



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:41 PM GMT

PDB ID : 4IND  
Title : The Triple Jelly Roll Fold and Turret Assembly in an Archaeal Virus  
Authors : Eilers, B.J.; Kraft, D.; Burgess, M.C.; Young, M.J.; Lawrence, C.M.  
Deposited on : 2013-01-04  
Resolution : 1.80 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

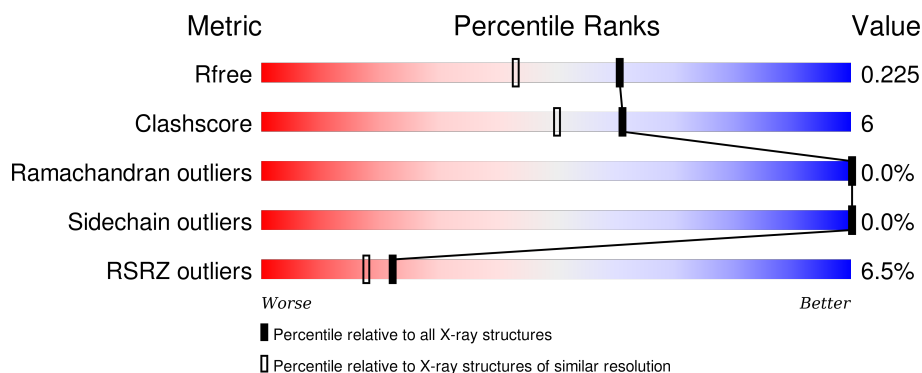
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	387	
1	B	387	
1	C	387	
1	D	387	
1	E	387	

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Mol	Chain	Length	Quality of chain	
1	F	387	5%	87% 11% .
1	G	387	3%	88% 10% .
1	H	387	5%	88% 9% .
1	I	387	4%	90% 8% .
1	J	387	9%	90% 8% .
1	K	387	6%	90% 7% .
1	L	387	9%	89% 9% .
1	M	387	6%	90% 7% .
1	N	387	5%	89% 9% .
1	O	387	6%	89% 8% .
1	P	387	6%	89% 9% .
1	Q	387	8%	88% 9% .
1	R	387	8%	89% 8% .
1	S	387	7%	90% 7% .
1	T	387	4%	88% 9% .

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
2	2HP	A	401	-	-	X	-
2	2HP	A	403	-	-	-	X
2	2HP	B	403	-	-	X	X
2	2HP	C	401	-	-	X	-
2	2HP	C	402	-	-	-	X
2	2HP	D	403	-	-	-	X
2	2HP	E	403	-	-	-	X
2	2HP	F	401	-	-	X	-
2	2HP	F	403	-	-	X	X
2	2HP	G	401	-	-	X	-
2	2HP	G	403	-	-	-	X
2	2HP	H	403	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2HP	I	403	-	-	-	X
2	2HP	J	402	-	-	-	X
2	2HP	L	403	-	-	-	X
2	2HP	M	403	-	-	-	X
2	2HP	N	403	-	-	-	X
2	2HP	O	403	-	-	-	X
2	2HP	P	402	-	-	X	-
2	2HP	Q	403	-	-	-	X
2	2HP	R	401	-	-	X	-
2	2HP	R	402	-	-	-	X
2	2HP	S	401	-	-	X	-
2	2HP	T	403	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 64220 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 C381 turret protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	6	0
			2970	1905	477	584	4			
1	B	377	Total	C	N	O	S	0	6	0
			2970	1905	477	584	4			
1	C	377	Total	C	N	O	S	0	6	0
			2970	1905	477	584	4			
1	D	377	Total	C	N	O	S	0	6	0
			2970	1905	477	584	4			
1	E	377	Total	C	N	O	S	0	6	0
			2970	1905	477	584	4			
1	F	377	Total	C	N	O	S	0	6	0
			2970	1905	477	584	4			
1	G	377	Total	C	N	O	S	0	6	0
			2970	1905	477	584	4			
1	H	377	Total	C	N	O	S	0	6	0
			2970	1905	477	584	4			
1	I	377	Total	C	N	O	S	0	6	0
			2970	1905	477	584	4			
1	J	377	Total	C	N	O	S	0	6	0
			2970	1905	477	584	4			
1	K	377	Total	C	N	O	S	0	6	0
			2970	1905	477	584	4			
1	L	377	Total	C	N	O	S	0	6	0
			2970	1905	477	584	4			
1	M	377	Total	C	N	O	S	0	6	0
			2970	1905	477	584	4			
1	N	377	Total	C	N	O	S	0	6	0
			2970	1905	477	584	4			
1	O	377	Total	C	N	O	S	0	6	0
			2970	1905	477	584	4			
1	P	377	Total	C	N	O	S	0	6	0
			2970	1905	477	584	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	377	Total	C	N	O	S	0	6	0
			2970	1905	477	584	4			
1	R	377	Total	C	N	O	S	0	6	0
			2970	1905	477	584	4			
1	S	377	Total	C	N	O	S	0	6	0
			2970	1905	477	584	4			
1	T	377	Total	C	N	O	S	0	6	0
			2970	1905	477	584	4			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
A	383	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
A	384	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
A	385	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
A	386	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
A	387	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
B	382	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
B	383	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
B	384	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
B	385	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
B	386	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
B	387	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
C	382	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
C	383	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
C	384	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
C	385	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
C	386	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
C	387	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
D	382	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
D	383	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
D	384	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
D	385	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
D	386	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
D	387	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
E	382	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
E	383	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
E	384	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
E	385	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
E	386	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
E	387	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
F	382	HIS	-	EXPRESSION TAG	UNP Q6Q0L3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	383	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
F	384	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
F	385	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
F	386	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
F	387	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
G	382	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
G	383	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
G	384	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
G	385	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
G	386	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
G	387	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
H	382	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
H	383	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
H	384	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
H	385	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
H	386	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
H	387	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
I	382	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
I	383	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
I	384	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
I	385	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
I	386	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
I	387	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
J	382	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
J	383	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
J	384	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
J	385	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
J	386	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
J	387	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
K	382	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
K	383	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
K	384	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
K	385	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
K	386	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
K	387	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
L	382	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
L	383	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
L	384	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
L	385	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
L	386	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
L	387	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
M	382	HIS	-	EXPRESSION TAG	UNP Q6Q0L3

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Chain	Residue	Modelled	Actual	Comment	Reference
M	383	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
M	384	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
M	385	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
M	386	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
M	387	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
N	382	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
N	383	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
N	384	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
N	385	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
N	386	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
N	387	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
O	382	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
O	383	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
O	384	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
O	385	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
O	386	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
O	387	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
P	382	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
P	383	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
P	384	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
P	385	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
P	386	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
P	387	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
Q	382	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
Q	383	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
Q	384	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
Q	385	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
Q	386	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
Q	387	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
R	382	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
R	383	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
R	384	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
R	385	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
R	386	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
R	387	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
S	382	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
S	383	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
S	384	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
S	385	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
S	386	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
S	387	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
T	382	HIS	-	EXPRESSION TAG	UNP Q6Q0L3

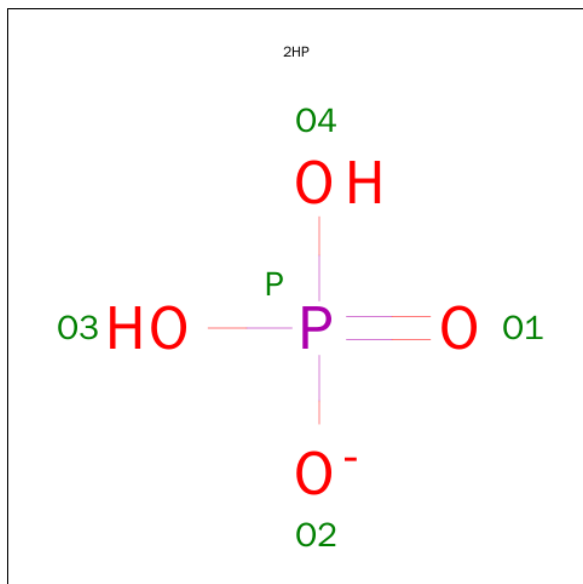
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Chain	Residue	Modelled	Actual	Comment	Reference
T	383	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
T	384	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
T	385	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
T	386	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
T	387	HIS	-	EXPRESSION TAG	UNP Q6Q0L3

- Molecule 2 is DIHYDROGENPHOSPHATE ION (three-letter code: 2HP) (formula:  $\text{H}_2\text{O}_4\text{P}$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	K	1	Total	O	P	0	0
			5	4	1		
2	K	1	Total	O	P	0	0
			5	4	1		
2	K	1	Total	O	P	0	0
			5	4	1		
2	L	1	Total	O	P	0	0
			5	4	1		
2	L	1	Total	O	P	0	0
			5	4	1		
2	L	1	Total	O	P	0	0
			5	4	1		
2	M	1	Total	O	P	0	0
			5	4	1		
2	M	1	Total	O	P	0	0
			5	4	1		
2	M	1	Total	O	P	0	0
			5	4	1		
2	N	1	Total	O	P	0	0
			5	4	1		
2	N	1	Total	O	P	0	0
			5	4	1		
2	N	1	Total	O	P	0	0
			5	4	1		
2	O	1	Total	O	P	0	0
			5	4	1		
2	O	1	Total	O	P	0	0
			5	4	1		
2	O	1	Total	O	P	0	0
			5	4	1		
2	P	1	Total	O	P	0	0
			5	4	1		
2	P	1	Total	O	P	0	0
			5	4	1		
2	P	1	Total	O	P	0	0
			5	4	1		
2	Q	1	Total	O	P	0	0
			5	4	1		
2	Q	1	Total	O	P	0	0
			5	4	1		
2	Q	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	Q	1	Total	O	P	0	0
			5	4	1		
2	R	1	Total	O	P	0	0
			5	4	1		
2	R	1	Total	O	P	0	0
			5	4	1		
2	S	1	Total	O	P	0	0
			5	4	1		
2	S	1	Total	O	P	0	0
			5	4	1		
2	S	1	Total	O	P	0	0
			5	4	1		
2	T	1	Total	O	P	0	0
			5	4	1		
2	T	1	Total	O	P	0	0
			5	4	1		
2	T	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	213	Total	O	0	0
			213	213		
3	B	207	Total	O	0	0
			207	207		
3	C	214	Total	O	0	0
			214	214		
3	D	244	Total	O	0	0
			244	244		
3	E	233	Total	O	0	0
			233	233		
3	F	230	Total	O	0	0
			230	230		
3	G	251	Total	O	0	0
			251	251		
3	H	259	Total	O	0	0
			259	259		
3	I	213	Total	O	0	0
			213	213		
3	J	229	Total	O	0	0
			229	229		

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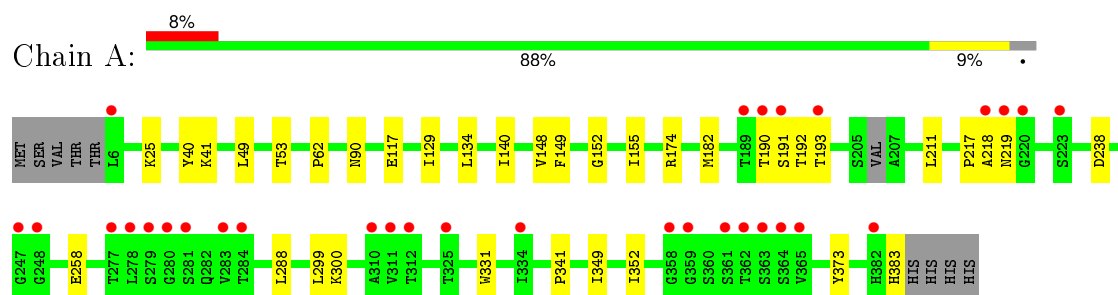
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	K	207	Total 207	O 207	0	0
3	L	197	Total 197	O 197	0	0
3	M	233	Total 233	O 233	0	0
3	N	238	Total 238	O 238	0	0
3	O	240	Total 240	O 240	0	0
3	P	233	Total 233	O 233	0	0
3	Q	216	Total 216	O 216	0	0
3	R	191	Total 191	O 191	0	0
3	S	239	Total 239	O 239	0	0
3	T	233	Total 233	O 233	0	0

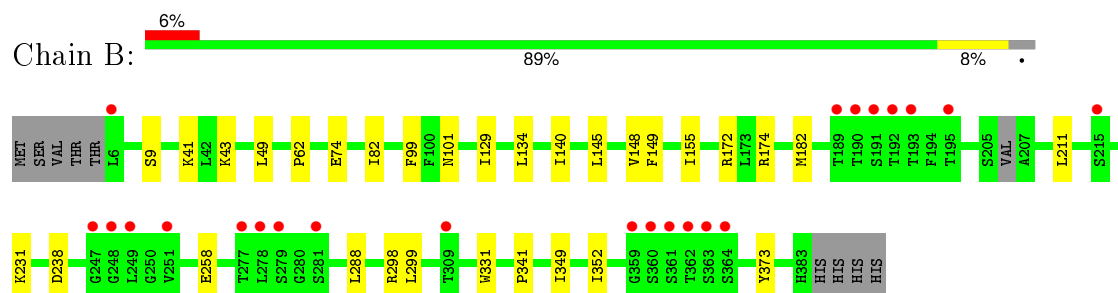
### 3 Residue-property plots [i](#)

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

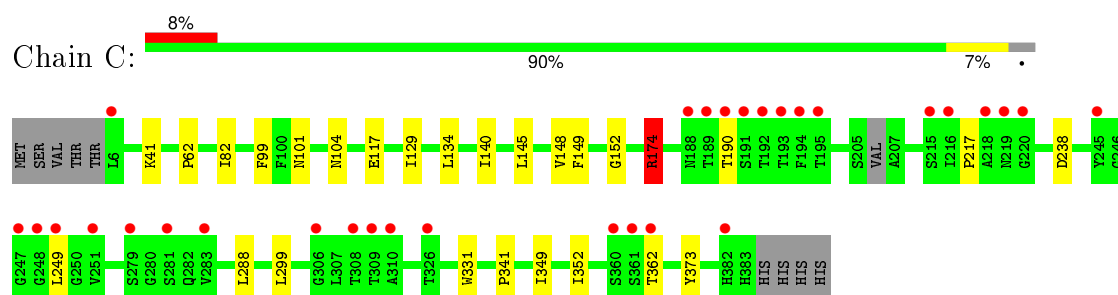
#### • Molecule 1: C381 turret protein



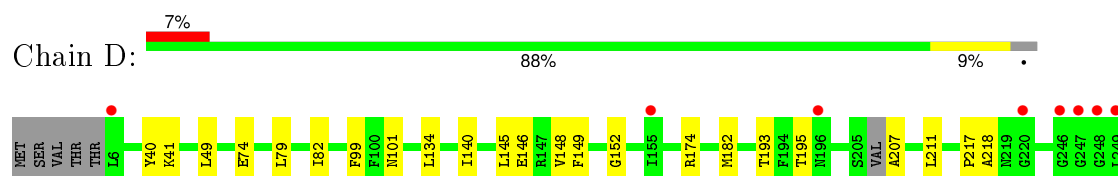
#### • Molecule 1: C381 turret protein

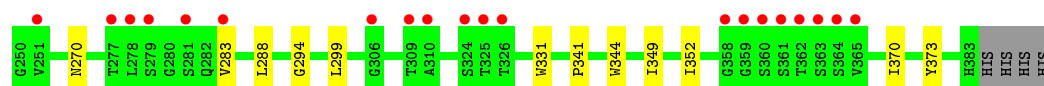


#### • Molecule 1: C381 turret protein

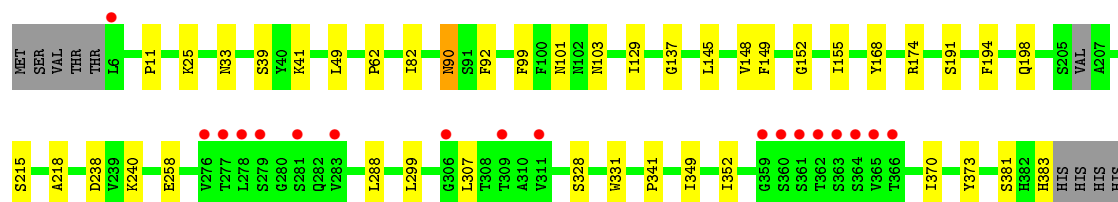
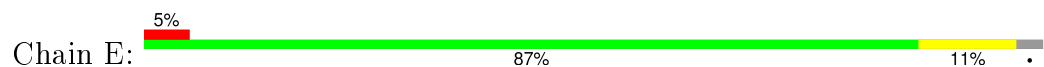


#### • Molecule 1: C381 turret protein

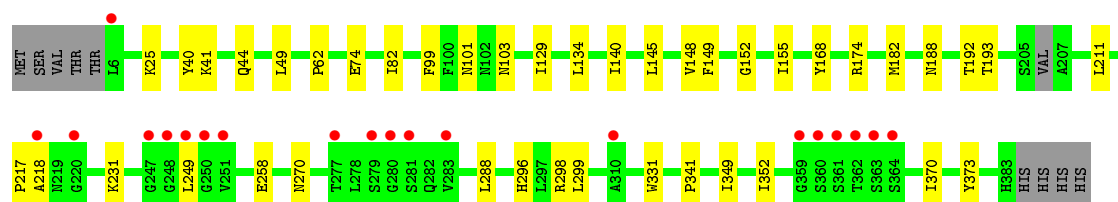
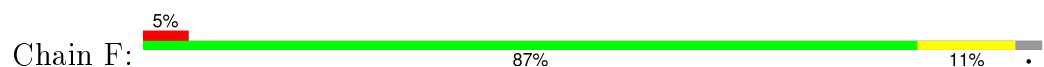




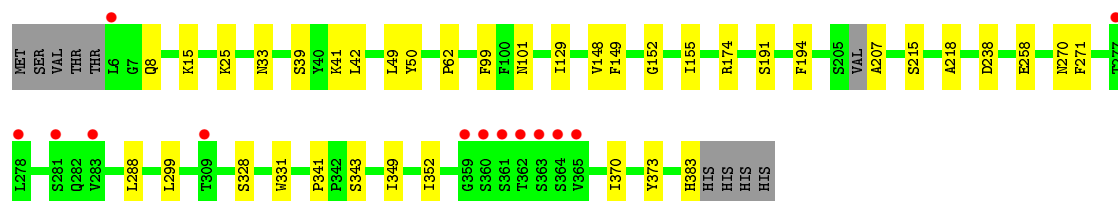
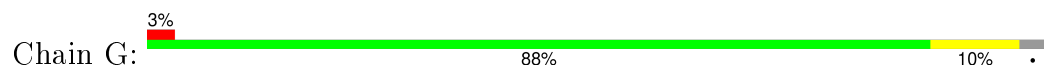
• Molecule 1: C381 turret protein



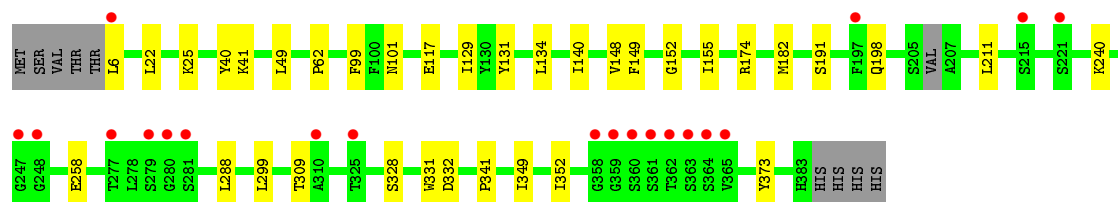
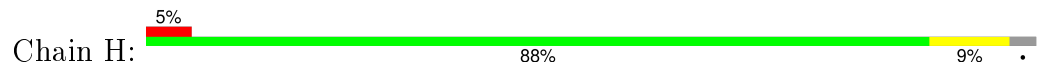
• Molecule 1: C381 turret protein



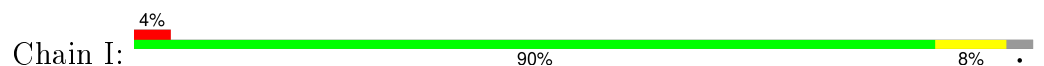
• Molecule 1: C381 turret protein



• Molecule 1: C381 turret protein

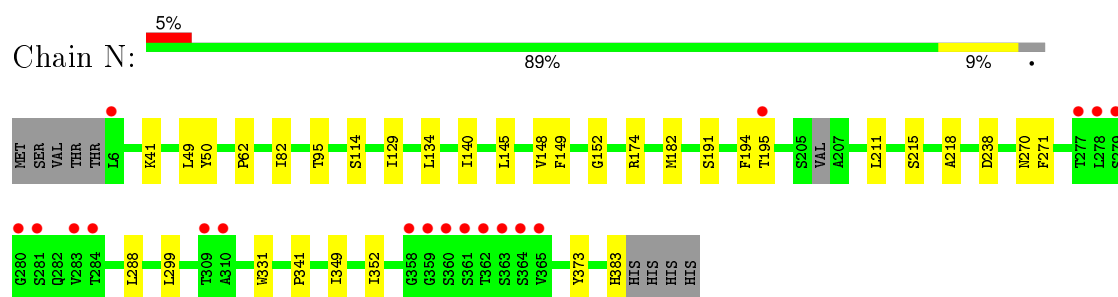


• Molecule 1: C381 turret protein

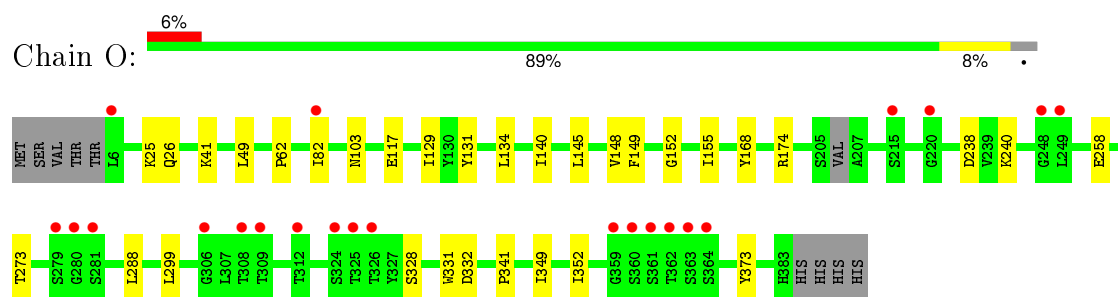




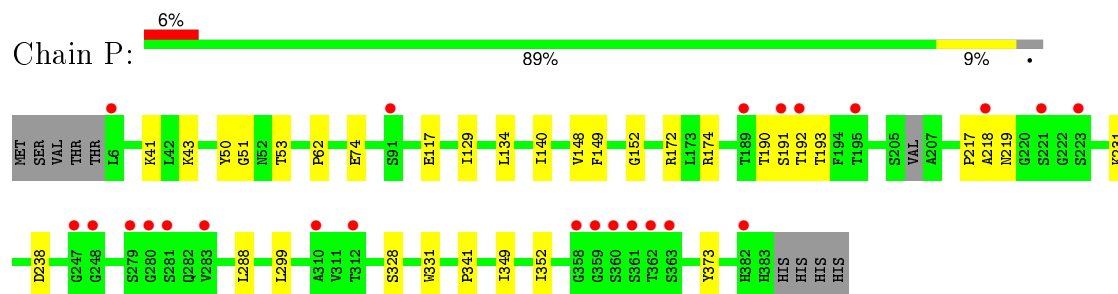




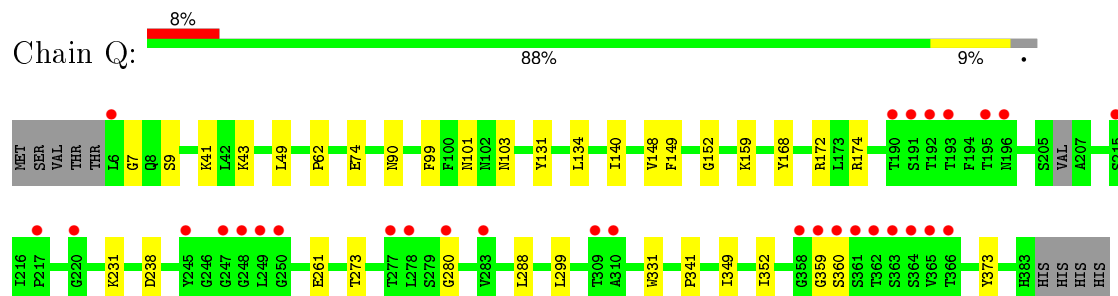
- Molecule 1: C381 turret protein



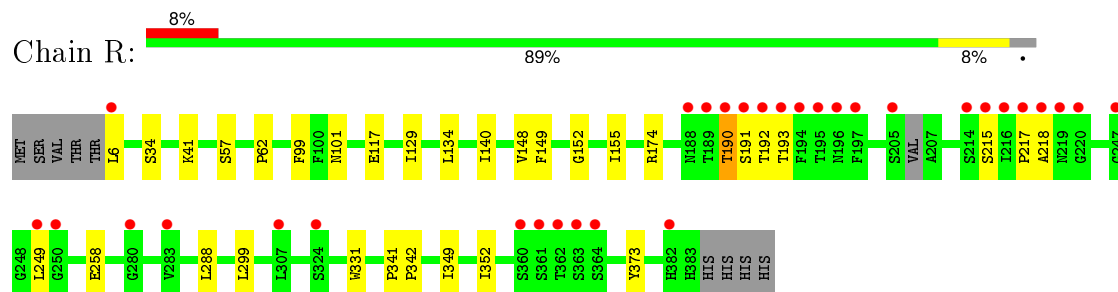
- Molecule 1: C381 turret protein



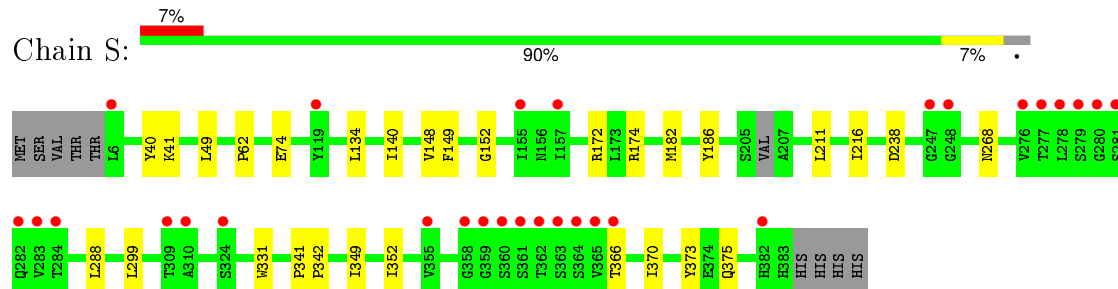
- Molecule 1: C381 turret protein



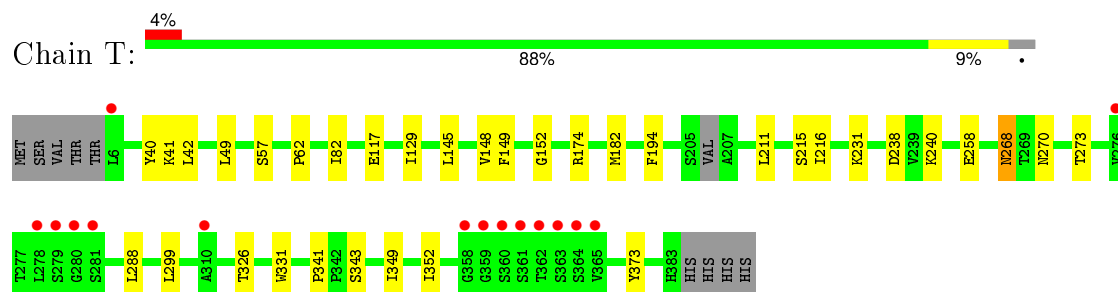
- Molecule 1: C381 turret protein



## ● Molecule 1: C381 turret protein



## ● Molecule 1: C381 turret protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.77Å 167.00Å 186.97Å 81.84° 82.17° 81.44°	Depositor
Resolution (Å)	39.19 – 1.80 39.18 – 1.76	Depositor EDS
% Data completeness (in resolution range)	86.9 (39.19-1.80) 81.8 (39.18-1.76)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 1.76Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.188 , 0.217 0.200 , 0.225	Depositor DCC
$R_{free}$ test set	38913 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 779346 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	64220	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 2HP

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	0.48	2/3032 (0.1%)	0.59	0/4127
1	B	0.43	0/3032	0.58	0/4127
1	C	0.43	0/3032	0.80	3/4127 (0.1%)
1	D	0.44	0/3032	0.59	0/4127
1	E	0.52	4/3032 (0.1%)	0.60	0/4127
1	F	0.46	0/3032	0.59	0/4127
1	G	0.46	0/3032	0.60	0/4127
1	H	0.46	0/3032	0.60	0/4127
1	I	0.42	0/3032	0.58	0/4127
1	J	0.44	0/3032	0.59	0/4127
1	K	0.42	0/3032	0.58	0/4127
1	L	0.42	0/3032	0.58	0/4127
1	M	0.44	0/3032	0.58	0/4127
1	N	0.45	0/3032	0.59	0/4127
1	O	0.43	0/3032	0.58	0/4127
1	P	0.43	0/3032	0.58	0/4127
1	Q	0.48	2/3032 (0.1%)	0.58	0/4127
1	R	0.44	0/3032	0.59	0/4127
1	S	0.46	0/3032	0.59	0/4127
1	T	0.49	2/3032 (0.1%)	0.59	0/4127
All	All	0.45	10/60640 (0.0%)	0.60	3/82540 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	ASN	CG-ND2	-8.86	1.10	1.32
1	Q	90	ASN	CG-ND2	-8.79	1.10	1.32
1	T	268	ASN	CG-ND2	-8.63	1.11	1.32
1	E	198	GLN	CD-NE2	-8.58	1.11	1.32
1	Q	90	ASN	CG-OD1	-8.44	1.05	1.24
1	E	90	ASN	CG-ND2	-7.97	1.12	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	268	ASN	CG-OD1	-7.72	1.06	1.24
1	A	90	ASN	CG-OD1	-7.55	1.07	1.24
1	E	198	GLN	CD-OE1	-7.21	1.08	1.24
1	E	90	ASN	CG-OD1	-6.70	1.09	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	174	ARG	NE-CZ-NH1	-24.25	108.17	120.30
1	C	174	ARG	NE-CZ-NH2	23.42	132.01	120.30
1	C	174	ARG	CD-NE-CZ	10.42	138.19	123.60

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	2970	0	2938	54	0
1	B	2970	0	2938	30	0
1	C	2970	0	2938	26	1
1	D	2970	0	2938	44	1
1	E	2970	0	2938	49	0
1	F	2970	0	2938	72	0
1	G	2970	0	2938	52	0
1	H	2970	0	2938	45	1
1	I	2970	0	2938	31	0
1	J	2970	0	2938	30	0
1	K	2970	0	2938	28	0
1	L	2970	0	2938	40	2
1	M	2970	0	2938	27	0
1	N	2970	0	2938	34	1
1	O	2970	0	2938	30	3
1	P	2970	0	2938	37	0
1	Q	2970	0	2938	40	0
1	R	2970	0	2938	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S	2970	0	2938	28	1
1	T	2970	0	2938	34	1
2	A	15	0	0	3	0
2	B	20	0	0	5	0
2	C	10	0	0	2	0
2	D	15	0	0	2	0
2	E	15	0	0	2	0
2	F	15	0	0	5	0
2	G	15	0	0	3	0
2	H	15	0	0	1	0
2	I	20	0	0	2	0
2	J	10	0	0	1	0
2	K	15	0	0	2	0
2	L	15	0	0	2	0
2	M	15	0	0	2	0
2	N	15	0	0	2	0
2	O	15	0	0	1	0
2	P	15	0	0	4	0
2	Q	20	0	0	3	0
2	R	10	0	0	2	0
2	S	15	0	0	3	0
2	T	15	0	0	3	0
3	A	213	0	0	2	0
3	B	207	0	0	5	0
3	C	214	0	0	4	0
3	D	244	0	0	9	0
3	E	233	0	0	5	0
3	F	230	0	0	11	0
3	G	251	0	0	6	0
3	H	259	0	0	5	0
3	I	213	0	0	5	0
3	J	229	0	0	6	0
3	K	207	0	0	4	0
3	L	197	0	0	2	0
3	M	233	0	0	3	0
3	N	238	0	0	4	1
3	O	240	0	0	4	0
3	P	233	0	0	4	0
3	Q	216	0	0	5	0
3	R	191	0	0	3	0
3	S	239	0	0	5	2
3	T	233	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	64220	0	58760	654	7

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 6.

All (654) 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:40:TYR:CZ	1:H:25:LYS:HE3	1.35	1.57
1:A:25:LYS:HE3	1:F:40:TYR:CZ	1.41	1.55
1:A:25:LYS:HE3	1:F:40:TYR:CE1	1.62	1.33
1:F:249:LEU:HD12	1:R:215:SER:OG	1.31	1.29
1:L:361:SER:OG	1:Q:360:SER:HB3	1.08	1.25
1:D:40:TYR:CE1	1:H:25:LYS:HE3	1.72	1.24
1:D:40:TYR:CZ	1:H:25:LYS:CE	2.24	1.20
1:A:25:LYS:CE	1:F:40:TYR:CZ	2.25	1.19
1:L:361:SER:OG	1:Q:360:SER:CB	1.90	1.19
1:F:296:HIS:NE2	2:F:403:2HP:O2	1.75	1.18
1:E:25:LYS:HE2	1:G:33:ASN:HB2	1.27	1.15
1:F:249:LEU:HD12	1:R:215:SER:CB	1.81	1.10
1:E:33:ASN:HB2	1:G:25:LYS:HE2	1.32	1.10
1:E:39[B]:SER:OG	1:G:41:LYS:HG2	1.51	1.10
1:H:349:ILE:HD12	1:H:352:ILE:HD11	1.37	1.06
1:E:41:LYS:HG2	1:G:39[B]:SER:OG	1.56	1.05
1:A:349:ILE:HD12	1:A:352:ILE:HD11	1.38	1.05
1:K:349:ILE:HD12	1:K:352:ILE:HD11	1.37	1.04
1:G:349:ILE:HD12	1:G:352:ILE:HD11	1.38	1.03
1:E:349:ILE:HD12	1:E:352:ILE:HD11	1.40	1.03
1:J:349:ILE:HD12	1:J:352:ILE:HD11	1.41	1.03
1:F:249:LEU:HA	1:R:215:SER:OG	1.57	1.02
1:O:349:ILE:HD12	1:O:352:ILE:HD11	1.40	1.02
1:Q:349:ILE:HD12	1:Q:352:ILE:HD11	1.42	1.02
1:A:25:LYS:CE	1:F:40:TYR:CE1	2.43	1.01
1:D:349:ILE:HD12	1:D:352:ILE:HD11	1.43	1.01
1:F:349:ILE:HD12	1:F:352:ILE:HD11	1.43	1.00
1:M:349:ILE:HD12	1:M:352:ILE:HD11	1.40	1.00
1:P:349:ILE:HD12	1:P:352:ILE:HD11	1.43	1.00
1:C:349:ILE:HD12	1:C:352:ILE:HD11	1.40	1.00
1:T:349:ILE:HD12	1:T:352:ILE:HD11	1.44	0.99
1:R:349:ILE:HD12	1:R:352:ILE:HD11	1.40	0.99
1:S:349:ILE:HD12	1:S:352:ILE:HD11	1.40	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ILE:HD12	1:B:352:ILE:HD11	1.41	0.98
2:B:403:2HP:O4	3:B:635:HOH:O	1.80	0.98
1:I:349:ILE:HD12	1:I:352:ILE:HD11	1.42	0.97
1:N:349:ILE:HD12	1:N:352:ILE:HD11	1.44	0.97
1:L:349:ILE:HD12	1:L:352:ILE:HD11	1.45	0.96
1:F:249:LEU:HA	1:R:215:SER:CB	1.95	0.96
1:R:192:THR:O	1:R:218:ALA:HA	1.66	0.95
1:L:361:SER:HG	1:Q:360:SER:HB3	1.30	0.95
1:F:249:LEU:CD1	1:R:215:SER:OG	2.17	0.93
1:D:40:TYR:CE2	1:H:25:LYS:CE	2.52	0.92
1:D:40:TYR:CE1	1:H:25:LYS:CE	2.51	0.92
1:P:231:LYS:NZ	2:P:403:2HP:O2	2.01	0.92
1:L:361:SER:HG	1:Q:360:SER:CB	1.82	0.92
1:L:188:ASN:OD1	1:L:190:THR:OG1	1.86	0.91
1:E:25:LYS:HE2	1:G:33:ASN:CB	2.01	0.91
1:T:231:LYS:NZ	2:T:403:2HP:O3	2.05	0.90
1:D:40:TYR:CE2	1:H:25:LYS:HE3	2.06	0.89
1:E:33:ASN:CB	1:G:25:LYS:HE2	2.04	0.88
1:D:40:TYR:O	1:H:25:LYS:NZ	2.06	0.88
1:F:249:LEU:CD2	1:R:217:PRO:HG3	2.03	0.88
1:B:231:LYS:NZ	2:B:403:2HP:O2	2.06	0.88
1:A:25:LYS:NZ	1:F:40:TYR:O	2.05	0.87
1:C:349:ILE:CD1	1:C:352:ILE:HD11	2.05	0.85
1:R:349:ILE:CD1	1:R:352:ILE:HD11	2.07	0.85
1:H:349:ILE:CD1	1:H:352:ILE:HD11	2.06	0.85
1:G:349:ILE:CD1	1:G:352:ILE:HD11	2.06	0.85
1:T:349:ILE:CD1	1:T:352:ILE:HD11	2.06	0.84
1:S:349:ILE:CD1	1:S:352:ILE:HD11	2.07	0.84
1:Q:349:ILE:CD1	1:Q:352:ILE:HD11	2.07	0.84
1:E:25:LYS:CE	1:G:33:ASN:HB2	2.07	0.84
1:M:349:ILE:CD1	1:M:352:ILE:HD11	2.07	0.84
1:A:25:LYS:CE	1:F:40:TYR:CE2	2.61	0.84
1:K:349:ILE:CD1	1:K:352:ILE:HD11	2.08	0.83
1:E:349:ILE:CD1	1:E:352:ILE:HD11	2.08	0.83
1:D:40:TYR:CE2	1:H:25:LYS:HE2	2.13	0.83
1:F:349:ILE:CD1	1:F:352:ILE:HD11	2.08	0.82
1:O:349:ILE:CD1	1:O:352:ILE:HD11	2.09	0.82
1:D:349:ILE:CD1	1:D:352:ILE:HD11	2.08	0.82
1:A:349:ILE:CD1	1:A:352:ILE:HD11	2.09	0.82
1:N:349:ILE:CD1	1:N:352:ILE:HD11	2.09	0.82
1:A:25:LYS:HE2	1:F:40:TYR:CE2	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:191:SER:O	1:R:218:ALA:HB1	1.80	0.81
1:B:349:ILE:CD1	1:B:352:ILE:HD11	2.11	0.81
1:F:249:LEU:HD21	1:R:217:PRO:HG3	1.63	0.81
1:E:33:ASN:HB2	1:G:25:LYS:CE	2.10	0.81
1:P:349:ILE:CD1	1:P:352:ILE:HD11	2.11	0.81
1:I:349:ILE:CD1	1:I:352:ILE:HD11	2.11	0.81
1:J:349:ILE:CD1	1:J:352:ILE:HD11	2.10	0.80
1:L:361:SER:CB	1:Q:360:SER:HB3	2.13	0.79
1:L:349:ILE:CD1	1:L:352:ILE:HD11	2.13	0.79
1:A:190:THR:O	1:A:219:ASN:N	2.17	0.76
1:F:249:LEU:CA	1:R:215:SER:OG	2.34	0.75
2:D:403:2HP:O4	3:D:727:HOH:O	2.03	0.75
1:L:361:SER:CB	1:Q:360:SER:CB	2.65	0.74
1:A:191:SER:C	1:A:218:ALA:HB1	2.09	0.73
1:F:231:LYS:NZ	2:F:403:2HP:O4	2.20	0.73
1:P:174:ARG:CZ	3:P:725:HOH:O	2.35	0.73
1:R:192:THR:HG22	1:R:193:THR:N	2.04	0.72
1:H:349:ILE:HD12	1:H:352:ILE:CD1	2.18	0.72
1:F:25:LYS:NZ	3:F:693:HOH:O	2.00	0.72
1:R:148:VAL:O	2:R:401:2HP:O4	2.08	0.71
1:E:381:SER:HB2	3:E:688:HOH:O	1.91	0.71
1:A:191:SER:HA	1:A:218:ALA:HB1	1.72	0.70
1:F:249:LEU:HD11	1:R:217:PRO:HD3	1.73	0.70
1:M:148:VAL:O	2:M:401:2HP:O4	2.10	0.70
1:G:41:LYS:NZ	3:G:568:HOH:O	2.18	0.70
1:A:349:ILE:HD12	1:A:352:ILE:CD1	2.20	0.70
1:T:268:ASN:HD22	1:T:270:ASN:HD21	1.37	0.69
1:E:349:ILE:HD12	1:E:352:ILE:CD1	2.20	0.69
1:K:349:ILE:HD12	1:K:352:ILE:CD1	2.19	0.69
1:G:349:ILE:HD12	1:G:352:ILE:CD1	2.21	0.69
1:Q:261[B]:GLU:OE2	3:Q:607:HOH:O	2.10	0.69
1:L:362:THR:HG21	1:Q:359:GLY:O	1.92	0.69
1:F:298:ARG:HD2	3:F:713:HOH:O	1.93	0.68
1:C:349:ILE:HD12	1:C:352:ILE:CD1	2.19	0.68
1:L:362:THR:CG2	1:Q:359:GLY:O	2.41	0.68
1:I:148:VAL:O	2:I:401:2HP:O4	2.11	0.68
1:J:148:VAL:O	2:J:401:2HP:O4	2.11	0.68
1:G:148:VAL:O	2:G:401:2HP:O4	2.12	0.68
1:R:349:ILE:HD12	1:R:352:ILE:CD1	2.20	0.68
2:F:403:2HP:O3	3:F:713:HOH:O	2.11	0.67
1:B:349:ILE:HD12	1:B:352:ILE:CD1	2.21	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:349:ILE:HD12	1:N:352:ILE:CD1	2.24	0.67
1:A:191:SER:CA	1:A:218:ALA:HB1	2.23	0.67
1:E:41:LYS:HG2	1:G:39[B]:SER:HG	1.59	0.67
1:A:129:ILE:HD13	1:E:49:LEU:HD22	1.75	0.67
1:N:195:THR:HG23	3:N:736:HOH:O	1.94	0.67
1:L:148:VAL:O	2:L:401:2HP:O4	2.13	0.66
1:M:349:ILE:HD12	1:M:352:ILE:CD1	2.21	0.66
1:K:41:LYS:NZ	3:K:640:HOH:O	2.23	0.66
1:F:249:LEU:HD12	1:R:215:SER:HB2	1.73	0.66
1:G:207:ALA:N	3:G:690:HOH:O	2.28	0.66
1:J:25:LYS:HD3	3:J:718:HOH:O	1.95	0.66
1:B:148:VAL:O	2:B:401:2HP:O4	2.14	0.65
1:C:148:VAL:O	2:C:401:2HP:O4	2.14	0.65
1:D:349:ILE:HD12	1:D:352:ILE:CD1	2.24	0.65
1:I:174:ARG:HG2	3:I:647:HOH:O	1.96	0.65
1:P:193:THR:HG23	1:P:217:PRO:HA	1.77	0.65
1:Q:148:VAL:O	2:Q:401:2HP:O4	2.13	0.65
1:N:49:LEU:HD22	1:O:129:ILE:HD13	1.79	0.65
1:I:349:ILE:HD12	1:I:352:ILE:CD1	2.25	0.65
1:F:299:LEU:HD11	1:F:352:ILE:HD12	1.79	0.65
1:E:39[B]:SER:HG	1:G:41:LYS:HG2	1.55	0.64
1:F:349:ILE:HD12	1:F:352:ILE:CD1	2.25	0.64
1:A:148:VAL:O	2:A:401:2HP:O4	2.16	0.64
1:S:349:ILE:HD12	1:S:352:ILE:CD1	2.23	0.64
1:T:326:THR:O	3:T:729:HOH:O	2.15	0.64
1:J:349:ILE:HD12	1:J:352:ILE:CD1	2.23	0.64
1:C:299:LEU:HD11	1:C:352:ILE:HD12	1.78	0.64
1:K:148:VAL:O	2:K:401:2HP:O4	2.16	0.64
1:R:299:LEU:HD11	1:R:352:ILE:HD12	1.80	0.64
1:F:193:THR:HG23	1:F:217:PRO:HA	1.80	0.63
1:O:240:LYS:NZ	3:O:612:HOH:O	2.26	0.63
1:D:146:GLU:HB3	3:D:720:HOH:O	1.98	0.63
1:B:299:LEU:HD11	1:B:352:ILE:HD12	1.80	0.63
1:F:193:THR:OG1	1:F:218:ALA:N	2.31	0.63
1:E:299:LEU:HD11	1:E:352:ILE:HD12	1.82	0.62
1:D:299:LEU:HD11	1:D:352:ILE:HD12	1.80	0.62
1:D:40:TYR:CD1	1:H:25:LYS:NZ	2.67	0.62
1:N:299:LEU:HD11	1:N:352:ILE:HD12	1.81	0.62
1:D:207:ALA:N	3:D:675:HOH:O	2.32	0.62
1:R:192:THR:O	1:R:218:ALA:CA	2.45	0.62
1:T:42:LEU:HD11	3:T:699:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:349:ILE:HD12	1:L:352:ILE:CD1	2.27	0.61
1:R:191:SER:O	1:R:218:ALA:CB	2.48	0.61
1:O:299:LEU:HD11	1:O:352:ILE:HD12	1.82	0.61
1:Q:349:ILE:HD12	1:Q:352:ILE:CD1	2.24	0.61
1:H:152:GLY:HA3	1:I:174:ARG:HD3	1.82	0.61
1:G:299:LEU:HD11	1:G:352:ILE:HD12	1.82	0.61
1:G:49:LEU:HD22	1:H:129:ILE:HD13	1.83	0.61
1:T:299:LEU:HD11	1:T:352:ILE:HD12	1.83	0.61
1:L:148:VAL:O	1:L:149:PHE:HB2	2.01	0.60
2:B:404:2HP:O3	1:C:238:ASP:OD2	2.19	0.60
1:A:299:LEU:HD11	1:A:352:ILE:HD12	1.83	0.60
1:B:43:LYS:NZ	3:B:638:HOH:O	2.34	0.60
1:K:174:ARG:HD3	1:O:152:GLY:HA3	1.82	0.60
1:R:192:THR:CG2	1:R:193:THR:N	2.65	0.60
1:K:159:LYS:HD2	3:K:547:HOH:O	2.00	0.60
1:H:6:LEU:HD11	3:H:734:HOH:O	2.02	0.60
1:A:148:VAL:O	1:A:149:PHE:HB2	2.02	0.59
1:N:148:VAL:O	2:N:401:2HP:O4	2.19	0.59
1:M:299:LEU:HD11	1:M:352:ILE:HD12	1.82	0.59
1:F:249:LEU:HD22	1:R:217:PRO:HG3	1.85	0.59
1:Q:299:LEU:HD11	1:Q:352:ILE:HD12	1.83	0.59
1:J:299:LEU:HD11	1:J:352:ILE:HD12	1.84	0.59
1:F:25:LYS:CD	3:F:693:HOH:O	2.50	0.59
1:T:349:ILE:HD12	1:T:352:ILE:CD1	2.25	0.59
1:O:349:ILE:HD12	1:O:352:ILE:CD1	2.23	0.59
1:S:299:LEU:HD11	1:S:352:ILE:HD12	1.84	0.58
1:T:268:ASN:ND2	1:T:270:ASN:HD21	2.01	0.58
1:D:193:THR:HG23	1:D:217:PRO:HA	1.85	0.58
1:F:174:ARG:HD3	1:J:152:GLY:HA3	1.85	0.58
1:G:191:SER:HA	1:G:218:ALA:HB1	1.86	0.58
1:F:148:VAL:O	1:F:149:PHE:HB2	2.03	0.58
1:P:299:LEU:HD11	1:P:352:ILE:HD12	1.85	0.58
1:C:217:PRO:HD2	3:C:611:HOH:O	2.03	0.58
1:E:25:LYS:HG2	1:G:33:ASN:ND2	2.19	0.58
1:A:191:SER:O	1:A:218:ALA:CB	2.51	0.58
1:D:40:TYR:CE1	1:H:25:LYS:NZ	2.71	0.58
1:L:299:LEU:HD11	1:L:352:ILE:HD12	1.85	0.58
1:M:152:GLY:HA3	1:N:174:ARG:HD3	1.84	0.58
1:F:129:ILE:HD13	1:J:49:LEU:HD22	1.86	0.57
1:F:152:GLY:HA3	1:G:174:ARG:HD3	1.85	0.57
1:G:15:LYS:CD	3:G:719:HOH:O	2.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:288[A]:LEU:HD11	1:O:373:TYR:CE2	2.40	0.57
1:I:299:LEU:HD11	1:I:352:ILE:HD12	1.85	0.57
1:S:148:VAL:O	2:S:401:2HP:O4	2.22	0.57
1:H:49:LEU:HD22	1:I:129:ILE:HD13	1.87	0.57
1:A:191:SER:C	1:A:218:ALA:CB	2.72	0.57
1:G:15:LYS:HD2	3:G:719:HOH:O	2.04	0.57
1:P:238:ASP:OD2	2:P:402:2HP:O3	2.22	0.57
1:E:33:ASN:ND2	1:G:25:LYS:HG2	2.20	0.57
1:N:288[A]:LEU:HD11	1:N:373:TYR:CE2	2.40	0.57
1:G:288[A]:LEU:HD11	1:G:373:TYR:CE2	2.40	0.57
1:L:191:SER:O	1:L:218:ALA:CB	2.53	0.57
1:H:299:LEU:HD11	1:H:352:ILE:HD12	1.86	0.56
1:A:148:VAL:HG23	1:A:149:PHE:CD2	2.40	0.56
1:F:288[A]:LEU:HD11	1:F:373:TYR:CE2	2.40	0.56
1:P:148:VAL:O	1:P:149:PHE:HB2	2.04	0.56
1:Q:159:LYS:HD2	3:Q:610:HOH:O	2.05	0.56
1:E:288[A]:LEU:HD11	1:E:373:TYR:CE2	2.40	0.56
1:L:207:ALA:N	3:L:646:HOH:O	2.38	0.56
1:S:148:VAL:O	1:S:149:PHE:HB2	2.04	0.56
1:P:191:SER:O	1:P:218:ALA:CB	2.53	0.56
1:M:49:LEU:HD22	1:N:129:ILE:HD13	1.87	0.56
1:P:41:LYS:HE3	1:P:62:PRO:HB3	1.88	0.56
1:H:148:VAL:O	2:H:401:2HP:O4	2.23	0.56
1:R:117:GLU:OE1	1:S:74:GLU:OE1	2.24	0.56
1:D:288[A]:LEU:HD11	1:D:373:TYR:CE2	2.41	0.56
1:L:152:GLY:HA3	1:M:174:ARG:HD3	1.88	0.56
1:K:288[A]:LEU:HD11	1:K:373:TYR:CE2	2.41	0.56
1:A:25:LYS:NZ	1:F:40:TYR:CD1	2.74	0.55
1:J:148:VAL:O	1:J:149:PHE:HB2	2.05	0.55
1:B:148:VAL:O	1:B:149:PHE:HB2	2.05	0.55
1:H:41:LYS:HE3	1:H:62:PRO:HB3	1.87	0.55
1:D:294:GLY:HA3	3:D:723:HOH:O	2.06	0.55
1:R:288[A]:LEU:HD11	1:R:373:TYR:CE2	2.41	0.55
1:K:299:LEU:HD11	1:K:352:ILE:HD12	1.87	0.55
1:P:349:ILE:HD12	1:P:352:ILE:CD1	2.26	0.55
1:A:288[A]:LEU:HD11	1:A:373:TYR:CE2	2.42	0.55
1:M:174:ARG:HG2	3:M:672:HOH:O	2.06	0.55
1:M:288[A]:LEU:HD11	1:M:373:TYR:CE2	2.41	0.55
1:H:288[A]:LEU:HD11	1:H:373:TYR:CE2	2.42	0.55
1:E:238:ASP:OD2	2:E:402:2HP:O3	2.23	0.55
1:R:148:VAL:O	1:R:149:PHE:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:148:VAL:O	1:N:149:PHE:HB2	2.07	0.55
1:T:288[A]:LEU:HD11	1:T:373:TYR:CE2	2.42	0.55
1:F:44:GLN:HB2	3:F:705:HOH:O	2.06	0.55
1:L:288[A]:LEU:HD11	1:L:373:TYR:CE2	2.42	0.55
1:M:148:VAL:O	1:M:149:PHE:HB2	2.06	0.55
1:H:148:VAL:HG23	1:H:149:PHE:CD2	2.42	0.55
1:A:152:GLY:HA3	1:B:174:ARG:HD3	1.89	0.55
1:O:240:LYS:NZ	3:O:653:HOH:O	2.39	0.54
1:E:148:VAL:O	1:E:149:PHE:HB2	2.06	0.54
1:E:148:VAL:HG23	1:E:149:PHE:CD2	2.42	0.54
1:Q:41:LYS:HE3	1:Q:62:PRO:HB3	1.89	0.54
1:S:288[A]:LEU:HD11	1:S:373:TYR:CE2	2.42	0.54
1:M:148:VAL:HG23	1:M:149:PHE:CD2	2.42	0.54
1:Q:148:VAL:O	1:Q:149:PHE:HB2	2.07	0.54
1:P:148:VAL:HG23	1:P:149:PHE:CD2	2.42	0.54
1:E:370:ILE:HD11	3:E:585:HOH:O	2.08	0.54
1:O:148:VAL:O	1:O:149:PHE:HB2	2.07	0.54
1:D:41:LYS:HG2	1:H:40:TYR:OH	2.07	0.54
1:A:25:LYS:NZ	1:F:40:TYR:CE1	2.74	0.54
1:Q:231:LYS:NZ	2:Q:403:2HP:O2	2.25	0.54
1:B:174:ARG:HG2	3:B:658:HOH:O	2.08	0.54
1:O:41:LYS:HE3	1:O:62:PRO:HB3	1.90	0.54
1:C:288[A]:LEU:HD11	1:C:373:TYR:CE2	2.43	0.54
1:S:268:ASN:OD1	1:S:375:GLN:HB3	2.07	0.54
1:E:191:SER:HA	1:E:218:ALA:HB1	1.89	0.54
1:T:268:ASN:HD22	1:T:270:ASN:ND2	2.06	0.54
1:G:148:VAL:O	1:G:149:PHE:HB2	2.07	0.54
1:H:148:VAL:O	1:H:149:PHE:HB2	2.08	0.54
1:F:148:VAL:O	2:F:401:2HP:O4	2.26	0.53
1:S:172:ARG:NH1	3:S:536:HOH:O	2.40	0.53
1:A:41:LYS:HE3	1:A:62:PRO:HB3	1.90	0.53
1:A:174:ARG:HD3	1:E:152:GLY:HA3	1.88	0.53
1:G:148:VAL:HG23	1:G:149:PHE:CD2	2.43	0.53
1:S:152:GLY:HA3	1:T:174:ARG:HD3	1.90	0.53
1:P:117:GLU:OE1	1:Q:74:GLU:OE1	2.26	0.53
1:Q:288[A]:LEU:HD11	1:Q:373:TYR:CE2	2.44	0.53
1:G:270:ASN:OD1	1:H:328:SER:HB2	2.09	0.53
1:K:41:LYS:HE3	1:K:62:PRO:HB3	1.89	0.53
1:E:194:PHE:O	1:E:215:SER:HA	2.07	0.53
1:I:49:LEU:HD22	1:J:129:ILE:HD13	1.89	0.53
1:F:249:LEU:HD21	1:R:217:PRO:CG	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:GLY:HA3	1:D:174:ARG:HD3	1.89	0.53
1:C:148:VAL:O	1:C:149:PHE:HB2	2.08	0.53
1:L:41:LYS:HE3	1:L:62:PRO:HB3	1.90	0.53
1:J:288[A]:LEU:HD11	1:J:373:TYR:CE2	2.44	0.53
1:P:288[A]:LEU:HD11	1:P:373:TYR:CE2	2.44	0.53
1:S:366:THR:HG22	3:S:720:HOH:O	2.09	0.52
1:N:191:SER:HA	1:N:218:ALA:HB1	1.90	0.52
1:P:43:LYS:NZ	3:P:640:HOH:O	2.42	0.52
1:D:40:TYR:OH	1:H:25:LYS:HE3	1.99	0.52
1:T:240:LYS:NZ	3:T:704:HOH:O	2.43	0.52
1:C:148:VAL:HG23	1:C:149:PHE:CD2	2.44	0.52
2:I:404:2HP:O1	1:J:238:ASP:OD2	2.28	0.52
1:I:41:LYS:NZ	3:I:648:HOH:O	2.28	0.52
1:J:148:VAL:HG23	1:J:149:PHE:CD2	2.45	0.52
1:Q:49:LEU:HD22	1:R:129:ILE:HD13	1.92	0.51
1:B:41:LYS:HE3	1:B:62:PRO:HB3	1.90	0.51
1:A:191:SER:O	1:A:218:ALA:HB2	2.10	0.51
1:O:148:VAL:HG23	1:O:149:PHE:CD2	2.46	0.51
1:B:172:ARG:NH1	3:B:686:HOH:O	2.43	0.51
1:B:288[A]:LEU:HD11	1:B:373:TYR:CE2	2.45	0.51
1:P:174:ARG:NH1	3:P:725:HOH:O	2.40	0.51
1:P:191:SER:O	1:P:218:ALA:HB1	2.10	0.51
1:D:148:VAL:O	1:D:149:PHE:HB2	2.10	0.51
1:N:194:PHE:O	1:N:215:SER:HA	2.10	0.51
1:R:41:LYS:HE3	1:R:62:PRO:HB3	1.93	0.51
1:G:238:ASP:OD2	2:G:402:2HP:O1	2.28	0.51
1:E:90:ASN:OD1	1:E:137:GLY:HA3	2.10	0.51
1:N:238:ASP:OD2	2:N:402:2HP:O1	2.29	0.51
1:D:40:TYR:CD2	1:H:25:LYS:HE2	2.46	0.51
1:L:362:THR:HG21	1:Q:280:GLY:HA2	1.93	0.51
1:I:148:VAL:O	1:I:149:PHE:HB2	2.10	0.51
1:R:152:GLY:HA3	1:S:174:ARG:HD3	1.93	0.51
1:P:129:ILE:HD13	1:T:49:LEU:HD22	1.92	0.51
1:T:148:VAL:O	1:T:149:PHE:HB2	2.11	0.51
1:H:198:GLN:NE2	3:H:572:HOH:O	2.38	0.51
1:K:49:LEU:HD22	1:L:129:ILE:HD13	1.93	0.50
1:K:148:VAL:O	1:K:149:PHE:HB2	2.11	0.50
1:F:44:GLN:CB	3:F:705:HOH:O	2.59	0.50
1:S:148:VAL:HG23	1:S:149:PHE:CD2	2.46	0.50
1:E:41:LYS:HE3	1:E:62:PRO:HB3	1.92	0.50
1:O:238:ASP:OD2	2:O:402:2HP:O1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:LYS:HE3	1:C:62:PRO:HB3	1.92	0.50
1:T:194:PHE:O	1:T:215:SER:HA	2.12	0.50
1:S:370:ILE:HD11	3:S:561:HOH:O	2.11	0.50
1:L:191:SER:O	1:L:218:ALA:HB1	2.12	0.50
1:P:74:GLU:OE1	1:T:117:GLU:OE1	2.30	0.50
1:D:152:GLY:HA3	1:E:174:ARG:HD3	1.94	0.50
1:A:25:LYS:CG	1:F:40:TYR:OH	2.60	0.50
1:L:148:VAL:HG23	1:L:149:PHE:CD2	2.47	0.50
1:N:148:VAL:HG23	1:N:149:PHE:CD2	2.45	0.50
1:K:129:ILE:HD13	1:O:49:LEU:HD22	1.94	0.50
1:H:41:LYS:HG2	3:H:696:HOH:O	2.11	0.49
1:D:79:LEU:O	2:D:401:2HP:O4	2.31	0.49
1:B:238:ASP:OD2	2:B:402:2HP:O3	2.30	0.49
1:F:288[A]:LEU:HD11	1:F:373:TYR:CZ	2.47	0.49
1:G:152:GLY:HA3	1:H:174:ARG:HD3	1.94	0.49
1:A:25:LYS:CE	1:F:40:TYR:CD1	2.95	0.49
1:F:25:LYS:HD2	3:F:693:HOH:O	2.11	0.49
1:F:148:VAL:HG23	1:F:149:PHE:CD2	2.47	0.49
1:L:172:ARG:NH1	3:L:567:HOH:O	2.45	0.49
1:C:190:THR:HG21	1:C:249:LEU:O	2.13	0.49
1:P:152:GLY:HA3	1:Q:174:ARG:HD3	1.93	0.49
1:R:190:THR:HG21	1:R:249:LEU:O	2.13	0.49
1:A:49:LEU:HD22	1:B:129:ILE:HD13	1.94	0.49
1:I:288[A]:LEU:HD11	1:I:373:TYR:CE2	2.47	0.49
1:G:288[A]:LEU:HD11	1:G:373:TYR:CZ	2.47	0.49
1:P:191:SER:C	1:P:218:ALA:HB1	2.33	0.49
1:C:104:ASN:ND2	3:C:587:HOH:O	2.45	0.49
1:J:41:LYS:HE3	1:J:62:PRO:HB3	1.93	0.49
1:O:288[A]:LEU:HD11	1:O:373:TYR:CZ	2.48	0.48
1:I:41:LYS:HE3	1:I:62:PRO:HB3	1.94	0.48
1:T:41:LYS:HE3	1:T:62:PRO:HB3	1.95	0.48
1:F:249:LEU:CD1	1:R:215:SER:CB	2.74	0.48
1:N:288[A]:LEU:HD11	1:N:373:TYR:CZ	2.48	0.48
1:J:190:THR:HG21	1:J:249:LEU:O	2.14	0.48
1:P:148:VAL:O	2:P:401:2HP:O4	2.32	0.48
1:E:148:VAL:O	2:E:401:2HP:O4	2.31	0.48
1:N:152:GLY:HA3	1:O:174:ARG:HD3	1.95	0.48
1:P:191:SER:O	1:P:218:ALA:HB2	2.14	0.48
1:G:194:PHE:O	1:G:215:SER:HA	2.12	0.48
1:A:191:SER:O	1:A:218:ALA:HB1	2.13	0.48
1:P:328:SER:HB2	1:T:270:ASN:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:SER:CA	1:G:218:ALA:HB1	2.43	0.48
1:K:74:GLU:OE1	1:O:117:GLU:OE1	2.32	0.48
1:D:146:GLU:CB	3:D:720:HOH:O	2.60	0.48
1:P:288[A]:LEU:HD11	1:P:373:TYR:CZ	2.49	0.48
3:F:584:HOH:O	1:G:383:HIS:HB3	2.14	0.48
1:P:190:THR:O	1:P:219:ASN:N	2.44	0.48
1:A:25:LYS:HE3	1:F:40:TYR:OH	2.01	0.47
1:R:148:VAL:HG23	1:R:149:PHE:CD2	2.49	0.47
1:Q:148:VAL:HG23	1:Q:149:PHE:CD2	2.49	0.47
1:S:41:LYS:HB3	3:S:630:HOH:O	2.13	0.47
1:A:288[A]:LEU:HD11	1:A:373:TYR:CZ	2.49	0.47
1:P:53:THR:O	1:Q:9:SER:HA	2.15	0.47
1:N:270:ASN:OD1	1:O:328:SER:HB2	2.14	0.47
1:T:148:VAL:O	2:T:401:2HP:O4	2.32	0.47
1:F:41:LYS:HE3	1:F:62:PRO:HB3	1.97	0.47
1:R:217:PRO:HD2	3:R:593:HOH:O	2.13	0.47
1:N:191:SER:O	1:N:218:ALA:HB2	2.15	0.47
1:K:43:LYS:NZ	3:K:538:HOH:O	2.43	0.47
1:N:41:LYS:HE3	1:N:62:PRO:HB3	1.96	0.47
1:D:49:LEU:HD22	1:E:129:ILE:HD13	1.97	0.47
1:P:172:ARG:NH1	3:P:534:HOH:O	2.46	0.47
1:Q:273:THR:HG22	3:Q:659:HOH:O	2.14	0.47
1:E:288[A]:LEU:HD11	1:E:373:TYR:CZ	2.49	0.47
1:E:331:TRP:CH2	1:E:341:PRO:HD3	2.50	0.47
1:K:134:LEU:HD13	1:K:140[A]:ILE:CD1	2.45	0.47
1:A:117:GLU:OE1	1:B:74:GLU:OE1	2.32	0.47
1:F:218:ALA:HB2	3:F:598:HOH:O	2.14	0.47
1:P:174:ARG:HD3	1:T:152:GLY:HA3	1.96	0.47
1:S:41:LYS:HE3	1:S:62:PRO:HB3	1.97	0.47
1:O:134:LEU:HD13	1:O:140[A]:ILE:CD1	2.45	0.47
1:D:40:TYR:CD1	1:H:25:LYS:CE	2.98	0.47
1:F:249:LEU:CD1	1:R:217:PRO:HG3	2.45	0.47
1:M:288[A]:LEU:HD11	1:M:373:TYR:CZ	2.50	0.47
1:N:191:SER:O	1:N:218:ALA:CB	2.63	0.47
1:K:148:VAL:HG23	1:K:149:PHE:CD2	2.51	0.46
1:C:288[A]:LEU:HD11	1:C:373:TYR:CZ	2.50	0.46
1:A:238:ASP:OD2	2:A:402:2HP:O3	2.34	0.46
1:C:117:GLU:OE1	1:D:74:GLU:OE1	2.32	0.46
1:J:288[A]:LEU:HD11	1:J:373:TYR:CZ	2.50	0.46
1:F:249:LEU:CD1	1:R:215:SER:HB2	2.44	0.46
1:K:288[A]:LEU:HD11	1:K:373:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:191:SER:C	1:N:218:ALA:HB1	2.36	0.46
1:Q:43:LYS:NZ	3:Q:568:HOH:O	2.47	0.46
1:R:134:LEU:HD13	1:R:140[A]:ILE:CD1	2.45	0.46
1:G:41:LYS:HE3	1:G:62:PRO:HB3	1.96	0.46
1:L:288[A]:LEU:HD11	1:L:373:TYR:CZ	2.51	0.46
1:G:8:GLN:HG2	3:G:712:HOH:O	2.16	0.46
1:L:362:THR:HG23	1:Q:359:GLY:O	2.14	0.46
1:K:134:LEU:HD13	1:K:140[A]:ILE:HD12	1.97	0.46
1:C:174:ARG:NH2	3:C:699:HOH:O	2.48	0.46
1:D:193:THR:OG1	1:D:218:ALA:N	2.43	0.46
1:N:191:SER:CA	1:N:218:ALA:HB1	2.46	0.46
1:H:99:PHE:CE2	1:H:101:ASN:HA	2.51	0.46
1:E:11:PRO:HG3	1:G:42:LEU:CD2	2.45	0.46
1:S:49:LEU:HD22	1:T:129:ILE:HD13	1.97	0.46
1:T:288[A]:LEU:HD11	1:T:373:TYR:CZ	2.50	0.46
1:E:39[B]:SER:OG	1:G:41:LYS:CG	2.42	0.46
1:F:249:LEU:HD11	1:R:217:PRO:CD	2.42	0.46
1:A:182[A]:MET:HE1	1:A:211:LEU:HD11	1.98	0.46
1:A:193:THR:HG23	1:A:217:PRO:HA	1.98	0.46
1:L:117:GLU:OE1	1:M:74:GLU:OE1	2.34	0.46
1:O:273:THR:HG22	3:O:716:HOH:O	2.15	0.46
1:Q:172:ARG:NH1	3:Q:586:HOH:O	2.49	0.46
1:A:25:LYS:HE2	1:F:40:TYR:CD2	2.51	0.46
1:A:191:SER:HA	1:A:219:ASN:OD1	2.15	0.46
1:D:288[A]:LEU:HD11	1:D:373:TYR:CZ	2.51	0.46
1:M:370:ILE:HD11	3:N:616:HOH:O	2.15	0.46
1:K:238:ASP:OD2	2:K:402:2HP:O1	2.33	0.45
1:K:172:ARG:NH1	3:K:532:HOH:O	2.48	0.45
1:L:182[A]:MET:HE1	1:L:211:LEU:HD11	1.98	0.45
1:J:134:LEU:HD13	1:J:140[A]:ILE:CD1	2.46	0.45
1:H:182[A]:MET:HE1	1:H:211:LEU:HD11	1.98	0.45
1:I:148:VAL:HG23	1:I:149:PHE:CD2	2.51	0.45
1:D:148:VAL:HG23	1:D:149:PHE:CD2	2.51	0.45
1:P:134:LEU:HD13	1:P:140[A]:ILE:CD1	2.46	0.45
1:E:39[A]:SER:HB3	1:G:41:LYS:HG2	1.98	0.45
1:T:238:ASP:OD2	2:T:402:2HP:O3	2.35	0.45
1:G:370:ILE:HD11	3:H:546:HOH:O	2.16	0.45
1:B:298:ARG:HD2	3:B:569:HOH:O	2.16	0.45
1:J:148:VAL:O	1:J:149:PHE:CB	2.65	0.45
1:P:192:THR:O	1:P:218:ALA:HA	2.17	0.45
1:F:188:ASN:ND2	1:F:192:THR:O	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182[A]:MET:HE1	1:D:211:LEU:HD11	1.98	0.45
1:D:370:ILE:HD11	3:D:599:HOH:O	2.15	0.45
1:S:148:VAL:O	1:S:149:PHE:CB	2.65	0.45
1:T:82:ILE:HG12	1:T:145:LEU:HD23	1.99	0.45
1:O:26:GLN:HB3	3:O:665:HOH:O	2.16	0.45
1:F:134:LEU:HD13	1:F:140[A]:ILE:CD1	2.47	0.45
1:D:82:ILE:HG12	1:D:145:LEU:HD23	1.99	0.45
1:A:134:LEU:HD13	1:A:140[A]:ILE:CD1	2.46	0.45
1:I:331:TRP:CH2	1:I:341:PRO:HD3	2.52	0.45
1:S:134:LEU:HD13	1:S:140[A]:ILE:CD1	2.47	0.45
1:G:148:VAL:O	2:G:401:2HP:P	2.74	0.44
1:P:50:TYR:CE2	1:Q:131:TYR:HB2	2.52	0.44
1:B:148:VAL:HG23	1:B:149:PHE:CD2	2.52	0.44
1:F:182[A]:MET:HE1	1:F:211:LEU:HD11	1.99	0.44
1:A:53:THR:O	1:B:9:SER:HA	2.17	0.44
2:P:402:2HP:O4	1:T:258:GLU:OE1	2.36	0.44
1:L:134:LEU:HD13	1:L:140[A]:ILE:CD1	2.47	0.44
1:C:134:LEU:HD13	1:C:140[A]:ILE:CD1	2.48	0.44
1:G:155:ILE:O	1:G:258:GLU:HA	2.18	0.44
1:R:193:THR:OG1	1:R:218:ALA:HB2	2.18	0.44
1:F:249:LEU:CG	1:R:215:SER:OG	2.64	0.44
1:R:288[A]:LEU:HD11	1:R:373:TYR:CZ	2.53	0.44
1:B:288[A]:LEU:HD11	1:B:373:TYR:CZ	2.53	0.44
1:L:49:LEU:HD22	1:M:129:ILE:HD13	2.00	0.44
1:G:50:TYR:CE2	1:H:131:TYR:HB2	2.52	0.44
1:M:331:TRP:CH2	1:M:341:PRO:HD3	2.52	0.44
1:I:299:LEU:HG	1:I:349:ILE:HD11	2.00	0.44
1:I:43:LYS:NZ	3:I:585:HOH:O	2.51	0.44
1:C:331:TRP:CH2	1:C:341:PRO:HD3	2.53	0.44
1:J:174:ARG:HD2	3:J:645:HOH:O	2.18	0.44
1:S:238:ASP:OD2	2:S:402:2HP:O3	2.36	0.44
1:T:331:TRP:CH2	1:T:341:PRO:HD3	2.52	0.44
1:H:331:TRP:CH2	1:H:341:PRO:HD3	2.52	0.44
1:M:134:LEU:HD13	1:M:140[A]:ILE:CD1	2.47	0.44
1:H:299:LEU:HG	1:H:349:ILE:HD11	2.00	0.44
1:A:192:THR:O	1:A:218:ALA:HA	2.18	0.44
1:S:148:VAL:O	2:S:401:2HP:P	2.76	0.44
1:G:331:TRP:CH2	1:G:341:PRO:HD3	2.53	0.44
1:L:99:PHE:CE2	1:L:101:ASN:HA	2.53	0.44
1:Q:134:LEU:HD13	1:Q:140[A]:ILE:CD1	2.48	0.44
1:J:17:LYS:HD3	3:J:700:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LYS:HG3	1:F:40:TYR:OH	2.18	0.43
1:O:299:LEU:HG	1:O:349:ILE:HD11	2.00	0.43
1:A:148:VAL:O	1:A:149:PHE:CB	2.63	0.43
1:B:331:TRP:CH2	1:B:341:PRO:HD3	2.53	0.43
1:D:270:ASN:OD1	1:E:328:SER:HB2	2.18	0.43
1:L:191:SER:O	1:L:218:ALA:HB2	2.17	0.43
1:H:288[A]:LEU:HD11	1:H:373:TYR:CZ	2.53	0.43
1:E:90:ASN:ND2	1:E:92:PHE:CZ	2.85	0.43
1:I:172:ARG:NH1	3:I:640:HOH:O	2.50	0.43
1:K:152:GLY:HA3	1:L:174:ARG:HD3	2.00	0.43
1:A:219:ASN:HB3	3:A:692:HOH:O	2.17	0.43
1:L:148:VAL:O	1:L:149:PHE:CB	2.63	0.43
1:D:99:PHE:CE2	1:D:101:ASN:HA	2.53	0.43
3:F:615:HOH:O	1:G:343:SER:HB2	2.18	0.43
1:Q:99:PHE:CE2	1:Q:101:ASN:HA	2.53	0.43
1:K:99:PHE:CE2	1:K:101:ASN:HA	2.53	0.43
1:L:331:TRP:CH2	1:L:341:PRO:HD3	2.53	0.43
1:T:57:SER:HB2	3:T:701:HOH:O	2.18	0.43
1:H:134:LEU:HD13	1:H:140[A]:ILE:CD1	2.48	0.43
1:N:95:THR:HG22	3:N:615:HOH:O	2.16	0.43
1:E:41:LYS:HG2	1:G:39[A]:SER:HB3	2.00	0.43
1:T:148:VAL:HG23	1:T:149:PHE:CD2	2.52	0.43
1:A:40:TYR:OH	1:F:41:LYS:HG2	2.17	0.43
1:N:82:ILE:HG12	1:N:145:LEU:HD23	2.00	0.43
1:M:82:ILE:HG12	1:M:145:LEU:HD23	2.00	0.43
1:Q:331:TRP:CH2	1:Q:341:PRO:HD3	2.53	0.43
1:M:148:VAL:O	1:M:149:PHE:CB	2.66	0.43
1:O:134:LEU:HD13	1:O:140[A]:ILE:HD12	2.00	0.43
1:R:57:SER:HB2	3:R:645:HOH:O	2.17	0.43
1:E:307:LEU:HB2	3:E:647:HOH:O	2.18	0.43
1:D:134:LEU:HD13	1:D:140[A]:ILE:CD1	2.48	0.43
1:F:82:ILE:HG12	1:F:145:LEU:HD23	2.01	0.43
1:O:103:ASN:HB2	1:O:168:TYR:O	2.19	0.43
1:H:117:GLU:OE1	1:I:74:GLU:OE1	2.36	0.43
1:L:361:SER:HB2	1:Q:360:SER:CB	2.45	0.43
1:C:174:ARG:HD3	3:C:692:HOH:O	2.18	0.43
1:J:331:TRP:CH2	1:J:341:PRO:HD3	2.54	0.43
1:C:148:VAL:O	2:C:401:2HP:P	2.77	0.43
1:T:194:PHE:HB2	1:T:216:ILE:HB	2.01	0.43
1:M:359:GLY:HA2	3:M:690:HOH:O	2.19	0.43
1:M:99:PHE:CE2	1:M:101:ASN:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:LEU:HG	1:B:349:ILE:HD11	2.01	0.43
1:C:148:VAL:O	1:C:149:PHE:CB	2.67	0.43
1:Q:288[A]:LEU:HD11	1:Q:373:TYR:CZ	2.54	0.43
1:N:331:TRP:CH2	1:N:341:PRO:HD3	2.53	0.43
1:N:182[A]:MET:HE1	1:N:211:LEU:HD11	2.01	0.43
1:I:155:ILE:O	1:I:258:GLU:HA	2.19	0.43
1:D:331:TRP:CH2	1:D:341:PRO:HD3	2.53	0.43
1:B:49:LEU:HD22	1:C:129:ILE:HD13	1.99	0.43
1:I:99:PHE:CE2	1:I:101:ASN:HA	2.54	0.43
1:T:273:THR:HG22	3:T:650:HOH:O	2.17	0.43
1:J:382:HIS:NE2	3:J:697:HOH:O	2.37	0.43
1:A:331:TRP:CH2	1:A:341:PRO:HD3	2.54	0.42
1:M:155:ILE:O	1:M:258:GLU:HA	2.19	0.42
1:B:134:LEU:HD13	1:B:140[A]:ILE:CD1	2.48	0.42
1:H:155:ILE:O	1:H:258:GLU:HA	2.19	0.42
1:R:331:TRP:CH2	1:R:341:PRO:HD3	2.54	0.42
1:R:342:PRO:HG3	1:S:342:PRO:HG2	2.01	0.42
1:T:182[A]:MET:HE1	1:T:211:LEU:HD11	2.02	0.42
1:M:238:ASP:OD2	2:M:402:2HP:O1	2.38	0.42
1:B:148:VAL:O	1:B:149:PHE:CB	2.65	0.42
1:F:148:VAL:O	2:F:401:2HP:P	2.78	0.42
1:S:288[A]:LEU:HD11	1:S:373:TYR:CZ	2.54	0.42
1:O:82:ILE:HG12	1:O:145:LEU:HD23	2.02	0.42
1:E:99:PHE:CE2	1:E:101:ASN:HA	2.54	0.42
1:J:99:PHE:CE2	1:J:101:ASN:HA	2.54	0.42
1:K:299:LEU:HG	1:K:349:ILE:HD11	2.01	0.42
1:F:44:GLN:CG	3:F:705:HOH:O	2.68	0.42
1:N:134:LEU:HD13	1:N:140[A]:ILE:CD1	2.50	0.42
1:H:240:LYS:NZ	3:H:729:HOH:O	2.53	0.42
1:C:82:ILE:HG12	1:C:145:LEU:HD23	2.01	0.42
1:R:6:LEU:HA	3:R:668:HOH:O	2.19	0.42
1:D:283:VAL:HA	3:D:605:HOH:O	2.19	0.42
1:F:249:LEU:O	1:R:215:SER:OG	2.38	0.42
1:J:299:LEU:HG	1:J:349:ILE:HD11	2.00	0.42
1:I:174:ARG:CZ	3:I:702:HOH:O	2.67	0.42
1:F:49:LEU:HD22	1:G:129:ILE:HD13	2.02	0.42
1:K:331:TRP:CH2	1:K:341:PRO:HD3	2.55	0.42
1:Q:152:GLY:HA3	1:R:174:ARG:HD3	2.02	0.42
1:L:299:LEU:HG	1:L:349:ILE:HD11	2.01	0.42
1:H:22:LEU:HD12	1:H:140[B]:ILE:HG22	2.02	0.42
1:N:114:SER:HB3	3:N:683:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:ILE:HG12	1:E:145:LEU:HD23	2.02	0.42
1:E:155:ILE:O	1:E:258:GLU:HA	2.19	0.42
1:I:288[A]:LEU:HD11	1:I:373:TYR:CZ	2.55	0.42
1:B:155:ILE:O	1:B:258:GLU:HA	2.20	0.42
1:A:300:LYS:HE3	3:A:673:HOH:O	2.19	0.41
1:A:383:HIS:HB3	3:E:590:HOH:O	2.20	0.41
1:A:155:ILE:O	1:A:258:GLU:HA	2.20	0.41
1:S:331:TRP:CH2	1:S:341:PRO:HD3	2.54	0.41
1:G:271:PHE:CE2	1:H:332:ASP:HB3	2.54	0.41
1:F:99:PHE:CE2	1:F:101:ASN:HA	2.55	0.41
1:L:238:ASP:OD2	2:L:402:2HP:O1	2.38	0.41
1:P:51:GLY:O	1:Q:7:GLY:HA3	2.20	0.41
1:D:40:TYR:CD2	1:H:25:LYS:CE	3.00	0.41
1:F:134:LEU:HD13	1:F:140[A]:ILE:HD12	2.02	0.41
1:I:103:ASN:HB2	1:I:168:TYR:O	2.20	0.41
1:Q:238:ASP:OD2	2:Q:402:2HP:O4	2.38	0.41
1:N:50:TYR:CE2	1:O:131:TYR:HB2	2.55	0.41
1:P:299:LEU:HG	1:P:349:ILE:HD11	2.02	0.41
1:P:148:VAL:O	1:P:149:PHE:CB	2.64	0.41
1:R:134:LEU:HD13	1:R:140[A]:ILE:HD12	2.01	0.41
1:I:82:ILE:HG12	1:I:145:LEU:HD23	2.03	0.41
1:D:344:TRP:HA	3:D:572:HOH:O	2.20	0.41
1:R:99:PHE:CE2	1:R:101:ASN:HA	2.56	0.41
1:E:240:LYS:NZ	3:E:732:HOH:O	2.54	0.41
1:F:331:TRP:CH2	1:F:341:PRO:HD3	2.55	0.41
1:I:146:GLU:O	1:I:146:GLU:HG3	2.20	0.41
1:R:148:VAL:O	2:R:401:2HP:P	2.79	0.41
1:F:270:ASN:OD1	1:G:328:SER:HB2	2.20	0.41
1:Q:103:ASN:HB2	1:Q:168:TYR:O	2.20	0.41
1:O:155:ILE:O	1:O:258:GLU:HA	2.21	0.41
1:P:331:TRP:CH2	1:P:341:PRO:HD3	2.55	0.41
1:R:193:THR:HG23	1:R:217:PRO:HA	2.02	0.41
1:R:299:LEU:HG	1:R:349:ILE:HD11	2.02	0.41
1:Q:148:VAL:O	1:Q:149:PHE:CB	2.67	0.41
1:S:182[A]:MET:HE1	1:S:211:LEU:HD11	2.01	0.41
1:M:182[A]:MET:HE1	1:M:211:LEU:HD11	2.03	0.41
1:I:186:TYR:C	1:I:186:TYR:CD1	2.94	0.41
1:S:186:TYR:CE1	1:S:216:ILE:HG23	2.56	0.41
1:N:299:LEU:HG	1:N:349:ILE:HD11	2.03	0.41
1:A:134:LEU:HD13	1:A:140[A]:ILE:HD12	2.03	0.41
1:B:82:ILE:HG12	1:B:145:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:300:LYS:HE3	3:J:649:HOH:O	2.21	0.41
1:B:182[A]:MET:HE1	1:B:211:LEU:HD11	2.03	0.41
1:C:99:PHE:CE2	1:C:101:ASN:HA	2.56	0.41
1:J:103:ASN:HB2	1:J:168:TYR:O	2.20	0.41
1:A:148:VAL:O	2:A:401:2HP:P	2.79	0.41
1:I:134:LEU:HD13	1:I:140[A]:ILE:HD12	2.03	0.41
1:O:331:TRP:CH2	1:O:341:PRO:HD3	2.55	0.41
1:K:82:ILE:HG12	1:K:145:LEU:HD23	2.03	0.41
1:R:155:ILE:O	1:R:258:GLU:HA	2.21	0.41
1:E:33:ASN:CG	1:G:25:LYS:HE2	2.42	0.40
1:E:299:LEU:HG	1:E:349:ILE:HD11	2.02	0.40
1:R:148:VAL:O	1:R:149:PHE:CB	2.66	0.40
1:J:134:LEU:HD13	1:J:140[A]:ILE:HD12	2.02	0.40
1:I:134:LEU:HD13	1:I:140[A]:ILE:CD1	2.50	0.40
1:F:103:ASN:HB2	1:F:168:TYR:O	2.21	0.40
1:J:147:ARG:HG3	3:J:658:HOH:O	2.20	0.40
1:I:138:LEU:HD23	1:I:138:LEU:HA	1.95	0.40
1:M:134:LEU:HD13	1:M:140[A]:ILE:HD12	2.03	0.40
1:B:99:PHE:CE2	1:B:101:ASN:HA	2.56	0.40
3:D:711:HOH:O	1:E:383:HIS:HB3	2.22	0.40
1:K:148:VAL:O	1:K:149:PHE:CB	2.69	0.40
1:E:103:ASN:HB2	1:E:168:TYR:O	2.22	0.40
1:F:370:ILE:HD11	3:G:582:HOH:O	2.20	0.40
1:G:99:PHE:CE2	1:G:101:ASN:HA	2.56	0.40
1:F:155:ILE:O	1:F:258:GLU:HA	2.21	0.40
1:N:148:VAL:O	1:N:149:PHE:CB	2.67	0.40
3:S:697:HOH:O	1:T:343:SER:HB2	2.22	0.40
1:N:271:PHE:CE2	1:O:332:ASP:HB3	2.57	0.40
1:F:74:GLU:OE1	1:J:117:GLU:OE1	2.39	0.40
3:M:573:HOH:O	1:N:383:HIS:HB3	2.22	0.40
1:M:124:LYS:HA	1:M:124:LYS:HD2	1.93	0.40
1:K:188:ASN:O	1:K:219:ASN:HA	2.21	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:25:LYS:NZ	3:S:706:HOH:O[1_554]	1.75	0.45
1:D:195:THR:OG1	1:L:221:SER:OG[1_565]	1.92	0.28
1:C:362:THR:CG2	1:H:309:THR:OG1[1_654]	1.96	0.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:40:TYR:OH	3:N:695:HOH:O[1_556]	2.02	0.18
1:O:25:LYS:CE	1:S:40:TYR:CZ[1_554]	2.15	0.05
1:O:25:LYS:CD	3:S:706:HOH:O[1_554]	2.16	0.04
1:L:205:SER:OG	1:N:191:SER:OG[1_655]	2.18	0.02

## 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	379/387 (98%)	364 (96%)	15 (4%)	0	100	100
1	B	379/387 (98%)	366 (97%)	13 (3%)	0	100	100
1	C	379/387 (98%)	368 (97%)	11 (3%)	0	100	100
1	D	379/387 (98%)	367 (97%)	12 (3%)	0	100	100
1	E	379/387 (98%)	367 (97%)	12 (3%)	0	100	100
1	F	379/387 (98%)	364 (96%)	15 (4%)	0	100	100
1	G	379/387 (98%)	367 (97%)	12 (3%)	0	100	100
1	H	379/387 (98%)	366 (97%)	13 (3%)	0	100	100
1	I	379/387 (98%)	365 (96%)	14 (4%)	0	100	100
1	J	379/387 (98%)	367 (97%)	12 (3%)	0	100	100
1	K	379/387 (98%)	366 (97%)	13 (3%)	0	100	100
1	L	379/387 (98%)	365 (96%)	14 (4%)	0	100	100
1	M	379/387 (98%)	363 (96%)	16 (4%)	0	100	100
1	N	379/387 (98%)	368 (97%)	11 (3%)	0	100	100
1	O	379/387 (98%)	367 (97%)	12 (3%)	0	100	100
1	P	379/387 (98%)	367 (97%)	12 (3%)	0	100	100
1	Q	379/387 (98%)	368 (97%)	11 (3%)	0	100	100
1	R	379/387 (98%)	365 (96%)	13 (3%)	1 (0%)	46	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	379/387 (98%)	366 (97%)	13 (3%)	0	100	100
1	T	379/387 (98%)	367 (97%)	12 (3%)	0	100	100
All	All	7580/7740 (98%)	7323 (97%)	256 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	34	SER

### 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	336/340 (99%)	336 (100%)	0	100	100
1	B	336/340 (99%)	336 (100%)	0	100	100
1	C	336/340 (99%)	335 (100%)	1 (0%)	94	94
1	D	336/340 (99%)	336 (100%)	0	100	100
1	E	336/340 (99%)	336 (100%)	0	100	100
1	F	336/340 (99%)	336 (100%)	0	100	100
1	G	336/340 (99%)	336 (100%)	0	100	100
1	H	336/340 (99%)	335 (100%)	1 (0%)	94	94
1	I	336/340 (99%)	336 (100%)	0	100	100
1	J	336/340 (99%)	336 (100%)	0	100	100
1	K	336/340 (99%)	336 (100%)	0	100	100
1	L	336/340 (99%)	336 (100%)	0	100	100
1	M	336/340 (99%)	336 (100%)	0	100	100
1	N	336/340 (99%)	336 (100%)	0	100	100
1	O	336/340 (99%)	336 (100%)	0	100	100
1	P	336/340 (99%)	336 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	336/340 (99%)	336 (100%)	0	100	100
1	R	336/340 (99%)	335 (100%)	1 (0%)	94	94
1	S	336/340 (99%)	336 (100%)	0	100	100
1	T	336/340 (99%)	336 (100%)	0	100	100
All	All	6720/6800 (99%)	6717 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	174	ARG
1	H	191	SER
1	R	190	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	T	268	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

60 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	2HP	A	401	-	4,4,4	0.20	0	6,6,6	2.20	1 (16%)
2	2HP	A	402	-	4,4,4	1.12	0	6,6,6	1.52	1 (16%)
2	2HP	A	403	-	4,4,4	0.21	0	6,6,6	1.85	1 (16%)
2	2HP	B	401	-	4,4,4	0.18	0	6,6,6	1.82	2 (33%)
2	2HP	B	402	-	4,4,4	1.12	0	6,6,6	1.41	1 (16%)
2	2HP	B	403	-	4,4,4	1.13	0	6,6,6	1.60	1 (16%)
2	2HP	B	404	-	4,4,4	1.03	0	6,6,6	1.03	0
2	2HP	C	401	-	4,4,4	0.19	0	6,6,6	1.52	1 (16%)
2	2HP	C	402	-	4,4,4	1.19	0	6,6,6	1.49	1 (16%)
2	2HP	D	401	-	4,4,4	0.24	0	6,6,6	1.88	2 (33%)
2	2HP	D	402	-	4,4,4	1.06	0	6,6,6	1.49	2 (33%)
2	2HP	D	403	-	4,4,4	1.19	0	6,6,6	1.54	1 (16%)
2	2HP	E	401	-	4,4,4	0.20	0	6,6,6	1.59	1 (16%)
2	2HP	E	402	-	4,4,4	1.16	0	6,6,6	1.11	0
2	2HP	E	403	-	4,4,4	1.16	0	6,6,6	1.22	1 (16%)
2	2HP	F	401	-	4,4,4	0.28	0	6,6,6	1.98	2 (33%)
2	2HP	F	402	-	4,4,4	0.16	0	6,6,6	2.07	1 (16%)
2	2HP	F	403	-	4,4,4	1.16	0	6,6,6	1.92	2 (33%)
2	2HP	G	401	-	4,4,4	0.30	0	6,6,6	1.76	2 (33%)
2	2HP	G	402	-	4,4,4	0.21	0	6,6,6	1.56	1 (16%)
2	2HP	G	403	-	4,4,4	1.01	0	6,6,6	1.66	1 (16%)
2	2HP	H	401	-	4,4,4	0.27	0	6,6,6	1.94	2 (33%)
2	2HP	H	402	-	4,4,4	0.28	0	6,6,6	1.44	1 (16%)
2	2HP	H	403	-	4,4,4	1.18	0	6,6,6	1.25	1 (16%)
2	2HP	I	401	-	4,4,4	0.15	0	6,6,6	1.69	1 (16%)
2	2HP	I	402	-	4,4,4	0.21	0	6,6,6	1.77	1 (16%)
2	2HP	I	403	-	4,4,4	1.17	0	6,6,6	1.50	1 (16%)
2	2HP	I	404	-	4,4,4	0.15	0	6,6,6	1.82	2 (33%)
2	2HP	J	401	-	4,4,4	0.18	0	6,6,6	1.79	2 (33%)
2	2HP	J	402	-	4,4,4	1.03	0	6,6,6	1.39	0
2	2HP	K	401	-	4,4,4	0.05	0	6,6,6	1.68	2 (33%)
2	2HP	K	402	-	4,4,4	0.19	0	6,6,6	1.66	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	2HP	K	403	-	4,4,4	1.03	0	6,6,6	1.45	1 (16%)
2	2HP	L	401	-	4,4,4	0.12	0	6,6,6	1.99	1 (16%)
2	2HP	L	402	-	4,4,4	0.34	0	6,6,6	1.55	2 (33%)
2	2HP	L	403	-	4,4,4	1.13	0	6,6,6	1.56	1 (16%)
2	2HP	M	401	-	4,4,4	0.23	0	6,6,6	2.16	2 (33%)
2	2HP	M	402	-	4,4,4	0.31	0	6,6,6	1.68	1 (16%)
2	2HP	M	403	-	4,4,4	0.95	0	6,6,6	1.49	1 (16%)
2	2HP	N	401	-	4,4,4	0.13	0	6,6,6	2.01	2 (33%)
2	2HP	N	402	-	4,4,4	0.29	0	6,6,6	1.44	2 (33%)
2	2HP	N	403	-	4,4,4	1.12	0	6,6,6	1.11	1 (16%)
2	2HP	O	401	-	4,4,4	0.16	0	6,6,6	1.94	2 (33%)
2	2HP	O	402	-	4,4,4	0.23	0	6,6,6	1.54	1 (16%)
2	2HP	O	403	-	4,4,4	1.01	0	6,6,6	1.58	2 (33%)
2	2HP	P	401	-	4,4,4	0.21	0	6,6,6	1.83	1 (16%)
2	2HP	P	402	-	4,4,4	1.00	0	6,6,6	0.95	0
2	2HP	P	403	-	4,4,4	1.05	0	6,6,6	1.66	1 (16%)
2	2HP	Q	401	-	4,4,4	0.27	0	6,6,6	1.93	2 (33%)
2	2HP	Q	402	-	4,4,4	1.09	0	6,6,6	1.40	1 (16%)
2	2HP	Q	403	-	4,4,4	1.12	0	6,6,6	1.78	1 (16%)
2	2HP	Q	404	-	4,4,4	1.07	0	6,6,6	1.35	1 (16%)
2	2HP	R	401	-	4,4,4	0.23	0	6,6,6	2.21	1 (16%)
2	2HP	R	402	-	4,4,4	1.14	0	6,6,6	1.60	1 (16%)
2	2HP	S	401	-	4,4,4	0.35	0	6,6,6	1.83	1 (16%)
2	2HP	S	402	-	4,4,4	1.17	0	6,6,6	1.12	0
2	2HP	S	403	-	4,4,4	1.26	1 (25%)	6,6,6	1.52	1 (16%)
2	2HP	T	401	-	4,4,4	0.19	0	6,6,6	1.97	2 (33%)
2	2HP	T	402	-	4,4,4	1.19	0	6,6,6	1.43	1 (16%)
2	2HP	T	403	-	4,4,4	1.06	0	6,6,6	1.56	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2HP	A	401	-	-	0/0/0/0	0/0/0/0
2	2HP	A	402	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2HP	A	403	-	-	0/0/0/0	0/0/0/0
2	2HP	B	401	-	-	0/0/0/0	0/0/0/0
2	2HP	B	402	-	-	0/0/0/0	0/0/0/0
2	2HP	B	403	-	-	0/0/0/0	0/0/0/0
2	2HP	B	404	-	-	0/0/0/0	0/0/0/0
2	2HP	C	401	-	-	0/0/0/0	0/0/0/0
2	2HP	C	402	-	-	0/0/0/0	0/0/0/0
2	2HP	D	401	-	-	0/0/0/0	0/0/0/0
2	2HP	D	402	-	-	0/0/0/0	0/0/0/0
2	2HP	D	403	-	-	0/0/0/0	0/0/0/0
2	2HP	E	401	-	-	0/0/0/0	0/0/0/0
2	2HP	E	402	-	-	0/0/0/0	0/0/0/0
2	2HP	E	403	-	-	0/0/0/0	0/0/0/0
2	2HP	F	401	-	-	0/0/0/0	0/0/0/0
2	2HP	F	402	-	-	0/0/0/0	0/0/0/0
2	2HP	F	403	-	-	0/0/0/0	0/0/0/0
2	2HP	G	401	-	-	0/0/0/0	0/0/0/0
2	2HP	G	402	-	-	0/0/0/0	0/0/0/0
2	2HP	G	403	-	-	0/0/0/0	0/0/0/0
2	2HP	H	401	-	-	0/0/0/0	0/0/0/0
2	2HP	H	402	-	-	0/0/0/0	0/0/0/0
2	2HP	H	403	-	-	0/0/0/0	0/0/0/0
2	2HP	I	401	-	-	0/0/0/0	0/0/0/0
2	2HP	I	402	-	-	0/0/0/0	0/0/0/0
2	2HP	I	403	-	-	0/0/0/0	0/0/0/0
2	2HP	I	404	-	-	0/0/0/0	0/0/0/0
2	2HP	J	401	-	-	0/0/0/0	0/0/0/0
2	2HP	J	402	-	-	0/0/0/0	0/0/0/0
2	2HP	K	401	-	-	0/0/0/0	0/0/0/0
2	2HP	K	402	-	-	0/0/0/0	0/0/0/0
2	2HP	K	403	-	-	0/0/0/0	0/0/0/0
2	2HP	L	401	-	-	0/0/0/0	0/0/0/0
2	2HP	L	402	-	-	0/0/0/0	0/0/0/0
2	2HP	L	403	-	-	0/0/0/0	0/0/0/0
2	2HP	M	401	-	-	0/0/0/0	0/0/0/0
2	2HP	M	402	-	-	0/0/0/0	0/0/0/0
2	2HP	M	403	-	-	0/0/0/0	0/0/0/0
2	2HP	N	401	-	-	0/0/0/0	0/0/0/0
2	2HP	N	402	-	-	0/0/0/0	0/0/0/0
2	2HP	N	403	-	-	0/0/0/0	0/0/0/0
2	2HP	O	401	-	-	0/0/0/0	0/0/0/0
2	2HP	O	402	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2HP	O	403	-	-	0/0/0/0	0/0/0/0
2	2HP	P	401	-	-	0/0/0/0	0/0/0/0
2	2HP	P	402	-	-	0/0/0/0	0/0/0/0
2	2HP	P	403	-	-	0/0/0/0	0/0/0/0
2	2HP	Q	401	-	-	0/0/0/0	0/0/0/0
2	2HP	Q	402	-	-	0/0/0/0	0/0/0/0
2	2HP	Q	403	-	-	0/0/0/0	0/0/0/0
2	2HP	Q	404	-	-	0/0/0/0	0/0/0/0
2	2HP	R	401	-	-	0/0/0/0	0/0/0/0
2	2HP	R	402	-	-	0/0/0/0	0/0/0/0
2	2HP	S	401	-	-	0/0/0/0	0/0/0/0
2	2HP	S	402	-	-	0/0/0/0	0/0/0/0
2	2HP	S	403	-	-	0/0/0/0	0/0/0/0
2	2HP	T	401	-	-	0/0/0/0	0/0/0/0
2	2HP	T	402	-	-	0/0/0/0	0/0/0/0
2	2HP	T	403	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	403	2HP	P-O1	2.01	1.58	1.50

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	401	2HP	O2-P-O1	-4.82	99.92	113.74
2	F	402	2HP	O2-P-O1	-4.57	100.64	113.74
2	A	401	2HP	O2-P-O1	-4.53	100.75	113.74
2	M	401	2HP	O2-P-O1	-4.46	100.96	113.74
2	L	401	2HP	O2-P-O1	-4.33	101.34	113.74
2	N	401	2HP	O2-P-O1	-4.06	102.09	113.74
2	T	401	2HP	O2-P-O1	-4.05	102.14	113.74
2	F	401	2HP	O2-P-O1	-4.00	102.28	113.74
2	H	401	2HP	O2-P-O1	-3.93	102.47	113.74
2	Q	401	2HP	O2-P-O1	-3.90	102.56	113.74
2	I	404	2HP	O2-P-O1	-3.81	102.81	113.74
2	S	401	2HP	O2-P-O1	-3.81	102.83	113.74
2	A	403	2HP	O2-P-O1	-3.80	102.86	113.74
2	I	402	2HP	O2-P-O1	-3.76	102.96	113.74
2	P	401	2HP	O2-P-O1	-3.74	103.01	113.74
2	J	401	2HP	O2-P-O1	-3.72	103.08	113.74
2	D	401	2HP	O2-P-O1	-3.70	103.14	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	402	2HP	O2-P-O1	-3.68	103.18	113.74
2	O	401	2HP	O2-P-O1	-3.58	103.49	113.74
2	F	403	2HP	O3-P-O2	-3.52	99.24	109.06
2	I	401	2HP	O2-P-O1	-3.48	103.77	113.74
2	B	401	2HP	O2-P-O1	-3.47	103.79	113.74
2	Q	403	2HP	O4-P-O2	-3.42	99.53	109.06
2	K	401	2HP	O2-P-O1	-3.40	103.98	113.74
2	K	402	2HP	O2-P-O1	-3.39	104.02	113.74
2	E	401	2HP	O2-P-O1	-3.27	104.38	113.74
2	O	402	2HP	O2-P-O1	-3.24	104.45	113.74
2	B	403	2HP	O4-P-O2	-3.23	100.05	109.06
2	G	401	2HP	O2-P-O1	-3.23	104.49	113.74
2	R	402	2HP	O4-P-O2	-3.17	100.21	109.06
2	G	403	2HP	O4-P-O2	-3.15	100.28	109.06
2	C	401	2HP	O2-P-O1	-3.04	105.02	113.74
2	C	402	2HP	O4-P-O2	-3.02	100.64	109.06
2	T	403	2HP	O4-P-O2	-3.01	100.65	109.06
2	D	403	2HP	O4-P-O2	-3.01	100.66	109.06
2	L	402	2HP	O2-P-O1	-3.01	105.12	113.74
2	H	402	2HP	O2-P-O1	-2.99	105.17	113.74
2	P	403	2HP	O4-P-O2	-2.94	100.86	109.06
2	A	402	2HP	O3-P-O2	-2.91	100.95	109.06
2	L	403	2HP	O4-P-O2	-2.89	101.00	109.06
2	S	403	2HP	O4-P-O2	-2.85	101.10	109.06
2	D	402	2HP	O4-P-O2	-2.78	101.29	109.06
2	T	402	2HP	O3-P-O2	-2.74	101.41	109.06
2	I	403	2HP	O4-P-O2	-2.74	101.43	109.06
2	O	403	2HP	O3-P-O2	-2.73	101.45	109.06
2	N	402	2HP	O2-P-O1	-2.62	106.24	113.74
2	H	403	2HP	O3-P-O2	-2.57	101.88	109.06
2	G	402	2HP	O2-P-O1	-2.56	106.40	113.74
2	E	403	2HP	O4-P-O2	-2.50	102.07	109.06
2	K	403	2HP	O4-P-O2	-2.49	102.12	109.06
2	Q	402	2HP	O4-P-O2	-2.49	102.12	109.06
2	B	402	2HP	O3-P-O2	-2.46	102.19	109.06
2	M	403	2HP	O4-P-O2	-2.42	102.30	109.06
2	N	403	2HP	O3-P-O2	-2.16	103.04	109.06
2	G	401	2HP	O4-P-O3	2.04	112.28	106.36
2	I	404	2HP	O4-P-O3	2.06	112.34	106.36
2	J	401	2HP	O4-P-O3	2.08	112.38	106.36
2	Q	404	2HP	O4-P-O3	2.12	112.51	106.36
2	O	401	2HP	O4-P-O3	2.16	112.63	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	401	2HP	O4-P-O3	2.17	112.64	106.36
2	K	401	2HP	O4-P-O3	2.17	112.66	106.36
2	L	402	2HP	O4-P-O3	2.19	112.70	106.36
2	O	403	2HP	O4-P-O3	2.20	112.75	106.36
2	N	402	2HP	O4-P-O3	2.25	112.88	106.36
2	D	401	2HP	O4-P-O3	2.26	112.92	106.36
2	D	402	2HP	O4-P-O3	2.29	113.00	106.36
2	Q	401	2HP	O4-P-O3	2.31	113.07	106.36
2	T	401	2HP	O4-P-O3	2.34	113.14	106.36
2	H	401	2HP	O4-P-O3	2.36	113.20	106.36
2	B	401	2HP	O4-P-O3	2.38	113.25	106.36
2	F	403	2HP	O3-P-O1	2.42	115.99	109.06
2	F	401	2HP	O4-P-O3	2.47	113.53	106.36
2	N	401	2HP	O4-P-O3	2.66	114.08	106.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

40 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	2HP	2	0
2	A	402	2HP	1	0
2	B	401	2HP	1	0
2	B	402	2HP	1	0
2	B	403	2HP	2	0
2	B	404	2HP	1	0
2	C	401	2HP	2	0
2	D	401	2HP	1	0
2	D	403	2HP	1	0
2	E	401	2HP	1	0
2	E	402	2HP	1	0
2	F	401	2HP	2	0
2	F	403	2HP	3	0
2	G	401	2HP	2	0
2	G	402	2HP	1	0
2	H	401	2HP	1	0
2	I	401	2HP	1	0
2	I	404	2HP	1	0
2	J	401	2HP	1	0
2	K	401	2HP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	402	2HP	1	0
2	L	401	2HP	1	0
2	L	402	2HP	1	0
2	M	401	2HP	1	0
2	M	402	2HP	1	0
2	N	401	2HP	1	0
2	N	402	2HP	1	0
2	O	402	2HP	1	0
2	P	401	2HP	1	0
2	P	402	2HP	2	0
2	P	403	2HP	1	0
2	Q	401	2HP	1	0
2	Q	402	2HP	1	0
2	Q	403	2HP	1	0
2	R	401	2HP	2	0
2	S	401	2HP	2	0
2	S	402	2HP	1	0
2	T	401	2HP	1	0
2	T	402	2HP	1	0
2	T	403	2HP	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 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	377/387 (97%)	0.14	31 (8%)	14 11	23, 36, 68, 95	0
1	B	377/387 (97%)	0.02	23 (6%)	25 20	25, 36, 62, 86	0
1	C	377/387 (97%)	0.06	31 (8%)	14 11	23, 38, 68, 105	0
1	D	377/387 (97%)	0.14	28 (7%)	17 14	23, 36, 67, 103	0
1	E	377/387 (97%)	-0.11	18 (4%)	34 28	22, 35, 67, 101	0
1	F	377/387 (97%)	0.00	20 (5%)	30 25	22, 34, 62, 117	0
1	G	377/387 (97%)	-0.22	13 (3%)	49 43	22, 32, 63, 98	0
1	H	377/387 (97%)	0.04	20 (5%)	30 25	23, 33, 62, 92	0
1	I	377/387 (97%)	-0.07	17 (4%)	37 31	24, 35, 66, 103	0
1	J	377/387 (97%)	0.11	34 (9%)	12 9	23, 36, 64, 107	0
1	K	377/387 (97%)	-0.01	22 (5%)	26 21	24, 38, 65, 107	0
1	L	377/387 (97%)	0.21	36 (9%)	10 8	24, 39, 76, 114	0
1	M	377/387 (97%)	0.11	25 (6%)	22 17	23, 35, 64, 91	0
1	N	377/387 (97%)	-0.17	19 (5%)	32 27	21, 34, 60, 92	0
1	O	377/387 (97%)	0.05	22 (5%)	26 21	24, 35, 65, 121	0
1	P	377/387 (97%)	0.18	24 (6%)	23 18	24, 36, 67, 94	0
1	Q	377/387 (97%)	0.18	30 (7%)	15 12	24, 36, 64, 103	0
1	R	377/387 (97%)	0.12	32 (8%)	13 10	22, 37, 71, 99	0
1	S	377/387 (97%)	0.19	29 (7%)	16 13	22, 35, 64, 88	0
1	T	377/387 (97%)	-0.18	15 (3%)	42 36	22, 34, 60, 91	0
All	All	7540/7740 (97%)	0.04	489 (6%)	22 18	21, 36, 66, 121	0

All (489) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	249	LEU	12.4
1	F	249	LEU	9.0
1	F	220	GLY	8.4
1	D	362	THR	8.0
1	R	219	ASN	7.7
1	M	362	THR	7.2
1	Q	359	GLY	7.0
1	M	281	SER	7.0
1	Q	365	VAL	6.9
1	L	361	SER	6.6
1	M	6	LEU	6.6
1	G	362	THR	6.5
1	R	189	THR	6.5
1	O	361	SER	6.3
1	L	193	THR	6.1
1	D	363	SER	6.1
1	P	248	GLY	6.0
1	B	362	THR	6.0
1	S	6	LEU	5.9
1	C	362	THR	5.9
1	C	248	GLY	5.8
1	R	220	GLY	5.7
1	E	362	THR	5.7
1	R	193	THR	5.6
1	A	191	SER	5.6
1	D	359	GLY	5.6
1	B	191	SER	5.5
1	S	362	THR	5.5
1	N	362	THR	5.5
1	N	360	SER	5.5
1	R	190	THR	5.4
1	L	248	GLY	5.4
1	D	364	SER	5.4
1	R	249	LEU	5.4
1	H	6	LEU	5.4
1	S	363	SER	5.3
1	S	283	VAL	5.3
1	L	189	THR	5.3
1	Q	363	SER	5.3
1	S	281	SER	5.2
1	S	360	SER	5.2
1	J	361	SER	5.2
1	F	362	THR	5.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	247	GLY	5.2
1	J	249	LEU	5.2
1	F	363	SER	5.1
1	M	363	SER	5.1
1	N	361	SER	5.1
1	R	324	SER	5.1
1	D	6	LEU	5.0
1	A	248	GLY	5.0
1	L	219	ASN	5.0
1	D	360	SER	5.0
1	P	362	THR	5.0
1	L	191	SER	4.9
1	R	191	SER	4.9
1	Q	360	SER	4.9
1	G	361	SER	4.9
1	T	361	SER	4.9
1	C	249	LEU	4.9
1	L	190	THR	4.8
1	L	362	THR	4.8
1	J	248	GLY	4.8
1	E	361	SER	4.8
1	Q	364	SER	4.8
1	J	190	THR	4.8
1	M	280	GLY	4.7
1	L	220	GLY	4.7
1	M	360	SER	4.7
1	A	363	SER	4.7
1	L	324	SER	4.6
1	Q	362	THR	4.6
1	D	220	GLY	4.6
1	B	248	GLY	4.5
1	A	361	SER	4.5
1	O	362	THR	4.5
1	T	362	THR	4.5
1	K	365	VAL	4.5
1	B	361	SER	4.5
1	F	6	LEU	4.5
1	L	194	PHE	4.5
1	N	278	LEU	4.4
1	M	283	VAL	4.4
1	N	363	SER	4.4
1	P	280	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	R	280	GLY	4.3
1	M	361	SER	4.3
1	P	361	SER	4.3
1	C	190	THR	4.3
1	G	360	SER	4.2
1	P	358	GLY	4.2
1	B	195	THR	4.2
1	S	365	VAL	4.2
1	K	362	THR	4.1
1	D	361	SER	4.1
1	F	360	SER	4.1
1	H	362	THR	4.1
1	O	360	SER	4.1
1	Q	361	SER	4.1
1	J	362	THR	4.1
1	P	247	GLY	4.1
1	O	364	SER	4.1
1	Q	6	LEU	4.1
1	J	309	THR	4.0
1	S	280	GLY	4.0
1	E	6	LEU	4.0
1	E	363	SER	4.0
1	D	358	GLY	4.0
1	I	362	THR	4.0
1	R	363	SER	4.0
1	S	361	SER	4.0
1	T	360	SER	4.0
1	O	6	LEU	4.0
1	A	279	SER	3.9
1	E	364	SER	3.9
1	K	281	SER	3.9
1	P	6	LEU	3.9
1	B	363	SER	3.9
1	C	191	SER	3.9
1	Q	247	GLY	3.9
1	R	247	GLY	3.9
1	J	360	SER	3.9
1	L	360	SER	3.9
1	A	219	ASN	3.9
1	N	358	GLY	3.9
1	R	382	HIS	3.9
1	A	362	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	276	VAL	3.8
1	F	364	SER	3.8
1	B	249	LEU	3.8
1	Q	249	LEU	3.8
1	A	358	GLY	3.8
1	F	281	SER	3.8
1	E	360	SER	3.8
1	J	191	SER	3.8
1	K	361	SER	3.8
1	H	361	SER	3.7
1	N	279	SER	3.7
1	K	249	LEU	3.7
1	C	309	THR	3.7
1	J	307	LEU	3.7
1	C	279	SER	3.7
1	R	194	PHE	3.7
1	G	6	LEU	3.7
1	L	249	LEU	3.7
1	E	365	VAL	3.6
1	A	223	SER	3.6
1	S	364	SER	3.6
1	D	248	GLY	3.6
1	J	363	SER	3.6
1	G	363	SER	3.6
1	L	382	HIS	3.6
1	L	359	GLY	3.6
1	M	358	GLY	3.6
1	P	363	SER	3.6
1	C	189	THR	3.6
1	C	218	ALA	3.6
1	R	283	VAL	3.6
1	A	281	SER	3.5
1	Q	280	GLY	3.5
1	C	360	SER	3.5
1	M	284	THR	3.5
1	K	310	ALA	3.5
1	C	194	PHE	3.5
1	T	365	VAL	3.5
1	O	281	SER	3.5
1	R	360	SER	3.5
1	G	278	LEU	3.5
1	F	361	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	M	365	VAL	3.4
1	P	360	SER	3.4
1	Q	366	THR	3.4
1	B	247	GLY	3.4
1	L	326	THR	3.4
1	A	190	THR	3.4
1	A	280	GLY	3.4
1	G	283	VAL	3.4
1	D	283	VAL	3.4
1	L	283	VAL	3.4
1	E	277	THR	3.3
1	L	192	THR	3.3
1	R	307	LEU	3.3
1	T	363	SER	3.3
1	G	365	VAL	3.3
1	Q	248	GLY	3.3
1	T	359	GLY	3.3
1	R	362	THR	3.3
1	E	281	SER	3.3
1	R	218	ALA	3.3
1	K	306	GLY	3.3
1	N	280	GLY	3.3
1	C	219	ASN	3.3
1	H	364	SER	3.3
1	N	359	GLY	3.3
1	D	279	SER	3.3
1	D	310	ALA	3.2
1	D	306	GLY	3.2
1	L	218	ALA	3.2
1	L	363	SER	3.2
1	E	278	LEU	3.2
1	Q	309	THR	3.2
1	F	359	GLY	3.2
1	M	359	GLY	3.2
1	K	283	VAL	3.2
1	I	191	SER	3.2
1	Q	191	SER	3.2
1	L	310	ALA	3.2
1	J	219	ASN	3.2
1	P	359	GLY	3.2
1	H	215	SER	3.2
1	O	324	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	O	363	SER	3.2
1	A	310	ALA	3.1
1	I	247	GLY	3.1
1	P	310	ALA	3.1
1	I	281	SER	3.1
1	T	364	SER	3.1
1	B	6	LEU	3.1
1	L	309	THR	3.1
1	P	195	THR	3.1
1	J	334	ILE	3.1
1	C	247	GLY	3.1
1	D	247	GLY	3.1
1	I	309	THR	3.1
1	J	310	ALA	3.1
1	S	310	ALA	3.1
1	E	283	VAL	3.1
1	T	6	LEU	3.1
1	K	363	SER	3.1
1	J	283	VAL	3.1
1	H	280	GLY	3.1
1	M	248	GLY	3.1
1	H	281	SER	3.0
1	K	364	SER	3.0
1	S	276	VAL	3.0
1	M	364	SER	3.0
1	R	361	SER	3.0
1	S	366	THR	3.0
1	P	223	SER	3.0
1	M	309	THR	3.0
1	Q	217	PRO	3.0
1	C	361	SER	3.0
1	S	248	GLY	3.0
1	C	382	HIS	3.0
1	B	360	SER	3.0
1	R	196	ASN	3.0
1	P	191	SER	3.0
1	A	359	GLY	2.9
1	R	192	THR	2.9
1	C	188	ASN	2.9
1	G	364	SER	2.9
1	I	279	SER	2.9
1	H	358	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	N	281	SER	2.9
1	A	6	LEU	2.9
1	P	281	SER	2.9
1	T	281	SER	2.9
1	N	6	LEU	2.9
1	T	358	GLY	2.9
1	R	188	ASN	2.8
1	C	281	SER	2.8
1	N	365	VAL	2.8
1	F	250	GLY	2.8
1	I	6	LEU	2.8
1	A	189	THR	2.8
1	I	193	THR	2.8
1	R	215	SER	2.8
1	M	325	THR	2.8
1	S	277	THR	2.8
1	S	284	THR	2.8
1	L	247	GLY	2.8
1	M	278	LEU	2.8
1	N	310	ALA	2.8
1	P	279	SER	2.8
1	C	193	THR	2.8
1	J	308	THR	2.8
1	O	325	THR	2.8
1	D	251	VAL	2.8
1	T	279	SER	2.8
1	A	325	THR	2.7
1	R	195	THR	2.7
1	D	246	GLY	2.7
1	L	188	ASN	2.7
1	Q	215	SER	2.7
1	I	195	THR	2.7
1	M	277	THR	2.7
1	K	309	THR	2.7
1	M	310	ALA	2.7
1	A	220	GLY	2.7
1	Q	195	THR	2.7
1	C	6	LEU	2.7
1	G	359	GLY	2.7
1	J	358	GLY	2.7
1	L	195	THR	2.7
1	N	195	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	187	ASN	2.7
1	I	249	LEU	2.7
1	L	216	ILE	2.6
1	M	326	THR	2.6
1	F	310	ALA	2.6
1	H	279	SER	2.6
1	R	197	PHE	2.6
1	F	247	GLY	2.6
1	H	277	THR	2.6
1	B	279	SER	2.6
1	C	215	SER	2.6
1	F	279	SER	2.6
1	I	219	ASN	2.6
1	R	250	GLY	2.6
1	J	189	THR	2.6
1	K	277	THR	2.6
1	N	284	THR	2.6
1	Q	277	THR	2.6
1	J	382	HIS	2.6
1	S	247	GLY	2.6
1	D	309	THR	2.6
1	H	360	SER	2.6
1	I	361	SER	2.6
1	K	191	SER	2.6
1	L	215	SER	2.6
1	L	364	SER	2.6
1	J	218	ALA	2.6
1	R	216	ILE	2.6
1	S	358	GLY	2.6
1	T	280	GLY	2.6
1	P	382	HIS	2.6
1	K	6	LEU	2.6
1	H	248	GLY	2.6
1	K	248	GLY	2.6
1	P	283	VAL	2.6
1	J	279	SER	2.6
1	E	366	THR	2.6
1	L	358	GLY	2.5
1	O	359	GLY	2.5
1	S	278	LEU	2.5
1	D	365	VAL	2.5
1	Q	283	VAL	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	190	THR	2.5
1	H	325	THR	2.5
1	Q	190	THR	2.5
1	Q	193	THR	2.5
1	J	247	GLY	2.5
1	A	218	ALA	2.5
1	F	218	ALA	2.5
1	N	364	SER	2.5
1	P	312	THR	2.5
1	B	364	SER	2.5
1	E	279	SER	2.5
1	I	360	SER	2.5
1	M	279	SER	2.5
1	B	192	THR	2.5
1	N	283	VAL	2.5
1	A	334	ILE	2.5
1	D	324	SER	2.5
1	G	281	SER	2.5
1	K	286	SER	2.5
1	J	312	THR	2.5
1	O	280	GLY	2.5
1	Q	358	GLY	2.5
1	P	218	ALA	2.5
1	C	306	GLY	2.5
1	E	359	GLY	2.5
1	I	248	GLY	2.5
1	A	312	THR	2.5
1	B	278	LEU	2.5
1	L	187	ASN	2.4
1	L	196	ASN	2.4
1	I	382	HIS	2.4
1	A	193	THR	2.4
1	K	366	THR	2.4
1	J	6	LEU	2.4
1	A	364	SER	2.4
1	S	282	GLN	2.4
1	A	277	THR	2.4
1	B	189	THR	2.4
1	C	326	THR	2.4
1	R	205	SER	2.4
1	C	220	GLY	2.4
1	J	280	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	O	248	GLY	2.4
1	Q	196	ASN	2.4
1	F	251	VAL	2.4
1	Q	310	ALA	2.4
1	J	326	THR	2.4
1	K	325	THR	2.4
1	F	280	GLY	2.4
1	A	311	VAL	2.4
1	M	308	THR	2.4
1	P	189	THR	2.4
1	O	249	LEU	2.3
1	R	6	LEU	2.3
1	H	363	SER	2.3
1	K	195	THR	2.3
1	P	221	SER	2.3
1	H	247	GLY	2.3
1	S	119	TYR	2.3
1	B	309	THR	2.3
1	S	157	ILE	2.3
1	J	281	SER	2.3
1	L	214	SER	2.3
1	S	279	SER	2.3
1	O	308	THR	2.3
1	T	310	ALA	2.3
1	A	283	VAL	2.3
1	C	251	VAL	2.3
1	D	281	SER	2.3
1	S	324	SER	2.3
1	F	283	VAL	2.3
1	M	276	VAL	2.3
1	H	221	SER	2.3
1	R	214	SER	2.3
1	H	197	PHE	2.3
1	J	194	PHE	2.3
1	B	193	THR	2.3
1	F	248	GLY	2.3
1	J	195	THR	2.3
1	T	278	LEU	2.2
1	M	282	GLN	2.2
1	O	306	GLY	2.2
1	B	277	THR	2.2
1	Q	245	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	195	THR	2.2
1	E	309	THR	2.2
1	Q	192	THR	2.2
1	C	216	ILE	2.2
1	H	359	GLY	2.2
1	Q	220	GLY	2.2
1	L	365	VAL	2.2
1	C	192	THR	2.2
1	J	193	THR	2.2
1	N	309	THR	2.2
1	R	364	SER	2.2
1	S	155	ILE	2.2
1	C	283	VAL	2.2
1	B	215	SER	2.2
1	K	247	GLY	2.2
1	A	365	VAL	2.2
1	J	324	SER	2.2
1	E	306	GLY	2.1
1	O	220	GLY	2.1
1	O	82	ILE	2.1
1	K	192	THR	2.1
1	N	277	THR	2.1
1	A	278	LEU	2.1
1	O	215	SER	2.1
1	Q	278	LEU	2.1
1	E	311	VAL	2.1
1	J	220	GLY	2.1
1	S	382	HIS	2.1
1	D	155	ILE	2.1
1	O	279	SER	2.1
1	P	91	SER	2.1
1	C	245	TYR	2.1
1	L	280	GLY	2.1
1	R	217	PRO	2.1
1	C	310	ALA	2.1
1	H	365	VAL	2.1
1	S	355	VAL	2.1
1	T	276	VAL	2.1
1	L	281	SER	2.1
1	G	277	THR	2.1
1	A	382	HIS	2.1
1	B	251	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	219	ASN	2.1
1	P	192	THR	2.1
1	S	309	THR	2.1
1	B	359	GLY	2.1
1	J	359	GLY	2.1
1	D	196	ASN	2.1
1	I	365	VAL	2.1
1	M	311	VAL	2.1
1	F	277	THR	2.1
1	I	196	ASN	2.0
1	L	197	PHE	2.0
1	A	284	THR	2.0
1	C	308	THR	2.0
1	D	326	THR	2.0
1	G	309	THR	2.0
1	O	312	THR	2.0
1	B	281	SER	2.0
1	J	205	SER	2.0
1	D	278	LEU	2.0
1	D	277	THR	2.0
1	D	325	THR	2.0
1	O	309	THR	2.0
1	O	326	THR	2.0
1	H	310	ALA	2.0
1	Q	250	GLY	2.0
1	S	359	GLY	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( $\text{\AA}^2$ )	Q<0.9
2	2HP	B	403	5/5	0.84	0.23	12.63	67,102,106,108	0
2	2HP	I	403	5/5	0.58	0.22	10.49	67,95,110,111	0
2	2HP	J	402	5/5	0.83	0.22	9.40	68,92,97,117	0
2	2HP	L	403	5/5	0.57	0.22	7.93	82,97,121,122	0
2	2HP	A	403	5/5	0.62	0.23	7.58	89,92,120,120	0
2	2HP	M	403	5/5	0.77	0.21	6.49	102,104,109,121	0
2	2HP	E	403	5/5	0.43	0.30	6.19	73,116,122,124	0
2	2HP	C	402	5/5	0.83	0.19	6.19	59,91,113,117	0
2	2HP	G	403	5/5	0.66	0.20	5.37	91,96,117,117	0
2	2HP	H	403	5/5	0.62	0.18	5.21	63,85,96,103	0
2	2HP	O	403	5/5	0.87	0.12	5.05	63,84,99,100	0
2	2HP	Q	403	5/5	0.86	0.14	4.66	67,92,102,103	0
2	2HP	F	403	5/5	0.75	0.19	4.23	54,111,114,114	0
2	2HP	R	402	5/5	0.90	0.15	4.21	80,84,98,101	0
2	2HP	N	403	5/5	0.80	0.15	4.14	53,91,95,98	0
2	2HP	T	403	5/5	0.80	0.17	3.48	70,100,107,135	0
2	2HP	D	403	5/5	0.86	0.13	2.56	64,66,100,101	0
2	2HP	K	401	5/5	0.95	0.16	1.30	51,55,62,102	0
2	2HP	O	402	5/5	0.98	0.09	1.20	40,43,49,93	0
2	2HP	L	401	5/5	0.97	0.14	0.83	50,52,55,115	0
2	2HP	S	402	5/5	0.99	0.12	0.79	41,47,53,83	0
2	2HP	I	401	5/5	0.96	0.14	0.51	38,57,59,81	0
2	2HP	M	402	5/5	0.99	0.12	0.47	50,51,58,62	0
2	2HP	P	402	5/5	0.97	0.10	0.42	39,47,50,79	0
2	2HP	K	403	5/5	0.91	0.10	0.25	87,93,98,99	0
2	2HP	B	401	5/5	0.98	0.12	0.18	34,41,53,82	0
2	2HP	H	402	5/5	0.98	0.09	0.17	39,40,44,65	0
2	2HP	A	402	5/5	0.98	0.09	0.11	44,48,52,77	0
2	2HP	L	402	5/5	0.98	0.09	0.09	45,46,61,68	0
2	2HP	Q	401	5/5	0.96	0.13	0.06	47,47,51,76	0
2	2HP	A	401	5/5	0.97	0.12	0.04	35,46,54,55	0
2	2HP	N	401	5/5	0.96	0.12	0.00	43,51,61,140	0
2	2HP	R	401	5/5	0.98	0.11	-0.06	40,46,52,60	0
2	2HP	B	404	5/5	0.99	0.11	-0.16	43,44,55,86	0
2	2HP	F	401	5/5	0.97	0.11	-0.18	46,46,54,65	0
2	2HP	P	401	5/5	0.97	0.10	-0.26	43,49,54,66	0
2	2HP	J	401	5/5	0.97	0.11	-0.27	47,48,51,64	0
2	2HP	C	401	5/5	0.98	0.11	-0.35	44,46,68,74	0
2	2HP	G	402	5/5	0.98	0.09	-0.37	39,45,58,59	0
2	2HP	D	402	5/5	0.96	0.09	-0.38	37,49,57,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	2HP	N	402	5/5	0.99	0.09	-0.39	40,41,56,58	0
2	2HP	T	401	5/5	0.98	0.11	-0.53	42,52,68,160	0
2	2HP	Q	402	5/5	0.97	0.08	-0.62	43,44,55,83	0
2	2HP	Q	404	5/5	0.99	0.08	-0.71	41,43,49,95	0
2	2HP	M	401	5/5	0.99	0.09	-0.73	38,44,52,77	0
2	2HP	I	404	5/5	0.99	0.06	-0.82	38,39,50,55	0
2	2HP	E	401	5/5	0.98	0.09	-0.86	49,49,70,135	0
2	2HP	G	401	5/5	0.97	0.08	-0.86	37,48,71,74	0
2	2HP	E	402	5/5	0.98	0.08	-0.90	45,45,54,63	0
2	2HP	B	402	5/5	0.98	0.08	-0.95	41,47,54,74	0
2	2HP	T	402	5/5	0.99	0.10	-0.96	39,39,52,81	0
2	2HP	D	401	5/5	0.97	0.08	-1.04	43,45,62,69	0
2	2HP	I	402	5/5	0.98	0.08	-1.06	43,45,57,58	0
2	2HP	O	401	5/5	0.97	0.10	-1.15	42,45,53,78	0
2	2HP	F	402	5/5	0.98	0.07	-1.22	39,46,58,79	0
2	2HP	S	401	5/5	0.98	0.07	-1.31	34,40,44,64	0
2	2HP	K	402	5/5	0.98	0.06	-1.90	42,45,51,53	0
2	2HP	H	401	5/5	0.99	0.06	-2.25	34,38,43,55	0
2	2HP	S	403	5/5	0.87	0.13	-	57,82,105,107	0
2	2HP	P	403	5/5	0.83	0.16	-	64,94,107,108	0

## 6.5 Other polymers

There are no such residues in this entry.