.43
1:C:14:VAL:O	1:C:57:PRO:HD3	2.19	0.43
1:C:275:LEU:HB2	1:C:293:GLU:HA	2.01	0.43
1:A:284:LEU:HD23	1:A:324:LYS:HE3	2.01	0.43
1:A:275:LEU:HA	1:A:275:LEU:HD12	1.94	0.42
1:A:283:TYR:CD1	1:A:332:VAL:HG21	2.53	0.42
1:F:35:THR:HG21	1:F:40:ILE:HD13	2.01	0.42
1:D:251:ARG:HA	1:D:251:ARG:HD2	1.85	0.42
1:D:92:TYR:CZ	1:D:124:TYR:HB3	2.54	0.42
1:E:96:PRO:HD2	1:E:97:LEU:HD23	2.02	0.42
1:E:427:THR:HB	1:E:435:TYR:HB3	2.00	0.42
1:B:413:SER:HB3	1:B:416:VAL:HG23	2.02	0.42
1:B:71:ARG:HD3	1:B:74:TRP:CZ2	2.54	0.42
1:F:6:LEU:HD11	1:F:48:ILE:HG12	2.01	0.42
1:D:93:PHE:CD1	1:D:125:ARG:HB2	2.55	0.42
1:B:425:LYS:HA	1:B:437:ASP:HB2	2.02	0.42
1:B:181:SER:OG	1:B:182:ILE:N	2.50	0.41
1:A:113:ARG:NH1	1:A:144:GLY:O	2.53	0.41
1:D:169:LEU:HB3	1:D:173:MET:HE3	2.02	0.41
1:A:59:MET:HB2	1:A:89:VAL:HG22	2.01	0.41
1:D:433:HIS:HE1	1:D:436:GLN:HG3	1.85	0.41
1:C:18:THR:HG21	1:D:383:GLN:NE2	2.35	0.41
1:F:71:ARG:HD3	1:F:74:TRP:CZ2	2.55	0.41
1:C:193:VAL:HG22	1:C:215:ARG:HA	2.01	0.41
1:C:316:HIS:HB2	1:C:339:CYS:HB3	2.01	0.41
1:B:6:LEU:HD12	1:B:46:PRO:HB2	2.01	0.41
1:A:67:ASN:ND2	1:A:98:ASN:HB3	2.35	0.41
1:C:176:ILE:HG23	1:C:181:SER:HB3	2.01	0.41
1:E:50:GLY:HA2	1:E:53:LEU:HD12	2.03	0.41
1:D:238:ILE:HG23	1:D:262:VAL:HG13	2.02	0.41
1:A:153:MET:HE2	1:A:223:ALA:HB1	2.02	0.41
1:A:251:ARG:HA	1:A:251:ARG:HD2	1.94	0.41
1:D:347:LEU:HD12	1:D:347:LEU:HA	1.86	0.41
1:C:413:SER:HB3	1:C:416:VAL:HG23	2.02	0.41
1:C:65:HIS:HE1	1:C:97:LEU:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:PHE:CD1	1:B:125:ARG:HB2	2.56	0.40
1:C:16[B]:GLU:HG3	1:C:17:THR:HG23	2.02	0.40
1:C:73:GLU:H	1:C:73:GLU:HG2	1.66	0.40
1:B:341:ASN:O	1:B:345:VAL:HG12	2.21	0.40
1:A:283:TYR:CE1	1:A:332:VAL:HG21	2.57	0.40
1:F:366:SER:OG	1:F:380:GLY:HA2	2.21	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	438/448 (98%)	410 (94%)	25 (6%)	3 (1%)	26	51
1	B	440/448 (98%)	425 (97%)	13 (3%)	2 (0%)	34	60
1	C	436/448 (97%)	397 (91%)	35 (8%)	4 (1%)	21	42
1	D	436/448 (97%)	416 (95%)	18 (4%)	2 (0%)	34	60
1	E	436/448 (97%)	419 (96%)	15 (3%)	2 (0%)	34	60
1	F	438/448 (98%)	424 (97%)	12 (3%)	2 (0%)	34	60
All	All	2624/2688 (98%)	2491 (95%)	118 (4%)	15 (1%)	30	56

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	PRO
1	A	242	HIS
1	B	242	HIS
1	C	242	HIS
1	D	242	HIS
1	E	242	HIS

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Mol	Chain	Res	Type
1	F	242	HIS
1	D	338	GLY
1	F	338	GLY
1	C	145	GLY
1	E	338	GLY
1	B	132	PRO
1	C	132	PRO
1	A	338	GLY
1	C	69	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	375/382 (98%)	343 (92%)	32 (8%)	13	25
1	B	377/382 (99%)	351 (93%)	26 (7%)	19	38
1	C	373/382 (98%)	336 (90%)	37 (10%)	10	18
1	D	373/382 (98%)	340 (91%)	33 (9%)	12	24
1	E	373/382 (98%)	350 (94%)	23 (6%)	23	45
1	F	375/382 (98%)	347 (92%)	28 (8%)	17	33
All	All	2246/2292 (98%)	2067 (92%)	179 (8%)	15	29

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	73	GLU
1	A	97	LEU
1	A	105	THR
1	A	107	GLU
1	A	115	LEU
1	A	119	LYS
1	A	136	ASP
1	A	150	LYS

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Mol	Chain	Res	Type
1	A	154	SER
1	A	156	CYS
1	A	160	ASP
1	A	166	ASP
1	A	171	LYS
1	A	194	ASN
1	A	202	GLU
1	A	233	LEU
1	A	238	ILE
1	A	262	VAL
1	A	272	LEU
1	A	278	PHE
1	A	295	GLN
1	A	322	GLN
1	A	323	MET
1	A	345	VAL
1	A	347	LEU
1	A	361	ILE
1	A	390	PHE
1	A	402	ASN
1	A	412	ILE
1	A	424	VAL
1	A	434	VAL
1	B	7	ILE
1	B	14	VAL
1	B	27	ARG
1	B	44	ASP
1	B	97	LEU
1	B	99	SER
1	B	119	LYS
1	B	135	ILE
1	B	136	ASP
1	B	150	LYS
1	B	156	CYS
1	B	202	GLU
1	B	233	LEU
1	B	238	ILE
1	B	272	LEU
1	B	278	PHE
1	B	295	GLN
1	B	345	VAL
1	B	347	LEU

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Mol	Chain	Res	Type
1	B	355	LYS
1	B	390	PHE
1	B	402	ASN
1	B	404	SER
1	B	412	ILE
1	B	421	ARG
1	B	424	VAL
1	C	27	ARG
1	C	36	GLU
1	C	43	ASP
1	C	75	GLU
1	C	97	LEU
1	C	105	THR
1	C	108	GLU
1	C	119	LYS
1	C	135	ILE
1	C	136	ASP
1	C	150	LYS
1	C	154	SER
1	C	156	CYS
1	C	160	ASP
1	C	227	ILE
1	C	233	LEU
1	C	238	ILE
1	C	242	HIS
1	C	262	VAL
1	C	272	LEU
1	C	278	PHE
1	C	295	GLN
1	C	304	LEU
1	C	310	ASP
1	C	312	ILE
1	C	328	THR
1	C	343	LEU
1	C	355	LYS
1	C	359	THR
1	C	361	ILE
1	C	378	GLN
1	C	390	PHE
1	C	393	ILE
1	C	402	ASN
1	C	418	GLN

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Mol	Chain	Res	Type
1	C	424	VAL
1	C	434	VAL
1	D	40	ILE
1	D	44	ASP
1	D	73	GLU
1	D	103	THR
1	D	112	LYS
1	D	113	ARG
1	D	119	LYS
1	D	134	ASN
1	D	135	ILE
1	D	136	ASP
1	D	140	ASP
1	D	150	LYS
1	D	154	SER
1	D	158	THR
1	D	166	ASP
1	D	202	GLU
1	D	218	VAL
1	D	233	LEU
1	D	238	ILE
1	D	262	VAL
1	D	272	LEU
1	D	278	PHE
1	D	295	GLN
1	D	322	GLN
1	D	347	LEU
1	D	390	PHE
1	D	395	LEU
1	D	402	ASN
1	D	418	GLN
1	D	421	ARG
1	D	424	VAL
1	D	434	VAL
1	D	436	GLN
1	E	14	VAL
1	E	57	PRO
1	E	97	LEU
1	E	99	SER
1	E	105	THR
1	E	113	ARG
1	E	119	LYS

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Mol	Chain	Res	Type
1	E	134	ASN
1	E	135	ILE
1	E	150	LYS
1	E	160	ASP
1	E	175	LYS
1	E	181	SER
1	E	219	SER
1	E	242	HIS
1	E	272	LEU
1	E	275	LEU
1	E	295	GLN
1	E	322	GLN
1	E	390	PHE
1	E	402	ASN
1	E	404	SER
1	E	434	VAL
1	F	14	VAL
1	F	75	GLU
1	F	97	LEU
1	F	108	GLU
1	F	113	ARG
1	F	114	GLN
1	F	119	LYS
1	F	134	ASN
1	F	136	ASP
1	F	150	LYS
1	F	160	ASP
1	F	171	LYS
1	F	202	GLU
1	F	233	LEU
1	F	242	HIS
1	F	262	VAL
1	F	272	LEU
1	F	275	LEU
1	F	322	GLN
1	F	331	GLU
1	F	347	LEU
1	F	356	MET
1	F	390	PHE
1	F	402	ASN
1	F	412	ILE
1	F	419	ARG

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Mol	Chain	Res	Type
1	F	424	VAL
1	F	434	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	114	GLN
1	A	142	HIS
1	A	378	GLN
1	A	383	GLN
1	A	433	HIS
1	B	67	ASN
1	B	98	ASN
1	B	242	HIS
1	B	378	GLN
1	B	418	GLN
1	C	67	ASN
1	C	98	ASN
1	C	114	GLN
1	C	142	HIS
1	C	418	GLN
1	D	67	ASN
1	D	162	GLN
1	D	242	HIS
1	D	352	HIS
1	D	378	GLN
1	D	418	GLN
1	D	433	HIS
1	E	67	ASN
1	E	142	HIS
1	E	352	HIS
1	E	378	GLN
1	F	67	ASN
1	F	98	ASN
1	F	142	HIS
1	F	322	GLN
1	F	383	GLN
1	F	418	GLN
1	F	436	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 6 ligands modelled in this entry, 6 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	436/448 (97%)	0.33	32 (7%) 18 12	22, 38, 54, 77	0
1	B	437/448 (97%)	0.12	25 (5%) 27 20	28, 37, 52, 66	0
1	C	435/448 (97%)	1.53	127 (29%) 1 0	22, 39, 51, 74	0
1	D	436/448 (97%)	0.26	32 (7%) 18 12	26, 38, 53, 70	0
1	E	436/448 (97%)	0.01	12 (2%) 56 49	25, 37, 47, 68	0
1	F	436/448 (97%)	-0.03	8 (1%) 71 66	26, 37, 48, 64	0
All	All	2616/2688 (97%)	0.37	236 (9%) 12 8	22, 37, 52, 77	0

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	158	THR	9.5
1	C	402	ASN	7.6
1	A	157	GLY	7.5
1	C	156	CYS	7.0
1	C	144	GLY	5.9
1	C	113	ARG	5.8
1	C	400	THR	5.7
1	A	322	GLN	5.6
1	C	159	ASP	5.5
1	C	322	GLN	5.4
1	A	111	LYS	5.1
1	C	157	GLY	5.1
1	C	111	LYS	5.1
1	C	31	VAL	5.0
1	C	109	LEU	4.9
1	C	210	ASP	4.8
1	C	141	LEU	4.8
1	C	121	LEU	4.7
1	C	241	CYS	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	205	ARG	4.7
1	A	204	GLN	4.6
1	C	122	VAL	4.6
1	C	4	PHE	4.6
1	C	334	GLY	4.5
1	D	202	GLU	4.5
1	D	43	ASP	4.5
1	C	21	ARG	4.5
1	A	325	THR	4.4
1	C	411	PRO	4.3
1	C	70	GLY	4.3
1	D	38	GLY	4.3
1	C	206	LEU	4.3
1	C	43	ASP	4.3
1	D	201	ILE	4.3
1	C	431	GLY	4.2
1	C	403	ALA	4.2
1	C	412	ILE	4.2
1	E	157	GLY	4.2
1	C	28	ASN	4.2
1	C	416	VAL	4.1
1	C	327	LYS	4.1
1	C	339	CYS	4.1
1	E	322	GLN	4.0
1	A	327	LYS	4.0
1	C	138	LEU	4.0
1	B	201	ILE	3.9
1	B	2	LYS	3.9
1	D	326	GLY	3.9
1	C	325	THR	3.9
1	C	375	LEU	3.9
1	A	43	ASP	3.9
1	C	130	LEU	3.8
1	C	179	LEU	3.8
1	A	160	ASP	3.8
1	C	328	THR	3.8
1	C	172	GLY	3.8
1	C	155	GLU	3.7
1	C	38	GLY	3.7
1	C	319	SER	3.7
1	C	145	GLY	3.7
1	E	402	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	199	ILE	3.7
1	B	322	GLN	3.6
1	E	159	ASP	3.6
1	C	32	SER	3.6
1	B	158	THR	3.6
1	D	159	ASP	3.6
1	C	203	GLU	3.6
1	C	186	HIS	3.6
1	C	429	CYS	3.5
1	B	43	ASP	3.5
1	A	158	THR	3.5
1	C	313	SER	3.4
1	C	199	ILE	3.4
1	C	137	HIS	3.4
1	A	321	PRO	3.4
1	C	92	TYR	3.3
1	B	160	ASP	3.3
1	D	327	LYS	3.3
1	C	299	ASP	3.3
1	E	160	ASP	3.3
1	C	355	LYS	3.2
1	C	115	LEU	3.2
1	C	60	VAL	3.2
1	D	205	ARG	3.2
1	B	178	ALA	3.2
1	D	328	THR	3.2
1	C	399	TYR	3.1
1	C	30	ILE	3.1
1	D	160	ASP	3.1
1	C	126	PHE	3.1
1	D	203	GLU	3.1
1	C	195	ALA	3.1
1	C	340	GLN	3.1
1	E	43	ASP	3.1
1	C	267	CYS	3.1
1	F	43	ASP	3.1
1	C	10	SER	3.0
1	A	406	LEU	3.0
1	A	241	CYS	3.0
1	C	45	GLY	3.0
1	C	42	SER	3.0
1	B	41	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	101	PRO	3.0
1	C	200	ALA	3.0
1	C	184	ALA	3.0
1	C	41	SER	2.9
1	B	156	CYS	2.9
1	A	159	ASP	2.9
1	C	100	ASN	2.9
1	C	401	LEU	2.9
1	E	325	THR	2.9
1	C	3	ARG	2.9
1	D	320	LEU	2.9
1	C	87	GLY	2.9
1	C	13	VAL	2.8
1	B	325	THR	2.8
1	C	63	HIS	2.8
1	C	147	ILE	2.8
1	C	204	GLN	2.8
1	C	342	THR	2.8
1	C	99	SER	2.8
1	D	400	THR	2.8
1	D	279	ALA	2.7
1	D	325	THR	2.7
1	B	28	ASN	2.7
1	A	203	GLU	2.7
1	D	404	SER	2.7
1	B	416	VAL	2.7
1	D	37	PRO	2.7
1	B	327	LYS	2.7
1	C	118	GLU	2.7
1	C	55	LEU	2.7
1	C	114	GLN	2.7
1	C	160	ASP	2.7
1	C	353	LYS	2.7
1	C	408	TYR	2.7
1	C	14	VAL	2.6
1	C	242	HIS	2.6
1	B	202	GLU	2.6
1	D	330	PHE	2.6
1	F	419	ARG	2.6
1	C	207	THR	2.6
1	B	136	ASP	2.6
1	D	70	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	242	HIS	2.6
1	A	74	TRP	2.6
1	F	279	ALA	2.5
1	B	333	TRP	2.5
1	D	21	ARG	2.5
1	C	197	THR	2.5
1	D	207	THR	2.5
1	D	206	LEU	2.5
1	C	337	ALA	2.5
1	C	165	HIS	2.5
1	C	74	TRP	2.5
1	D	44	ASP	2.5
1	D	321	PRO	2.5
1	A	205	ARG	2.5
1	A	411	PRO	2.5
1	B	241	CYS	2.5
1	D	322	GLN	2.5
1	A	144	GLY	2.4
1	A	199	ILE	2.4
1	A	207	THR	2.4
1	A	314	SER	2.4
1	D	342	THR	2.4
1	E	241	CYS	2.4
1	D	185	VAL	2.4
1	A	137	HIS	2.4
1	C	320	LEU	2.4
1	D	419	ARG	2.4
1	C	426	HIS	2.4
1	C	396	ASN	2.4
1	E	204	GLN	2.4
1	C	151	ALA	2.4
1	E	158	THR	2.4
1	C	343	LEU	2.3
1	A	200	ALA	2.3
1	B	314	SER	2.3
1	C	243	VAL	2.3
1	A	44	ASP	2.3
1	C	162	GLN	2.3
1	D	241	CYS	2.3
1	A	116	ALA	2.3
1	C	176	ILE	2.3
1	C	276	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	159	ASP	2.3
1	F	402	ASN	2.3
1	C	61	ASP	2.3
1	C	95	MET	2.3
1	C	127	TRP	2.3
1	C	173	MET	2.3
1	F	158	THR	2.3
1	F	241	CYS	2.3
1	A	155	GLU	2.2
1	C	29	GLY	2.2
1	A	412	ILE	2.2
1	C	183	LEU	2.2
1	A	71	ARG	2.2
1	C	326	GLY	2.2
1	E	144	GLY	2.2
1	C	15	THR	2.2
1	C	86	ALA	2.2
1	B	64	VAL	2.2
1	E	382	ILE	2.2
1	C	279	ALA	2.2
1	C	436	GLN	2.2
1	C	208	VAL	2.2
1	B	382	ILE	2.1
1	A	342	THR	2.1
1	B	206	LEU	2.1
1	C	420	PHE	2.1
1	A	315	ASP	2.1
1	C	112	LYS	2.1
1	C	185	VAL	2.1
1	A	100	ASN	2.1
1	C	268	PRO	2.1
1	C	373	PHE	2.1
1	C	244	SER	2.1
1	C	365	LEU	2.1
1	D	432	LYS	2.1
1	C	34	ILE	2.1
1	C	37	PRO	2.1
1	B	44	ASP	2.1
1	F	157	GLY	2.1
1	C	123[A]	ASP	2.1
1	C	417	GLY	2.1
1	D	45	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	314	SER	2.1
1	C	19	THR	2.0
1	C	170	LEU	2.0
1	B	417	GLY	2.0
1	B	70	GLY	2.0
1	B	3	ARG	2.0
1	C	73	GLU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	D	447	1/1	0.83	0.20	-0.80	40,40,40,40	1
2	ZN	C	447	1/1	0.93	0.21	-1.82	50,50,50,50	1
2	ZN	B	447	1/1	0.96	0.08	-2.84	39,39,39,39	1
2	ZN	E	447	1/1	0.97	0.08	-4.25	39,39,39,39	1
2	ZN	A	447	1/1	0.97	0.06	-	43,43,43,43	1
2	ZN	F	447	1/1	0.94	0.22	-	39,39,39,39	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.