



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 12:04 am BST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

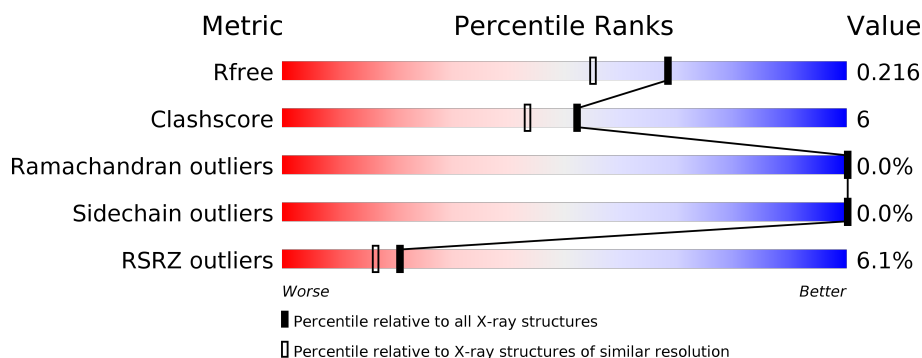
1 Overall quality at a glance

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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	387	<div> <div>7%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	B	387	<div> <div>5%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	C	387	<div> <div>7%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>
1	D	387	<div> <div>6%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	E	387	<div> <div>4%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	F	387	<div> <div>5%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	387	
1	H	387	
1	I	387	
1	J	387	
1	K	387	
1	L	387	
1	M	387	
1	N	387	
1	O	387	
1	P	387	
1	Q	387	
1	R	387	
1	S	387	
1	T	387	

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	B	403	-	-	X	-
2	2HP	C	401	-	-	X	-
2	2HP	F	401	-	-	X	-
2	2HP	F	403	-	-	X	-
2	2HP	G	401	-	-	X	-
2	2HP	P	402	-	-	X	-
2	2HP	R	401	-	-	X	-
2	2HP	S	401	-	-	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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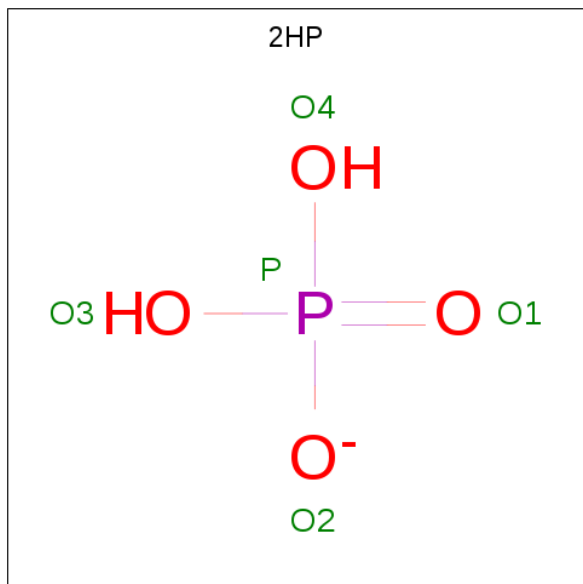
Chain	Residue	Modelled	Actual	Comment	Reference
M	383	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
M	384	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
M	385	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
M	386	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
M	387	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
N	382	HIS	-	EXPRESSION TAG	UNP Q6Q0L3
N	383	HIS	-	EXPRESSION TAG	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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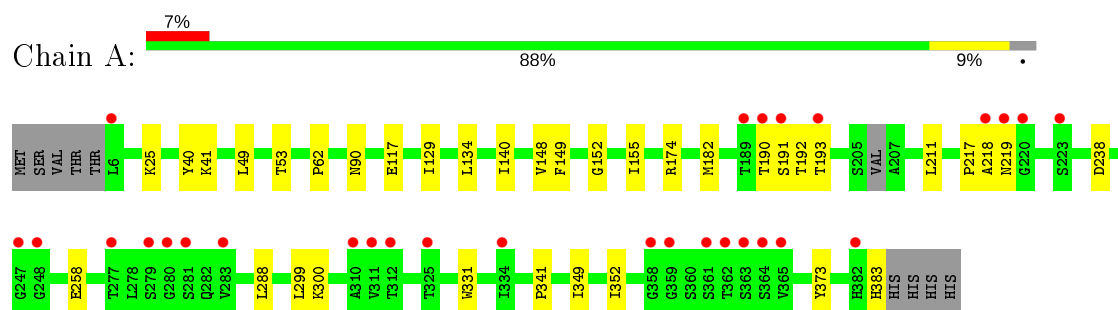
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	K	207	Total 207	O 207	0	0
3	L	197	Total 197	O 197	0	0
3	M	233	Total 233	O 233	0	0
3	N	238	Total 238	O 238	0	0
3	O	240	Total 240	O 240	0	0
3	P	233	Total 233	O 233	0	0
3	Q	216	Total 216	O 216	0	0
3	R	191	Total 191	O 191	0	0
3	S	239	Total 239	O 239	0	0
3	T	233	Total 233	O 233	0	0

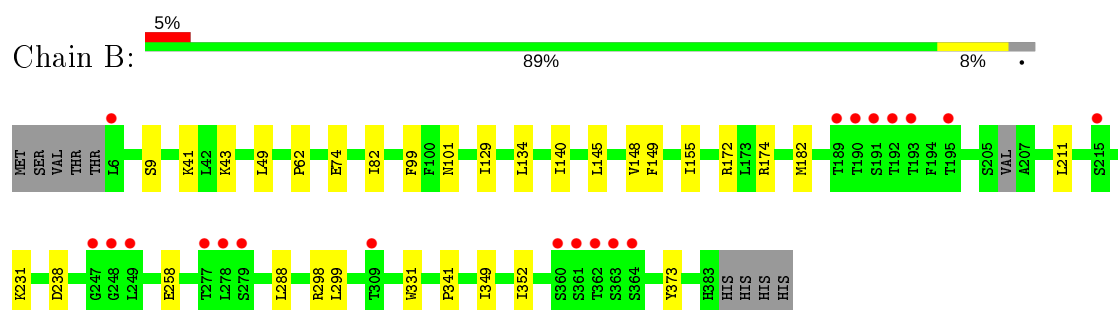
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

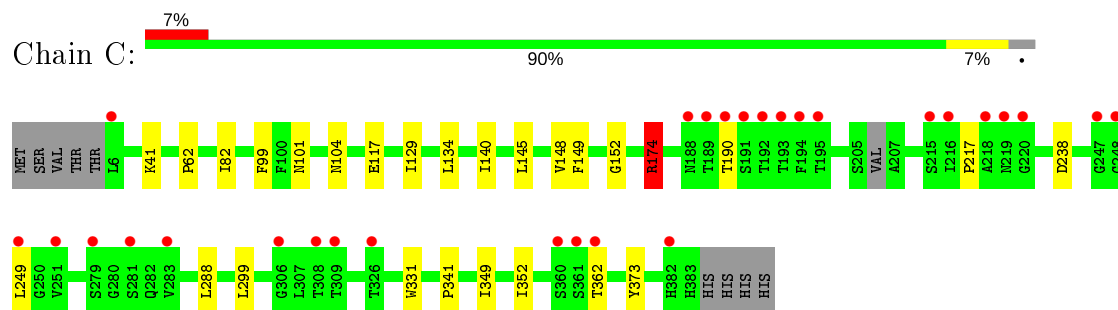
• Molecule 1: C381 turret protein



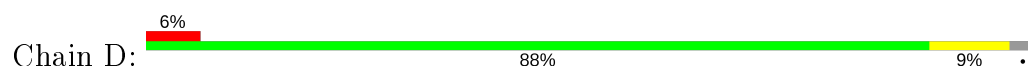
• Molecule 1: C381 turret protein

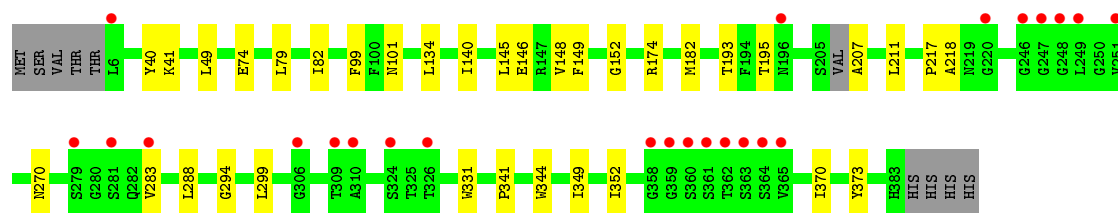


• Molecule 1: C381 turret protein

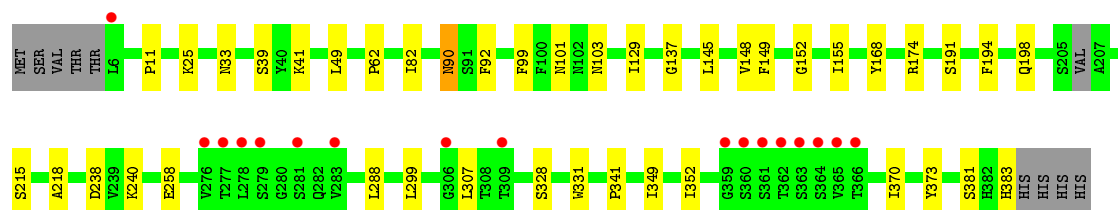
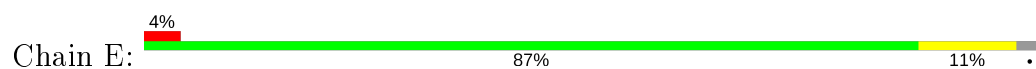


• Molecule 1: C381 turret protein

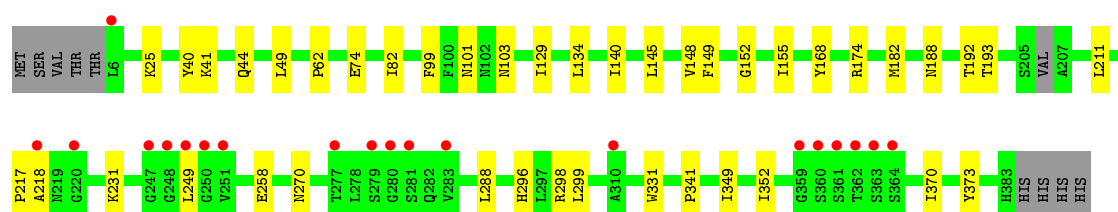
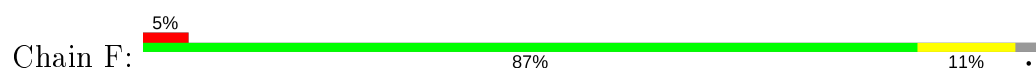




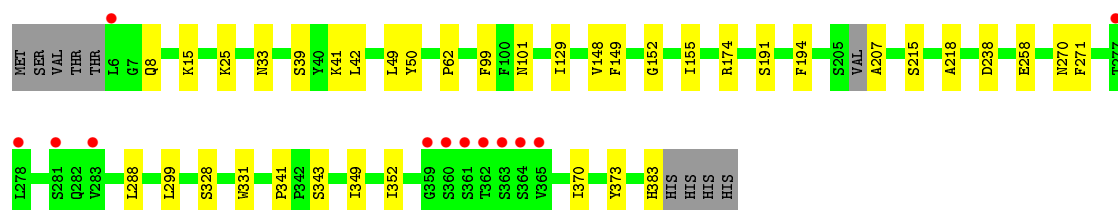
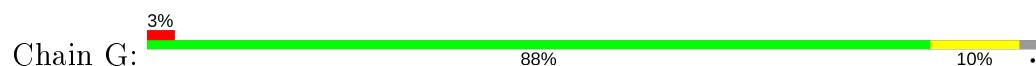
• Molecule 1: C381 turret protein



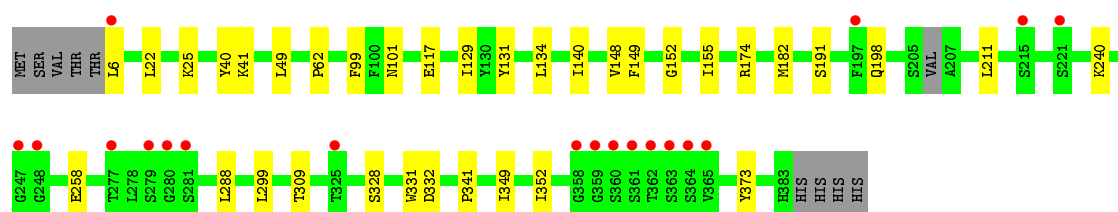
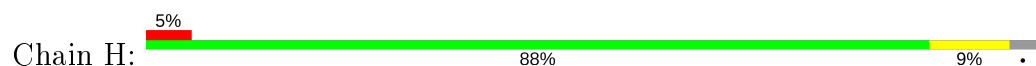
• Molecule 1: C381 turret protein



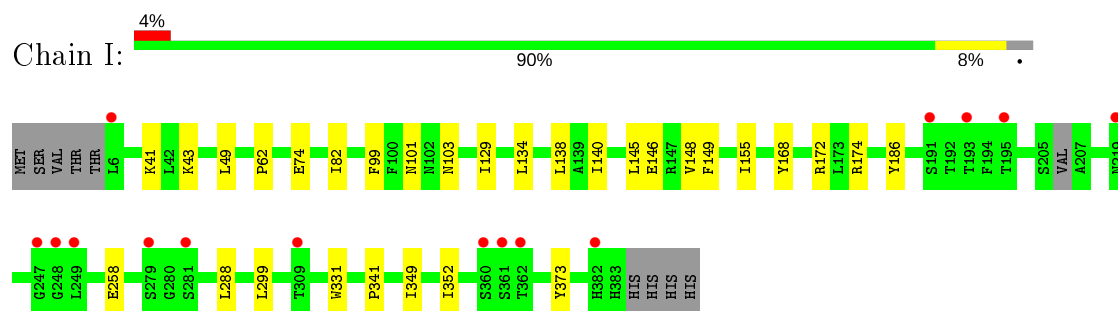
• Molecule 1: C381 turret protein



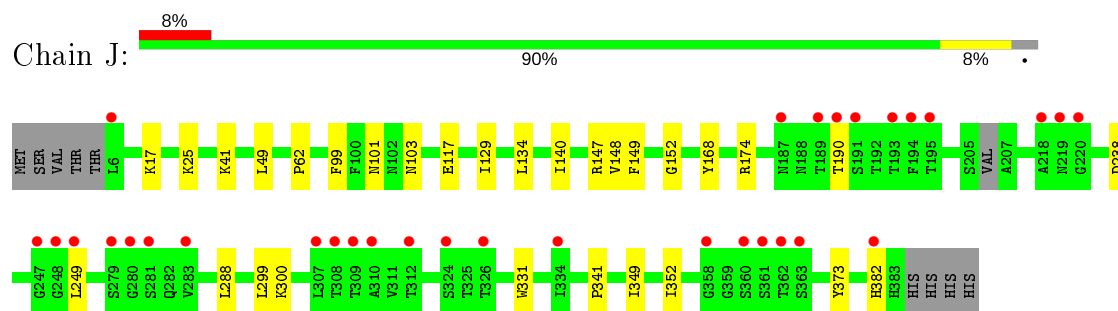
• Molecule 1: C381 turret protein



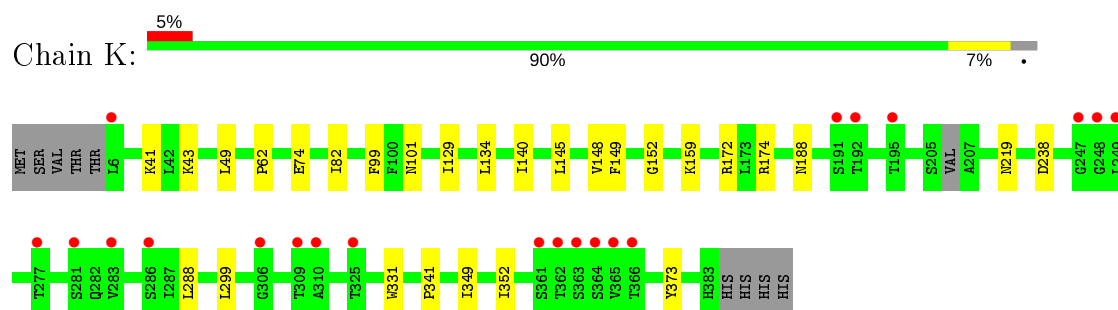
- Molecule 1: C381 turret protein



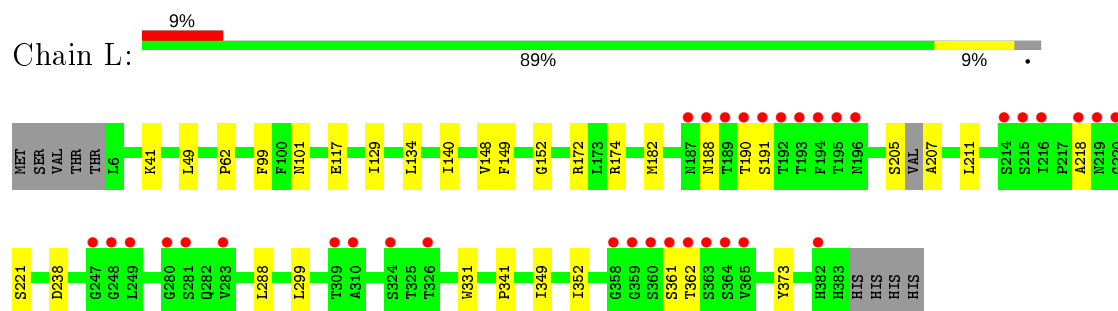
- Molecule 1: C381 turret protein



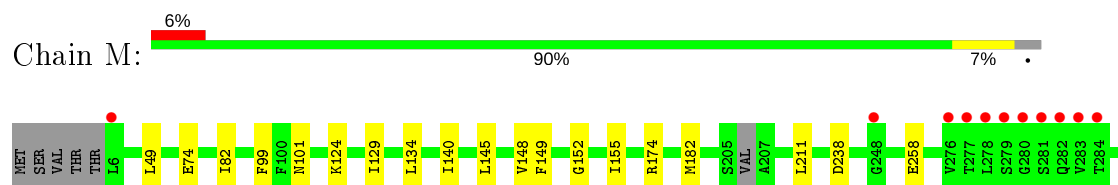
- Molecule 1: C381 turret protein




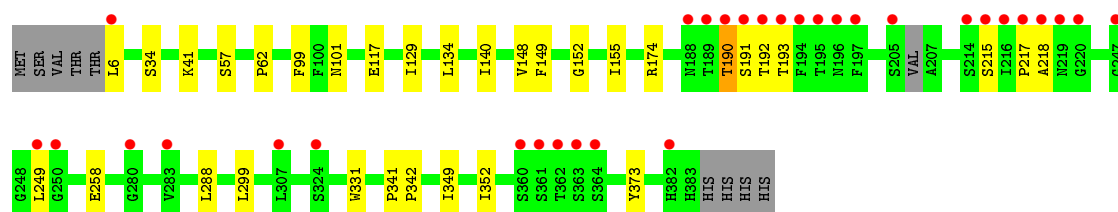
- Molecule 1: C381 turret protein




- Molecule 1: C381 turret protein

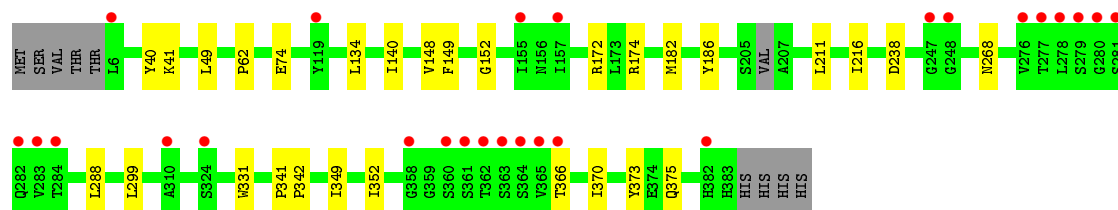


Chain R: 




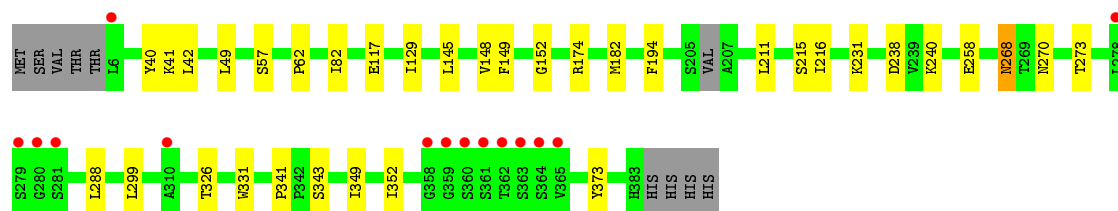
• Molecule 1: C381 turret protein

Chain S: 



• Molecule 1: C381 turret protein

Chain T: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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) 81.9 (39.18-1.76)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.188 , 0.217 0.190 , 0.216	Depositor DCC
R_{free} test set	39151 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	64220	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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:O:349:ILE:HD12	1:O:352:ILE:HD11	1.40	1.02
1:F:249:LEU:HA	1:R:215:SER:OG	1.57	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:R:349:ILE:HD12	1:R:352:ILE:HD11	1.40	0.99
1:T:349:ILE:HD12	1:T:352:ILE:HD11	1.44	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:S:349:ILE:CD1	1:S:352:ILE:HD11	2.07	0.84
1:T:349:ILE:CD1	1:T:352:ILE:HD11	2.06	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:B:349:ILE:CD1	1:B:352:ILE:HD11	2.11	0.81
1:R:191:SER:O	1:R:218:ALA:HB1	1.80	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:I:349:ILE:CD1	1:I:352:ILE:HD11	2.11	0.81
1:P:349:ILE:CD1	1:P:352:ILE:HD11	2.11	0.81
1:J:349:ILE:CD1	1:J:352:ILE:HD11	2.10	0.80
1:L:349:ILE:CD1	1:L:352:ILE:HD11	2.13	0.79
1:L:361:SER:CB	1:Q:360:SER:HB3	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:M:148:VAL:O	2:M:401:2HP:O4	2.10	0.70
1:F:249:LEU:HD11	1:R:217:PRO:HD3	1.73	0.70
1:A:349:ILE:HD12	1:A:352:ILE:CD1	2.20	0.70
1:G:41:LYS:NZ	3:G:568:HOH:O	2.18	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:G:349:ILE:HD12	1:G:352:ILE:CD1	2.21	0.69
1:K:349:ILE:HD12	1:K:352:ILE:CD1	2.19	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:C:349:ILE:HD12	1:C:352:ILE:CD1	2.19	0.68
1:F:298:ARG:HD2	3:F:713:HOH:O	1.93	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:G:148:VAL:O	2:G:401:2HP:O4	2.12	0.68
1:J:148:VAL:O	2:J:401:2HP:O4	2.11	0.68
1:R:349:ILE:HD12	1:R:352:ILE:CD1	2.20	0.68
1:A:191:SER:CA	1:A:218:ALA:HB1	2.23	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)
2:F:403:2HP:O3	3:F:713:HOH:O	2.11	0.67
1:N:349:ILE:HD12	1:N:352:ILE:CD1	2.24	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:A:148:VAL:O	2:A:401:2HP:O4	2.16	0.64
1:F:349:ILE:HD12	1:F:352:ILE:CD1	2.25	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:C:299:LEU:HD11	1:C:352:ILE:HD12	1.78	0.64
1:J:349:ILE:HD12	1:J:352:ILE:CD1	2.23	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:D:299:LEU:HD11	1:D:352:ILE:HD12	1.80	0.62
1:E:299:LEU:HD11	1:E:352:ILE:HD12	1.82	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:H:152:GLY:HA3	1:I:174:ARG:HD3	1.82	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: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
2:B:404:2HP:O3	1:C:238:ASP:OD2	2.19	0.60
1:L:148:VAL:O	1:L:149:PHE:HB2	2.01	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:K:159:LYS:HD2	3:K:547:HOH:O	2.00	0.60
1:R:192:THR:CG2	1:R:193:THR:N	2.65	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:F:25:LYS:CD	3:F:693:HOH:O	2.50	0.59
1:J:299:LEU:HD11	1:J:352:ILE:HD12	1.84	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:D:193:THR:HG23	1:D:217:PRO:HA	1.85	0.58
1:T:268:ASN:ND2	1:T:270:ASN:HD21	2.01	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:C:217:PRO:HD2	3:C:611:HOH:O	2.03	0.58
1:P:299:LEU:HD11	1:P:352:ILE:HD12	1.85	0.58
1:A:191:SER:O	1:A:218:ALA:CB	2.51	0.58
1:E:25:LYS:HG2	1:G:33:ASN:ND2	2.19	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:H:49:LEU:HD22	1:I:129:ILE:HD13	1.87	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: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: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:H:299:LEU:HD11	1:H:352:ILE:HD12	1.86	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:P:191:SER:O	1:P:218:ALA:CB	2.53	0.56
1:S:148:VAL:O	1:S:149:PHE:HB2	2.04	0.56
1:M:49:LEU:HD22	1:N:129:ILE:HD13	1.87	0.56
1:H:148:VAL:O	2:H:401:2HP:O4	2.23	0.56
1:P:41:LYS:HE3	1:P:62:PRO:HB3	1.88	0.56
1:D:288[A]:LEU:HD11	1:D:373:TYR:CE2	2.41	0.56
1:R:117:GLU:OE1	1:S:74:GLU:OE1	2.24	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:B:148:VAL:O	1:B:149:PHE:HB2	2.05	0.55
1:D:294:GLY:HA3	3:D:723:HOH:O	2.06	0.55
1:H:41:LYS:HE3	1:H:62:PRO:HB3	1.87	0.55
1:J:148:VAL:O	1:J:149:PHE:HB2	2.05	0.55
1:R:288[A]:LEU:HD11	1:R:373:TYR:CE2	2.41	0.55
1:A:288[A]:LEU:HD11	1:A:373:TYR:CE2	2.42	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:E:238:ASP:OD2	2:E:402:2HP:O3	2.23	0.55
1:H:288[A]:LEU:HD11	1:H: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:N:148:VAL:O	1:N:149:PHE:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:148:VAL:O	1:R: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:A:152:GLY:HA3	1:B:174:ARG:HD3	1.89	0.55
1:H:148:VAL:HG23	1:H:149:PHE:CD2	2.42	0.55
1:M:148:VAL:O	1:M:149:PHE:HB2	2.06	0.55
1:E:148:VAL:O	1:E:149:PHE:HB2	2.06	0.54
1:O:240:LYS:NZ	3:O:653:HOH:O	2.39	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:D:41:LYS:HG2	1:H:40:TYR:OH	2.07	0.54
1:E:370:ILE:HD11	3:E:585:HOH:O	2.08	0.54
1:M:148:VAL:HG23	1:M:149:PHE:CD2	2.42	0.54
1:O:148:VAL:O	1:O:149:PHE:HB2	2.07	0.54
1:P:148:VAL:HG23	1:P:149:PHE:CD2	2.42	0.54
1:Q:148:VAL:O	1:Q:149:PHE:HB2	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:C:288[A]:LEU:HD11	1:C:373:TYR:CE2	2.43	0.54
1:O:41:LYS:HE3	1:O:62:PRO:HB3	1.90	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: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:T:268:ASN:HD22	1:T:270:ASN:ND2	2.06	0.54
1:A:174:ARG:HD3	1:E:152:GLY:HA3	1.88	0.53
1:A:41:LYS:HE3	1:A:62:PRO:HB3	1.90	0.53
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: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:Q:288[A]:LEU:HD11	1:Q:373:TYR:CE2	2.44	0.53
1:P:117:GLU:OE1	1:Q:74:GLU:OE1	2.26	0.53
1:G:270:ASN:OD1	1:H:328:SER:HB2	2.09	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:K:41:LYS:HE3	1:K:62:PRO:HB3	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:J:288[A]:LEU:HD11	1:J:373:TYR:CE2	2.44	0.53
1:L:41:LYS:HE3	1:L:62:PRO:HB3	1.90	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:B:41:LYS:HE3	1:B:62:PRO:HB3	1.90	0.51
1:Q:49:LEU:HD22	1:R:129:ILE:HD13	1.92	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:E:90:ASN:OD1	1:E:137:GLY:HA3	2.10	0.51
1:G:238:ASP:OD2	2:G:402:2HP:O1	2.28	0.51
1:R:41:LYS:HE3	1:R:62:PRO:HB3	1.93	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:I:148:VAL:O	1:I:149:PHE:HB2	2.10	0.51
1:P:129:ILE:HD13	1:T:49:LEU:HD22	1.92	0.51
1:L:362:THR:HG21	1:Q:280:GLY:HA2	1.93	0.51
1:R:152:GLY:HA3	1:S:174:ARG:HD3	1.93	0.51
1:H:198:GLN:NE2	3:H:572:HOH:O	2.38	0.51
1:T:148:VAL:O	1:T:149:PHE:HB2	2.11	0.51
1:K:49:LEU:HD22	1:L:129:ILE:HD13	1.93	0.50
1:F:44:GLN:CB	3:F:705:HOH:O	2.59	0.50
1:K:148:VAL:O	1:K:149:PHE:HB2	2.11	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:D:152:GLY:HA3	1:E:174:ARG:HD3	1.94	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:A:25:LYS:CG	1:F:40:TYR:OH	2.60	0.50
1:K:129:ILE:HD13	1:O:49:LEU:HD22	1.94	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:D:79:LEU:O	2:D:401:2HP:O4	2.31	0.49
1:H:41:LYS:HG2	3:H:696:HOH:O	2.11	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:148:VAL:HG23	1:F:149:PHE:CD2	2.47	0.49
1:F:25:LYS:HD2	3:F:693:HOH:O	2.11	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: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:R:190:THR:HG21	1:R:249:LEU:O	2.13	0.49
1:C:104:ASN:ND2	3:C:587:HOH:O	2.45	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: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:J:190:THR:HG21	1:J:249:LEU:O	2.14	0.48
1:N:288[A]:LEU:HD11	1:N:373:TYR:CZ	2.48	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:148:VAL:O	2:P:401:2HP:O4	2.32	0.48
1:G:194:PHE:O	1:G:215:SER:HA	2.12	0.48
1:P:191:SER:O	1:P:218:ALA:HB2	2.14	0.48
1:A:191:SER:O	1:A:218:ALA:HB1	2.13	0.48
1:G:191:SER:CA	1:G:218:ALA:HB1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:328:SER:HB2	1:T:270:ASN:OD1	2.14	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
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:P:288[A]:LEU:HD11	1:P:373:TYR:CZ	2.49	0.48
1:A:25:LYS:HE3	1:F:40:TYR:OH	2.01	0.47
1:Q:148:VAL:HG23	1:Q:149:PHE:CD2	2.49	0.47
1:R:148:VAL:HG23	1:R: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:N:270:ASN:OD1	1:O:328:SER:HB2	2.14	0.47
1:P:53:THR:O	1:Q:9:SER:HA	2.15	0.47
1:F:41:LYS:HE3	1:F:62:PRO:HB3	1.97	0.47
1:T:148:VAL:O	2:T:401:2HP:O4	2.32	0.47
1:D:49:LEU:HD22	1:E:129:ILE:HD13	1.97	0.47
1:K:43:LYS:NZ	3:K:538:HOH:O	2.43	0.47
1:N:191:SER:O	1:N:218:ALA:HB2	2.15	0.47
1:N:41:LYS:HE3	1:N:62:PRO:HB3	1.96	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:R:217:PRO:HD2	3:R:593:HOH:O	2.13	0.47
1:A:117:GLU:OE1	1:B:74:GLU:OE1	2.32	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:E:288[A]:LEU:HD11	1:E:373:TYR:CZ	2.49	0.47
1:F:218:ALA:HB2	3:F:598:HOH:O	2.14	0.47
1:O:134:LEU:HD13	1:O:140[A]:ILE:CD1	2.45	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:D:40:TYR:CD1	1:H:25:LYS:CE	2.98	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:F:249:LEU:CD1	1:R:217:PRO:HG3	2.45	0.47
1:A:238:ASP:OD2	2:A:402:2HP:O3	2.34	0.46
1:C:288[A]:LEU:HD11	1:C:373:TYR:CZ	2.50	0.46
1:C:117:GLU:OE1	1:D:74:GLU:OE1	2.32	0.46
1:K:148:VAL:HG23	1:K:149:PHE:CD2	2.51	0.46
1:J:288[A]:LEU:HD11	1:J:373:TYR:CZ	2.50	0.46
1:K:288[A]:LEU:HD11	1:K:373:TYR:CZ	2.51	0.46
1:N:191:SER:C	1:N:218:ALA:HB1	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:249:LEU:CD1	1:R:215:SER:HB2	2.44	0.46
1:G:41:LYS:HE3	1:G:62:PRO:HB3	1.96	0.46
1:G:8:GLN:HG2	3:G:712:HOH:O	2.16	0.46
1:L:288[A]:LEU:HD11	1:L:373:TYR:CZ	2.51	0.46
1:C:174:ARG:NH2	3:C:699:HOH:O	2.48	0.46
1:K:134:LEU:HD13	1:K:140[A]:ILE:HD12	1.97	0.46
1:L:362:THR:HG23	1:Q:359:GLY:O	2.14	0.46
1:D:193:THR:OG1	1:D:218:ALA:N	2.43	0.46
1:E:11:PRO:HG3	1:G:42:LEU:CD2	2.45	0.46
1:H:99:PHE:CE2	1:H:101:ASN:HA	2.51	0.46
1:N:191:SER:CA	1:N:218:ALA:HB1	2.46	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:A:193:THR:HG23	1:A:217:PRO:HA	1.98	0.46
1:A:182[A]:MET:HE1	1:A:211:LEU:HD11	1.98	0.46
1:F:249:LEU:HD11	1:R:217:PRO:CD	2.42	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:191:SER:HA	1:A:219:ASN:OD1	2.15	0.46
1:A:25:LYS:HE2	1:F:40:TYR:CD2	2.51	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:172:ARG:NH1	3:K:532:HOH:O	2.48	0.45
1:K:238:ASP:OD2	2:K:402:2HP:O1	2.33	0.45
1:H:182[A]:MET:HE1	1:H:211:LEU:HD11	1.98	0.45
1:J:134:LEU:HD13	1:J:140[A]:ILE:CD1	2.46	0.45
1:L:182[A]:MET:HE1	1:L:211:LEU:HD11	1.98	0.45
1:D:148:VAL:HG23	1:D:149:PHE:CD2	2.51	0.45
1:I:148:VAL:HG23	1:I: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:B:298:ARG:HD2	3:B:569:HOH:O	2.16	0.45
1:G:370:ILE:HD11	3:H:546:HOH:O	2.16	0.45
1:T:238:ASP:OD2	2:T:402:2HP:O3	2.35	0.45
1:F:188:ASN:ND2	1:F:192:THR:O	2.39	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

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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:O:26:GLN:HB3	3:O:665:HOH:O	2.16	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:A:134:LEU:HD13	1:A:140[A]:ILE:CD1	2.46	0.45
1:D:82:ILE:HG12	1:D:145:LEU:HD23	1.99	0.45
1:F:134:LEU:HD13	1:F:140[A]:ILE:CD1	2.47	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:A:53:THR:O	1:B:9:SER:HA	2.17	0.44
1:F:182[A]:MET:HE1	1:F:211:LEU:HD11	1.99	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:L:134:LEU:HD13	1:L:140[A]:ILE:CD1	2.47	0.44
2:P:402:2HP:O4	1:T:258:GLU:OE1	2.36	0.44
1:B:288[A]:LEU:HD11	1:B:373:TYR:CZ	2.53	0.44
1:G:50:TYR:CE2	1:H:131:TYR:HB2	2.52	0.44
1:L:49:LEU:HD22	1:M:129:ILE:HD13	2.00	0.44
1:M:331:TRP:CH2	1:M:341:PRO:HD3	2.52	0.44
1:F:249:LEU:CG	1:R:215:SER:OG	2.64	0.44
1:R:193:THR:OG1	1:R:218:ALA:HB2	2.18	0.44
1:R:288[A]:LEU:HD11	1:R:373:TYR:CZ	2.53	0.44
1:C:331:TRP:CH2	1:C:341:PRO:HD3	2.53	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: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: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:T:331:TRP:CH2	1:T:341:PRO:HD3	2.52	0.44
1:A:192:THR:O	1:A:218:ALA:HA	2.18	0.44
1:G:331:TRP:CH2	1:G:341:PRO:HD3	2.53	0.44
1:H:299:LEU:HG	1:H:349:ILE:HD11	2.00	0.44
1:J:17:LYS:HD3	3:J:700:HOH:O	2.18	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:S:148:VAL:O	2:S:401:2HP:P	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:VAL:O	1:A:149:PHE:CB	2.63	0.43
1:A:25:LYS:HG3	1:F:40:TYR:OH	2.18	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:O:299:LEU:HG	1:O:349:ILE:HD11	2.00	0.43
1:E:90:ASN:ND2	1:E:92:PHE:CZ	2.85	0.43
1:H:288[A]:LEU:HD11	1:H:373:TYR:CZ	2.53	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:L:191:SER:O	1:L:218:ALA:HB2	2.17	0.43
1:A:219:ASN:HB3	3:A:692:HOH:O	2.17	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:H:134:LEU:HD13	1:H:140[A]:ILE:CD1	2.48	0.43
1:K:99:PHE:CE2	1:K:101:ASN:HA	2.53	0.43
1:L:148:VAL:O	1:L:149:PHE:CB	2.63	0.43
1:L:331:TRP:CH2	1:L:341:PRO:HD3	2.53	0.43
1:N:95:THR:HG22	3:N:615:HOH:O	2.16	0.43
1:Q:99:PHE:CE2	1:Q:101:ASN:HA	2.53	0.43
1:T:57:SER:HB2	3:T:701:HOH:O	2.18	0.43
1:A:40:TYR:OH	1:F:41:LYS:HG2	2.17	0.43
1:E:41:LYS:HG2	1:G:39[A]:SER:HB3	2.00	0.43
1:M:82:ILE:HG12	1:M:145:LEU:HD23	2.00	0.43
1:N:82:ILE:HG12	1:N:145:LEU:HD23	2.00	0.43
1:Q:331:TRP:CH2	1:Q:341:PRO:HD3	2.53	0.43
1:T:148:VAL:HG23	1:T:149:PHE:CD2	2.52	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:D:134:LEU:HD13	1:D:140[A]:ILE:CD1	2.48	0.43
1:E:307:LEU:HB2	3:E:647:HOH:O	2.18	0.43
1:F:82:ILE:HG12	1:F:145:LEU:HD23	2.01	0.43
1:H:117:GLU:OE1	1:I:74:GLU:OE1	2.36	0.43
1:O:103:ASN:HB2	1:O:168:TYR:O	2.19	0.43
1:R:57:SER:HB2	3:R:645:HOH:O	2.17	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:L:361:SER:HB2	1:Q:360:SER:CB	2.45	0.43
1:C:148:VAL:O	2:C:401:2HP:P	2.77	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
1:T:194:PHE:HB2	1:T:216:ILE:HB	2.01	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:B:49:LEU:HD22	1:C:129:ILE:HD13	1.99	0.43
1:C:148:VAL:O	1:C:149:PHE:CB	2.67	0.43
1:D:331:TRP:CH2	1:D:341:PRO:HD3	2.53	0.43
1:I:155:ILE:O	1:I:258:GLU:HA	2.19	0.43
1:N:182[A]:MET:HE1	1:N:211:LEU:HD11	2.01	0.43
1:N:331:TRP:CH2	1:N:341:PRO:HD3	2.53	0.43
1:Q:288[A]:LEU:HD11	1:Q:373:TYR:CZ	2.54	0.43
1:I:99:PHE:CE2	1:I:101:ASN:HA	2.54	0.43
1:J:382:HIS:NE2	3:J:697:HOH:O	2.37	0.43
1:T:273:THR:HG22	3:T:650:HOH:O	2.17	0.43
1:A:331:TRP:CH2	1:A:341:PRO:HD3	2.54	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:M:155:ILE:O	1:M: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:M:238:ASP:OD2	2:M:402:2HP:O1	2.38	0.42
1:T:182[A]:MET:HE1	1:T:211:LEU:HD11	2.02	0.42
1:B:148:VAL:O	1:B:149:PHE:CB	2.65	0.42
1:E:99:PHE:CE2	1:E:101:ASN:HA	2.54	0.42
1:F:148:VAL:O	2:F:401:2HP:P	2.78	0.42
1:J:99:PHE:CE2	1:J:101:ASN:HA	2.54	0.42
1:O:82:ILE:HG12	1:O:145:LEU:HD23	2.02	0.42
1:S:288[A]:LEU:HD11	1:S:373:TYR:CZ	2.54	0.42
1:F:44:GLN:CG	3:F:705:HOH:O	2.68	0.42
1:K:299:LEU:HG	1:K:349:ILE:HD11	2.01	0.42
1:C:82:ILE:HG12	1:C:145:LEU:HD23	2.01	0.42
1:D:283:VAL:HA	3:D:605:HOH:O	2.19	0.42
1:H:240:LYS:NZ	3:H:729:HOH:O	2.53	0.42
1:N:134:LEU:HD13	1:N:140[A]:ILE:CD1	2.50	0.42
1:R:6:LEU:HA	3:R:668: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:F:49:LEU:HD22	1:G:129:ILE:HD13	2.02	0.42
1:I:174:ARG:CZ	3:I:702:HOH:O	2.67	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:E:155:ILE:O	1:E:258:GLU:HA	2.19	0.42
1:E:82:ILE:HG12	1:E:145:LEU:HD23	2.02	0.42
1:H:22:LEU:HD12	1:H:140[B]:ILE:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:299:LEU:HG	1:L:349:ILE:HD11	2.01	0.42
1:N:114:SER:HB3	3:N:683:HOH:O	2.20	0.42
1:B:155:ILE:O	1:B:258:GLU:HA	2.20	0.42
1:I:288[A]:LEU:HD11	1:I:373:TYR:CZ	2.55	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:F:99:PHE:CE2	1:F:101:ASN:HA	2.55	0.41
1:G:271:PHE:CE2	1:H:332:ASP:HB3	2.54	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:S:331:TRP:CH2	1:S:341:PRO:HD3	2.54	0.41
1:F:134:LEU:HD13	1:F:140[A]:ILE:HD12	2.02	0.41
1:D:40:TYR:CD2	1:H:25:LYS:CE	3.00	0.41
1:I:103:ASN:HB2	1:I:168:TYR:O	2.20	0.41
1:N:50:TYR:CE2	1:O:131:TYR:HB2	2.55	0.41
1:Q:238:ASP:OD2	2:Q:402:2HP:O4	2.38	0.41
1:D:344:TRP:HA	3:D:572:HOH:O	2.20	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:82:ILE:HG12	1:I:145:LEU:HD23	2.03	0.41
1:I:146:GLU:O	1:I:146:GLU:HG3	2.20	0.41
1:P:148:VAL:O	1:P:149:PHE:CB	2.64	0.41
1:P:299:LEU:HG	1:P:349:ILE:HD11	2.02	0.41
1:R:134:LEU:HD13	1:R:140[A]:ILE:HD12	2.01	0.41
1:R:99:PHE:CE2	1:R:101:ASN:HA	2.56	0.41
1:F:270:ASN:OD1	1:G:328:SER:HB2	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:Q:103:ASN:HB2	1:Q:168:TYR:O	2.20	0.41
1:R:148:VAL:O	2:R:401:2HP:P	2.79	0.41
1:I:186:TYR:CD1	1:I:186:TYR:C	2.94	0.41
1:M:182[A]:MET:HE1	1:M:211:LEU:HD11	2.03	0.41
1:Q:148:VAL:O	1:Q:149:PHE:CB	2.67	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:S:182[A]:MET:HE1	1:S:211:LEU:HD11	2.01	0.41
1:S:186:TYR:CE1	1:S:216:ILE:HG23	2.56	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
1:B:182[A]:MET:HE1	1:B:211:LEU:HD11	2.03	0.41

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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	41	27

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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%)	92	91
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%)	92	91
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%)	92	91
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	C	401	-	4,4,4	0.86	0	6,6,6	0.93	0
2	2HP	Q	403	-	4,4,4	1.73	1 (25%)	6,6,6	1.28	1 (16%)
2	2HP	M	402	-	4,4,4	0.87	0	6,6,6	1.03	1 (16%)
2	2HP	I	403	-	4,4,4	1.81	1 (25%)	6,6,6	0.98	1 (16%)
2	2HP	T	402	-	4,4,4	1.66	1 (25%)	6,6,6	1.12	1 (16%)
2	2HP	E	402	-	4,4,4	1.66	1 (25%)	6,6,6	0.76	0
2	2HP	A	403	-	4,4,4	0.83	0	6,6,6	1.19	1 (16%)
2	2HP	M	401	-	4,4,4	0.88	0	6,6,6	1.47	1 (16%)
2	2HP	D	402	-	4,4,4	1.55	1 (25%)	6,6,6	1.12	1 (16%)
2	2HP	S	403	-	4,4,4	1.95	1 (25%)	6,6,6	0.99	1 (16%)
2	2HP	B	403	-	4,4,4	1.73	1 (25%)	6,6,6	1.14	1 (16%)
2	2HP	R	401	-	4,4,4	0.85	0	6,6,6	1.41	1 (16%)
2	2HP	J	401	-	4,4,4	0.85	0	6,6,6	1.21	1 (16%)
2	2HP	M	403	-	4,4,4	1.49	1 (25%)	6,6,6	1.03	0
2	2HP	J	402	-	4,4,4	1.50	1 (25%)	6,6,6	0.96	0
2	2HP	S	401	-	4,4,4	0.94	0	6,6,6	1.07	1 (16%)
2	2HP	K	402	-	4,4,4	0.87	0	6,6,6	1.03	0
2	2HP	G	403	-	4,4,4	1.52	1 (25%)	6,6,6	1.32	1 (16%)
2	2HP	B	401	-	4,4,4	0.76	0	6,6,6	1.24	0
2	2HP	E	403	-	4,4,4	1.77	1 (25%)	6,6,6	0.86	0
2	2HP	D	401	-	4,4,4	0.92	0	6,6,6	1.18	1 (16%)
2	2HP	D	403	-	4,4,4	1.83	1 (25%)	6,6,6	1.04	1 (16%)
2	2HP	A	402	-	4,4,4	1.62	1 (25%)	6,6,6	1.11	1 (16%)
2	2HP	N	403	-	4,4,4	1.68	1 (25%)	6,6,6	0.81	0
2	2HP	E	401	-	4,4,4	0.84	0	6,6,6	0.99	0
2	2HP	R	402	-	4,4,4	1.74	1 (25%)	6,6,6	1.13	1 (16%)
2	2HP	P	401	-	4,4,4	0.81	0	6,6,6	1.14	1 (16%)
2	2HP	S	402	-	4,4,4	1.60	1 (25%)	6,6,6	0.66	0
2	2HP	O	403	-	4,4,4	1.59	1 (25%)	6,6,6	1.12	1 (16%)
2	2HP	P	403	-	4,4,4	1.62	1 (25%)	6,6,6	1.11	1 (16%)
2	2HP	L	401	-	4,4,4	0.74	0	6,6,6	1.32	1 (16%)
2	2HP	L	403	-	4,4,4	1.74	1 (25%)	6,6,6	1.07	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2HP	H	402	-	4,4,4	0.84	0	6,6,6	0.92	0
2	2HP	T	401	-	4,4,4	0.85	0	6,6,6	1.33	1 (16%)
2	2HP	I	402	-	4,4,4	0.85	0	6,6,6	1.17	1 (16%)
2	2HP	F	401	-	4,4,4	0.85	0	6,6,6	1.36	1 (16%)
2	2HP	B	402	-	4,4,4	1.64	1 (25%)	6,6,6	1.02	0
2	2HP	C	402	-	4,4,4	1.84	1 (25%)	6,6,6	1.02	1 (16%)
2	2HP	O	401	-	4,4,4	0.50	0	6,6,6	1.37	1 (16%)
2	2HP	Q	404	-	4,4,4	1.52	1 (25%)	6,6,6	0.81	0
2	2HP	I	404	-	4,4,4	0.81	0	6,6,6	1.12	1 (16%)
2	2HP	G	401	-	4,4,4	0.59	0	6,6,6	1.23	0
2	2HP	F	403	-	4,4,4	1.77	1 (25%)	6,6,6	1.44	1 (16%)
2	2HP	K	403	-	4,4,4	1.57	1 (25%)	6,6,6	0.98	0
2	2HP	T	403	-	4,4,4	1.61	1 (25%)	6,6,6	1.24	1 (16%)
2	2HP	P	402	-	4,4,4	1.55	0	6,6,6	0.63	0
2	2HP	H	401	-	4,4,4	0.72	0	6,6,6	1.35	1 (16%)
2	2HP	Q	402	-	4,4,4	1.61	1 (25%)	6,6,6	1.01	0
2	2HP	B	404	-	4,4,4	1.52	1 (25%)	6,6,6	0.45	0
2	2HP	Q	401	-	4,4,4	0.67	0	6,6,6	1.30	1 (16%)
2	2HP	N	402	-	4,4,4	0.94	0	6,6,6	0.98	0
2	2HP	L	402	-	4,4,4	0.95	0	6,6,6	0.92	0
2	2HP	O	402	-	4,4,4	0.88	0	6,6,6	0.97	0
2	2HP	I	401	-	4,4,4	0.65	0	6,6,6	1.14	0
2	2HP	K	401	-	4,4,4	0.67	0	6,6,6	1.04	0
2	2HP	F	402	-	4,4,4	0.58	0	6,6,6	1.38	1 (16%)
2	2HP	H	403	-	4,4,4	1.80	1 (25%)	6,6,6	0.88	0
2	2HP	G	402	-	4,4,4	0.80	0	6,6,6	1.19	0
2	2HP	A	401	-	4,4,4	0.88	0	6,6,6	1.42	1 (16%)
2	2HP	N	401	-	4,4,4	0.69	0	6,6,6	1.32	1 (16%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	403	2HP	P-O1	3.19	1.58	1.50
2	H	403	2HP	P-O1	3.03	1.58	1.50
2	C	402	2HP	P-O1	3.01	1.57	1.50
2	D	403	2HP	P-O1	2.90	1.57	1.50
2	E	403	2HP	P-O1	2.89	1.57	1.50
2	I	403	2HP	P-O1	2.82	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	402	2HP	P-O1	2.77	1.57	1.50
2	N	403	2HP	P-O1	2.76	1.57	1.50
2	B	403	2HP	P-O1	2.75	1.57	1.50
2	F	403	2HP	P-O1	2.74	1.57	1.50
2	L	403	2HP	P-O1	2.72	1.57	1.50
2	Q	403	2HP	P-O1	2.66	1.57	1.50
2	T	403	2HP	P-O1	2.53	1.56	1.50
2	O	403	2HP	P-O1	2.52	1.56	1.50
2	T	402	2HP	P-O1	2.49	1.56	1.50
2	K	403	2HP	P-O1	2.47	1.56	1.50
2	P	403	2HP	P-O1	2.47	1.56	1.50
2	Q	402	2HP	P-O1	2.45	1.56	1.50
2	B	402	2HP	P-O1	2.33	1.56	1.50
2	E	402	2HP	P-O1	2.30	1.56	1.50
2	A	402	2HP	P-O1	2.26	1.56	1.50
2	M	403	2HP	P-O1	2.25	1.56	1.50
2	G	403	2HP	P-O1	2.22	1.56	1.50
2	D	402	2HP	P-O1	2.13	1.55	1.50
2	S	402	2HP	P-O3	-2.10	1.48	1.54
2	B	404	2HP	P-O1	2.08	1.55	1.50
2	Q	404	2HP	P-O1	2.06	1.55	1.50
2	J	402	2HP	P-O1	2.05	1.55	1.50

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	401	2HP	O2-P-O1	-3.00	99.92	110.89
2	F	402	2HP	O2-P-O1	-2.80	100.64	110.89
2	A	401	2HP	O2-P-O1	-2.77	100.75	110.89
2	F	403	2HP	O3-P-O2	-2.72	99.24	107.97
2	M	401	2HP	O2-P-O1	-2.71	100.96	110.89
2	Q	403	2HP	O4-P-O2	-2.63	99.53	107.97
2	L	401	2HP	O2-P-O1	-2.61	101.34	110.89
2	B	403	2HP	O4-P-O2	-2.47	100.05	107.97
2	R	402	2HP	O4-P-O2	-2.42	100.21	107.97
2	N	401	2HP	O2-P-O1	-2.41	102.09	110.89
2	G	403	2HP	O4-P-O2	-2.40	100.28	107.97
2	T	401	2HP	O2-P-O1	-2.39	102.14	110.89
2	F	401	2HP	O2-P-O1	-2.36	102.28	110.89
2	H	401	2HP	O2-P-O1	-2.30	102.47	110.89
2	C	402	2HP	O4-P-O2	-2.28	100.64	107.97
2	T	403	2HP	O4-P-O2	-2.28	100.65	107.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	401	2HP	O2-P-O1	-2.28	102.56	110.89
2	D	403	2HP	O4-P-O2	-2.28	100.66	107.97
2	P	403	2HP	O4-P-O2	-2.22	100.86	107.97
2	I	404	2HP	O2-P-O1	-2.21	102.81	110.89
2	S	401	2HP	O2-P-O1	-2.20	102.83	110.89
2	A	403	2HP	O2-P-O1	-2.20	102.86	110.89
2	A	402	2HP	O3-P-O2	-2.19	100.95	107.97
2	L	403	2HP	O4-P-O2	-2.17	101.00	107.97
2	I	402	2HP	O2-P-O1	-2.17	102.96	110.89
2	P	401	2HP	O2-P-O1	-2.16	103.01	110.89
2	S	403	2HP	O4-P-O2	-2.14	101.10	107.97
2	J	401	2HP	O2-P-O1	-2.14	103.08	110.89
2	D	401	2HP	O2-P-O1	-2.12	103.14	110.89
2	M	402	2HP	O2-P-O1	-2.11	103.18	110.89
2	D	402	2HP	O4-P-O2	-2.08	101.29	107.97
2	T	402	2HP	O3-P-O2	-2.04	101.41	107.97
2	I	403	2HP	O4-P-O2	-2.04	101.43	107.97
2	O	403	2HP	O3-P-O2	-2.03	101.45	107.97
2	O	401	2HP	O2-P-O1	-2.02	103.49	110.89

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	C	401	2HP	2	0
2	Q	403	2HP	1	0
2	M	402	2HP	1	0
2	T	402	2HP	1	0
2	E	402	2HP	1	0
2	M	401	2HP	1	0
2	B	403	2HP	2	0
2	R	401	2HP	2	0
2	J	401	2HP	1	0
2	S	401	2HP	2	0
2	K	402	2HP	1	0
2	B	401	2HP	1	0
2	D	401	2HP	1	0
2	D	403	2HP	1	0
2	A	402	2HP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	2HP	1	0
2	P	401	2HP	1	0
2	S	402	2HP	1	0
2	P	403	2HP	1	0
2	L	401	2HP	1	0
2	T	401	2HP	1	0
2	F	401	2HP	2	0
2	B	402	2HP	1	0
2	I	404	2HP	1	0
2	G	401	2HP	2	0
2	F	403	2HP	3	0
2	T	403	2HP	1	0
2	P	402	2HP	2	0
2	H	401	2HP	1	0
2	Q	402	2HP	1	0
2	B	404	2HP	1	0
2	Q	401	2HP	1	0
2	N	402	2HP	1	0
2	L	402	2HP	1	0
2	O	402	2HP	1	0
2	I	401	2HP	1	0
2	K	401	2HP	1	0
2	G	402	2HP	1	0
2	A	401	2HP	2	0
2	N	401	2HP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	377/387 (97%)	0.09	29 (7%)	13	10	23, 36, 68, 95	0
1	B	377/387 (97%)	-0.03	20 (5%)	26	21	25, 36, 62, 86	0
1	C	377/387 (97%)	0.01	29 (7%)	13	10	23, 38, 68, 105	0
1	D	377/387 (97%)	0.09	24 (6%)	19	15	23, 36, 67, 103	0
1	E	377/387 (97%)	-0.16	17 (4%)	33	27	22, 35, 67, 101	0
1	F	377/387 (97%)	-0.04	20 (5%)	26	21	22, 34, 62, 117	0
1	G	377/387 (97%)	-0.26	12 (3%)	47	41	22, 32, 63, 98	0
1	H	377/387 (97%)	-0.01	19 (5%)	28	23	23, 33, 62, 92	0
1	I	377/387 (97%)	-0.12	15 (3%)	38	32	24, 35, 66, 103	0
1	J	377/387 (97%)	0.06	32 (8%)	10	8	23, 36, 64, 107	0
1	K	377/387 (97%)	-0.06	21 (5%)	24	19	24, 38, 65, 107	0
1	L	377/387 (97%)	0.16	35 (9%)	8	6	24, 39, 76, 114	0
1	M	377/387 (97%)	0.06	24 (6%)	19	15	23, 35, 64, 91	0
1	N	377/387 (97%)	-0.21	19 (5%)	28	23	21, 34, 60, 92	0
1	O	377/387 (97%)	0.00	19 (5%)	28	23	24, 35, 65, 121	0
1	P	377/387 (97%)	0.13	25 (6%)	18	14	24, 36, 67, 94	0
1	Q	377/387 (97%)	0.12	29 (7%)	13	10	24, 36, 64, 103	0
1	R	377/387 (97%)	0.07	32 (8%)	10	8	22, 37, 71, 99	0
1	S	377/387 (97%)	0.13	26 (6%)	16	13	22, 35, 64, 88	0
1	T	377/387 (97%)	-0.22	14 (3%)	41	36	22, 34, 60, 91	0
All	All	7540/7740 (97%)	-0.01	461 (6%)	21	16	21, 36, 66, 121	0

All (461) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	249	LEU	12.0
1	F	249	LEU	8.7
1	F	220	GLY	8.3
1	D	362	THR	7.8
1	R	219	ASN	7.6
1	M	362	THR	7.0
1	Q	359	GLY	6.8
1	M	281	SER	6.8
1	Q	365	VAL	6.7
1	L	361	SER	6.5
1	M	6	LEU	6.4
1	R	189	THR	6.4
1	G	362	THR	6.4
1	O	361	SER	6.3
1	D	363	SER	6.0
1	P	248	GLY	6.0
1	L	193	THR	5.9
1	B	362	THR	5.9
1	C	362	THR	5.8
1	S	6	LEU	5.8
1	C	248	GLY	5.7
1	R	220	GLY	5.7
1	E	362	THR	5.6
1	R	193	THR	5.5
1	D	359	GLY	5.5
1	A	191	SER	5.5
1	N	362	THR	5.4
1	R	190	THR	5.4
1	B	191	SER	5.4
1	L	248	GLY	5.3
1	S	362	THR	5.3
1	D	364	SER	5.3
1	N	360	SER	5.3
1	Q	363	SER	5.3
1	S	363	SER	5.3
1	L	189	THR	5.3
1	R	249	LEU	5.2
1	H	6	LEU	5.2
1	S	283	VAL	5.2
1	S	281	SER	5.1
1	S	360	SER	5.1
1	F	362	THR	5.1
1	A	247	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	F	363	SER	5.1
1	N	361	SER	5.0
1	J	361	SER	5.0
1	M	363	SER	5.0
1	A	248	GLY	5.0
1	R	324	SER	4.9
1	L	191	SER	4.9
1	J	249	LEU	4.9
1	Q	360	SER	4.9
1	R	191	SER	4.8
1	L	219	ASN	4.8
1	D	6	LEU	4.8
1	L	362	THR	4.8
1	P	362	THR	4.8
1	D	360	SER	4.8
1	L	190	THR	4.8
1	T	361	SER	4.7
1	G	361	SER	4.7
1	C	249	LEU	4.7
1	J	248	GLY	4.7
1	M	280	GLY	4.7
1	J	190	THR	4.6
1	Q	364	SER	4.6
1	E	361	SER	4.6
1	A	363	SER	4.6
1	Q	362	THR	4.5
1	M	360	SER	4.5
1	L	324	SER	4.5
1	L	220	GLY	4.5
1	A	361	SER	4.5
1	O	362	THR	4.4
1	D	220	GLY	4.4
1	B	248	GLY	4.4
1	B	361	SER	4.4
1	T	362	THR	4.4
1	F	6	LEU	4.3
1	K	365	VAL	4.3
1	N	363	SER	4.3
1	N	278	LEU	4.3
1	P	280	GLY	4.3
1	M	361	SER	4.3
1	R	280	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	P	361	SER	4.2
1	K	362	THR	4.2
1	M	283	VAL	4.2
1	L	194	PHE	4.2
1	C	190	THR	4.2
1	G	360	SER	4.1
1	B	195	THR	4.1
1	P	247	GLY	4.1
1	H	362	THR	4.1
1	D	361	SER	4.0
1	J	362	THR	4.0
1	S	365	VAL	4.0
1	P	358	GLY	4.0
1	O	364	SER	4.0
1	Q	361	SER	4.0
1	O	360	SER	4.0
1	P	6	LEU	4.0
1	S	280	GLY	4.0
1	F	360	SER	3.9
1	S	361	SER	3.9
1	I	362	THR	3.9
1	E	363	SER	3.9
1	J	309	THR	3.9
1	O	6	LEU	3.9
1	R	363	SER	3.9
1	E	6	LEU	3.9
1	D	358	GLY	3.9
1	C	191	SER	3.9
1	K	281	SER	3.9
1	T	360	SER	3.9
1	Q	6	LEU	3.8
1	R	247	GLY	3.8
1	A	362	THR	3.8
1	N	358	GLY	3.8
1	Q	247	GLY	3.8
1	B	363	SER	3.8
1	E	276	VAL	3.8
1	A	219	ASN	3.8
1	A	279	SER	3.8
1	E	364	SER	3.8
1	J	360	SER	3.8
1	R	382	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	364	SER	3.7
1	J	191	SER	3.7
1	B	249	LEU	3.7
1	Q	249	LEU	3.7
1	A	358	GLY	3.7
1	F	281	SER	3.7
1	E	360	SER	3.7
1	H	361	SER	3.7
1	K	361	SER	3.7
1	K	249	LEU	3.6
1	J	363	SER	3.6
1	L	360	SER	3.6
1	J	307	LEU	3.6
1	N	279	SER	3.6
1	S	364	SER	3.6
1	D	248	GLY	3.6
1	E	365	VAL	3.6
1	C	279	SER	3.5
1	M	358	GLY	3.5
1	C	309	THR	3.5
1	A	281	SER	3.5
1	C	189	THR	3.5
1	A	223	SER	3.5
1	G	6	LEU	3.5
1	K	310	ALA	3.5
1	L	359	GLY	3.5
1	L	382	HIS	3.5
1	R	194	PHE	3.5
1	G	363	SER	3.5
1	P	363	SER	3.5
1	Q	280	GLY	3.4
1	C	218	ALA	3.4
1	R	283	VAL	3.4
1	M	284	THR	3.4
1	C	360	SER	3.4
1	L	249	LEU	3.4
1	B	247	GLY	3.4
1	O	281	SER	3.4
1	A	280	GLY	3.4
1	F	361	SER	3.4
1	R	360	SER	3.4
1	C	194	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	T	365	VAL	3.4
1	G	278	LEU	3.3
1	Q	366	THR	3.3
1	E	281	SER	3.3
1	M	365	VAL	3.3
1	T	359	GLY	3.3
1	A	190	THR	3.3
1	L	192	THR	3.3
1	L	326	THR	3.3
1	P	360	SER	3.3
1	N	359	GLY	3.2
1	T	363	SER	3.2
1	R	307	LEU	3.2
1	R	218	ALA	3.2
1	Q	248	GLY	3.2
1	R	362	THR	3.2
1	D	279	SER	3.2
1	E	277	THR	3.2
1	D	310	ALA	3.2
1	D	283	VAL	3.2
1	G	365	VAL	3.2
1	L	283	VAL	3.2
1	M	359	GLY	3.2
1	C	219	ASN	3.2
1	G	283	VAL	3.2
1	L	363	SER	3.2
1	K	306	GLY	3.2
1	N	280	GLY	3.2
1	H	364	SER	3.1
1	I	247	GLY	3.1
1	O	363	SER	3.1
1	C	247	GLY	3.1
1	E	278	LEU	3.1
1	H	280	GLY	3.1
1	Q	309	THR	3.1
1	L	310	ALA	3.1
1	P	359	GLY	3.1
1	J	219	ASN	3.1
1	L	218	ALA	3.1
1	F	359	GLY	3.1
1	M	364	SER	3.1
1	S	310	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	215	SER	3.0
1	Q	191	SER	3.0
1	A	310	ALA	3.0
1	P	310	ALA	3.0
1	I	191	SER	3.0
1	K	283	VAL	3.0
1	T	364	SER	3.0
1	P	195	THR	3.0
1	D	306	GLY	3.0
1	O	324	SER	3.0
1	I	281	SER	3.0
1	J	310	ALA	3.0
1	K	363	SER	3.0
1	P	191	SER	3.0
1	R	361	SER	3.0
1	B	6	LEU	3.0
1	Q	217	PRO	3.0
1	L	309	THR	3.0
1	D	247	GLY	3.0
1	M	248	GLY	3.0
1	J	283	VAL	3.0
1	R	196	ASN	3.0
1	S	366	THR	2.9
1	C	361	SER	2.9
1	K	364	SER	2.9
1	C	382	HIS	2.9
1	I	309	THR	2.9
1	R	192	THR	2.9
1	H	281	SER	2.9
1	J	334	ILE	2.9
1	M	309	THR	2.9
1	B	360	SER	2.9
1	P	223	SER	2.9
1	S	276	VAL	2.9
1	A	359	GLY	2.9
1	S	248	GLY	2.9
1	C	188	ASN	2.9
1	E	283	VAL	2.9
1	I	279	SER	2.8
1	T	281	SER	2.8
1	A	6	LEU	2.8
1	G	364	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	N	281	SER	2.8
1	T	358	GLY	2.8
1	T	6	LEU	2.8
1	P	281	SER	2.8
1	C	281	SER	2.8
1	A	189	THR	2.8
1	H	358	GLY	2.8
1	F	250	GLY	2.7
1	I	193	THR	2.7
1	L	247	GLY	2.7
1	N	365	VAL	2.7
1	I	6	LEU	2.7
1	N	6	LEU	2.7
1	P	279	SER	2.7
1	R	188	ASN	2.7
1	N	310	ALA	2.7
1	Q	215	SER	2.7
1	T	279	SER	2.7
1	J	187	ASN	2.7
1	J	308	THR	2.7
1	L	188	ASN	2.7
1	M	325	THR	2.7
1	R	215	SER	2.7
1	C	193	THR	2.7
1	S	277	THR	2.7
1	S	284	THR	2.7
1	A	220	GLY	2.6
1	D	246	GLY	2.6
1	O	325	THR	2.6
1	Q	195	THR	2.6
1	H	279	SER	2.6
1	I	195	THR	2.6
1	R	195	THR	2.6
1	F	310	ALA	2.6
1	M	310	ALA	2.6
1	F	247	GLY	2.6
1	K	309	THR	2.6
1	M	277	THR	2.6
1	M	278	LEU	2.6
1	J	358	GLY	2.6
1	L	216	ILE	2.6
1	R	216	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	189	THR	2.6
1	Q	277	THR	2.6
1	G	359	GLY	2.6
1	S	247	GLY	2.6
1	B	279	SER	2.6
1	A	325	THR	2.6
1	I	219	ASN	2.6
1	D	251	VAL	2.6
1	R	250	GLY	2.6
1	S	358	GLY	2.6
1	I	249	LEU	2.5
1	F	279	SER	2.5
1	K	248	GLY	2.5
1	K	277	THR	2.5
1	L	195	THR	2.5
1	N	195	THR	2.5
1	C	215	SER	2.5
1	H	277	THR	2.5
1	M	326	THR	2.5
1	N	284	THR	2.5
1	H	360	SER	2.5
1	I	361	SER	2.5
1	J	382	HIS	2.5
1	B	190	THR	2.5
1	D	309	THR	2.5
1	L	364	SER	2.5
1	A	218	ALA	2.5
1	H	248	GLY	2.5
1	J	247	GLY	2.5
1	C	6	LEU	2.5
1	K	6	LEU	2.5
1	E	366	THR	2.5
1	Q	193	THR	2.5
1	K	191	SER	2.5
1	N	364	SER	2.5
1	J	218	ALA	2.5
1	T	280	GLY	2.5
1	G	281	SER	2.5
1	L	215	SER	2.5
1	D	365	VAL	2.4
1	P	312	THR	2.4
1	R	197	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	S	278	LEU	2.4
1	L	358	GLY	2.4
1	O	359	GLY	2.4
1	Q	358	GLY	2.4
1	P	218	ALA	2.4
1	E	279	SER	2.4
1	H	325	THR	2.4
1	I	360	SER	2.4
1	J	279	SER	2.4
1	M	279	SER	2.4
1	L	196	ASN	2.4
1	F	218	ALA	2.4
1	B	364	SER	2.4
1	D	324	SER	2.4
1	B	192	THR	2.4
1	J	312	THR	2.4
1	K	366	THR	2.4
1	N	283	VAL	2.4
1	P	382	HIS	2.4
1	A	193	THR	2.4
1	A	312	THR	2.4
1	Q	190	THR	2.4
1	C	306	GLY	2.4
1	I	248	GLY	2.4
1	P	283	VAL	2.4
1	A	364	SER	2.4
1	O	248	GLY	2.4
1	O	280	GLY	2.4
1	Q	196	ASN	2.4
1	A	334	ILE	2.4
1	Q	283	VAL	2.4
1	A	277	THR	2.3
1	B	189	THR	2.3
1	L	187	ASN	2.3
1	C	220	GLY	2.3
1	S	282	GLN	2.3
1	S	324	SER	2.3
1	B	278	LEU	2.3
1	I	382	HIS	2.3
1	C	326	THR	2.3
1	H	247	GLY	2.3
1	E	359	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	280	GLY	2.3
1	J	280	GLY	2.3
1	Q	310	ALA	2.3
1	J	326	THR	2.3
1	P	189	THR	2.3
1	R	205	SER	2.3
1	R	6	LEU	2.3
1	J	281	SER	2.3
1	P	221	SER	2.3
1	S	119	TYR	2.3
1	M	308	THR	2.3
1	H	363	SER	2.3
1	K	286	SER	2.3
1	A	311	VAL	2.2
1	K	195	THR	2.2
1	K	325	THR	2.2
1	O	308	THR	2.2
1	T	310	ALA	2.2
1	D	281	SER	2.2
1	L	214	SER	2.2
1	S	279	SER	2.2
1	F	248	GLY	2.2
1	F	251	VAL	2.2
1	H	221	SER	2.2
1	M	282	GLN	2.2
1	H	197	PHE	2.2
1	K	247	GLY	2.2
1	C	283	VAL	2.2
1	C	216	ILE	2.2
1	J	6	LEU	2.2
1	T	278	LEU	2.2
1	B	193	THR	2.2
1	E	309	THR	2.2
1	J	195	THR	2.2
1	J	194	PHE	2.2
1	C	251	VAL	2.2
1	M	276	VAL	2.2
1	B	277	THR	2.1
1	B	309	THR	2.1
1	C	192	THR	2.1
1	J	193	THR	2.1
1	N	309	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	359	GLY	2.1
1	B	215	SER	2.1
1	A	283	VAL	2.1
1	C	195	THR	2.1
1	O	220	GLY	2.1
1	Q	192	THR	2.1
1	S	157	ILE	2.1
1	O	249	LEU	2.1
1	O	215	SER	2.1
1	O	279	SER	2.1
1	O	82	ILE	2.1
1	J	324	SER	2.1
1	R	214	SER	2.1
1	R	364	SER	2.1
1	L	280	GLY	2.1
1	F	283	VAL	2.1
1	N	277	THR	2.1
1	D	196	ASN	2.1
1	Q	220	GLY	2.1
1	Q	245	TYR	2.1
1	L	365	VAL	2.1
1	P	91	SER	2.1
1	Q	278	LEU	2.1
1	R	217	PRO	2.1
1	S	155	ILE	2.1
1	O	306	GLY	2.1
1	A	365	VAL	2.0
1	H	365	VAL	2.0
1	E	306	GLY	2.0
1	J	220	GLY	2.0
1	F	277	THR	2.0
1	K	192	THR	2.0
1	P	192	THR	2.0
1	P	196	ASN	2.0
1	A	382	HIS	2.0
1	C	308	THR	2.0
1	D	326	THR	2.0
1	G	277	THR	2.0
1	L	281	SER	2.0
1	S	382	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	2HP	E	403	5/5	0.42	0.30	73,116,122,124	0
2	2HP	L	403	5/5	0.57	0.22	82,97,121,122	0
2	2HP	I	403	5/5	0.58	0.22	67,95,110,111	0
2	2HP	H	403	5/5	0.62	0.18	63,85,96,103	0
2	2HP	A	403	5/5	0.63	0.23	89,92,120,120	0
2	2HP	G	403	5/5	0.65	0.20	91,96,117,117	0
2	2HP	F	403	5/5	0.74	0.19	54,111,114,114	0
2	2HP	M	403	5/5	0.77	0.21	102,104,109,121	0
2	2HP	N	403	5/5	0.80	0.15	53,91,95,98	0
2	2HP	T	403	5/5	0.80	0.17	70,100,107,135	0
2	2HP	C	402	5/5	0.83	0.19	59,91,113,117	0
2	2HP	P	403	5/5	0.83	0.17	64,94,107,108	0
2	2HP	J	402	5/5	0.83	0.22	68,92,97,117	0
2	2HP	B	403	5/5	0.84	0.23	67,102,106,108	0
2	2HP	Q	403	5/5	0.86	0.15	67,92,102,103	0
2	2HP	S	403	5/5	0.87	0.13	57,82,105,107	0
2	2HP	D	403	5/5	0.87	0.13	64,66,100,101	0
2	2HP	O	403	5/5	0.88	0.12	63,84,99,100	0
2	2HP	R	402	5/5	0.90	0.15	80,84,98,101	0
2	2HP	K	403	5/5	0.91	0.10	87,93,98,99	0
2	2HP	K	401	5/5	0.95	0.16	51,55,62,102	0
2	2HP	I	401	5/5	0.96	0.14	38,57,59,81	0
2	2HP	D	402	5/5	0.96	0.09	37,49,57,73	0
2	2HP	Q	401	5/5	0.96	0.13	47,47,51,76	0
2	2HP	N	401	5/5	0.96	0.12	43,51,61,140	0
2	2HP	L	401	5/5	0.97	0.13	50,52,55,115	0
2	2HP	F	401	5/5	0.97	0.11	46,46,54,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	2HP	P	402	5/5	0.97	0.10	39,47,50,79	0
2	2HP	Q	402	5/5	0.97	0.08	43,44,55,83	0
2	2HP	P	401	5/5	0.97	0.10	43,49,54,66	0
2	2HP	D	401	5/5	0.97	0.08	43,45,62,69	0
2	2HP	O	401	5/5	0.97	0.10	42,45,53,78	0
2	2HP	G	401	5/5	0.97	0.08	37,48,71,74	0
2	2HP	A	401	5/5	0.97	0.12	35,46,54,55	0
2	2HP	J	401	5/5	0.97	0.11	47,48,51,64	0
2	2HP	C	401	5/5	0.98	0.11	44,46,68,74	0
2	2HP	B	401	5/5	0.98	0.12	34,41,53,82	0
2	2HP	E	402	5/5	0.98	0.08	45,45,54,63	0
2	2HP	R	401	5/5	0.98	0.11	40,46,52,60	0
2	2HP	S	401	5/5	0.98	0.07	34,40,44,64	0
2	2HP	A	402	5/5	0.98	0.09	44,48,52,77	0
2	2HP	H	402	5/5	0.98	0.09	39,40,44,65	0
2	2HP	L	402	5/5	0.98	0.09	45,46,61,68	0
2	2HP	O	402	5/5	0.98	0.09	40,43,49,93	0
2	2HP	T	401	5/5	0.98	0.11	42,52,68,160	0
2	2HP	I	402	5/5	0.98	0.08	43,45,57,58	0
2	2HP	F	402	5/5	0.98	0.07	39,46,58,79	0
2	2HP	B	402	5/5	0.98	0.08	41,47,54,74	0
2	2HP	G	402	5/5	0.98	0.09	39,45,58,59	0
2	2HP	K	402	5/5	0.98	0.06	42,45,51,53	0
2	2HP	E	401	5/5	0.98	0.09	49,49,70,135	0
2	2HP	M	401	5/5	0.99	0.09	38,44,52,77	0
2	2HP	M	402	5/5	0.99	0.12	50,51,58,62	0
2	2HP	T	402	5/5	0.99	0.10	39,39,52,81	0
2	2HP	Q	404	5/5	0.99	0.08	41,43,49,95	0
2	2HP	H	401	5/5	0.99	0.06	34,38,43,55	0
2	2HP	I	404	5/5	0.99	0.06	38,39,50,55	0
2	2HP	B	404	5/5	0.99	0.11	43,44,55,86	0
2	2HP	S	402	5/5	0.99	0.12	41,47,53,83	0
2	2HP	N	402	5/5	0.99	0.09	40,41,56,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.