



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 06:49 AM EDT

PDB ID : 3H6I  
Title : Crystal Structure of Mycobacterium Tuberculosis Proteasome Modified by inhibitor GL1  
Authors : Li, D.; Li, H.; Lin, G.  
Deposited on : 2009-04-23  
Resolution : 2.43 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

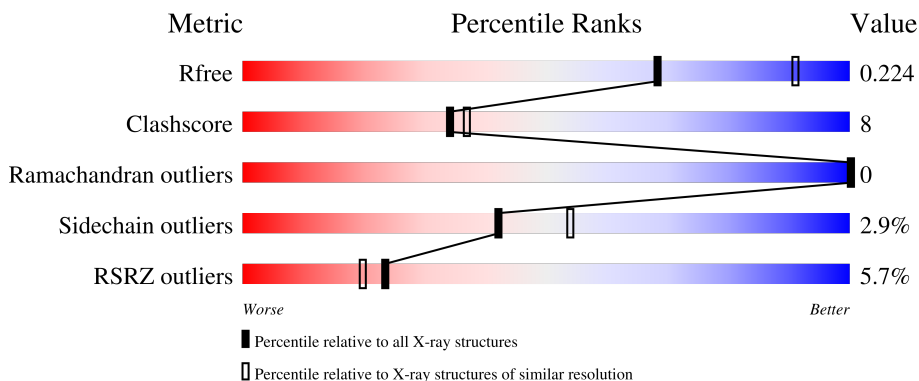
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.43 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.



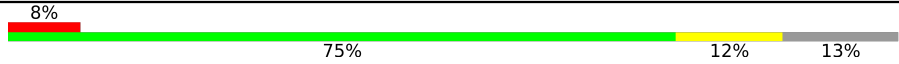

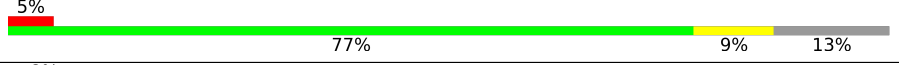



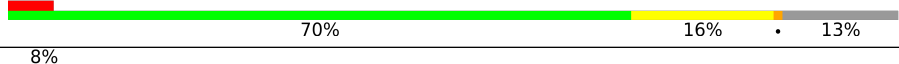

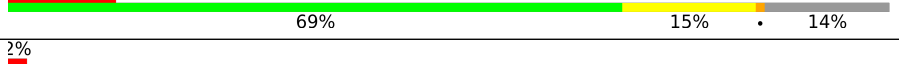


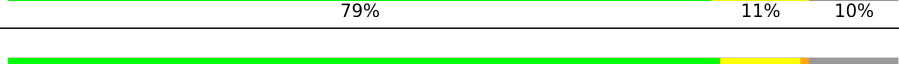

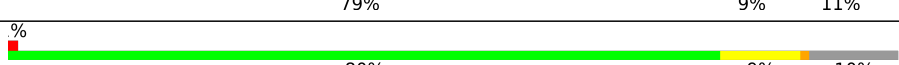

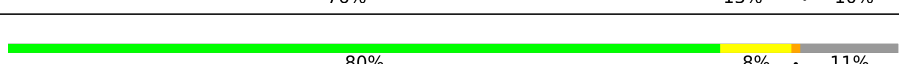
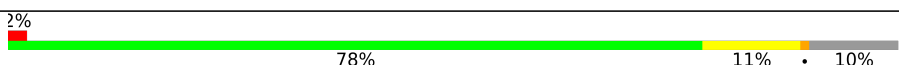
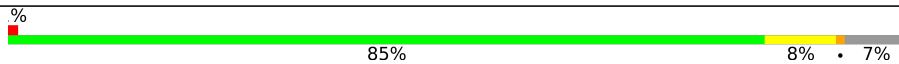
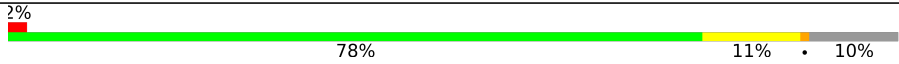




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	248	 8% 75% 10% • 13%
1	A	248	 14% 75% 11% 13%
1	B	248	 6% 74% 12% • 14%
1	D	248	 11% 71% 12% • 14%
1	F	248	 6% 73% 14% • 12%

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Mol	Chain	Length	Quality of chain
1	I	248	
1	K	248	
1	M	248	
1	O	248	
1	Q	248	
1	S	248	
1	U	248	
1	W	248	
1	Y	248	
2	2	240	
2	C	240	
2	E	240	
2	G	240	
2	H	240	
2	J	240	
2	L	240	
2	N	240	
2	P	240	
2	R	240	
2	T	240	
2	V	240	
2	X	240	
2	Z	240	

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	OZT	P	301	-	-	X	-
3	DMF	C	5	-	-	X	-
3	DMF	C	64	-	-	X	-
3	DMF	C	73	-	-	X	-
3	DMF	D	249	-	-	-	X
3	DMF	E	32	-	-	-	X
3	DMF	H	19	-	-	X	-
3	DMF	H	31	-	-	-	X
3	DMF	J	6	-	-	X	-
3	DMF	O	250	-	-	X	-
3	DMF	T	35	-	-	X	-
3	DMF	T	94	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 48540 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 Proteasome (Alpha subunit) PrcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	Total 1662	C 1041	N 304	O 314	S 3	0	0	0
1	B	214	Total 1650	C 1033	N 302	O 312	S 3	0	0	0
1	D	213	Total 1644	C 1030	N 301	O 310	S 3	0	0	0
1	F	217	Total 1669	C 1045	N 305	O 316	S 3	0	0	0
1	I	215	Total 1656	C 1038	N 303	O 312	S 3	0	0	0
1	K	217	Total 1670	C 1047	N 305	O 315	S 3	0	0	0
1	M	216	Total 1662	C 1041	N 304	O 314	S 3	0	0	0
1	O	215	Total 1654	C 1035	N 303	O 313	S 3	0	0	0
1	Q	218	Total 1677	C 1051	N 306	O 317	S 3	0	0	0
1	S	215	Total 1654	C 1035	N 303	O 313	S 3	0	0	0
1	U	215	Total 1654	C 1035	N 303	O 313	S 3	0	0	0
1	W	217	Total 1670	C 1047	N 305	O 315	S 3	0	0	0
1	Y	213	Total 1644	C 1030	N 301	O 310	S 3	0	0	0
1	1	215	Total 1656	C 1038	N 303	O 312	S 3	0	0	0

- Molecule 2 is a protein called Proteasome (Beta subunit) PrcB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	215	Total 1593	C 998	N 274	O 317	S 4	0	0	0
2	E	216	Total 1601	C 1004	N 275	O 318	S 4	0	0	0
2	G	216	Total 1601	C 1004	N 275	O 318	S 4	0	0	0
2	H	213	Total 1583	C 992	N 272	O 315	S 4	0	0	0
2	J	216	Total 1601	C 1004	N 275	O 318	S 4	0	0	0
2	L	216	Total 1601	C 1004	N 275	O 318	S 4	0	0	0
2	N	213	Total 1580	C 989	N 272	O 315	S 4	0	0	0
2	P	216	Total 1601	C 1004	N 275	O 318	S 4	0	0	0
2	R	223	Total 1646	C 1031	N 282	O 329	S 4	0	0	0
2	T	216	Total 1601	C 1004	N 275	O 318	S 4	0	0	0
2	V	221	Total 1632	C 1022	N 280	O 326	S 4	0	0	0
2	X	216	Total 1601	C 1004	N 275	O 318	S 4	0	0	0
2	Z	215	Total 1593	C 998	N 274	O 317	S 4	0	0	0
2	2	215	Total 1593	C 998	N 274	O 317	S 4	0	0	0

There are 98 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	301	OZT	-	insertion	UNP O33245
C	535	HIS	-	expression tag	UNP O33245
C	536	HIS	-	expression tag	UNP O33245
C	537	HIS	-	expression tag	UNP O33245
C	538	HIS	-	expression tag	UNP O33245
C	539	HIS	-	expression tag	UNP O33245
C	540	HIS	-	expression tag	UNP O33245
E	301	OZT	-	insertion	UNP O33245
E	535	HIS	-	expression tag	UNP O33245
E	536	HIS	-	expression tag	UNP O33245
E	537	HIS	-	expression tag	UNP O33245
E	538	HIS	-	expression tag	UNP O33245

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Chain	Residue	Modelled	Actual	Comment	Reference
E	539	HIS	-	expression tag	UNP O33245
E	540	HIS	-	expression tag	UNP O33245
G	301	OZT	-	insertion	UNP O33245
G	535	HIS	-	expression tag	UNP O33245
G	536	HIS	-	expression tag	UNP O33245
G	537	HIS	-	expression tag	UNP O33245
G	538	HIS	-	expression tag	UNP O33245
G	539	HIS	-	expression tag	UNP O33245
G	540	HIS	-	expression tag	UNP O33245
H	301	OZT	-	insertion	UNP O33245
H	535	HIS	-	expression tag	UNP O33245
H	536	HIS	-	expression tag	UNP O33245
H	537	HIS	-	expression tag	UNP O33245
H	538	HIS	-	expression tag	UNP O33245
H	539	HIS	-	expression tag	UNP O33245
H	540	HIS	-	expression tag	UNP O33245
J	301	OZT	-	insertion	UNP O33245
J	535	HIS	-	expression tag	UNP O33245
J	536	HIS	-	expression tag	UNP O33245
J	537	HIS	-	expression tag	UNP O33245
J	538	HIS	-	expression tag	UNP O33245
J	539	HIS	-	expression tag	UNP O33245
J	540	HIS	-	expression tag	UNP O33245
L	301	OZT	-	insertion	UNP O33245
L	535	HIS	-	expression tag	UNP O33245
L	536	HIS	-	expression tag	UNP O33245
L	537	HIS	-	expression tag	UNP O33245
L	538	HIS	-	expression tag	UNP O33245
L	539	HIS	-	expression tag	UNP O33245
L	540	HIS	-	expression tag	UNP O33245
N	301	OZT	-	insertion	UNP O33245
N	535	HIS	-	expression tag	UNP O33245
N	536	HIS	-	expression tag	UNP O33245
N	537	HIS	-	expression tag	UNP O33245
N	538	HIS	-	expression tag	UNP O33245
N	539	HIS	-	expression tag	UNP O33245
N	540	HIS	-	expression tag	UNP O33245
P	301	OZT	-	insertion	UNP O33245
P	535	HIS	-	expression tag	UNP O33245
P	536	HIS	-	expression tag	UNP O33245
P	537	HIS	-	expression tag	UNP O33245
P	538	HIS	-	expression tag	UNP O33245

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Chain	Residue	Modelled	Actual	Comment	Reference
P	539	HIS	-	expression tag	UNP O33245
P	540	HIS	-	expression tag	UNP O33245
R	301	OZT	-	insertion	UNP O33245
R	535	HIS	-	expression tag	UNP O33245
R	536	HIS	-	expression tag	UNP O33245
R	537	HIS	-	expression tag	UNP O33245
R	538	HIS	-	expression tag	UNP O33245
R	539	HIS	-	expression tag	UNP O33245
R	540	HIS	-	expression tag	UNP O33245
T	301	OZT	-	insertion	UNP O33245
T	535	HIS	-	expression tag	UNP O33245
T	536	HIS	-	expression tag	UNP O33245
T	537	HIS	-	expression tag	UNP O33245
T	538	HIS	-	expression tag	UNP O33245
T	539	HIS	-	expression tag	UNP O33245
T	540	HIS	-	expression tag	UNP O33245
V	301	OZT	-	insertion	UNP O33245
V	535	HIS	-	expression tag	UNP O33245
V	536	HIS	-	expression tag	UNP O33245
V	537	HIS	-	expression tag	UNP O33245
V	538	HIS	-	expression tag	UNP O33245
V	539	HIS	-	expression tag	UNP O33245
V	540	HIS	-	expression tag	UNP O33245
X	301	OZT	-	insertion	UNP O33245
X	535	HIS	-	expression tag	UNP O33245
X	536	HIS	-	expression tag	UNP O33245
X	537	HIS	-	expression tag	UNP O33245
X	538	HIS	-	expression tag	UNP O33245
X	539	HIS	-	expression tag	UNP O33245
X	540	HIS	-	expression tag	UNP O33245
Z	301	OZT	-	insertion	UNP O33245
Z	535	HIS	-	expression tag	UNP O33245
Z	536	HIS	-	expression tag	UNP O33245
Z	537	HIS	-	expression tag	UNP O33245
Z	538	HIS	-	expression tag	UNP O33245
Z	539	HIS	-	expression tag	UNP O33245
Z	540	HIS	-	expression tag	UNP O33245
2	301	OZT	-	insertion	UNP O33245
2	535	HIS	-	expression tag	UNP O33245
2	536	HIS	-	expression tag	UNP O33245
2	537	HIS	-	expression tag	UNP O33245
2	538	HIS	-	expression tag	UNP O33245

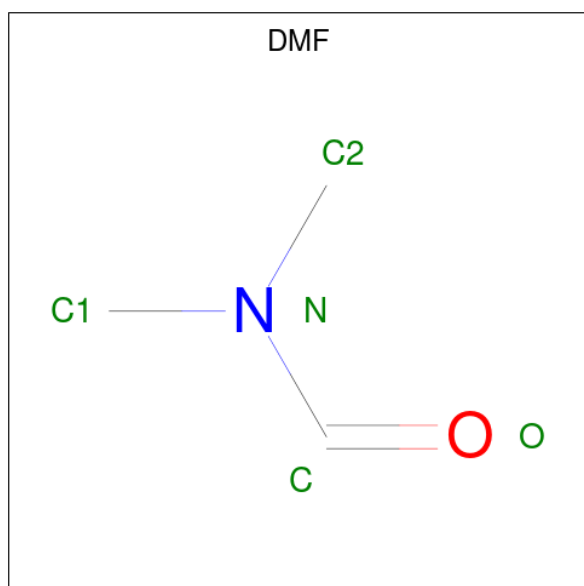
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Chain	Residue	Modelled	Actual	Comment	Reference
2	539	HIS	-	expression tag	UNP O33245
2	540	HIS	-	expression tag	UNP O33245

- Molecule 3 is DIMETHYLFORMAMIDE (three-letter code: DMF) (formula: C<sub>3</sub>H<sub>7</sub>NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total	C	N	O	0	0
			5	3	1	1		
3	A	1	Total	C	N	O	0	0
			5	3	1	1		
3	B	1	Total	C	N	O	0	0
			5	3	1	1		
3	B	1	Total	C	N	O	0	0
			5	3	1	1		
3	B	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	D	1	Total	C	N	O	0	0
			5	3	1	1		
3	D	1	Total	C	N	O	0	0
			5	3	1	1		
3	D	1	Total	C	N	O	0	0
			5	3	1	1		
3	D	1	Total	C	N	O	0	0
			5	3	1	1		
3	E	1	Total	C	N	O	0	0
			5	3	1	1		
3	E	1	Total	C	N	O	0	0
			5	3	1	1		
3	E	1	Total	C	N	O	0	0
			5	3	1	1		
3	E	1	Total	C	N	O	0	0
			5	3	1	1		
3	E	1	Total	C	N	O	0	0
			5	3	1	1		
3	E	1	Total	C	N	O	0	0
			5	3	1	1		
3	E	1	Total	C	N	O	0	0
			5	3	1	1		
3	F	1	Total	C	N	O	0	0
			5	3	1	1		
3	F	1	Total	C	N	O	0	0
			5	3	1	1		
3	G	1	Total	C	N	O	0	0
			5	3	1	1		
3	G	1	Total	C	N	O	0	0
			5	3	1	1		
3	G	1	Total	C	N	O	0	0
			5	3	1	1		
3	G	1	Total	C	N	O	0	0
			5	3	1	1		
3	H	1	Total	C	N	O	0	0
			5	3	1	1		
3	H	1	Total	C	N	O	0	0
			5	3	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			5	3	1	1		
3	H	1	Total	C	N	O	0	0
			5	3	1	1		
3	H	1	Total	C	N	O	0	0
			5	3	1	1		
3	H	1	Total	C	N	O	0	0
			5	3	1	1		
3	H	1	Total	C	N	O	0	0
			5	3	1	1		
3	I	1	Total	C	N	O	0	0
			5	3	1	1		
3	I	1	Total	C	N	O	0	0
			5	3	1	1		
3	J	1	Total	C	N	O	0	0
			5	3	1	1		
3	J	1	Total	C	N	O	0	0
			5	3	1	1		
3	J	1	Total	C	N	O	0	0
			5	3	1	1		
3	K	1	Total	C	N	O	0	0
			5	3	1	1		
3	K	1	Total	C	N	O	0	0
			5	3	1	1		
3	L	1	Total	C	N	O	0	0
			5	3	1	1		
3	L	1	Total	C	N	O	0	0
			5	3	1	1		
3	L	1	Total	C	N	O	0	0
			5	3	1	1		
3	M	1	Total	C	N	O	0	0
			5	3	1	1		
3	M	1	Total	C	N	O	0	0
			5	3	1	1		
3	N	1	Total	C	N	O	0	0
			5	3	1	1		
3	N	1	Total	C	N	O	0	0
			5	3	1	1		
3	N	1	Total	C	N	O	0	0
			5	3	1	1		
3	N	1	Total	C	N	O	0	0
			5	3	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	N	1	Total 5	C 3	N 1	O 1	0	0
3	N	1	Total 5	C 3	N 1	O 1	0	0
3	N	1	Total 5	C 3	N 1	O 1	0	0
3	O	1	Total 5	C 3	N 1	O 1	0	0
3	O	1	Total 5	C 3	N 1	O 1	0	0
3	P	1	Total 5	C 3	N 1	O 1	0	0
3	P	1	Total 5	C 3	N 1	O 1	0	0
3	P	1	Total 5	C 3	N 1	O 1	0	0
3	P	1	Total 5	C 3	N 1	O 1	0	0
3	P	1	Total 5	C 3	N 1	O 1	0	0
3	Q	1	Total 5	C 3	N 1	O 1	0	0
3	Q	1	Total 5	C 3	N 1	O 1	0	0
3	R	1	Total 5	C 3	N 1	O 1	0	0
3	R	1	Total 5	C 3	N 1	O 1	0	0
3	R	1	Total 5	C 3	N 1	O 1	0	0
3	R	1	Total 5	C 3	N 1	O 1	0	0
3	S	1	Total 5	C 3	N 1	O 1	0	0
3	S	1	Total 5	C 3	N 1	O 1	0	0
3	S	1	Total 5	C 3	N 1	O 1	0	0
3	T	1	Total 5	C 3	N 1	O 1	0	0
3	T	1	Total 5	C 3	N 1	O 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	T	1	Total 5	C 3	N 1	O 1	0	0
3	T	1	Total 5	C 3	N 1	O 1	0	0
3	T	1	Total 5	C 3	N 1	O 1	0	0
3	U	1	Total 5	C 3	N 1	O 1	0	0
3	U	1	Total 5	C 3	N 1	O 1	0	0
3	U	1	Total 5	C 3	N 1	O 1	0	0
3	U	1	Total 5	C 3	N 1	O 1	0	0
3	V	1	Total 5	C 3	N 1	O 1	0	0
3	V	1	Total 5	C 3	N 1	O 1	0	0
3	V	1	Total 5	C 3	N 1	O 1	0	0
3	V	1	Total 5	C 3	N 1	O 1	0	0
3	W	1	Total 5	C 3	N 1	O 1	0	0
3	W	1	Total 5	C 3	N 1	O 1	0	0
3	X	1	Total 5	C 3	N 1	O 1	0	0
3	X	1	Total 5	C 3	N 1	O 1	0	0
3	X	1	Total 5	C 3	N 1	O 1	0	0
3	Y	1	Total 5	C 3	N 1	O 1	0	0
3	Z	1	Total 5	C 3	N 1	O 1	0	0
3	Z	1	Total 5	C 3	N 1	O 1	0	0
3	Z	1	Total 5	C 3	N 1	O 1	0	0
3	Z	1	Total 5	C 3	N 1	O 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	Z	1	Total	C	N	O	0	0
			5	3	1	1		
3	Z	1	Total	C	N	O	0	0
			5	3	1	1		
3	1	1	Total	C	N	O	0	0
			5	3	1	1		
3	1	1	Total	C	N	O	0	0
			5	3	1	1		
3	1	1	Total	C	N	O	0	0
			5	3	1	1		
3	2	1	Total	C	N	O	0	0
			5	3	1	1		
3	2	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	45	Total	O	0	0
			45	45		
4	C	142	Total	O	0	0
			142	142		
4	D	43	Total	O	0	0
			43	43		
4	E	124	Total	O	0	0
			124	124		
4	F	34	Total	O	0	0
			34	34		
4	G	136	Total	O	0	0
			136	136		
4	H	122	Total	O	0	0
			122	122		
4	I	37	Total	O	0	0
			37	37		
4	J	128	Total	O	0	0
			128	128		
4	K	45	Total	O	0	0
			45	45		

*Continued on next page...*

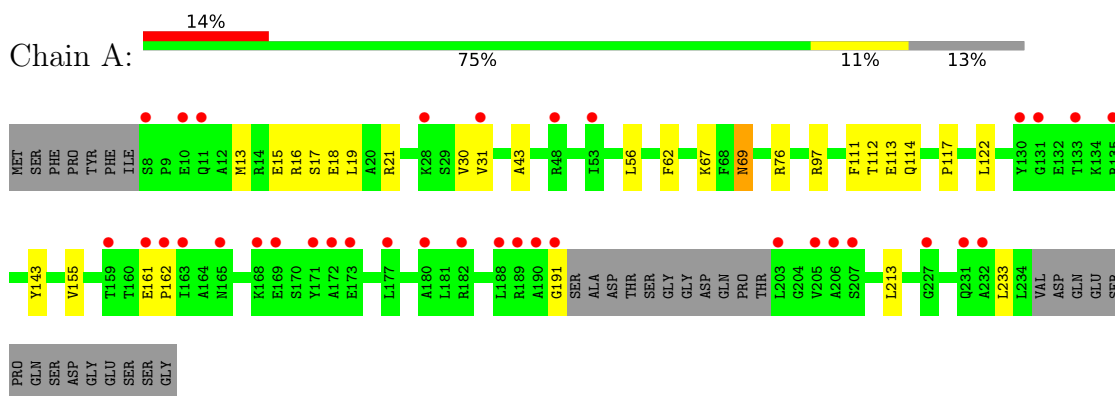
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	138	Total 138	O 138	0	0
4	M	52	Total 52	O 52	0	0
4	N	118	Total 118	O 118	0	0
4	O	51	Total 51	O 51	0	0
4	P	111	Total 111	O 111	0	0
4	Q	41	Total 41	O 41	0	0
4	R	141	Total 141	O 141	0	0
4	S	31	Total 31	O 31	0	0
4	T	112	Total 112	O 112	0	0
4	U	43	Total 43	O 43	0	0
4	V	154	Total 154	O 154	0	0
4	W	31	Total 31	O 31	0	0
4	X	130	Total 130	O 130	0	0
4	Y	41	Total 41	O 41	0	0
4	Z	113	Total 113	O 113	0	0
4	1	42	Total 42	O 42	0	0
4	2	133	Total 133	O 133	0	0

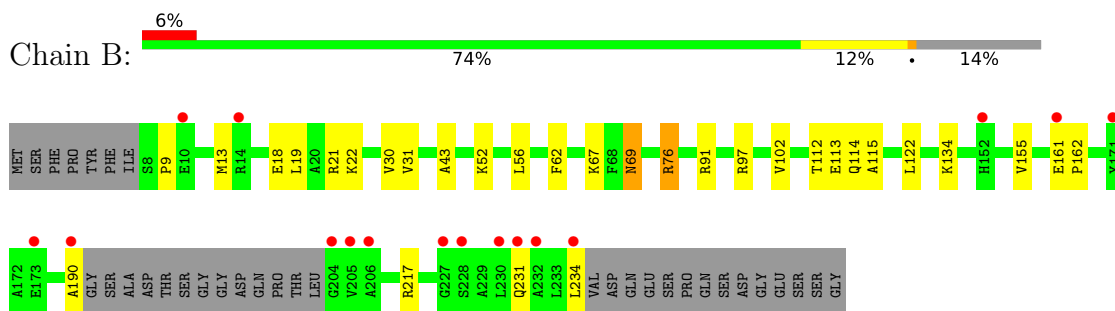
### 3 Residue-property plots [i](#)

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

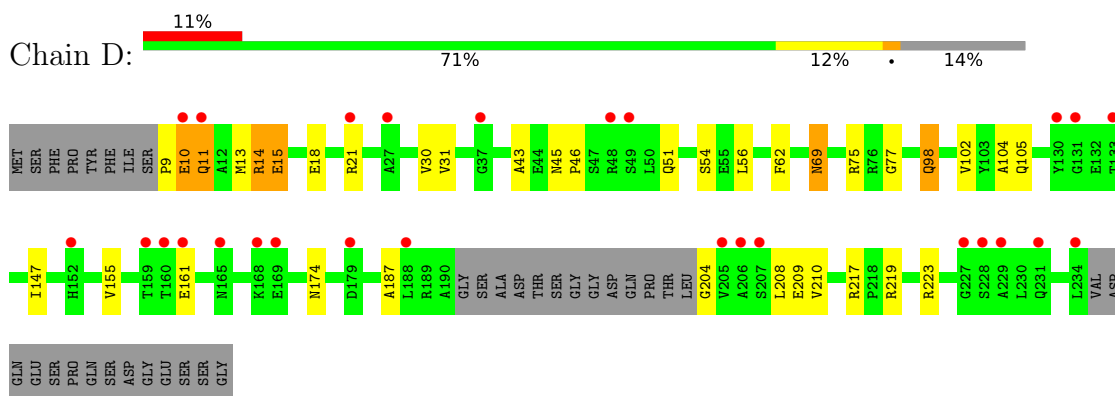
- Molecule 1: Proteasome (Alpha subunit) PrcA



- Molecule 1: Proteasome (Alpha subunit) PrcA

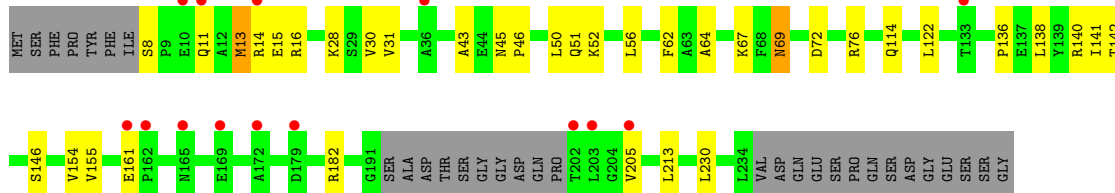
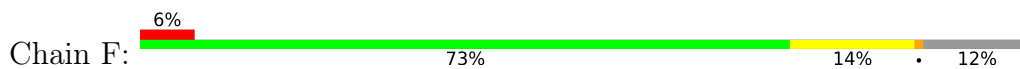


- Molecule 1: Proteasome (Alpha subunit) PrcA

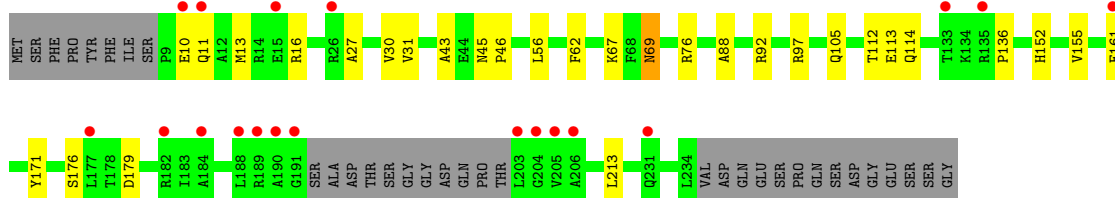
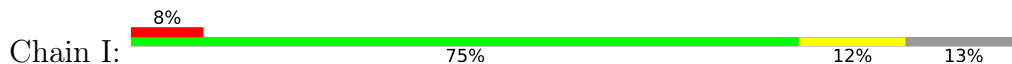


- Molecule 1: Proteasome (Alpha subunit) PrcA

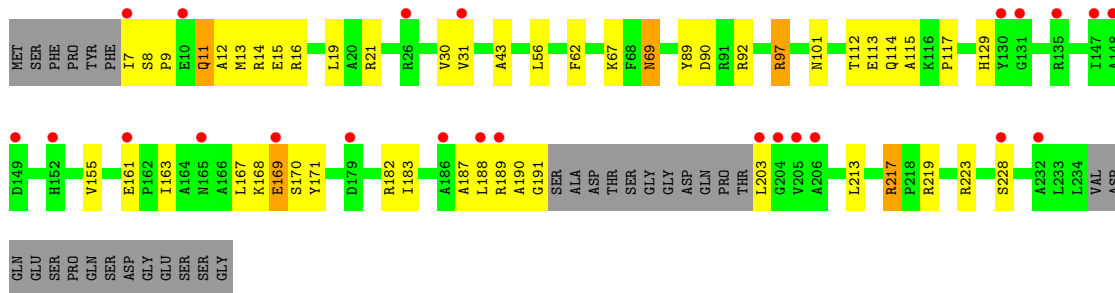




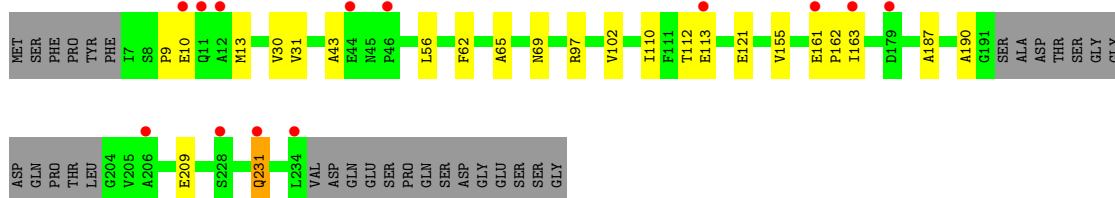
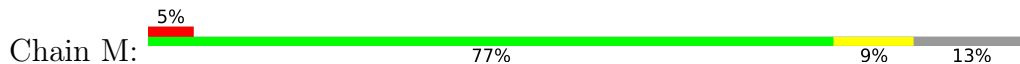
• Molecule 1: Proteasome (Alpha subunit) PrcA



• Molecule 1: Proteasome (Alpha subunit) PrcA

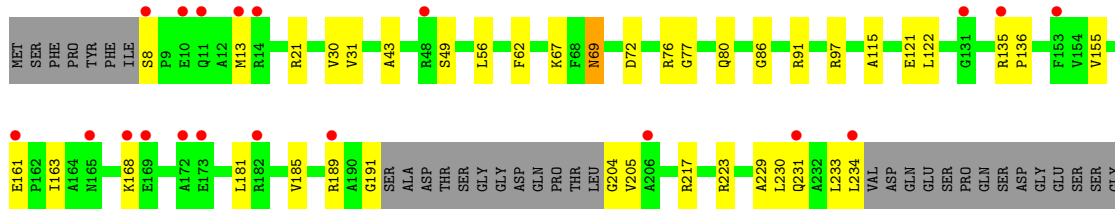


• Molecule 1: Proteasome (Alpha subunit) PrcA

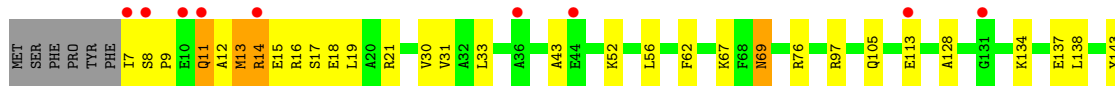


• Molecule 1: Proteasome (Alpha subunit) PrcA

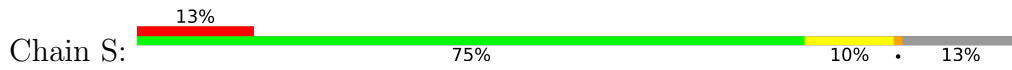




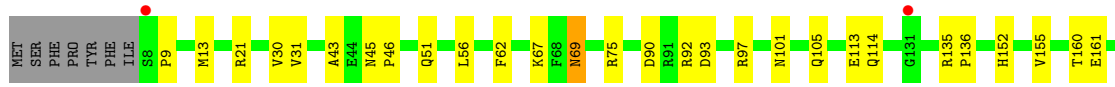
• Molecule 1: Proteasome (Alpha subunit) PrcA



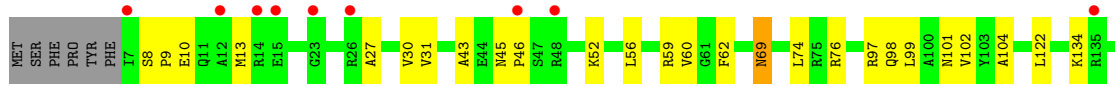
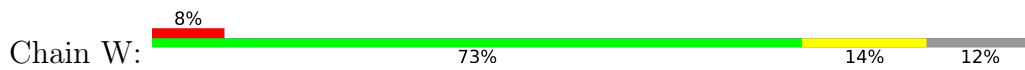
• Molecule 1: Proteasome (Alpha subunit) PrcA

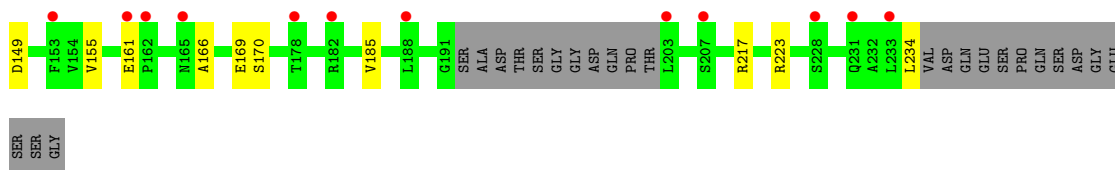


• Molecule 1: Proteasome (Alpha subunit) PrcA

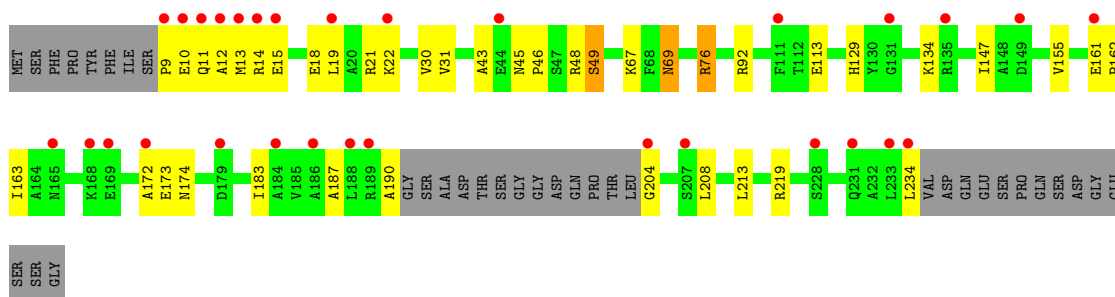


• Molecule 1: Proteasome (Alpha subunit) PrcA

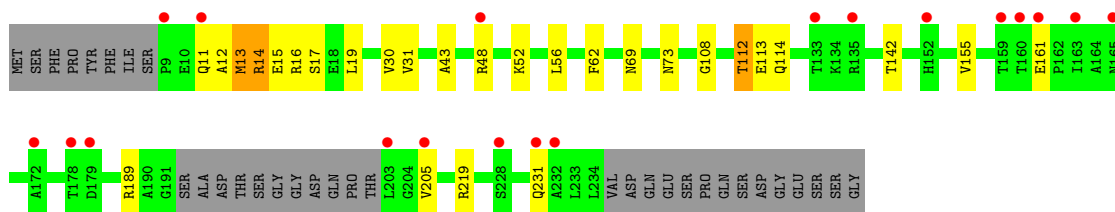
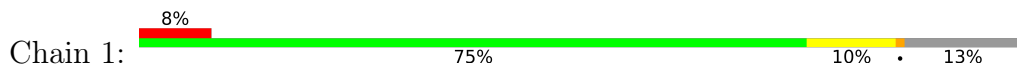




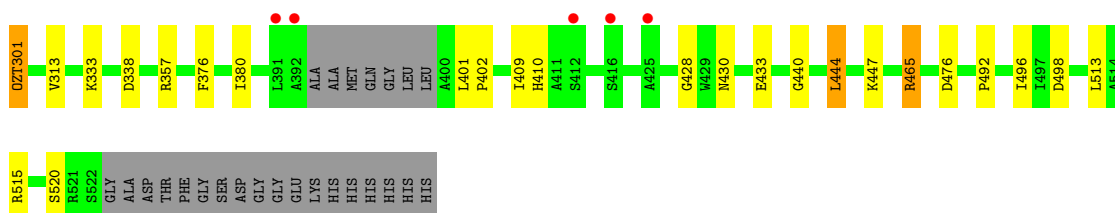
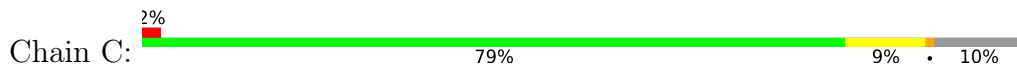
• Molecule 1: Proteasome (Alpha subunit) PrcA



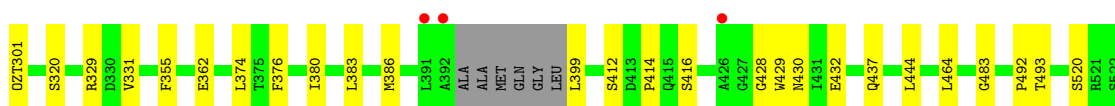
• Molecule 1: Proteasome (Alpha subunit) PrcA



• Molecule 2: Proteasome (Beta subunit) PrcB

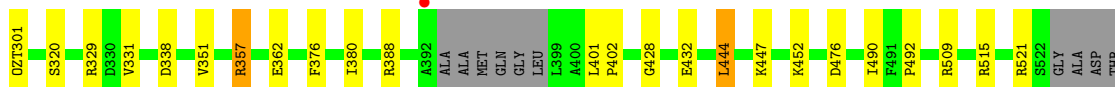
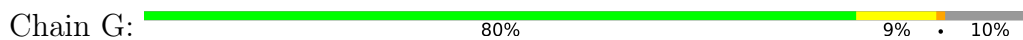


• Molecule 2: Proteasome (Beta subunit) PrcB



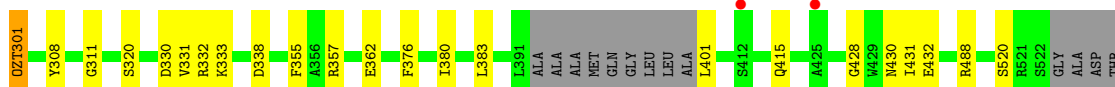
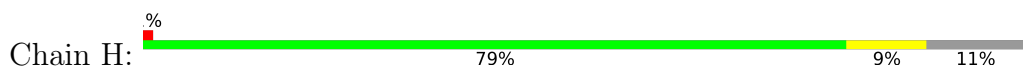
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ALA  
ASP  
THR  
PHE  
GLY  
SER  
ASP  
GLY  
GLY  
GLU  
LYS  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS

● Molecule 2: Proteasome (Beta subunit) PrcB



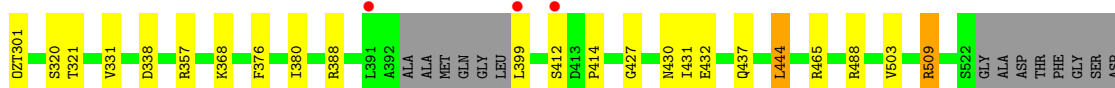
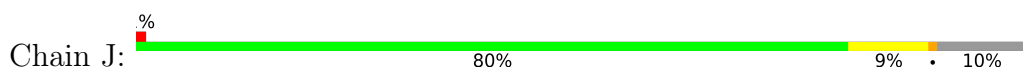
PHE  
GLY  
SER  
ASP  
GLY  
GLY  
GLU  
LYS  
HIS  
HIS  
HIS  
HIS

● Molecule 2: Proteasome (Beta subunit) PrcB



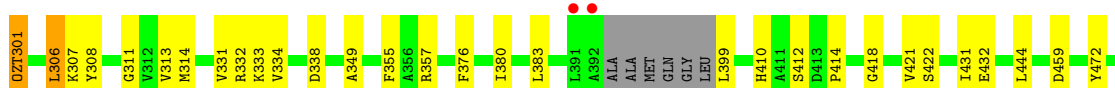
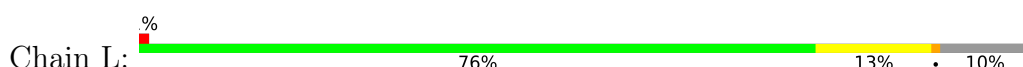
PHE  
GLY  
SER  
ASP  
GLY  
GLY  
GLU  
LYS  
HIS  
HIS  
HIS  
HIS

● Molecule 2: Proteasome (Beta subunit) PrcB



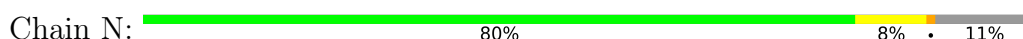
GLY  
GLY  
GLU  
LYS  
HIS  
HIS  
HIS  
HIS

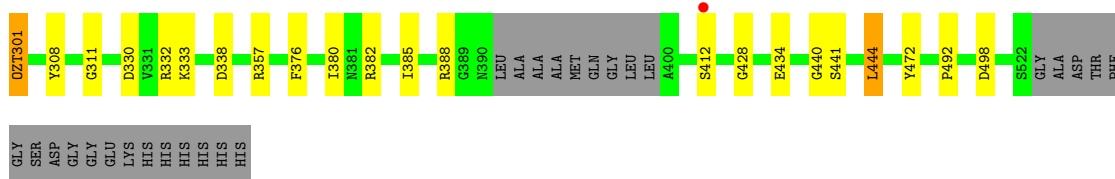
● Molecule 2: Proteasome (Beta subunit) PrcB



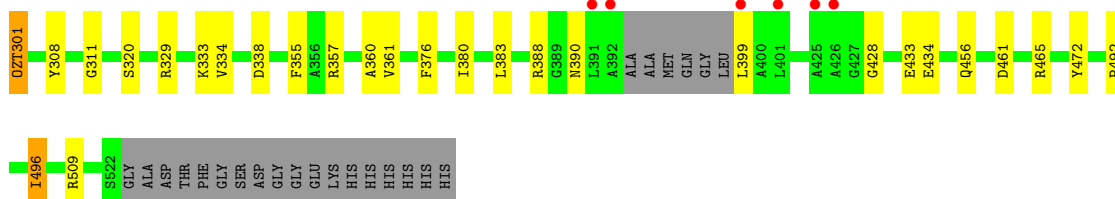
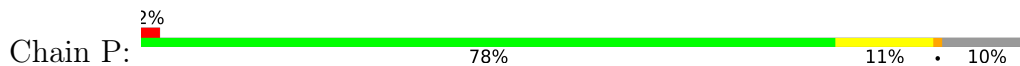
G482 P492 R509 R521 S522 GLY ALA ASP THR PHE GLY SER ASP GLY GLU LYS HIS HIS HIS HIS HIS HIS

● Molecule 2: Proteasome (Beta subunit) PrcB

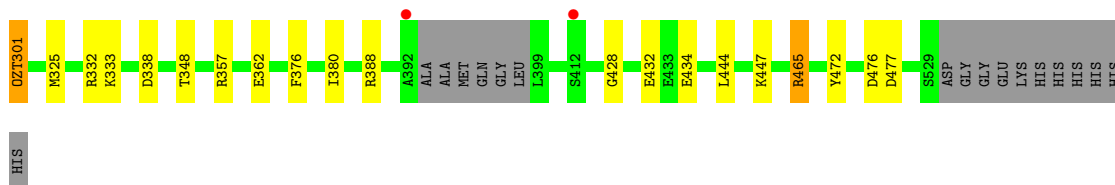
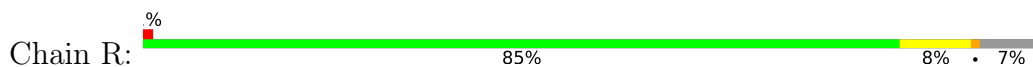




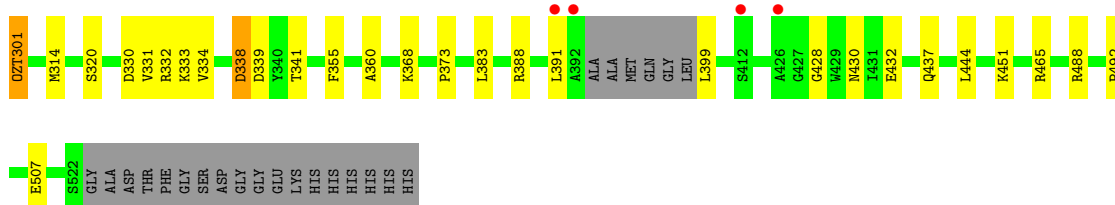
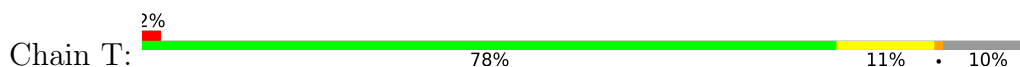
- Molecule 2: Proteasome (Beta subunit) PrcB



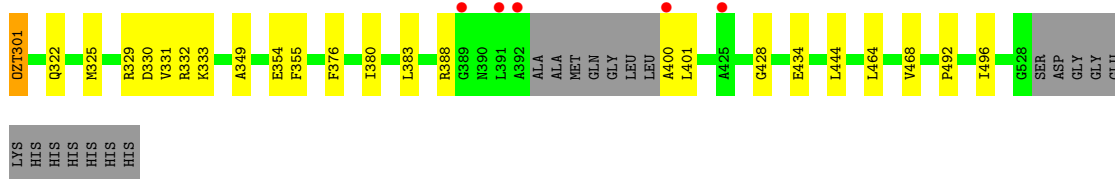
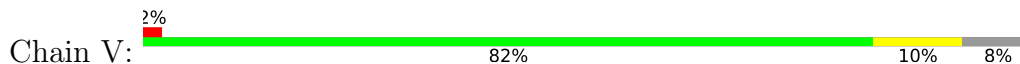
- Molecule 2: Proteasome (Beta subunit) PrcB



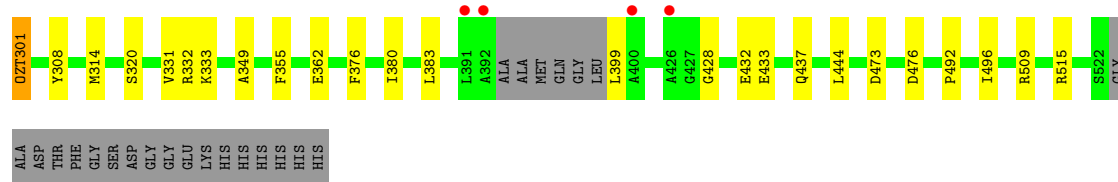
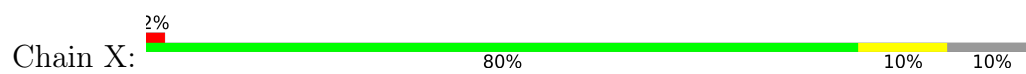
- Molecule 2: Proteasome (Beta subunit) PrcB



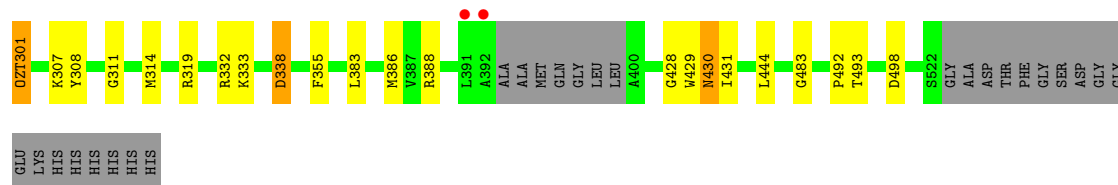
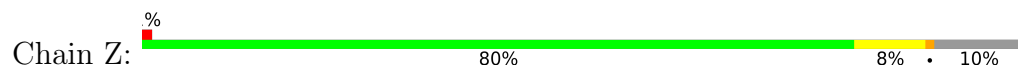
- Molecule 2: Proteasome (Beta subunit) PrcB



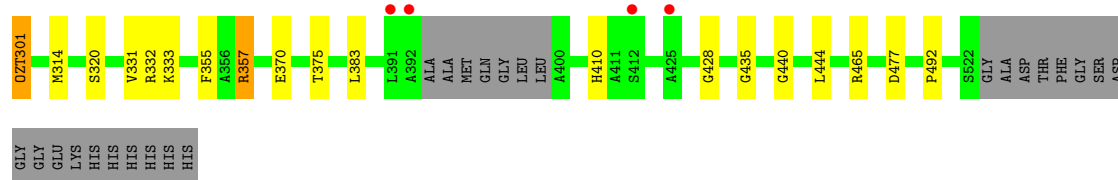
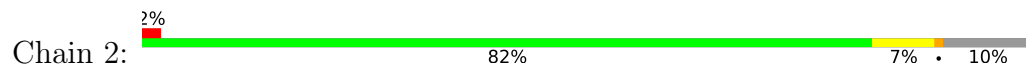
- Molecule 2: Proteasome (Beta subunit) PrcB



- Molecule 2: Proteasome (Beta subunit) PrcB



- Molecule 2: Proteasome (Beta subunit) PrcB



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	171.62Å 117.67Å 196.34Å 90.00° 113.65° 90.00°	Depositor
Resolution (Å)	29.75 – 2.43 30.57 – 2.44	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.75-2.43) 97.9 (30.57-2.44)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.82 (at 2.45Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.204 , 0.232 0.196 , 0.224	Depositor DCC
$R_{free}$ test set	13191 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtrriage
Anisotropy	0.198	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.003 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	48540	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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, 0.333 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: OZT, DMF

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	1	0.76	0/1681	0.85	0/2270
1	A	0.75	0/1687	0.83	1/2279 (0.0%)
1	B	0.76	0/1675	0.85	2/2263 (0.1%)
1	D	0.75	0/1669	0.84	1/2254 (0.0%)
1	F	0.76	0/1694	0.84	1/2289 (0.0%)
1	I	0.73	0/1681	0.87	2/2270 (0.1%)
1	K	0.74	0/1695	0.85	2/2290 (0.1%)
1	M	0.77	0/1687	0.86	0/2279
1	O	0.78	0/1679	0.84	1/2268 (0.0%)
1	Q	0.76	0/1702	0.81	2/2300 (0.1%)
1	S	0.74	0/1679	0.85	1/2268 (0.0%)
1	U	0.77	0/1679	0.85	2/2268 (0.1%)
1	W	0.76	0/1695	0.86	0/2290
1	Y	0.75	0/1669	0.85	2/2254 (0.1%)
2	2	0.89	1/1607 (0.1%)	0.84	1/2178 (0.0%)
2	C	0.87	1/1607 (0.1%)	0.88	2/2178 (0.1%)
2	E	0.91	0/1615	0.88	0/2189
2	G	0.89	0/1615	0.88	3/2189 (0.1%)
2	H	0.91	0/1597	0.87	2/2164 (0.1%)
2	J	0.92	1/1615 (0.1%)	0.87	1/2189 (0.0%)
2	L	0.91	0/1615	0.87	0/2189
2	N	0.89	0/1594	0.87	1/2160 (0.0%)
2	P	0.86	1/1615 (0.1%)	0.85	1/2189 (0.0%)
2	R	0.88	0/1661	0.86	0/2251
2	T	0.86	0/1615	0.86	1/2189 (0.0%)
2	V	0.92	0/1647	0.83	0/2232
2	X	0.91	1/1615 (0.1%)	0.88	1/2189 (0.0%)
2	Z	0.88	1/1607 (0.1%)	0.87	2/2178 (0.1%)
All	All	0.83	6/46197 (0.0%)	0.86	32/62506 (0.1%)

All (6) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	313	VAL	CB-CG1	-5.88	1.40	1.52
2	2	314	MET	SD-CE	-5.82	1.45	1.77
2	J	503	VAL	CA-CB	5.34	1.66	1.54
2	P	496	ILE	C-N	-5.29	1.21	1.34
2	X	308	TYR	CD2-CE2	5.19	1.47	1.39
2	Z	314	MET	SD-CE	-5.18	1.48	1.77

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	465	ARG	NE-CZ-NH2	-5.67	117.47	120.30
2	H	357	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	122	LEU	CA-CB-CG	5.61	128.20	115.30
1	K	21	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	76	ARG	NE-CZ-NH2	-5.51	117.55	120.30
2	H	488	ARG	NE-CZ-NH1	-5.46	117.57	120.30
2	G	357	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	S	75	ARG	NE-CZ-NH1	5.45	123.03	120.30
2	Z	319	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	D	208	LEU	CA-CB-CG	5.37	127.66	115.30
2	P	338	ASP	CB-CG-OD1	5.37	123.13	118.30
2	J	338	ASP	CB-CG-OD1	5.35	123.12	118.30
1	I	76	ARG	NE-CZ-NH2	-5.35	117.62	120.30
2	G	521	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	G	338	ASP	CB-CG-OD1	5.30	123.07	118.30
1	U	21	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	122	LEU	CA-CB-CG	5.25	127.37	115.30
2	Z	498	ASP	CB-CG-OD1	5.21	122.99	118.30
2	X	314	MET	CG-SD-CE	-5.18	91.91	100.20
1	Y	213	LEU	N-CA-C	-5.15	97.09	111.00
2	N	338	ASP	CB-CG-OD1	5.14	122.92	118.30
1	Q	213	LEU	N-CA-C	-5.12	97.17	111.00
1	F	213	LEU	N-CA-C	-5.09	97.25	111.00
1	K	213	LEU	N-CA-C	-5.09	97.25	111.00
2	2	357	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	O	122	LEU	CA-CB-CG	5.09	127.00	115.30
1	I	213	LEU	N-CA-C	-5.07	97.32	111.00
2	T	488	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	Y	76	ARG	NE-CZ-NH2	-5.05	117.77	120.30
2	C	338	ASP	CB-CG-OD1	5.04	122.84	118.30
1	Q	33	LEU	CA-CB-CG	5.04	126.90	115.30
1	U	21	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1656	0	1658	32	0
1	A	1662	0	1662	29	0
1	B	1650	0	1648	32	0
1	D	1644	0	1644	33	0
1	F	1669	0	1669	38	0
1	I	1656	0	1658	24	0
1	K	1670	0	1673	51	0
1	M	1662	0	1662	16	0
1	O	1654	0	1651	44	0
1	Q	1677	0	1680	38	0
1	S	1654	0	1651	20	0
1	U	1654	0	1651	37	0
1	W	1670	0	1673	27	0
1	Y	1644	0	1644	48	0
2	2	1593	0	1577	19	0
2	C	1593	0	1577	32	0
2	E	1601	0	1588	19	0
2	G	1601	0	1588	23	0
2	H	1583	0	1567	17	0
2	J	1601	0	1588	24	0
2	L	1601	0	1588	31	0
2	N	1580	0	1561	19	0
2	P	1601	0	1587	24	0
2	R	1646	0	1624	23	0
2	T	1601	0	1588	25	0
2	V	1632	0	1608	15	0
2	X	1601	0	1588	17	0
2	Z	1593	0	1577	17	0
3	1	15	0	21	3	0
3	2	15	0	21	1	0
3	A	10	0	14	2	0
3	B	15	0	21	2	0
3	C	40	0	56	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	20	0	28	2	0
3	E	30	0	42	5	0
3	F	10	0	14	1	0
3	G	20	0	28	8	0
3	H	35	0	49	8	0
3	I	10	0	14	0	0
3	J	15	0	21	5	0
3	K	10	0	14	2	0
3	L	15	0	21	5	0
3	M	10	0	14	1	0
3	N	35	0	49	7	0
3	O	10	0	14	6	0
3	P	25	0	35	2	0
3	Q	10	0	14	0	0
3	R	20	0	28	2	0
3	S	15	0	21	1	0
3	T	25	0	35	9	0
3	U	20	0	28	4	0
3	V	20	0	28	1	0
3	W	10	0	14	1	0
3	X	15	0	21	1	0
3	Y	5	0	7	0	0
3	Z	30	0	42	10	0
4	1	42	0	0	9	0
4	2	133	0	0	13	0
4	A	43	0	0	5	0
4	B	45	0	0	13	0
4	C	142	0	0	12	0
4	D	43	0	0	15	0
4	E	124	0	0	8	0
4	F	34	0	0	6	0
4	G	136	0	0	18	0
4	H	122	0	0	13	0
4	I	37	0	0	9	0
4	J	128	0	0	16	0
4	K	45	0	0	17	0
4	L	138	0	0	7	0
4	M	52	0	0	6	0
4	N	118	0	0	10	0
4	O	51	0	0	17	0
4	P	111	0	0	10	0
4	Q	41	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	141	0	0	14	0
4	S	31	0	0	5	0
4	T	112	0	0	9	0
4	U	43	0	0	13	0
4	V	154	0	0	8	0
4	W	31	0	0	5	0
4	X	130	0	0	5	0
4	Y	41	0	0	21	0
4	Z	113	0	0	17	0
All	All	48540	0	46144	775	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (775) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:400:ALA:HA	4:V:2033:HOH:O	1.27	1.32
2:C:430:ASN:HB2	4:C:2190:HOH:O	1.33	1.26
2:C:447:LYS:CD	3:C:5:DMF:H12	1.66	1.26
2:V:332:ARG:HB3	4:V:2317:HOH:O	1.32	1.25
1:U:160:THR:HG22	4:U:2365:HOH:O	1.34	1.24
2:C:447:LYS:HD2	3:C:5:DMF:C1	1.64	1.24
1:S:121:GLU:HG3	4:S:2023:HOH:O	1.34	1.23
1:A:162:PRO:HB2	4:A:2159:HOH:O	1.36	1.21
1:Y:18:GLU:OE1	1:Y:22:LYS:HE3	1.43	1.19
2:G:402:PRO:HD3	4:G:2237:HOH:O	1.41	1.18
2:X:332:ARG:HD2	4:X:2151:HOH:O	1.44	1.16
2:C:447:LYS:CD	3:C:5:DMF:C1	2.22	1.15
1:1:11:GLN:HA	1:1:14:ARG:HG2	1.21	1.12
1:W:134:LYS:HE2	4:W:2357:HOH:O	1.49	1.11
2:C:447:LYS:HD3	3:C:5:DMF:H12	1.13	1.10
1:S:76:ARG:HD3	4:S:2370:HOH:O	1.52	1.09
2:C:447:LYS:HD2	3:C:5:DMF:H11	1.29	1.08
1:1:11:GLN:HG3	1:1:14:ARG:NE	1.68	1.08
1:O:229:ALA:O	1:O:233:LEU:HD23	1.55	1.06
2:H:332:ARG:HD2	4:H:2352:HOH:O	1.55	1.06
1:1:11:GLN:HG3	1:1:14:ARG:HE	0.93	1.06
2:L:306:LEU:CD1	2:L:313:VAL:CG1	2.33	1.05
2:R:357:ARG:HD2	4:Z:2095:HOH:O	1.56	1.05
2:E:428:GLY:HA2	4:E:2161:HOH:O	1.57	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:388:ARG:HG2	4:T:2215:HOH:O	1.57	1.04
1:D:104:ALA:HB2	4:D:2360:HOH:O	1.58	1.04
2:L:306:LEU:HD12	2:L:313:VAL:CG1	1.89	1.03
1:B:52:LYS:HD3	4:B:2129:HOH:O	1.58	1.01
1:U:51:GLN:HB2	4:U:2105:HOH:O	1.59	1.01
2:G:351:VAL:HG13	4:G:2353:HOH:O	1.59	1.01
1:M:231:GLN:HG3	4:M:2387:HOH:O	1.58	1.01
1:Q:14:ARG:HH11	1:Q:14:ARG:HB3	1.24	1.00
2:L:306:LEU:HD12	2:L:313:VAL:HG13	1.40	1.00
2:2:465:ARG:HD3	4:2:2340:HOH:O	1.61	1.00
2:L:306:LEU:CD1	2:L:313:VAL:HG13	1.91	1.00
3:Z:91:DMF:HC	4:Z:1148:HOH:O	1.59	1.00
2:X:432:GLU:HB3	4:X:2235:HOH:O	1.62	1.00
3:U:252:DMF:H13	4:2:2315:HOH:O	1.62	0.99
1:F:28:LYS:HE2	4:F:2298:HOH:O	1.60	0.99
1:U:9:PRO:HD2	1:1:15:GLU:OE1	1.63	0.99
2:C:496:ILE:HD13	3:C:64:DMF:HC	1.43	0.99
1:O:76:ARG:HD3	4:O:2287:HOH:O	1.61	0.98
2:E:386:MET:SD	4:E:2398:HOH:O	2.21	0.97
1:D:54:SER:HB3	4:D:2426:HOH:O	1.63	0.97
3:E:55:DMF:HC	4:K:2288:HOH:O	1.65	0.96
1:Q:14:ARG:HB3	1:Q:14:ARG:NH1	1.81	0.95
2:J:388:ARG:HG2	4:J:2405:HOH:O	1.67	0.94
2:G:509:ARG:HG3	4:G:2167:HOH:O	1.69	0.92
2:P:433:GLU:HG3	4:P:2308:HOH:O	1.67	0.92
1:Q:97:ARG:HD2	1:Y:49:SER:OG	1.66	0.92
1:O:21:ARG:HD3	4:O:2361:HOH:O	1.69	0.92
1:Y:18:GLU:CD	1:Y:21:ARG:HH21	1.73	0.91
2:X:428:GLY:HA2	4:X:2092:HOH:O	1.71	0.91
2:T:399:LEU:HA	4:T:2342:HOH:O	1.71	0.90
3:L:60:DMF:H12	4:N:2035:HOH:O	1.71	0.90
1:D:147:ILE:HB	4:D:2360:HOH:O	1.70	0.90
1:D:11:GLN:HG2	1:D:14:ARG:NH2	1.87	0.89
2:J:509:ARG:HG2	4:J:2068:HOH:O	1.71	0.89
1:I:92:ARG:HB2	4:I:2214:HOH:O	1.73	0.88
1:A:76:ARG:HD3	4:A:2166:HOH:O	1.72	0.88
1:1:11:GLN:HA	1:1:14:ARG:CG	2.04	0.88
2:R:428:GLY:HA2	4:R:2208:HOH:O	1.72	0.88
2:Z:493:THR:HB	4:Z:2402:HOH:O	1.72	0.88
1:1:11:GLN:CA	1:1:14:ARG:HG2	2.03	0.88
2:R:447:LYS:HD3	4:R:2181:HOH:O	1.72	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:217:ARG:HD3	4:K:2228:HOH:O	1.73	0.87
2:X:433:GLU:HG3	4:Z:2252:HOH:O	1.73	0.87
2:C:444:LEU:HB2	3:C:73:DMF:H22	1.56	0.87
3:T:94:DMF:H23	4:T:2165:HOH:O	1.75	0.85
2:J:444:LEU:HD13	4:J:2376:HOH:O	1.77	0.85
2:2:465:ARG:CD	4:2:2340:HOH:O	2.21	0.85
3:G:20:DMF:H11	4:G:2328:HOH:O	1.77	0.85
3:N:2:DMF:HC	4:N:134:HOH:O	1.77	0.84
2:R:348:THR:HG23	4:R:2216:HOH:O	1.77	0.84
2:H:431:ILE:H	3:H:53:DMF:HC	1.43	0.84
2:H:430:ASN:HB2	4:H:2304:HOH:O	1.76	0.84
2:J:430:ASN:HB2	4:J:2411:HOH:O	1.77	0.84
1:F:76:ARG:HD3	4:F:2225:HOH:O	1.78	0.83
3:G:20:DMF:C1	4:G:2328:HOH:O	2.25	0.83
1:1:11:GLN:CG	1:1:14:ARG:HE	1.87	0.83
2:G:509:ARG:CG	4:G:2167:HOH:O	2.23	0.83
3:J:82:DMF:H12	4:J:2332:HOH:O	1.78	0.82
2:R:362:GLU:HB2	4:R:2079:HOH:O	1.78	0.82
1:1:11:GLN:O	1:1:14:ARG:HG3	1.79	0.82
2:C:428:GLY:HA2	4:C:2031:HOH:O	1.79	0.82
1:O:97:ARG:HD3	4:O:2218:HOH:O	1.78	0.82
2:L:306:LEU:HD11	2:L:313:VAL:CG1	2.09	0.81
1:1:12:ALA:O	1:1:16:ARG:HG3	1.80	0.81
1:D:217:ARG:NH2	1:D:223:ARG:HG3	1.95	0.81
1:Y:21:ARG:CG	4:Y:2251:HOH:O	2.29	0.81
3:V:16:DMF:H13	4:2:2372:HOH:O	1.81	0.81
1:K:217:ARG:CD	4:K:2228:HOH:O	2.30	0.80
1:O:97:ARG:CD	4:O:2218:HOH:O	2.28	0.80
2:P:334:VAL:HB	4:P:2373:HOH:O	1.81	0.80
1:U:155:VAL:HG12	4:U:2365:HOH:O	1.82	0.80
2:J:431:ILE:HD13	4:J:2185:HOH:O	1.82	0.80
1:S:60:VAL:HG11	1:S:99:LEU:HD12	1.64	0.80
1:A:19:LEU:C	1:A:19:LEU:HD23	2.02	0.80
1:Y:18:GLU:OE1	1:Y:22:LYS:CE	2.29	0.80
1:K:101:ASN:HB2	4:K:1174:HOH:O	1.80	0.79
1:Y:183:ILE:HD13	4:Y:2086:HOH:O	1.81	0.79
2:P:433:GLU:CG	4:P:2308:HOH:O	2.23	0.79
1:K:15:GLU:HG2	1:M:10:GLU:HG2	1.62	0.79
2:2:410:HIS:HE1	4:2:2267:HOH:O	1.65	0.79
2:L:308:TYR:CZ	2:L:311:GLY:HA3	2.18	0.79
1:U:168:LYS:CD	4:U:2067:HOH:O	2.31	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:428:GLY:HA2	4:T:2055:HOH:O	1.83	0.78
2:Z:430:ASN:HB2	4:Z:2171:HOH:O	1.82	0.78
2:2:301:OZT:H27	2:2:333:LYS:HE2	1.65	0.78
2:V:301:OZT:H27	2:V:333:LYS:HE2	1.66	0.78
1:K:12:ALA:O	1:K:16:ARG:HG3	1.83	0.78
2:T:373:PRO:HG2	3:T:35:DMF:HC	1.66	0.78
1:O:168:LYS:CD	4:O:2321:HOH:O	2.31	0.77
2:L:410:HIS:CE1	4:L:2102:HOH:O	2.37	0.77
2:P:301:OZT:C7	2:P:333:LYS:HE2	2.14	0.77
1:Y:183:ILE:CD1	4:Y:2086:HOH:O	2.31	0.77
2:G:401:LEU:HA	4:G:2237:HOH:O	1.83	0.77
2:R:332:ARG:HG3	4:R:2085:HOH:O	1.83	0.77
1:O:163:ILE:HG12	1:O:191:GLY:HA3	1.67	0.76
1:B:30:VAL:HG22	4:B:2129:HOH:O	1.86	0.76
2:2:428:GLY:HA2	4:2:2057:HOH:O	1.85	0.75
1:K:228:SER:HA	4:K:2191:HOH:O	1.87	0.75
2:T:373:PRO:HG2	3:T:35:DMF:C	2.17	0.75
1:Y:10:GLU:HA	1:Y:10:GLU:OE2	1.86	0.75
3:Z:69:DMF:C1	4:Z:2391:HOH:O	2.34	0.74
3:U:251:DMF:C1	4:V:2355:HOH:O	2.35	0.74
2:T:332:ARG:HH11	3:T:94:DMF:H22	1.51	0.74
1:O:168:LYS:HD2	4:O:2321:HOH:O	1.87	0.74
1:Q:19:LEU:O	1:Q:19:LEU:HD23	1.87	0.74
2:G:432:GLU:HG2	4:G:2096:HOH:O	1.86	0.74
1:Q:7:ILE:HD12	1:Q:11:GLN:HB3	1.70	0.74
1:Q:19:LEU:HD23	1:Q:19:LEU:C	2.06	0.74
1:1:11:GLN:HB3	4:1:2326:HOH:O	1.88	0.74
2:R:447:LYS:CD	4:R:2181:HOH:O	2.32	0.74
1:Y:12:ALA:O	1:Y:15:GLU:HB2	1.87	0.74
1:Y:21:ARG:HG2	4:Y:2251:HOH:O	1.86	0.73
3:G:96:DMF:HC	4:G:2327:HOH:O	1.88	0.73
2:H:401:LEU:HB3	4:H:2201:HOH:O	1.87	0.73
3:U:251:DMF:H13	4:V:2355:HOH:O	1.89	0.73
1:K:129:HIS:HE1	4:K:2227:HOH:O	1.72	0.73
1:S:205:VAL:HG21	1:S:231:GLN:HG2	1.71	0.73
1:K:15:GLU:HB3	1:M:9:PRO:HG2	1.70	0.72
1:U:152:HIS:NE2	1:U:173:GLU:OE2	2.22	0.72
1:D:104:ALA:CB	4:D:2360:HOH:O	2.27	0.72
3:H:31:DMF:H23	4:L:2384:HOH:O	1.89	0.71
1:U:105:GLN:NE2	4:U:925:HOH:O	2.23	0.71
2:E:355:PHE:CE2	4:E:2398:HOH:O	2.44	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:140:ARG:NH1	1:F:142:THR:HG22	2.05	0.71
1:Q:230:LEU:O	1:Q:234:LEU:HD12	1.91	0.71
1:S:44:GLU:HG3	1:S:188:LEU:HD12	1.72	0.71
1:I:97:ARG:HG2	4:I:2313:HOH:O	1.90	0.71
1:O:181:LEU:O	1:O:185:VAL:HG23	1.90	0.71
2:G:432:GLU:CG	4:G:2096:HOH:O	2.38	0.71
1:M:121:GLU:HG3	4:M:2114:HOH:O	1.91	0.70
3:G:96:DMF:C	4:G:2327:HOH:O	2.40	0.70
1:D:9:PRO:HD2	4:D:2330:HOH:O	1.92	0.70
1:K:15:GLU:HG2	1:M:10:GLU:CG	2.21	0.70
1:F:140:ARG:HH12	1:F:142:THR:HG22	1.57	0.70
2:J:321:THR:O	3:J:6:DMF:H21	1.91	0.70
1:D:11:GLN:HG2	1:D:14:ARG:CZ	2.21	0.70
2:E:376:PHE:CE2	2:E:380:ILE:HD11	2.26	0.70
1:I:11:GLN:O	1:I:15:GLU:HG3	1.92	0.70
2:G:444:LEU:HD13	4:G:2406:HOH:O	1.93	0.69
1:I:92:ARG:CG	4:I:2214:HOH:O	2.41	0.69
1:Y:172:ALA:CB	4:Y:2086:HOH:O	2.41	0.69
2:N:388:ARG:NH1	4:N:2048:HOH:O	2.24	0.69
1:K:217:ARG:HH21	1:K:223:ARG:HG3	1.58	0.69
2:C:357:ARG:HD2	4:C:2061:HOH:O	1.92	0.69
2:C:496:ILE:HD13	3:C:64:DMF:C	2.20	0.69
1:O:21:ARG:CD	4:O:2361:HOH:O	2.32	0.69
4:A:2243:HOH:O	1:B:112:THR:HG21	1.92	0.68
1:D:187:ALA:HB2	4:D:2331:HOH:O	1.93	0.68
2:J:321:THR:H	3:J:6:DMF:H22	1.56	0.68
1:U:168:LYS:HD2	4:U:2067:HOH:O	1.93	0.68
1:D:10:GLU:HA	1:D:10:GLU:OE1	1.94	0.68
1:Q:219:ARG:NH2	3:R:89:DMF:H22	2.08	0.68
1:Y:92:ARG:HG3	4:Y:2307:HOH:O	1.94	0.68
1:Y:172:ALA:HB3	4:Y:2086:HOH:O	1.94	0.67
1:I:73:ASN:CB	4:I:2207:HOH:O	2.41	0.67
2:N:444:LEU:H	3:N:97:DMF:H12	1.59	0.67
1:F:182:ARG:NH2	4:F:2248:HOH:O	2.26	0.67
1:W:60:VAL:HG11	1:W:99:LEU:HD12	1.77	0.67
3:H:19:DMF:H22	4:L:1904:HOH:O	1.94	0.67
3:Z:69:DMF:H13	4:Z:2391:HOH:O	1.94	0.67
1:B:19:LEU:C	1:B:19:LEU:HD23	2.15	0.67
2:J:357:ARG:HD3	4:J:2224:HOH:O	1.95	0.67
3:A:250:DMF:C1	4:H:2272:HOH:O	2.42	0.66
2:E:355:PHE:CZ	4:E:2398:HOH:O	2.47	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:308:TYR:CZ	2:N:311:GLY:HA3	2.30	0.66
1:A:111:PHE:HE1	1:A:143:TYR:CD2	2.14	0.66
3:Z:69:DMF:H12	4:Z:2391:HOH:O	1.96	0.66
2:C:498:ASP:OD2	3:C:64:DMF:C1	2.43	0.66
1:K:182:ARG:HG3	4:K:2028:HOH:O	1.96	0.66
1:F:140:ARG:NH1	1:F:142:THR:CG2	2.59	0.66
1:B:97:ARG:NH2	4:B:2348:HOH:O	2.28	0.65
1:U:168:LYS:HD3	4:U:2067:HOH:O	1.94	0.65
1:A:16:ARG:NH2	1:A:114:GLN:O	2.30	0.65
1:O:163:ILE:CG1	1:O:191:GLY:HA3	2.25	0.65
2:C:301:OZT:H27	2:C:333:LYS:HE2	1.78	0.65
2:P:301:OZT:H27	2:P:333:LYS:HE2	1.78	0.65
2:T:430:ASN:HB2	4:T:1606:HOH:O	1.97	0.65
1:Y:18:GLU:OE2	1:Y:21:ARG:NH2	2.30	0.65
1:A:18:GLU:OE1	1:A:21:ARG:NH2	2.29	0.65
1:D:147:ILE:CB	4:D:2360:HOH:O	2.37	0.65
2:C:444:LEU:HD22	3:C:73:DMF:H13	1.79	0.65
1:B:19:LEU:HD23	1:B:19:LEU:O	1.97	0.65
1:O:205:VAL:HG21	1:O:231:GLN:HG2	1.79	0.65
1:B:43:ALA:HB1	4:B:2129:HOH:O	1.97	0.64
1:A:113:GLU:N	1:A:113:GLU:OE1	2.30	0.64
3:H:19:DMF:H23	4:H:2377:HOH:O	1.95	0.64
1:Q:137:GLU:C	1:Q:138:LEU:HD12	2.17	0.64
1:U:31:VAL:HB	1:U:188:LEU:HD11	1.79	0.64
2:R:432:GLU:OE2	2:R:434:GLU:HB2	1.96	0.64
1:Y:19:LEU:C	1:Y:19:LEU:HD23	2.18	0.64
3:S:250:DMF:HC	2:T:360:ALA:HB1	1.78	0.64
1:B:114:GLN:NE2	4:B:2199:HOH:O	2.30	0.64
2:L:314:MET:HE3	2:L:334:VAL:HG13	1.80	0.64
1:D:18:GLU:OE1	1:D:21:ARG:NH2	2.30	0.64
2:G:452:LYS:HB3	3:G:39:DMF:H13	1.79	0.64
1:Y:18:GLU:OE2	1:Y:21:ARG:NE	2.30	0.64
1:Q:14:ARG:NH1	1:Q:14:ARG:CB	2.58	0.64
1:K:191:GLY:C	4:K:2150:HOH:O	2.35	0.63
2:2:332:ARG:NH2	4:2:1264:HOH:O	2.30	0.63
2:C:433:GLU:HG3	4:C:2311:HOH:O	1.98	0.63
2:G:388:ARG:NH1	4:G:2024:HOH:O	2.31	0.63
2:G:444:LEU:HB3	4:G:1218:HOH:O	1.98	0.63
1:Q:13:MET:HE2	1:Q:13:MET:HA	1.80	0.63
2:2:357:ARG:NE	4:2:2213:HOH:O	2.31	0.63
1:K:11:GLN:HE21	1:K:14:ARG:NH1	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:128:ALA:HB2	1:Q:134:LYS:HB3	1.81	0.63
1:U:92:ARG:HD2	2:2:375:THR:HG21	1.80	0.63
2:V:401:LEU:HB2	4:V:2153:HOH:O	1.99	0.63
2:N:332:ARG:NH2	4:N:2264:HOH:O	2.28	0.63
1:Y:147:ILE:HD13	4:Y:2303:HOH:O	1.98	0.63
1:K:163:ILE:HG23	1:K:187:ALA:O	1.98	0.63
1:B:162:PRO:HB2	1:B:190:ALA:HB1	1.81	0.63
1:A:111:PHE:HE1	1:A:143:TYR:HD2	1.46	0.62
1:D:204:GLY:N	4:D:2400:HOH:O	2.32	0.62
2:N:357:ARG:HD3	4:N:2035:HOH:O	1.97	0.62
1:A:15:GLU:HB3	1:B:9:PRO:HG2	1.81	0.62
3:H:19:DMF:C2	4:H:2377:HOH:O	2.47	0.62
1:K:228:SER:HB3	4:K:2191:HOH:O	1.99	0.62
2:Z:428:GLY:HA2	4:Z:2109:HOH:O	1.99	0.62
2:G:401:LEU:HB2	4:G:2255:HOH:O	1.99	0.62
2:L:306:LEU:HD12	2:L:313:VAL:HG12	1.77	0.62
1:M:102:VAL:HG12	3:M:249:DMF:H22	1.81	0.62
2:H:301:OZT:H27	2:H:333:LYS:HE2	1.80	0.62
1:Y:19:LEU:HD23	1:Y:19:LEU:O	2.00	0.62
1:Y:204:GLY:N	4:Y:1615:HOH:O	2.33	0.62
2:X:515:ARG:HD2	4:X:2081:HOH:O	2.00	0.62
1:F:8:SER:N	4:F:2029:HOH:O	2.33	0.62
1:F:140:ARG:HH12	1:F:142:THR:CG2	2.13	0.62
1:K:169:GLU:OE1	1:K:169:GLU:C	2.38	0.62
1:O:76:ARG:O	1:O:80:GLN:HG3	1.99	0.62
2:C:515:ARG:HD2	4:C:2187:HOH:O	2.00	0.62
1:D:219:ARG:NH2	3:D:252:DMF:HC	2.15	0.62
2:H:308:TYR:CZ	2:H:311:GLY:HA3	2.35	0.62
1:1:11:GLN:O	1:1:14:ARG:CG	2.47	0.62
2:N:444:LEU:HB2	3:N:97:DMF:H12	1.82	0.61
2:V:428:GLY:HA2	4:V:2197:HOH:O	1.99	0.61
1:W:76:ARG:NH2	3:W:249:DMF:H22	2.15	0.61
2:2:301:OZT:C7	2:2:333:LYS:HE2	2.29	0.61
1:Y:18:GLU:OE1	1:Y:21:ARG:NH2	2.30	0.61
1:A:112:THR:CG2	1:O:115:ALA:HB3	2.30	0.61
1:F:13:MET:HE2	1:F:16:ARG:HD3	1.82	0.61
1:D:210:VAL:N	4:D:2263:HOH:O	2.22	0.61
1:W:97:ARG:NH1	4:W:2056:HOH:O	2.30	0.61
1:Y:21:ARG:HG3	4:Y:2251:HOH:O	1.96	0.61
1:F:136:PRO:HG3	4:F:2210:HOH:O	1.99	0.61
2:V:325:MET:SD	2:2:444:LEU:HD21	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:163:ILE:HG23	1:K:187:ALA:C	2.21	0.61
1:I:92:ARG:CB	4:I:2214:HOH:O	2.36	0.61
1:U:179:ASP:O	1:U:183:ILE:HG13	2.01	0.61
2:Z:483:GLY:HA3	3:Z:27:DMF:O	2.01	0.61
1:B:134:LYS:NZ	4:B:2220:HOH:O	2.33	0.60
2:G:444:LEU:CD1	4:G:2406:HOH:O	2.48	0.60
1:M:209:GLU:HA	4:M:2429:HOH:O	2.00	0.60
2:G:428:GLY:HA2	4:G:2024:HOH:O	2.02	0.60
1:I:27:ALA:HB1	4:I:2062:HOH:O	2.00	0.60
1:W:166:ALA:O	1:W:169:GLU:HG3	2.01	0.60
2:J:509:ARG:CG	4:J:2068:HOH:O	2.41	0.60
1:I:16:ARG:NH2	1:I:114:GLN:O	2.30	0.60
1:K:182:ARG:CG	4:K:2028:HOH:O	2.49	0.60
2:Z:429:TRP:HZ3	2:Z:431:ILE:HG13	1.66	0.60
1:A:191:GLY:N	4:A:2159:HOH:O	2.35	0.60
1:F:141:ILE:HD12	1:F:141:ILE:N	2.17	0.60
1:O:233:LEU:N	1:O:233:LEU:HD22	2.16	0.60
1:D:147:ILE:CG2	4:D:2360:HOH:O	2.50	0.59
1:F:30:VAL:HG22	1:F:52:LYS:HZ3	1.67	0.59
2:L:331:VAL:HG13	2:L:349:ALA:HB2	1.84	0.59
1:B:52:LYS:CD	4:B:2129:HOH:O	2.32	0.59
1:A:111:PHE:CE1	1:A:143:TYR:HD2	2.20	0.59
3:A:250:DMF:H11	4:H:2272:HOH:O	2.02	0.59
2:C:444:LEU:H	3:C:73:DMF:H22	1.67	0.59
1:D:77:GLY:HA3	3:D:251:DMF:H13	1.83	0.59
1:O:121:GLU:HG3	4:O:2044:HOH:O	2.03	0.59
1:D:30:VAL:HG13	1:D:43:ALA:HB2	1.85	0.59
2:X:515:ARG:NH2	4:X:2341:HOH:O	2.28	0.59
2:H:428:GLY:HA2	4:H:2132:HOH:O	2.02	0.59
1:I:92:ARG:HG3	4:I:2214:HOH:O	2.01	0.59
2:Z:388:ARG:NH1	4:Z:2109:HOH:O	2.35	0.59
1:I:19:LEU:C	1:I:19:LEU:HD23	2.23	0.59
2:G:357:ARG:HA	3:G:1:DMF:HC	1.85	0.59
1:U:31:VAL:CG2	1:U:188:LEU:HD11	2.33	0.59
1:Y:147:ILE:CD1	4:Y:2303:HOH:O	2.49	0.59
1:D:11:GLN:HG2	1:D:14:ARG:HH22	1.68	0.58
2:H:332:ARG:HB2	4:H:2352:HOH:O	2.02	0.58
1:Y:129:HIS:HE1	4:Y:2152:HOH:O	1.86	0.58
2:J:321:THR:N	3:J:6:DMF:H22	2.18	0.58
2:N:332:ARG:HG3	4:N:2380:HOH:O	2.02	0.58
2:G:476:ASP:OD1	3:G:20:DMF:H12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:250:DMF:HC	3:L:4:DMF:H21	1.85	0.58
2:L:332:ARG:HB2	4:L:2140:HOH:O	2.02	0.58
1:Q:105:GLN:NE2	4:Q:2244:HOH:O	2.36	0.58
1:S:97:ARG:HG2	1:S:98:GLN:N	2.19	0.58
2:C:465:ARG:HD3	4:C:1567:HOH:O	2.03	0.58
1:Y:92:ARG:HG2	4:Y:2152:HOH:O	2.02	0.58
2:2:357:ARG:HD3	4:2:2213:HOH:O	2.03	0.58
2:C:409:ILE:HG22	4:C:2174:HOH:O	2.02	0.58
1:O:91:ARG:HH12	3:O:250:DMF:H13	1.69	0.58
4:A:2428:HOH:O	3:H:41:DMF:C2	2.52	0.58
1:K:189:ARG:HD3	1:K:203:LEU:HD12	1.85	0.58
2:L:306:LEU:HD11	2:L:313:VAL:HG13	1.72	0.58
2:H:401:LEU:N	4:H:1585:HOH:O	2.37	0.58
2:L:306:LEU:HD11	2:L:313:VAL:HG11	1.86	0.58
1:K:129:HIS:CE1	4:K:2227:HOH:O	2.52	0.58
1:O:76:ARG:O	1:O:80:GLN:CG	2.52	0.58
1:S:56:LEU:HD13	1:S:99:LEU:HD13	1.86	0.58
1:W:169:GLU:HG3	1:W:170:SER:H	1.69	0.58
2:T:332:ARG:NH1	3:T:94:DMF:H22	2.18	0.57
2:2:410:HIS:CE1	4:2:2267:HOH:O	2.45	0.57
1:O:77:GLY:HA3	3:O:249:DMF:C	2.34	0.57
2:2:357:ARG:CD	4:2:2213:HOH:O	2.52	0.57
1:Q:76:ARG:HD3	4:Q:527:HOH:O	2.04	0.57
2:V:464:LEU:O	2:V:468:VAL:HG23	2.03	0.57
1:F:31:VAL:HG22	1:F:155:VAL:HG22	1.86	0.57
1:B:217:ARG:NH1	4:B:2322:HOH:O	2.37	0.57
1:K:167:LEU:O	1:K:171:TYR:N	2.37	0.57
2:L:307:LYS:HE3	2:L:418:GLY:O	2.04	0.57
1:Y:129:HIS:CE1	4:Y:2152:HOH:O	2.56	0.57
2:J:412:SER:O	2:J:414:PRO:HD3	2.05	0.57
1:1:73:ASN:CG	4:1:2207:HOH:O	2.42	0.57
1:I:30:VAL:HG13	1:I:43:ALA:HB2	1.86	0.57
1:Q:230:LEU:HG	1:Q:234:LEU:HD11	1.85	0.57
2:R:465:ARG:HD3	4:R:1483:HOH:O	2.05	0.57
1:U:184:ALA:O	1:U:188:LEU:HD13	2.05	0.57
1:O:229:ALA:O	1:O:233:LEU:CD2	2.44	0.56
1:O:233:LEU:N	1:O:233:LEU:CD2	2.68	0.56
1:Q:67:LYS:HE3	4:Q:389:HOH:O	2.04	0.56
1:Q:69:ASN:HD22	1:Q:69:ASN:H	1.52	0.56
2:P:428:GLY:HA2	4:P:1465:HOH:O	2.05	0.56
1:B:18:GLU:OE1	1:B:21:ARG:NE	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:97:ARG:NH1	4:M:2407:HOH:O	2.38	0.56
2:T:451:LYS:HE2	2:X:473:ASP:OD1	2.05	0.56
1:K:228:SER:CB	4:K:2191:HOH:O	2.53	0.56
2:R:357:ARG:CD	4:Z:2095:HOH:O	2.30	0.56
2:C:465:ARG:HG3	2:C:513:LEU:HD22	1.87	0.56
2:J:321:THR:H	3:J:6:DMF:C2	2.18	0.56
1:F:30:VAL:CG2	1:F:52:LYS:NZ	2.69	0.56
1:M:110:ILE:HG22	4:M:2182:HOH:O	2.05	0.56
1:W:60:VAL:HG11	1:W:99:LEU:CD1	2.35	0.55
1:B:52:LYS:NZ	4:B:2129:HOH:O	2.35	0.55
1:I:12:ALA:N	4:I:2326:HOH:O	2.38	0.55
2:P:461:ASP:OD1	2:P:509:ARG:NH2	2.39	0.55
1:U:31:VAL:CB	1:U:188:LEU:HD11	2.36	0.55
3:C:17:DMF:H22	4:C:1355:HOH:O	2.06	0.55
1:A:19:LEU:C	1:A:19:LEU:CD2	2.73	0.55
1:O:97:ARG:HD2	4:O:2218:HOH:O	1.99	0.55
1:A:112:THR:HG22	1:O:115:ALA:HB3	1.87	0.55
1:Q:8:SER:HB2	1:Q:9:PRO:CD	2.37	0.55
1:F:69:ASN:H	1:F:69:ASN:HD22	1.55	0.55
1:K:16:ARG:NH2	1:K:114:GLN:O	2.40	0.55
1:B:91:ARG:HD2	4:B:2302:HOH:O	2.07	0.55
1:K:228:SER:CA	4:K:2191:HOH:O	2.50	0.55
1:Q:18:GLU:OE1	1:Q:21:ARG:NH2	2.30	0.55
2:T:432:GLU:HG3	2:T:437:GLN:HB2	1.89	0.55
3:1:251:DMF:HC	3:2:78:DMF:O	2.06	0.55
1:A:19:LEU:HD23	1:A:19:LEU:O	2.07	0.54
1:D:98:GLN:O	1:D:102:VAL:HG23	2.07	0.54
1:U:181:LEU:HD12	1:U:181:LEU:O	2.08	0.54
2:H:401:LEU:CB	4:H:2201:HOH:O	2.52	0.54
1:Y:92:ARG:CG	4:Y:2152:HOH:O	2.56	0.54
1:Y:92:ARG:CG	4:Y:2307:HOH:O	2.52	0.54
1:I:73:ASN:HB2	4:I:2207:HOH:O	2.04	0.54
1:F:46:PRO:HG3	4:F:2298:HOH:O	2.07	0.54
2:L:357:ARG:NH1	4:L:2273:HOH:O	2.30	0.54
2:E:416:SER:HA	4:E:2094:HOH:O	2.06	0.54
1:F:52:LYS:HE2	1:F:64:ALA:O	2.08	0.54
1:U:114:GLN:NE2	4:U:2039:HOH:O	2.41	0.54
2:E:429:TRP:CE2	3:E:70:DMF:H12	2.43	0.54
2:V:388:ARG:NH1	4:V:2197:HOH:O	2.41	0.54
1:I:219:ARG:CZ	3:I:251:DMF:H23	2.38	0.54
2:C:444:LEU:N	3:C:73:DMF:H22	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:320:SER:HB3	2:E:331:VAL:HG21	1.90	0.53
1:Q:181:LEU:HD23	1:Q:233:LEU:HB3	1.90	0.53
2:C:444:LEU:HB2	3:C:73:DMF:C2	2.33	0.53
2:C:498:ASP:OD2	3:C:64:DMF:H12	2.08	0.53
2:V:301:OZT:C7	2:V:333:LYS:HE2	2.36	0.53
1:Y:92:ARG:HB2	4:Y:2307:HOH:O	2.08	0.53
1:F:16:ARG:NH2	1:F:114:GLN:O	2.32	0.53
1:O:91:ARG:NH1	3:O:250:DMF:H13	2.23	0.53
1:1:30:VAL:HG13	1:1:43:ALA:HB2	1.90	0.53
2:L:314:MET:CE	2:L:334:VAL:HG13	2.38	0.53
2:R:332:ARG:NH2	4:R:1931:HOH:O	2.42	0.53
2:C:444:LEU:CB	3:C:73:DMF:H22	2.33	0.53
1:O:21:ARG:NE	4:O:2361:HOH:O	2.39	0.53
1:S:30:VAL:HG13	1:S:43:ALA:HB2	1.90	0.53
2:X:320:SER:HB3	2:X:331:VAL:HG21	1.91	0.53
1:Q:19:LEU:C	1:Q:19:LEU:CD2	2.77	0.52
1:M:162:PRO:HB2	1:M:190:ALA:O	2.10	0.52
1:Y:234:LEU:HA	4:Y:2005:HOH:O	2.08	0.52
2:Z:493:THR:CB	4:Z:2402:HOH:O	2.42	0.52
1:D:9:PRO:CD	4:D:2330:HOH:O	2.52	0.52
2:T:338:ASP:OD1	2:T:341:THR:OG1	2.21	0.52
1:U:97:ARG:NH2	2:2:370:GLU:O	2.43	0.52
1:I:69:ASN:H	1:I:69:ASN:HD22	1.58	0.52
1:O:136:PRO:HG3	4:O:2149:HOH:O	2.09	0.52
2:X:496:ILE:HD13	3:X:67:DMF:H13	1.92	0.52
2:J:357:ARG:CD	4:J:2224:HOH:O	2.56	0.52
1:S:163:ILE:HD11	1:S:191:GLY:HA3	1.92	0.52
1:U:178:THR:HG22	1:U:182:ARG:CZ	2.39	0.52
1:A:16:ARG:HB3	1:A:117:PRO:HG3	1.92	0.52
1:Y:69:ASN:HD22	1:Y:69:ASN:H	1.58	0.52
1:F:15:GLU:HB2	1:W:9:PRO:HG2	1.92	0.52
1:Q:52:LYS:NZ	4:Q:2084:HOH:O	2.27	0.52
1:B:67:LYS:HG2	1:B:69:ASN:HD21	1.76	0.51
2:L:357:ARG:HD3	4:L:2131:HOH:O	2.09	0.51
1:F:205:VAL:HG22	1:F:230:LEU:HD23	1.91	0.51
1:I:11:GLN:N	4:I:2112:HOH:O	2.43	0.51
1:Q:231:GLN:OE1	1:Q:231:GLN:HA	2.09	0.51
1:F:50:LEU:HD12	1:W:149:ASP:HB2	1.92	0.51
2:E:355:PHE:CD2	4:E:2398:HOH:O	2.60	0.51
1:K:190:ALA:CB	4:K:2004:HOH:O	2.58	0.51
1:Q:231:GLN:OE1	1:Q:231:GLN:CA	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:30:VAL:HG13	1:Y:43:ALA:HB2	1.92	0.51
1:B:21:ARG:NH2	1:B:22:LYS:CG	2.74	0.51
1:Q:8:SER:HB2	1:Q:9:PRO:HD2	1.91	0.51
3:O:250:DMF:H12	2:P:361:VAL:HA	1.92	0.51
1:S:177:LEU:HG	1:S:233:LEU:HD11	1.93	0.51
1:W:31:VAL:HG22	1:W:155:VAL:HG22	1.93	0.51
1:Y:31:VAL:HG22	1:Y:155:VAL:HG22	1.92	0.51
3:C:43:DMF:HC	1:I:88:ALA:HA	1.92	0.51
1:O:217:ARG:NH2	1:O:223:ARG:HG3	2.26	0.51
2:Z:308:TYR:CZ	2:Z:311:GLY:HA3	2.46	0.51
1:B:21:ARG:NH2	1:B:22:LYS:HG2	2.26	0.51
1:K:69:ASN:H	1:K:69:ASN:HD22	1.58	0.51
2:J:431:ILE:CD1	4:J:2185:HOH:O	2.50	0.50
4:U:2295:HOH:O	1:I:48:ARG:NH2	2.44	0.50
2:L:355:PHE:HE1	2:L:383:LEU:HD11	1.76	0.50
1:U:75:ARG:HD3	4:U:2058:HOH:O	2.09	0.50
1:Y:76:ARG:HD3	4:Y:1321:HOH:O	2.10	0.50
3:Z:91:DMF:C	4:Z:1148:HOH:O	2.37	0.50
1:K:169:GLU:OE1	1:K:169:GLU:O	2.30	0.50
1:K:170:SER:O	1:K:183:ILE:HD13	2.11	0.50
1:K:217:ARG:NH2	1:K:223:ARG:HG3	2.24	0.50
1:W:185:VAL:HG21	1:W:234:LEU:HD11	1.93	0.50
1:A:69:ASN:H	1:A:69:ASN:HD22	1.60	0.50
3:C:64:DMF:C	4:C:2195:HOH:O	2.60	0.50
2:P:355:PHE:HE2	4:P:2412:HOH:O	1.95	0.50
2:C:496:ILE:CD1	3:C:64:DMF:HC	2.28	0.50
1:F:13:MET:HE2	1:F:13:MET:HA	1.94	0.50
2:H:362:GLU:HG3	4:H:1702:HOH:O	2.12	0.50
2:R:376:PHE:CE2	2:R:380:ILE:HD11	2.46	0.50
1:S:69:ASN:HD22	1:S:69:ASN:H	1.59	0.50
1:S:163:ILE:CG1	1:S:191:GLY:HA3	2.42	0.50
1:Y:10:GLU:O	1:Y:13:MET:HB3	2.11	0.50
2:C:410:HIS:CE1	4:C:2344:HOH:O	2.64	0.50
1:A:111:PHE:CE1	1:A:143:TYR:CD2	2.96	0.50
1:B:115:ALA:HB3	1:I:112:THR:HG23	1.93	0.50
2:L:472:TYR:CE1	3:L:9:DMF:C1	2.95	0.50
1:Q:31:VAL:HG22	1:Q:155:VAL:HG22	1.94	0.50
1:U:101:ASN:HB3	3:U:250:DMF:HC	1.94	0.50
1:K:97:ARG:NH1	1:K:97:ARG:HG2	2.27	0.50
2:R:301:OZT:H27	2:R:333:LYS:HE2	1.94	0.49
1:B:22:LYS:NZ	1:I:10:GLU:OE2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:476:ASP:O	2:V:329:ARG:NH2	2.44	0.49
2:R:432:GLU:HB2	4:R:2012:HOH:O	2.12	0.49
2:T:373:PRO:HG2	3:T:35:DMF:C1	2.42	0.49
2:L:472:TYR:CE1	3:L:9:DMF:H13	2.48	0.49
2:N:301:OZT:H17	2:N:333:LYS:NZ	2.27	0.49
2:P:329:ARG:HD2	2:V:434:GLU:OE2	2.12	0.49
1:A:30:VAL:HG13	1:A:43:ALA:HB2	1.95	0.49
1:B:102:VAL:HG12	3:B:249:DMF:H12	1.93	0.49
2:J:368:LYS:NZ	4:J:2318:HOH:O	2.39	0.49
2:J:432:GLU:HG2	2:J:437:GLN:HB2	1.95	0.49
2:Z:332:ARG:NH2	4:Z:2163:HOH:O	2.45	0.49
1:D:56:LEU:HG	1:D:62:PHE:HB2	1.94	0.49
1:Y:173:GLU:O	1:Y:174:ASN:HB2	2.13	0.49
1:K:8:SER:OG	1:K:11:GLN:HB2	2.12	0.49
1:S:142:THR:HA	4:S:2023:HOH:O	2.12	0.49
2:2:320:SER:HB3	2:2:331:VAL:HG21	1.94	0.49
1:A:97:ARG:HD3	1:O:49:SER:HB2	1.95	0.49
2:H:320:SER:HB3	2:H:331:VAL:HG21	1.94	0.49
1:O:76:ARG:NH1	4:O:2287:HOH:O	2.30	0.49
2:P:376:PHE:CE2	2:P:380:ILE:HD11	2.48	0.49
1:Y:204:GLY:O	1:Y:208:LEU:HG	2.12	0.49
1:F:11:GLN:O	1:F:15:GLU:HG3	2.13	0.49
2:N:472:TYR:CZ	3:N:36:DMF:H22	2.48	0.48
4:O:2280:HOH:O	2:P:357:ARG:NH1	2.34	0.48
2:R:301:OZT:H17	2:R:333:LYS:NZ	2.28	0.48
2:T:430:ASN:HA	3:T:92:DMF:HC	1.94	0.48
1:I:176:SER:OG	1:I:179:ASP:HB2	2.13	0.48
2:R:388:ARG:NH1	4:R:2208:HOH:O	2.47	0.48
1:U:136:PRO:HG3	4:U:2145:HOH:O	2.13	0.48
1:U:51:GLN:CB	4:U:2105:HOH:O	2.38	0.48
1:Y:92:ARG:CB	4:Y:2307:HOH:O	2.61	0.48
2:Z:429:TRP:CZ3	2:Z:431:ILE:HG13	2.48	0.48
1:F:30:VAL:HG22	1:F:52:LYS:NZ	2.28	0.48
1:S:163:ILE:CG1	1:S:191:GLY:CA	2.92	0.48
2:L:376:PHE:CE2	2:L:380:ILE:HD11	2.48	0.48
1:I:205:VAL:HG21	1:I:231:GLN:HG2	1.95	0.48
1:D:10:GLU:HG2	1:Q:15:GLU:HG3	1.95	0.48
1:I:152:HIS:HB3	1:I:171:TYR:CZ	2.49	0.48
2:G:376:PHE:CE2	2:G:380:ILE:HD11	2.49	0.47
1:F:52:LYS:HE2	1:F:52:LYS:HB3	1.56	0.47
2:P:388:ARG:NH1	4:P:1465:HOH:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:456:GLN:OE1	2:P:465:ARG:NH1	2.46	0.47
1:A:15:GLU:HB3	1:B:9:PRO:CG	2.45	0.47
1:B:56:LEU:HG	1:B:62:PHE:HB2	1.97	0.47
2:L:308:TYR:CE1	2:L:311:GLY:HA3	2.48	0.47
2:H:301:OZT:H17	2:H:333:LYS:NZ	2.30	0.47
2:T:320:SER:HB3	2:T:331:VAL:HG21	1.96	0.47
1:W:76:ARG:HD2	4:W:2090:HOH:O	2.14	0.47
2:2:355:PHE:HE1	2:2:383:LEU:HD11	1.79	0.47
1:I:152:HIS:CD2	1:I:171:TYR:HE2	2.32	0.47
2:L:306:LEU:CD1	2:L:313:VAL:HG12	2.34	0.47
1:U:9:PRO:CD	1:I:15:GLU:OE1	2.48	0.47
2:Z:429:TRP:CE2	3:Z:71:DMF:H22	2.50	0.47
3:1:250:DMF:HC	4:1:1918:HOH:O	2.14	0.47
2:C:444:LEU:HD22	3:C:73:DMF:C1	2.45	0.47
1:K:190:ALA:HB3	4:K:2004:HOH:O	2.14	0.47
2:Z:301:OZT:H27	2:Z:333:LYS:HE2	1.96	0.47
4:B:2199:HOH:O	1:I:112:THR:HG21	2.14	0.47
1:K:97:ARG:HG2	1:K:97:ARG:HH11	1.80	0.47
2:N:301:OZT:H27	2:N:333:LYS:HE2	1.97	0.47
1:O:168:LYS:HD3	4:O:2321:HOH:O	2.08	0.47
2:R:332:ARG:CG	4:R:2085:HOH:O	2.51	0.47
1:W:30:VAL:HG13	1:W:43:ALA:HB2	1.97	0.47
1:I:105:GLN:NE2	4:I:2193:HOH:O	2.47	0.46
1:K:170:SER:OG	1:K:183:ILE:HG23	2.15	0.46
1:O:135:ARG:HD3	4:O:1427:HOH:O	2.15	0.46
2:T:451:LYS:NZ	2:X:476:ASP:OD2	2.42	0.46
1:B:69:ASN:HD22	1:B:69:ASN:H	1.64	0.46
1:Y:19:LEU:C	1:Y:19:LEU:CD2	2.82	0.46
2:2:477:ASP:OD2	4:2:1889:HOH:O	2.21	0.46
1:F:67:LYS:HG2	1:F:69:ASN:HD21	1.80	0.46
1:Y:219:ARG:NH2	3:Z:91:DMF:H22	2.30	0.46
3:N:2:DMF:H23	4:P:2424:HOH:O	2.14	0.46
2:E:430:ASN:HA	3:E:95:DMF:HC	1.96	0.46
1:F:30:VAL:CG2	1:F:52:LYS:HZ1	2.28	0.46
2:P:320:SER:CB	4:P:2168:HOH:O	2.63	0.46
2:E:483:GLY:HA3	3:E:32:DMF:H23	1.97	0.46
2:J:465:ARG:NH2	4:J:2247:HOH:O	2.41	0.46
1:K:19:LEU:HD23	1:K:19:LEU:C	2.36	0.46
2:L:355:PHE:CE1	2:L:383:LEU:HD11	2.51	0.46
1:W:98:GLN:O	1:W:102:VAL:HG23	2.16	0.46
1:Y:18:GLU:OE2	1:Y:21:ARG:CZ	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:31:VAL:HG22	1:M:155:VAL:HG22	1.98	0.46
2:E:429:TRP:CZ2	3:E:70:DMF:H12	2.50	0.46
1:F:138:LEU:HD23	1:F:154:VAL:HG23	1.98	0.46
3:H:19:DMF:H12	2:L:521:ARG:HB3	1.98	0.46
1:K:217:ARG:HD2	4:K:2228:HOH:O	2.05	0.46
1:1:52:LYS:NZ	4:1:2239:HOH:O	2.49	0.46
1:O:31:VAL:HG22	1:O:155:VAL:HG22	1.96	0.46
1:D:69:ASN:H	1:D:69:ASN:HD22	1.64	0.45
2:H:432:GLU:HB2	4:H:2119:HOH:O	2.15	0.45
1:M:30:VAL:HG13	1:M:43:ALA:HB2	1.98	0.45
2:P:301:OZT:H27	2:P:333:LYS:CE	2.47	0.45
1:S:56:LEU:HG	1:S:62:PHE:HB2	1.97	0.45
1:Y:163:ILE:HG23	1:Y:187:ALA:O	2.17	0.45
1:K:19:LEU:HD22	1:K:117:PRO:HG2	1.98	0.45
1:U:69:ASN:H	1:U:69:ASN:HD22	1.65	0.45
1:U:205:VAL:HG13	1:U:230:LEU:HD23	1.98	0.45
2:H:355:PHE:HE1	2:H:383:LEU:HD11	1.82	0.45
1:I:152:HIS:CD2	1:I:171:TYR:CE2	3.05	0.45
1:O:67:LYS:HG2	1:O:69:ASN:HD21	1.82	0.45
1:O:69:ASN:HD22	1:O:69:ASN:H	1.63	0.45
1:Q:12:ALA:O	1:Q:16:ARG:HG3	2.16	0.45
1:W:169:GLU:HG3	1:W:170:SER:N	2.31	0.45
1:1:108:GLY:O	1:1:112:THR:HG23	2.16	0.45
1:F:56:LEU:HG	1:F:62:PHE:HB2	1.99	0.45
2:N:428:GLY:HA2	4:N:2048:HOH:O	2.16	0.45
1:W:10:GLU:OE1	1:W:10:GLU:HA	2.16	0.45
1:W:74:LEU:HD13	1:W:122:LEU:HD21	1.99	0.45
3:Z:27:DMF:C2	4:Z:2076:HOH:O	2.64	0.45
2:H:431:ILE:H	3:H:53:DMF:C	2.22	0.45
1:Y:9:PRO:HD2	1:Y:11:GLN:HB3	1.99	0.45
1:D:9:PRO:N	4:D:2330:HOH:O	2.49	0.45
1:F:11:GLN:O	1:F:15:GLU:CG	2.64	0.45
1:I:31:VAL:HG22	1:I:155:VAL:HG22	1.98	0.45
2:J:444:LEU:CD1	4:J:2376:HOH:O	2.49	0.45
2:X:355:PHE:HE1	2:X:383:LEU:HD11	1.82	0.45
2:L:412:SER:O	2:L:414:PRO:HD3	2.17	0.45
1:I:67:LYS:HG2	1:I:69:ASN:HD21	1.81	0.45
1:O:30:VAL:HG13	1:O:43:ALA:HB2	1.97	0.45
2:P:390:ASN:CG	4:P:2412:HOH:O	2.55	0.45
2:T:368:LYS:NZ	4:T:2375:HOH:O	2.49	0.45
2:V:355:PHE:HE1	2:V:383:LEU:HD11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:52:LYS:NZ	4:W:2259:HOH:O	2.33	0.45
2:J:320:SER:HB3	2:J:331:VAL:HG21	1.99	0.44
2:J:427:GLY:HA3	4:J:2405:HOH:O	2.16	0.44
2:N:434:GLU:HB2	4:N:2211:HOH:O	2.17	0.44
1:Q:13:MET:HE2	1:Q:13:MET:CA	2.47	0.44
1:U:178:THR:CG2	1:U:182:ARG:CZ	2.95	0.44
1:W:56:LEU:HG	1:W:62:PHE:HB2	1.99	0.44
1:A:112:THR:HB	1:A:113:GLU:OE1	2.17	0.44
2:J:376:PHE:CE2	2:J:380:ILE:HD11	2.52	0.44
2:Z:307:LYS:HE2	2:Z:307:LYS:HB3	1.76	0.44
1:A:56:LEU:HG	1:A:62:PHE:HB2	2.00	0.44
1:D:147:ILE:HG21	4:D:2360:HOH:O	2.15	0.44
1:M:65:ALA:HB1	4:M:2177:HOH:O	2.17	0.44
2:P:472:TYR:CE1	3:P:23:DMF:H22	2.53	0.44
2:R:301:OZT:O6	4:R:2282:HOH:O	2.21	0.44
2:V:376:PHE:CE2	2:V:380:ILE:HD11	2.53	0.44
1:F:51:GLN:HB2	3:F:250:DMF:H21	1.98	0.44
2:J:488:ARG:NH2	2:R:476:ASP:OD1	2.49	0.44
2:P:308:TYR:CZ	2:P:311:GLY:HA3	2.53	0.44
2:X:376:PHE:CE2	2:X:380:ILE:HD11	2.52	0.44
1:A:112:THR:HG23	1:O:115:ALA:HB3	1.99	0.44
1:U:173:GLU:C	1:U:174:ASN:OD1	2.56	0.44
1:W:69:ASN:H	1:W:69:ASN:HD22	1.63	0.44
1:I:11:GLN:HG3	1:I:14:ARG:CD	2.46	0.44
2:C:444:LEU:HB3	4:C:281:HOH:O	2.16	0.44
1:F:45:ASN:HA	1:F:46:PRO:HD2	1.85	0.44
1:B:19:LEU:C	1:B:19:LEU:CD2	2.83	0.44
1:B:31:VAL:HG22	1:B:155:VAL:HG22	1.99	0.44
1:D:105:GLN:NE2	4:D:1127:HOH:O	2.50	0.44
2:G:320:SER:HB3	2:G:331:VAL:HG21	1.98	0.44
1:M:56:LEU:HG	1:M:62:PHE:HB2	2.00	0.44
1:I:56:LEU:HG	1:I:62:PHE:HB2	2.00	0.44
2:J:465:ARG:NE	4:J:2247:HOH:O	2.33	0.44
1:O:8:SER:N	4:O:1604:HOH:O	2.50	0.44
3:O:250:DMF:H23	2:P:360:ALA:HB3	2.00	0.44
1:Q:152:HIS:NE2	1:Q:173:GLU:OE1	2.51	0.44
2:L:472:TYR:CZ	3:L:9:DMF:H11	2.53	0.43
1:Q:13:MET:HE3	1:Q:13:MET:HB2	1.74	0.43
1:B:30:VAL:HG13	1:B:43:ALA:HB2	2.00	0.43
1:K:30:VAL:HG13	1:K:43:ALA:HB2	2.00	0.43
2:N:382:ARG:NH2	2:N:385:ILE:HD13	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:476:ASP:O	2:E:329:ARG:NH2	2.50	0.43
2:E:355:PHE:CE1	4:E:2398:HOH:O	2.70	0.43
2:E:355:PHE:HE1	2:E:383:LEU:HD11	1.83	0.43
2:E:374:LEU:HD21	1:K:89:TYR:HD1	1.83	0.43
1:M:163:ILE:HG23	1:M:187:ALA:O	2.18	0.43
1:S:90:ASP:HB2	4:S:901:HOH:O	2.17	0.43
2:T:355:PHE:HE1	2:T:383:LEU:HD11	1.82	0.43
2:T:373:PRO:HG2	3:T:35:DMF:N	2.33	0.43
1:B:52:LYS:CE	4:B:2129:HOH:O	2.62	0.43
1:F:72:ASP:O	1:F:76:ARG:HG3	2.19	0.43
1:Q:8:SER:O	1:Q:11:GLN:HB2	2.18	0.43
4:D:725:HOH:O	1:K:112:THR:HG21	2.19	0.43
2:P:301:OZT:H17	2:P:333:LYS:HE2	1.99	0.43
1:1:11:GLN:CB	4:1:2326:HOH:O	2.58	0.43
2:J:357:ARG:NE	4:J:2224:HOH:O	2.51	0.43
2:L:422:SER:OG	2:L:432:GLU:OE2	2.30	0.43
2:N:441:SER:O	3:N:97:DMF:H13	2.19	0.43
1:U:30:VAL:HG13	1:U:43:ALA:HB2	2.00	0.43
3:B:250:DMF:H13	4:C:1685:HOH:O	2.19	0.43
2:P:496:ILE:HD13	3:P:61:DMF:H13	2.01	0.43
2:X:432:GLU:HG3	2:X:437:GLN:HB2	2.00	0.43
1:A:31:VAL:HG22	1:A:155:VAL:HG22	2.01	0.43
2:C:401:LEU:HA	2:C:402:PRO:HD3	1.89	0.43
1:F:30:VAL:HG13	1:F:43:ALA:HB2	1.99	0.43
1:I:56:LEU:HG	1:I:62:PHE:HB2	2.01	0.43
1:O:56:LEU:HG	1:O:62:PHE:HB2	2.01	0.43
1:Q:30:VAL:HG13	1:Q:43:ALA:HB2	2.00	0.43
2:X:301:OZT:H27	2:X:333:LYS:HE2	2.01	0.43
1:D:51:GLN:HG2	1:D:209:GLU:OE2	2.18	0.43
1:I:16:ARG:NH2	1:I:114:GLN:O	2.42	0.43
2:C:376:PHE:CE2	2:C:380:ILE:HD11	2.54	0.43
1:O:72:ASP:O	1:O:76:ARG:HG3	2.19	0.43
2:T:399:LEU:CA	4:T:2342:HOH:O	2.47	0.43
1:Y:45:ASN:HA	1:Y:46:PRO:HD2	1.79	0.43
1:Y:134:LYS:N	4:Y:2396:HOH:O	2.47	0.43
1:D:98:GLN:HE21	1:D:98:GLN:HB3	1.69	0.42
1:W:97:ARG:O	1:W:101:ASN:HB2	2.19	0.42
2:G:401:LEU:HA	2:G:402:PRO:HD3	1.88	0.42
1:W:27:ALA:HB1	4:W:2259:HOH:O	2.18	0.42
1:D:15:GLU:HG2	1:K:9:PRO:HD2	2.01	0.42
1:K:97:ARG:HH11	1:K:97:ARG:CG	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:301:OZT:H27	2:T:333:LYS:HE2	2.01	0.42
1:D:54:SER:OG	1:D:75:ARG:HD2	2.20	0.42
1:K:11:GLN:O	1:K:12:ALA:C	2.56	0.42
1:K:219:ARG:NH2	3:K:250:DMF:H23	2.35	0.42
1:O:77:GLY:HA3	3:O:249:DMF:HC	2.02	0.42
2:R:325:MET:SD	2:Z:444:LEU:HD21	2.59	0.42
2:X:331:VAL:HG13	2:X:349:ALA:HB2	2.02	0.42
1:K:163:ILE:HD13	1:K:188:LEU:HA	2.02	0.42
1:U:31:VAL:HG21	1:U:188:LEU:HD11	2.01	0.42
2:Z:355:PHE:HE1	2:Z:383:LEU:HD11	1.85	0.42
2:P:433:GLU:HG2	4:P:2308:HOH:O	2.05	0.42
1:Q:56:LEU:HG	1:Q:62:PHE:HB2	2.02	0.42
2:Z:386:MET:CE	4:Z:2339:HOH:O	2.68	0.42
2:2:435:GLY:N	4:2:2018:HOH:O	2.32	0.42
1:A:17:SER:O	1:A:21:ARG:HB2	2.20	0.42
1:F:69:ASN:HB3	1:W:104:ALA:HB1	2.02	0.42
2:H:376:PHE:CE2	2:H:380:ILE:HD11	2.54	0.42
1:1:31:VAL:HG22	1:1:155:VAL:HG22	2.02	0.42
1:K:31:VAL:HG22	1:K:155:VAL:HG22	2.01	0.42
2:R:432:GLU:OE2	2:R:434:GLU:N	2.49	0.42
2:R:477:ASP:OD2	4:R:1890:HOH:O	2.21	0.42
1:U:67:LYS:HG2	1:U:69:ASN:HD21	1.85	0.42
2:Z:338:ASP:OD1	2:Z:338:ASP:C	2.58	0.42
1:A:15:GLU:HA	1:A:15:GLU:OE1	2.20	0.41
2:L:482:GLY:HA3	4:L:2221:HOH:O	2.20	0.41
2:N:498:ASP:HB2	4:N:543:HOH:O	2.19	0.41
2:V:354:GLU:OE1	4:V:2432:HOH:O	2.22	0.41
1:A:67:LYS:HG2	1:A:69:ASN:HD21	1.86	0.41
1:Q:138:LEU:HD12	1:Q:138:LEU:N	2.35	0.41
1:U:90:ASP:OD1	1:U:93:ASP:N	2.53	0.41
1:U:135:ARG:HD3	4:U:1432:HOH:O	2.20	0.41
1:B:21:ARG:NH2	1:B:22:LYS:HG3	2.35	0.41
1:D:31:VAL:HG22	1:D:155:VAL:HG22	2.01	0.41
1:I:45:ASN:HA	1:I:46:PRO:HD2	1.99	0.41
4:R:1034:HOH:O	3:Z:79:DMF:H22	2.19	0.41
1:F:122:LEU:O	1:F:140:ARG:HA	2.20	0.41
2:G:447:LYS:NZ	3:G:96:DMF:H23	2.35	0.41
2:N:376:PHE:CE2	2:N:380:ILE:HD11	2.55	0.41
2:P:355:PHE:HE1	2:P:383:LEU:HD11	1.84	0.41
2:T:339:ASP:HB2	3:T:35:DMF:H22	2.03	0.41
1:U:31:VAL:HG22	1:U:155:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:301:OZT:O	2:C:440:GLY:HA3	2.21	0.41
1:I:136:PRO:HG3	4:I:2245:HOH:O	2.21	0.41
1:K:11:GLN:O	1:K:14:ARG:N	2.49	0.41
1:K:115:ALA:HB3	1:M:112:THR:HG23	2.02	0.41
2:T:391:LEU:HB3	4:T:1428:HOH:O	2.20	0.41
2:T:507:GLU:HG3	4:T:1165:HOH:O	2.20	0.41
1:B:67:LYS:HG2	1:B:69:ASN:ND2	2.35	0.41
1:K:56:LEU:HG	1:K:62:PHE:HB2	2.03	0.41
2:N:357:ARG:CD	4:N:2035:HOH:O	2.63	0.41
1:U:56:LEU:HG	1:U:62:PHE:HB2	2.03	0.41
2:X:433:GLU:CG	4:Z:2252:HOH:O	2.47	0.41
1:Y:11:GLN:O	1:Y:14:ARG:HB3	2.20	0.41
1:B:76:ARG:HD3	4:B:2144:HOH:O	2.19	0.41
1:F:142:THR:OG1	1:F:146:SER:HB2	2.21	0.41
2:G:515:ARG:NE	4:G:2281:HOH:O	2.52	0.41
2:X:509:ARG:HA	2:X:509:ARG:HD2	1.91	0.41
1:Y:67:LYS:HG2	1:Y:69:ASN:HD21	1.85	0.41
2:N:301:OZT:O	2:N:440:GLY:HA3	2.21	0.41
2:N:472:TYR:CE1	3:N:36:DMF:H22	2.55	0.41
1:O:76:ARG:O	1:O:80:GLN:HG2	2.21	0.41
1:O:230:LEU:HD12	1:O:230:LEU:HA	1.81	0.41
1:Q:231:GLN:OE1	1:Q:231:GLN:O	2.38	0.41
1:S:181:LEU:O	1:S:185:VAL:HG23	2.20	0.41
1:Y:162:PRO:HB2	1:Y:190:ALA:O	2.21	0.41
1:1:142:THR:HA	4:1:2089:HOH:O	2.20	0.41
2:2:301:OZT:O	2:2:440:GLY:HA3	2.21	0.41
1:D:45:ASN:HA	1:D:46:PRO:HD2	1.99	0.41
2:E:493:THR:CB	4:E:2369:HOH:O	2.69	0.41
1:S:80:GLN:HB2	4:S:2270:HOH:O	2.21	0.41
2:V:331:VAL:HG13	2:V:349:ALA:HB2	2.02	0.41
1:A:213:LEU:HD23	1:A:213:LEU:HA	1.99	0.40
1:O:86:GLY:O	4:O:2280:HOH:O	2.22	0.40
1:Q:56:LEU:HD23	1:Q:56:LEU:HA	1.95	0.40
1:S:44:GLU:HG3	1:S:188:LEU:CD1	2.45	0.40
2:T:314:MET:HE3	2:T:334:VAL:HG13	2.02	0.40
2:E:412:SER:O	2:E:414:PRO:HD3	2.21	0.40
1:K:67:LYS:HG2	1:K:69:ASN:HD21	1.86	0.40
2:L:301:OZT:C7	2:L:333:LYS:NZ	2.84	0.40
1:W:217:ARG:NH2	1:W:223:ARG:HG3	2.36	0.40
2:E:432:GLU:HG3	2:E:437:GLN:HB2	2.04	0.40
1:K:90:ASP:HB2	4:K:750:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:17:SER:OG	1:Q:143:TYR:OH	2.31	0.40
1:S:116:LYS:HD2	1:1:13:MET:SD	2.60	0.40
1:U:45:ASN:HA	1:U:46:PRO:HD2	2.00	0.40
1:Y:48:ARG:H	1:Y:48:ARG:HG2	1.62	0.40
2:G:329:ARG:O	2:G:490:ILE:HG21	2.21	0.40
1:O:189:ARG:HH22	1:O:204:GLY:N	2.18	0.40
1:F:15:GLU:OE2	1:W:8:SER:OG	2.30	0.40
2:L:421:VAL:HG22	2:L:431:ILE:HG12	2.03	0.40
2:R:472:TYR:CE1	3:R:68:DMF:H12	2.56	0.40
1:U:187:ALA:O	1:U:190:ALA:HB3	2.21	0.40
1:W:45:ASN:HA	1:W:46:PRO:HD2	2.00	0.40
1:W:59:ARG:HA	1:W:59:ARG:HD2	1.98	0.40
1:1:11:GLN:HA	1:1:14:ARG:NE	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	211/248 (85%)	206 (98%)	5 (2%)	0	100	100
1	A	212/248 (86%)	207 (98%)	5 (2%)	0	100	100
1	B	210/248 (85%)	206 (98%)	4 (2%)	0	100	100
1	D	209/248 (84%)	205 (98%)	4 (2%)	0	100	100
1	F	213/248 (86%)	209 (98%)	4 (2%)	0	100	100
1	I	211/248 (85%)	207 (98%)	4 (2%)	0	100	100
1	K	213/248 (86%)	208 (98%)	5 (2%)	0	100	100
1	M	212/248 (86%)	206 (97%)	6 (3%)	0	100	100
1	O	211/248 (85%)	208 (99%)	3 (1%)	0	100	100
1	Q	214/248 (86%)	207 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	211/248 (85%)	208 (99%)	3 (1%)	0	100	100
1	U	211/248 (85%)	208 (99%)	3 (1%)	0	100	100
1	W	213/248 (86%)	209 (98%)	4 (2%)	0	100	100
1	Y	209/248 (84%)	205 (98%)	4 (2%)	0	100	100
2	2	211/240 (88%)	210 (100%)	1 (0%)	0	100	100
2	C	211/240 (88%)	210 (100%)	1 (0%)	0	100	100
2	E	212/240 (88%)	211 (100%)	1 (0%)	0	100	100
2	G	212/240 (88%)	211 (100%)	1 (0%)	0	100	100
2	H	209/240 (87%)	208 (100%)	1 (0%)	0	100	100
2	J	212/240 (88%)	211 (100%)	1 (0%)	0	100	100
2	L	212/240 (88%)	211 (100%)	1 (0%)	0	100	100
2	N	209/240 (87%)	209 (100%)	0	0	100	100
2	P	212/240 (88%)	211 (100%)	1 (0%)	0	100	100
2	R	219/240 (91%)	217 (99%)	2 (1%)	0	100	100
2	T	212/240 (88%)	211 (100%)	1 (0%)	0	100	100
2	V	217/240 (90%)	214 (99%)	3 (1%)	0	100	100
2	X	212/240 (88%)	210 (99%)	2 (1%)	0	100	100
2	Z	211/240 (88%)	210 (100%)	1 (0%)	0	100	100
All	All	5931/6832 (87%)	5853 (99%)	78 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	1	164/192 (85%)	156 (95%)	8 (5%)	25	33
1	A	165/192 (86%)	161 (98%)	4 (2%)	49	61
1	B	164/192 (85%)	158 (96%)	6 (4%)	34	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	163/192 (85%)	154 (94%)	9 (6%)	21	28
1	F	166/192 (86%)	162 (98%)	4 (2%)	49	61
1	I	164/192 (85%)	160 (98%)	4 (2%)	49	61
1	K	166/192 (86%)	155 (93%)	11 (7%)	16	20
1	M	165/192 (86%)	160 (97%)	5 (3%)	41	53
1	O	164/192 (85%)	160 (98%)	4 (2%)	49	61
1	Q	167/192 (87%)	161 (96%)	6 (4%)	35	46
1	S	164/192 (85%)	158 (96%)	6 (4%)	34	45
1	U	164/192 (85%)	159 (97%)	5 (3%)	41	53
1	W	166/192 (86%)	163 (98%)	3 (2%)	59	71
1	Y	163/192 (85%)	159 (98%)	4 (2%)	47	60
2	2	160/177 (90%)	159 (99%)	1 (1%)	86	91
2	C	160/177 (90%)	157 (98%)	3 (2%)	57	69
2	E	161/177 (91%)	155 (96%)	6 (4%)	34	45
2	G	161/177 (91%)	158 (98%)	3 (2%)	57	69
2	H	160/177 (90%)	156 (98%)	4 (2%)	47	60
2	J	161/177 (91%)	158 (98%)	3 (2%)	57	69
2	L	161/177 (91%)	154 (96%)	7 (4%)	29	38
2	N	159/177 (90%)	155 (98%)	4 (2%)	47	60
2	P	161/177 (91%)	158 (98%)	3 (2%)	57	69
2	R	165/177 (93%)	162 (98%)	3 (2%)	59	71
2	T	161/177 (91%)	156 (97%)	5 (3%)	40	52
2	V	163/177 (92%)	158 (97%)	5 (3%)	40	52
2	X	161/177 (91%)	157 (98%)	4 (2%)	47	60
2	Z	160/177 (90%)	157 (98%)	3 (2%)	57	69
All	All	4559/5166 (88%)	4426 (97%)	133 (3%)	42	54

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	MET
1	A	69	ASN
1	A	161	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	233	LEU
1	B	13	MET
1	B	69	ASN
1	B	113	GLU
1	B	161	GLU
1	B	231	GLN
1	B	234	LEU
2	C	444	LEU
2	C	492	PRO
2	C	520	SER
1	D	10	GLU
1	D	11	GLN
1	D	13	MET
1	D	14	ARG
1	D	15	GLU
1	D	69	ASN
1	D	98	GLN
1	D	161	GLU
1	D	174	ASN
2	E	362	GLU
2	E	399	LEU
2	E	444	LEU
2	E	464	LEU
2	E	492	PRO
2	E	520	SER
1	F	13	MET
1	F	14	ARG
1	F	69	ASN
1	F	161	GLU
2	G	362	GLU
2	G	444	LEU
2	G	492	PRO
2	H	330	ASP
2	H	338	ASP
2	H	415	GLN
2	H	520	SER
1	I	13	MET
1	I	69	ASN
1	I	113	GLU
1	I	161	GLU
2	J	399	LEU
2	J	444	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	J	509	ARG
1	K	7	ILE
1	K	11	GLN
1	K	13	MET
1	K	69	ASN
1	K	92	ARG
1	K	97	ARG
1	K	113	GLU
1	K	161	GLU
1	K	168	LYS
1	K	169	GLU
1	K	217	ARG
2	L	306	LEU
2	L	338	ASP
2	L	399	LEU
2	L	444	LEU
2	L	459	ASP
2	L	492	PRO
2	L	509	ARG
1	M	13	MET
1	M	69	ASN
1	M	113	GLU
1	M	161	GLU
1	M	231	GLN
2	N	330	ASP
2	N	412	SER
2	N	444	LEU
2	N	492	PRO
1	O	13	MET
1	O	69	ASN
1	O	161	GLU
1	O	234	LEU
2	P	399	LEU
2	P	434	GLU
2	P	492	PRO
1	Q	11	GLN
1	Q	13	MET
1	Q	14	ARG
1	Q	69	ASN
1	Q	113	GLU
1	Q	231	GLN
2	R	338	ASP

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Mol	Chain	Res	Type
2	R	444	LEU
2	R	465	ARG
1	S	13	MET
1	S	69	ASN
1	S	97	ARG
1	S	161	GLU
1	S	233	LEU
1	S	234	LEU
2	T	330	ASP
2	T	338	ASP
2	T	444	LEU
2	T	465	ARG
2	T	492	PRO
1	U	13	MET
1	U	69	ASN
1	U	113	GLU
1	U	161	GLU
1	U	174	ASN
2	V	322	GLN
2	V	330	ASP
2	V	444	LEU
2	V	492	PRO
2	V	496	ILE
1	W	13	MET
1	W	69	ASN
1	W	161	GLU
2	X	362	GLU
2	X	399	LEU
2	X	444	LEU
2	X	492	PRO
1	Y	49	SER
1	Y	69	ASN
1	Y	113	GLU
1	Y	161	GLU
2	Z	338	ASP
2	Z	430	ASN
2	Z	492	PRO
1	1	13	MET
1	1	14	ARG
1	1	17	SER
1	1	69	ASN
1	1	112	THR

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Mol	Chain	Res	Type
1	1	113	GLU
1	1	161	GLU
1	1	189	ARG
2	2	492	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	165	ASN
1	B	69	ASN
1	B	114	GLN
1	B	165	ASN
1	B	174	ASN
1	D	11	GLN
1	D	69	ASN
1	D	98	GLN
1	D	105	GLN
1	D	114	GLN
1	D	165	ASN
1	F	69	ASN
1	F	114	GLN
1	F	165	ASN
1	I	69	ASN
1	I	152	HIS
1	I	165	ASN
1	K	11	GLN
1	K	69	ASN
1	K	174	ASN
1	M	69	ASN
1	M	114	GLN
1	M	165	ASN
2	N	415	GLN
1	O	69	ASN
1	O	114	GLN
1	O	165	ASN
1	Q	69	ASN
1	Q	165	ASN
1	S	69	ASN
1	S	165	ASN
1	U	69	ASN
1	U	165	ASN

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Mol	Chain	Res	Type
1	W	69	ASN
1	W	98	GLN
1	W	114	GLN
1	W	165	ASN
2	X	415	GLN
2	X	430	ASN
1	Y	69	ASN
1	Y	98	GLN
1	Y	165	ASN
1	1	69	ASN
1	1	114	GLN
1	1	165	ASN
2	2	415	GLN
2	2	430	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](#)

14 non-standard protein/DNA/RNA residues 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	OZT	T	301	2	7,9,10	4.46	4 (57%)	9,12,14	5.55	6 (66%)
2	OZT	L	301	2	7,9,10	4.83	4 (57%)	9,12,14	5.50	6 (66%)
2	OZT	G	301	2	7,9,10	4.21	4 (57%)	9,12,14	5.37	7 (77%)
2	OZT	V	301	2	7,9,10	4.53	4 (57%)	9,12,14	5.67	7 (77%)
2	OZT	X	301	2	7,9,10	5.00	5 (71%)	9,12,14	5.40	7 (77%)
2	OZT	P	301	2	7,9,10	4.04	4 (57%)	9,12,14	5.29	6 (66%)
2	OZT	J	301	2	7,9,10	4.86	4 (57%)	9,12,14	5.42	6 (66%)
2	OZT	N	301	2	7,9,10	4.46	3 (42%)	9,12,14	5.21	6 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OZT	Z	301	2	7,9,10	4.67	4 (57%)	9,12,14	5.33	6 (66%)
2	OZT	E	301	2	7,9,10	4.36	4 (57%)	9,12,14	5.19	7 (77%)
2	OZT	C	301	2	7,9,10	4.75	4 (57%)	9,12,14	5.47	6 (66%)
2	OZT	R	301	2	7,9,10	5.08	5 (71%)	9,12,14	5.09	6 (66%)
2	OZT	2	301	2	7,9,10	4.88	6 (85%)	9,12,14	5.23	6 (66%)
2	OZT	H	301	2	7,9,10	4.60	4 (57%)	9,12,14	5.55	6 (66%)

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	OZT	T	301	2	-	1/1/14/16	0/1/1/1
2	OZT	L	301	2	-	0/1/14/16	0/1/1/1
2	OZT	G	301	2	-	1/1/14/16	0/1/1/1
2	OZT	V	301	2	-	0/1/14/16	0/1/1/1
2	OZT	X	301	2	-	0/1/14/16	0/1/1/1
2	OZT	P	301	2	-	1/1/14/16	0/1/1/1
2	OZT	J	301	2	-	1/1/14/16	0/1/1/1
2	OZT	N	301	2	-	1/1/14/16	0/1/1/1
2	OZT	Z	301	2	-	1/1/14/16	0/1/1/1
2	OZT	E	301	2	-	1/1/14/16	0/1/1/1
2	OZT	C	301	2	-	1/1/14/16	0/1/1/1
2	OZT	R	301	2	-	1/1/14/16	0/1/1/1
2	OZT	2	301	2	-	1/1/14/16	0/1/1/1
2	OZT	H	301	2	-	1/1/14/16	0/1/1/1

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	301	OZT	O1-C5	10.85	1.51	1.36
2	X	301	OZT	O1-C5	10.58	1.50	1.36
2	L	301	OZT	O1-C5	10.33	1.50	1.36
2	T	301	OZT	O1-C5	9.91	1.49	1.36
2	R	301	OZT	O1-C5	9.54	1.49	1.36
2	H	301	OZT	O1-C5	9.51	1.49	1.36
2	C	301	OZT	O1-C5	9.36	1.49	1.36
2	E	301	OZT	O1-C5	9.24	1.48	1.36
2	2	301	OZT	O1-C5	9.20	1.48	1.36
2	G	301	OZT	O1-C5	9.09	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	301	OZT	O1-C5	9.04	1.48	1.36
2	V	301	OZT	O1-C5	8.49	1.47	1.36
2	N	301	OZT	O1-C5	8.38	1.47	1.36
2	P	301	OZT	O1-C5	8.22	1.47	1.36
2	R	301	OZT	C5-N	6.87	1.43	1.33
2	C	301	OZT	C5-N	6.44	1.42	1.33
2	N	301	OZT	C5-N	6.33	1.42	1.33
2	2	301	OZT	C5-N	6.04	1.42	1.33
2	X	301	OZT	C5-N	5.63	1.41	1.33
2	H	301	OZT	C5-N	5.60	1.41	1.33
2	V	301	OZT	O1-C2	-5.24	1.38	1.46
2	Z	301	OZT	C5-N	5.17	1.40	1.33
2	L	301	OZT	C5-N	5.08	1.40	1.33
2	J	301	OZT	C5-N	4.93	1.40	1.33
2	N	301	OZT	O1-C2	-4.88	1.39	1.46
2	V	301	OZT	C5-N	4.74	1.40	1.33
2	2	301	OZT	O1-C2	-4.72	1.39	1.46
2	P	301	OZT	C5-N	4.64	1.40	1.33
2	R	301	OZT	O1-C2	-4.54	1.40	1.46
2	Z	301	OZT	O1-C2	-4.51	1.40	1.46
2	G	301	OZT	C5-N	4.46	1.39	1.33
2	L	301	OZT	O1-C2	-4.37	1.40	1.46
2	Z	301	OZT	C2-CA	-4.27	1.46	1.54
2	E	301	OZT	C5-N	4.26	1.39	1.33
2	X	301	OZT	O1-C2	-4.13	1.40	1.46
2	V	301	OZT	C2-CA	-3.96	1.46	1.54
2	T	301	OZT	C5-N	3.86	1.39	1.33
2	T	301	OZT	O1-C2	-3.86	1.41	1.46
2	P	301	OZT	O1-C2	-3.82	1.41	1.46
2	J	301	OZT	O1-C2	-3.78	1.41	1.46
2	C	301	OZT	O1-C2	-3.77	1.41	1.46
2	E	301	OZT	O1-C2	-3.71	1.41	1.46
2	H	301	OZT	O1-C2	-3.66	1.41	1.46
2	G	301	OZT	O1-C2	-3.61	1.41	1.46
2	2	301	OZT	C2-CA	-3.46	1.47	1.54
2	R	301	OZT	C2-CA	-3.40	1.48	1.54
2	E	301	OZT	C2-CA	-3.34	1.48	1.54
2	H	301	OZT	C2-CA	-2.92	1.48	1.54
2	X	301	OZT	C2-CA	-2.85	1.49	1.54
2	T	301	OZT	C2-CA	-2.74	1.49	1.54
2	C	301	OZT	C2-CA	-2.73	1.49	1.54
2	G	301	OZT	C2-CA	-2.66	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	301	OZT	C2-CA	-2.65	1.49	1.54
2	L	301	OZT	C2-CA	-2.56	1.49	1.54
2	R	301	OZT	O6-C5	2.42	1.26	1.21
2	2	301	OZT	O6-C5	2.36	1.26	1.21
2	X	301	OZT	C7-C2	-2.29	1.46	1.51
2	2	301	OZT	C7-C2	-2.25	1.46	1.51
2	J	301	OZT	C2-CA	-2.21	1.50	1.54

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	OZT	O1-C5-N	9.10	117.50	109.86
2	T	301	OZT	O1-C5-N	9.00	117.41	109.86
2	N	301	OZT	O1-C5-N	8.95	117.37	109.86
2	P	301	OZT	O1-C5-N	8.88	117.31	109.86
2	V	301	OZT	O1-C2-CA	8.78	112.05	103.58
2	H	301	OZT	O1-C5-N	8.78	117.22	109.86
2	C	301	OZT	O1-C5-N	8.72	117.17	109.86
2	X	301	OZT	O1-C5-N	8.69	117.15	109.86
2	J	301	OZT	O1-C5-N	8.69	117.15	109.86
2	Z	301	OZT	O1-C5-N	8.56	117.04	109.86
2	L	301	OZT	O1-C5-N	8.43	116.93	109.86
2	V	301	OZT	O1-C5-N	8.40	116.91	109.86
2	R	301	OZT	O1-C5-N	8.07	116.63	109.86
2	E	301	OZT	O1-C5-N	8.06	116.62	109.86
2	2	301	OZT	O1-C5-N	8.05	116.61	109.86
2	L	301	OZT	O1-C2-CA	8.03	111.33	103.58
2	H	301	OZT	O1-C2-CA	7.52	110.84	103.58
2	2	301	OZT	O1-C2-CA	7.41	110.73	103.58
2	X	301	OZT	O1-C2-CA	7.39	110.71	103.58
2	T	301	OZT	O6-C5-N	-7.32	120.67	129.22
2	P	301	OZT	O1-C2-CA	7.28	110.61	103.58
2	J	301	OZT	O6-C5-N	-7.17	120.84	129.22
2	N	301	OZT	O1-C2-CA	7.17	110.49	103.58
2	L	301	OZT	C2-O1-C5	-7.05	98.87	110.41
2	R	301	OZT	O1-C2-CA	7.04	110.37	103.58
2	C	301	OZT	O1-C2-CA	7.03	110.36	103.58
2	J	301	OZT	O1-C2-CA	7.00	110.33	103.58
2	J	301	OZT	C2-O1-C5	-6.90	99.12	110.41
2	H	301	OZT	C2-O1-C5	-6.89	99.13	110.41
2	T	301	OZT	C2-O1-C5	-6.86	99.18	110.41
2	V	301	OZT	C2-O1-C5	-6.86	99.19	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	OZT	O1-C2-CA	6.85	110.19	103.58
2	X	301	OZT	C2-O1-C5	-6.83	99.23	110.41
2	P	301	OZT	C2-O1-C5	-6.82	99.24	110.41
2	Z	301	OZT	O1-C2-CA	6.80	110.14	103.58
2	T	301	OZT	O1-C2-CA	6.78	110.12	103.58
2	G	301	OZT	O6-C5-N	-6.76	121.32	129.22
2	L	301	OZT	O6-C5-N	-6.68	121.41	129.22
2	C	301	OZT	C2-O1-C5	-6.66	99.52	110.41
2	G	301	OZT	C2-O1-C5	-6.61	99.60	110.41
2	2	301	OZT	C2-O1-C5	-6.53	99.72	110.41
2	E	301	OZT	O6-C5-N	-6.52	121.60	129.22
2	G	301	OZT	O1-C2-CA	6.49	109.84	103.58
2	Z	301	OZT	C2-O1-C5	-6.49	99.80	110.41
2	H	301	OZT	O6-C5-N	-6.41	121.73	129.22
2	P	301	OZT	O6-C5-N	-6.36	121.79	129.22
2	X	301	OZT	O6-C5-N	-6.35	121.80	129.22
2	E	301	OZT	C2-O1-C5	-6.28	100.13	110.41
2	N	301	OZT	C2-O1-C5	-6.26	100.17	110.41
2	R	301	OZT	C2-O1-C5	-6.23	100.21	110.41
2	Z	301	OZT	O6-C5-N	-6.18	122.00	129.22
2	C	301	OZT	O6-C5-N	-6.14	122.05	129.22
2	V	301	OZT	O6-C5-N	-5.93	122.30	129.22
2	C	301	OZT	C2-CA-C	-5.93	105.92	114.16
2	N	301	OZT	O6-C5-N	-5.64	122.63	129.22
2	2	301	OZT	C2-CA-C	-5.61	106.36	114.16
2	2	301	OZT	O6-C5-N	-5.57	122.72	129.22
2	H	301	OZT	C2-CA-C	-5.57	106.42	114.16
2	V	301	OZT	C2-CA-C	-5.37	106.69	114.16
2	R	301	OZT	C2-CA-C	-5.29	106.81	114.16
2	R	301	OZT	O6-C5-N	-5.20	123.14	129.22
2	Z	301	OZT	C2-CA-C	-5.19	106.94	114.16
2	T	301	OZT	C2-CA-C	-5.17	106.98	114.16
2	V	301	OZT	C7-C2-CA	-5.07	107.67	114.80
2	L	301	OZT	C7-C2-CA	-5.01	107.76	114.80
2	X	301	OZT	C7-C2-CA	-4.97	107.81	114.80
2	Z	301	OZT	C7-C2-CA	-4.96	107.82	114.80
2	N	301	OZT	C2-CA-C	-4.91	107.33	114.16
2	E	301	OZT	C7-C2-CA	-4.91	107.89	114.80
2	C	301	OZT	C7-C2-CA	-4.69	108.20	114.80
2	J	301	OZT	C7-C2-CA	-4.62	108.30	114.80
2	H	301	OZT	C7-C2-CA	-4.60	108.33	114.80
2	G	301	OZT	C7-C2-CA	-4.59	108.34	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	301	OZT	C7-C2-CA	-4.41	108.59	114.80
2	R	301	OZT	C7-C2-CA	-4.37	108.65	114.80
2	P	301	OZT	C7-C2-CA	-4.34	108.70	114.80
2	2	301	OZT	C7-C2-CA	-4.31	108.74	114.80
2	E	301	OZT	C2-CA-C	-4.27	108.22	114.16
2	G	301	OZT	C2-CA-C	-4.21	108.30	114.16
2	L	301	OZT	C2-CA-C	-3.96	108.65	114.16
2	J	301	OZT	C2-CA-C	-3.94	108.68	114.16
2	X	301	OZT	C2-CA-C	-3.85	108.80	114.16
2	N	301	OZT	C7-C2-CA	-3.54	109.82	114.80
2	P	301	OZT	C2-CA-C	-3.38	109.45	114.16
2	G	301	OZT	O-C-CA	-2.20	118.69	124.83
2	E	301	OZT	O-C-CA	-2.18	118.76	124.83
2	X	301	OZT	O-C-CA	-2.10	118.98	124.83
2	V	301	OZT	O-C-CA	-2.00	119.25	124.83

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	OZT	O-C-CA-C2
2	E	301	OZT	O-C-CA-C2
2	G	301	OZT	O-C-CA-C2
2	H	301	OZT	O-C-CA-C2
2	J	301	OZT	O-C-CA-C2
2	N	301	OZT	O-C-CA-C2
2	P	301	OZT	O-C-CA-C2
2	R	301	OZT	O-C-CA-C2
2	T	301	OZT	O-C-CA-C2
2	Z	301	OZT	O-C-CA-C2
2	2	301	OZT	O-C-CA-C2

There are no ring outliers.

11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	301	OZT	1	0
2	L	301	OZT	1	0
2	V	301	OZT	2	0
2	X	301	OZT	1	0
2	P	301	OZT	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	301	OZT	3	0
2	Z	301	OZT	1	0
2	C	301	OZT	2	0
2	R	301	OZT	3	0
2	2	301	OZT	3	0
2	H	301	OZT	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

102 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	$\# Z  > 2$
3	DMF	V	86	-	4,4,4	0.27	0	4,4,4	0.47	0
3	DMF	P	100	-	4,4,4	0.48	0	4,4,4	0.32	0
3	DMF	2	58	-	4,4,4	0.77	0	4,4,4	0.30	0
3	DMF	F	249	-	4,4,4	0.52	0	4,4,4	0.43	0
3	DMF	Z	71	-	4,4,4	0.47	0	4,4,4	0.33	0
3	DMF	T	92	-	4,4,4	0.82	0	4,4,4	0.35	0
3	DMF	2	66	-	4,4,4	0.70	0	4,4,4	0.26	0
3	DMF	E	32	-	4,4,4	0.68	0	4,4,4	0.33	0
3	DMF	C	43	-	4,4,4	0.91	0	4,4,4	0.34	0
3	DMF	R	3	-	4,4,4	0.26	0	4,4,4	0.43	0
3	DMF	1	250	-	4,4,4	0.35	0	4,4,4	0.27	0
3	DMF	U	251	-	4,4,4	0.85	0	4,4,4	0.27	0
3	DMF	N	24	-	4,4,4	0.45	0	4,4,4	0.32	0
3	DMF	C	73	-	4,4,4	0.26	0	4,4,4	0.34	0
3	DMF	E	70	-	4,4,4	0.32	0	4,4,4	0.51	0
3	DMF	O	250	-	4,4,4	0.29	0	4,4,4	0.44	0
3	DMF	X	25	-	4,4,4	0.57	0	4,4,4	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	DMF	H	102	-	4,4,4	0.46	0	4,4,4	0.38	0
3	DMF	T	35	-	4,4,4	0.33	0	4,4,4	0.37	0
3	DMF	V	16	-	4,4,4	0.35	0	4,4,4	0.55	0
3	DMF	2	78	-	4,4,4	0.20	0	4,4,4	0.39	0
3	DMF	L	9	-	4,4,4	0.20	0	4,4,4	0.44	0
3	DMF	K	249	-	4,4,4	0.70	0	4,4,4	0.27	0
3	DMF	C	15	-	4,4,4	0.38	0	4,4,4	0.41	0
3	DMF	F	250	-	4,4,4	0.33	0	4,4,4	0.39	0
3	DMF	X	88	-	4,4,4	0.46	0	4,4,4	0.45	0
3	DMF	I	249	-	4,4,4	0.72	0	4,4,4	0.37	0
3	DMF	Z	69	-	4,4,4	0.56	0	4,4,4	0.30	0
3	DMF	D	251	-	4,4,4	0.44	0	4,4,4	0.47	0
3	DMF	H	14	-	4,4,4	0.56	0	4,4,4	0.31	0
3	DMF	E	55	-	4,4,4	0.43	0	4,4,4	0.33	0
3	DMF	T	62	-	4,4,4	0.46	0	4,4,4	0.30	0
3	DMF	L	4	-	4,4,4	0.42	0	4,4,4	0.29	0
3	DMF	Z	79	-	4,4,4	0.85	0	4,4,4	0.45	0
3	DMF	D	250	-	4,4,4	0.65	0	4,4,4	0.32	0
3	DMF	A	249	-	4,4,4	0.55	0	4,4,4	0.34	0
3	DMF	Q	250	-	4,4,4	0.29	0	4,4,4	0.52	0
3	DMF	Y	249	-	4,4,4	0.63	0	4,4,4	0.44	0
3	DMF	S	251	-	4,4,4	0.30	0	4,4,4	0.40	0
3	DMF	G	96	-	4,4,4	0.77	0	4,4,4	0.31	0
3	DMF	V	90	-	4,4,4	0.25	0	4,4,4	0.34	0
3	DMF	Q	249	-	4,4,4	0.43	0	4,4,4	0.34	0
3	DMF	H	31	-	4,4,4	0.83	0	4,4,4	0.31	0
3	DMF	V	65	-	4,4,4	0.86	0	4,4,4	0.28	0
3	DMF	P	74	-	4,4,4	0.38	0	4,4,4	0.18	0
3	DMF	D	249	-	4,4,4	0.28	0	4,4,4	0.32	0
3	DMF	Z	91	-	4,4,4	0.30	0	4,4,4	0.56	0
3	DMF	R	68	-	4,4,4	0.25	0	4,4,4	0.50	0
3	DMF	U	250	-	4,4,4	0.29	0	4,4,4	0.47	0
3	DMF	Z	27	-	4,4,4	0.15	0	4,4,4	0.37	0
3	DMF	R	54	-	4,4,4	0.37	0	4,4,4	0.41	0
3	DMF	B	250	-	4,4,4	0.84	0	4,4,4	0.28	0
3	DMF	X	67	-	4,4,4	0.70	0	4,4,4	0.30	0
3	DMF	H	52	-	4,4,4	0.35	0	4,4,4	0.52	0
3	DMF	1	251	-	4,4,4	0.45	0	4,4,4	0.61	0
3	DMF	E	95	-	4,4,4	1.07	0	4,4,4	0.41	0
3	DMF	J	6	-	4,4,4	0.26	0	4,4,4	0.41	0
3	DMF	D	252	-	4,4,4	0.24	0	4,4,4	0.35	0
3	DMF	N	37	-	4,4,4	0.66	0	4,4,4	0.39	0
3	DMF	G	1	-	4,4,4	0.35	0	4,4,4	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	DMF	S	250	-	4,4,4	0.28	0	4,4,4	0.41	0
3	DMF	I	249	-	4,4,4	0.51	0	4,4,4	0.39	0
3	DMF	J	82	-	4,4,4	0.51	0	4,4,4	0.33	0
3	DMF	J	59	-	4,4,4	0.22	0	4,4,4	0.37	0
3	DMF	O	249	-	4,4,4	0.26	0	4,4,4	0.64	0
3	DMF	C	5	-	4,4,4	0.31	0	4,4,4	0.55	0
3	DMF	C	28	-	4,4,4	0.53	0	4,4,4	0.29	0
3	DMF	R	89	-	4,4,4	0.29	0	4,4,4	0.55	0
3	DMF	A	250	-	4,4,4	0.62	0	4,4,4	0.44	0
3	DMF	C	48	-	4,4,4	0.47	0	4,4,4	0.28	0
3	DMF	W	250	-	4,4,4	0.69	0	4,4,4	0.31	0
3	DMF	M	249	-	4,4,4	0.56	0	4,4,4	0.39	0
3	DMF	Z	50	-	4,4,4	0.23	0	4,4,4	0.40	0
3	DMF	B	251	-	4,4,4	0.66	0	4,4,4	0.22	0
3	DMF	S	249	-	4,4,4	0.57	0	4,4,4	0.20	0
3	DMF	U	249	-	4,4,4	0.51	0	4,4,4	0.22	0
3	DMF	M	250	-	4,4,4	0.70	0	4,4,4	0.51	0
3	DMF	L	60	-	4,4,4	0.45	0	4,4,4	0.30	0
3	DMF	C	64	-	4,4,4	0.26	0	4,4,4	0.44	0
3	DMF	W	249	-	4,4,4	0.33	0	4,4,4	0.37	0
3	DMF	B	249	-	4,4,4	0.19	0	4,4,4	0.40	0
3	DMF	K	250	-	4,4,4	0.56	0	4,4,4	0.35	0
3	DMF	N	99	-	4,4,4	0.89	0	4,4,4	0.45	0
3	DMF	I	250	-	4,4,4	0.45	0	4,4,4	0.26	0
3	DMF	N	36	-	4,4,4	0.32	0	4,4,4	0.44	0
3	DMF	T	46	-	4,4,4	0.51	0	4,4,4	0.35	0
3	DMF	C	17	-	4,4,4	0.26	0	4,4,4	0.40	0
3	DMF	P	61	-	4,4,4	0.73	0	4,4,4	0.29	0
3	DMF	N	2	-	4,4,4	0.17	0	4,4,4	0.41	0
3	DMF	G	20	-	4,4,4	0.49	0	4,4,4	0.34	0
3	DMF	P	85	-	4,4,4	0.80	0	4,4,4	0.37	0
3	DMF	E	83	-	4,4,4	0.28	0	4,4,4	0.72	0
3	DMF	H	53	-	4,4,4	0.32	0	4,4,4	0.36	0
3	DMF	T	94	-	4,4,4	0.51	0	4,4,4	0.35	0
3	DMF	U	252	-	4,4,4	0.82	0	4,4,4	0.36	0
3	DMF	H	41	-	4,4,4	0.53	0	4,4,4	0.35	0
3	DMF	E	44	-	4,4,4	0.28	0	4,4,4	0.52	0
3	DMF	H	19	-	4,4,4	0.47	0	4,4,4	0.29	0
3	DMF	N	21	-	4,4,4	0.24	0	4,4,4	0.41	0
3	DMF	G	39	-	4,4,4	0.70	0	4,4,4	0.33	0
3	DMF	P	23	-	4,4,4	0.21	0	4,4,4	0.35	0
3	DMF	N	97	-	4,4,4	0.87	0	4,4,4	0.44	0

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
3	DMF	V	86	-	-	0/2/2/2	-
3	DMF	P	100	-	-	0/2/2/2	-
3	DMF	2	58	-	-	0/2/2/2	-
3	DMF	F	249	-	-	0/2/2/2	-
3	DMF	Z	71	-	-	0/2/2/2	-
3	DMF	T	92	-	-	0/2/2/2	-
3	DMF	2	66	-	-	0/2/2/2	-
3	DMF	E	32	-	-	0/2/2/2	-
3	DMF	C	43	-	-	0/2/2/2	-
3	DMF	R	3	-	-	2/2/2/2	-
3	DMF	1	250	-	-	0/2/2/2	-
3	DMF	U	251	-	-	0/2/2/2	-
3	DMF	N	24	-	-	0/2/2/2	-
3	DMF	C	73	-	-	2/2/2/2	-
3	DMF	E	70	-	-	2/2/2/2	-
3	DMF	O	250	-	-	2/2/2/2	-
3	DMF	X	25	-	-	0/2/2/2	-
3	DMF	H	102	-	-	0/2/2/2	-
3	DMF	T	35	-	-	2/2/2/2	-
3	DMF	V	16	-	-	2/2/2/2	-
3	DMF	2	78	-	-	0/2/2/2	-
3	DMF	L	9	-	-	2/2/2/2	-
3	DMF	K	249	-	-	0/2/2/2	-
3	DMF	C	15	-	-	0/2/2/2	-
3	DMF	F	250	-	-	2/2/2/2	-
3	DMF	X	88	-	-	0/2/2/2	-
3	DMF	I	249	-	-	0/2/2/2	-
3	DMF	Z	69	-	-	0/2/2/2	-
3	DMF	D	251	-	-	0/2/2/2	-
3	DMF	H	14	-	-	0/2/2/2	-
3	DMF	E	55	-	-	0/2/2/2	-
3	DMF	T	62	-	-	0/2/2/2	-
3	DMF	L	4	-	-	0/2/2/2	-
3	DMF	Z	79	-	-	0/2/2/2	-
3	DMF	D	250	-	-	0/2/2/2	-
3	DMF	A	249	-	-	0/2/2/2	-
3	DMF	Q	250	-	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	Y	249	-	-	0/2/2/2	-
3	DMF	S	251	-	-	2/2/2/2	-
3	DMF	G	96	-	-	0/2/2/2	-
3	DMF	V	90	-	-	2/2/2/2	-
3	DMF	Q	249	-	-	0/2/2/2	-
3	DMF	H	31	-	-	0/2/2/2	-
3	DMF	V	65	-	-	0/2/2/2	-
3	DMF	P	74	-	-	0/2/2/2	-
3	DMF	D	249	-	-	2/2/2/2	-
3	DMF	Z	91	-	-	2/2/2/2	-
3	DMF	R	68	-	-	2/2/2/2	-
3	DMF	U	250	-	-	2/2/2/2	-
3	DMF	Z	27	-	-	2/2/2/2	-
3	DMF	R	54	-	-	0/2/2/2	-
3	DMF	B	250	-	-	0/2/2/2	-
3	DMF	X	67	-	-	0/2/2/2	-
3	DMF	H	52	-	-	2/2/2/2	-
3	DMF	I	251	-	-	0/2/2/2	-
3	DMF	E	95	-	-	0/2/2/2	-
3	DMF	J	6	-	-	2/2/2/2	-
3	DMF	D	252	-	-	2/2/2/2	-
3	DMF	N	37	-	-	0/2/2/2	-
3	DMF	G	1	-	-	2/2/2/2	-
3	DMF	S	250	-	-	2/2/2/2	-
3	DMF	I	249	-	-	0/2/2/2	-
3	DMF	J	82	-	-	0/2/2/2	-
3	DMF	J	59	-	-	2/2/2/2	-
3	DMF	O	249	-	-	2/2/2/2	-
3	DMF	C	5	-	-	2/2/2/2	-
3	DMF	C	28	-	-	0/2/2/2	-
3	DMF	R	89	-	-	2/2/2/2	-
3	DMF	A	250	-	-	0/2/2/2	-
3	DMF	C	48	-	-	0/2/2/2	-
3	DMF	W	250	-	-	0/2/2/2	-
3	DMF	M	249	-	-	0/2/2/2	-
3	DMF	Z	50	-	-	0/2/2/2	-
3	DMF	B	251	-	-	0/2/2/2	-
3	DMF	S	249	-	-	0/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	U	249	-	-	0/2/2/2	-
3	DMF	M	250	-	-	0/2/2/2	-
3	DMF	L	60	-	-	0/2/2/2	-
3	DMF	C	64	-	-	2/2/2/2	-
3	DMF	W	249	-	-	2/2/2/2	-
3	DMF	B	249	-	-	2/2/2/2	-
3	DMF	K	250	-	-	0/2/2/2	-
3	DMF	N	99	-	-	0/2/2/2	-
3	DMF	I	250	-	-	0/2/2/2	-
3	DMF	N	36	-	-	0/2/2/2	-
3	DMF	T	46	-	-	0/2/2/2	-
3	DMF	C	17	-	-	0/2/2/2	-
3	DMF	P	61	-	-	0/2/2/2	-
3	DMF	N	2	-	-	2/2/2/2	-
3	DMF	G	20	-	-	0/2/2/2	-
3	DMF	P	85	-	-	0/2/2/2	-
3	DMF	E	83	-	-	2/2/2/2	-
3	DMF	H	53	-	-	2/2/2/2	-
3	DMF	T	94	-	-	0/2/2/2	-
3	DMF	U	252	-	-	0/2/2/2	-
3	DMF	H	41	-	-	0/2/2/2	-
3	DMF	E	44	-	-	2/2/2/2	-
3	DMF	H	19	-	-	0/2/2/2	-
3	DMF	N	21	-	-	2/2/2/2	-
3	DMF	G	39	-	-	0/2/2/2	-
3	DMF	P	23	-	-	0/2/2/2	-
3	DMF	N	97	-	-	0/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	252	DMF	O-C-N-C1
3	D	252	DMF	O-C-N-C2
3	N	2	DMF	O-C-N-C1
3	R	89	DMF	O-C-N-C1
3	C	73	DMF	O-C-N-C2

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Mol	Chain	Res	Type	Atoms
3	C	73	DMF	O-C-N-C1
3	R	89	DMF	O-C-N-C2
3	E	70	DMF	O-C-N-C1
3	F	250	DMF	O-C-N-C2
3	R	68	DMF	O-C-N-C1
3	N	2	DMF	O-C-N-C2
3	V	90	DMF	O-C-N-C1
3	Z	91	DMF	O-C-N-C1
3	E	70	DMF	O-C-N-C2
3	F	250	DMF	O-C-N-C1
3	R	68	DMF	O-C-N-C2
3	V	16	DMF	O-C-N-C2
3	N	21	DMF	O-C-N-C1
3	V	16	DMF	O-C-N-C1
3	V	90	DMF	O-C-N-C2
3	Z	91	DMF	O-C-N-C2
3	N	21	DMF	O-C-N-C2
3	C	5	DMF	O-C-N-C1
3	U	250	DMF	O-C-N-C1
3	S	250	DMF	O-C-N-C1
3	B	249	DMF	O-C-N-C1
3	C	64	DMF	O-C-N-C1
3	D	249	DMF	O-C-N-C1
3	E	44	DMF	O-C-N-C1
3	E	83	DMF	O-C-N-C1
3	G	1	DMF	O-C-N-C1
3	H	52	DMF	O-C-N-C1
3	H	53	DMF	O-C-N-C1
3	J	6	DMF	O-C-N-C1
3	J	59	DMF	O-C-N-C1
3	L	9	DMF	O-C-N-C1
3	O	249	DMF	O-C-N-C1
3	O	250	DMF	O-C-N-C1
3	Q	250	DMF	O-C-N-C1
3	R	3	DMF	O-C-N-C1
3	S	251	DMF	O-C-N-C1
3	T	35	DMF	O-C-N-C1
3	W	249	DMF	O-C-N-C1
3	Z	27	DMF	O-C-N-C1
3	U	250	DMF	O-C-N-C2
3	C	5	DMF	O-C-N-C2
3	Q	250	DMF	O-C-N-C2

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Mol	Chain	Res	Type	Atoms
3	S	250	DMF	O-C-N-C2
3	Z	27	DMF	O-C-N-C2
3	J	6	DMF	O-C-N-C2
3	L	9	DMF	O-C-N-C2
3	O	250	DMF	O-C-N-C2
3	H	53	DMF	O-C-N-C2
3	T	35	DMF	O-C-N-C2
3	W	249	DMF	O-C-N-C2
3	D	249	DMF	O-C-N-C2
3	O	249	DMF	O-C-N-C2
3	J	59	DMF	O-C-N-C2
3	R	3	DMF	O-C-N-C2
3	C	64	DMF	O-C-N-C2
3	G	1	DMF	O-C-N-C2
3	E	44	DMF	O-C-N-C2
3	E	83	DMF	O-C-N-C2
3	H	52	DMF	O-C-N-C2
3	B	249	DMF	O-C-N-C2
3	S	251	DMF	O-C-N-C2

There are no ring outliers.

57 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Z	71	DMF	1	0
3	T	92	DMF	1	0
3	E	32	DMF	1	0
3	C	43	DMF	1	0
3	1	250	DMF	1	0
3	U	251	DMF	2	0
3	C	73	DMF	7	0
3	E	70	DMF	2	0
3	O	250	DMF	4	0
3	T	35	DMF	5	0
3	V	16	DMF	1	0
3	2	78	DMF	1	0
3	L	9	DMF	3	0
3	F	250	DMF	1	0
3	Z	69	DMF	3	0
3	D	251	DMF	1	0
3	E	55	DMF	1	0
3	L	4	DMF	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Z	79	DMF	1	0
3	G	96	DMF	3	0
3	H	31	DMF	1	0
3	Z	91	DMF	3	0
3	R	68	DMF	1	0
3	U	250	DMF	1	0
3	Z	27	DMF	2	0
3	B	250	DMF	1	0
3	X	67	DMF	1	0
3	1	251	DMF	2	0
3	E	95	DMF	1	0
3	J	6	DMF	4	0
3	D	252	DMF	1	0
3	G	1	DMF	1	0
3	S	250	DMF	1	0
3	J	82	DMF	1	0
3	O	249	DMF	2	0
3	C	5	DMF	5	0
3	R	89	DMF	1	0
3	A	250	DMF	2	0
3	M	249	DMF	1	0
3	L	60	DMF	1	0
3	C	64	DMF	6	0
3	W	249	DMF	1	0
3	B	249	DMF	1	0
3	K	250	DMF	2	0
3	N	36	DMF	2	0
3	C	17	DMF	1	0
3	P	61	DMF	1	0
3	N	2	DMF	2	0
3	G	20	DMF	3	0
3	H	53	DMF	2	0
3	T	94	DMF	3	0
3	U	252	DMF	1	0
3	H	41	DMF	1	0
3	H	19	DMF	4	0
3	G	39	DMF	1	0
3	P	23	DMF	1	0
3	N	97	DMF	3	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 i

### 6.1 Protein, DNA and RNA chains i

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	1	215/248 (86%)	0.41	19 (8%) 10 7	20, 55, 92, 101	0
1	A	216/248 (87%)	0.66	35 (16%) 1 1	21, 56, 100, 109	0
1	B	214/248 (86%)	0.43	16 (7%) 14 11	22, 56, 98, 108	0
1	D	213/248 (85%)	0.65	27 (12%) 3 2	21, 56, 96, 105	0
1	F	217/248 (87%)	0.44	14 (6%) 18 15	22, 55, 91, 102	0
1	I	215/248 (86%)	0.46	19 (8%) 10 7	23, 56, 98, 107	0
1	K	217/248 (87%)	0.53	24 (11%) 5 3	19, 57, 94, 109	0
1	M	216/248 (87%)	0.40	13 (6%) 21 18	21, 55, 92, 99	0
1	O	215/248 (86%)	0.49	20 (9%) 8 6	21, 56, 92, 102	0
1	Q	218/248 (87%)	0.39	16 (7%) 15 11	21, 55, 90, 101	0
1	S	215/248 (86%)	0.61	32 (14%) 2 1	21, 57, 102, 112	0
1	U	215/248 (86%)	0.45	13 (6%) 21 18	22, 55, 96, 106	0
1	W	217/248 (87%)	0.49	21 (9%) 7 5	22, 56, 93, 99	0
1	Y	213/248 (85%)	0.74	30 (14%) 2 1	23, 57, 99, 111	0
2	2	214/240 (89%)	-0.51	4 (1%) 66 63	10, 20, 43, 73	0
2	C	214/240 (89%)	-0.38	5 (2%) 60 56	8, 20, 46, 76	0
2	E	215/240 (89%)	-0.51	3 (1%) 75 73	10, 20, 45, 76	0
2	G	215/240 (89%)	-0.58	1 (0%) 91 91	10, 21, 47, 75	0
2	H	212/240 (88%)	-0.49	2 (0%) 84 83	11, 22, 45, 70	0
2	J	215/240 (89%)	-0.37	3 (1%) 75 73	10, 21, 46, 70	0
2	L	215/240 (89%)	-0.45	2 (0%) 84 83	10, 21, 45, 72	0
2	N	212/240 (88%)	-0.50	1 (0%) 91 91	9, 21, 43, 67	0
2	P	215/240 (89%)	-0.42	6 (2%) 53 49	10, 23, 47, 73	0
2	R	222/240 (92%)	-0.50	2 (0%) 84 83	8, 19, 44, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	T	215/240 (89%)	-0.35	4 (1%) 66 63	9, 22, 47, 80	0
2	V	220/240 (91%)	-0.57	5 (2%) 60 56	8, 20, 44, 74	0
2	X	215/240 (89%)	-0.48	4 (1%) 66 63	10, 22, 46, 79	0
2	Z	214/240 (89%)	-0.43	2 (0%) 84 83	10, 23, 46, 68	0
All	All	6029/6832 (88%)	0.02	343 (5%) 23 20	8, 34, 89, 112	0

All (343) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	12	ALA	9.2
1	S	188	LEU	7.4
1	F	202	THR	7.2
1	B	205	VAL	7.0
1	U	204	GLY	6.5
1	S	8	SER	6.2
1	U	206	ALA	6.0
1	A	172	ALA	5.8
1	B	204	GLY	5.7
1	D	169	GLU	5.7
1	U	205	VAL	5.5
1	Y	10	GLU	5.3
1	D	131	GLY	5.2
1	Y	11	GLN	5.1
2	T	392	ALA	5.1
1	U	231	GLN	5.0
1	Y	231	GLN	5.0
1	Y	188	LEU	4.9
1	Q	7	ILE	4.8
1	D	48	ARG	4.7
1	B	206	ALA	4.7
1	K	7	ILE	4.6
1	O	172	ALA	4.5
1	W	7	ILE	4.5
1	M	10	GLU	4.5
1	Y	131	GLY	4.3
1	K	169	GLU	4.2
1	F	169	GLU	4.2
1	Y	184	ALA	4.2
1	1	179	ASP	4.2
1	A	131	GLY	4.2
1	Y	186	ALA	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	Q	14	ARG	4.1
2	L	392	ALA	4.1
1	O	161	GLU	4.0
1	D	206	ALA	4.0
1	Y	169	GLU	4.0
1	O	14	ARG	4.0
2	P	425	ALA	4.0
1	A	10	GLU	4.0
2	R	412	SER	4.0
2	T	391	LEU	3.9
2	X	391	LEU	3.9
1	1	232	ALA	3.9
1	B	231	GLN	3.9
1	S	232	ALA	3.9
1	O	168	LYS	3.8
1	Q	202	THR	3.8
1	D	207	SER	3.8
2	H	425	ALA	3.8
1	A	168	LYS	3.8
1	A	191	GLY	3.8
1	Y	179	ASP	3.7
1	Y	9	PRO	3.7
1	S	172	ALA	3.7
1	D	10	GLU	3.7
1	O	8	SER	3.7
1	Q	172	ALA	3.7
1	D	165	ASN	3.7
1	K	179	ASP	3.7
1	D	228	SER	3.6
1	U	232	ALA	3.6
1	F	179	ASP	3.6
1	D	231	GLN	3.6
2	2	392	ALA	3.6
1	D	168	LYS	3.6
1	M	206	ALA	3.6
1	B	234	LEU	3.6
1	Y	234	LEU	3.6
1	K	232	ALA	3.5
1	A	227	GLY	3.5
1	B	232	ALA	3.5
2	Z	391	LEU	3.5
1	Y	44	GLU	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	W	161	GLU	3.4
1	I	203	LEU	3.4
1	D	159	THR	3.4
1	O	13	MET	3.4
1	D	227	GLY	3.3
1	O	234	LEU	3.3
1	Y	14	ARG	3.3
1	1	165	ASN	3.3
1	A	206	ALA	3.3
1	S	205	VAL	3.3
1	O	169	GLU	3.3
1	D	27	ALA	3.2
1	Y	165	ASN	3.2
1	A	161	GLU	3.2
2	X	392	ALA	3.2
2	N	412	SER	3.2
1	K	205	VAL	3.2
1	K	186	ALA	3.2
2	V	400	ALA	3.2
1	O	11	GLN	3.2
1	F	205	VAL	3.2
1	S	14	ARG	3.2
1	1	133	THR	3.1
1	A	231	GLN	3.1
1	I	11	GLN	3.1
1	A	207	SER	3.1
1	O	182	ARG	3.1
1	M	113	GLU	3.1
1	U	8	SER	3.1
1	Q	11	GLN	3.1
1	O	206	ALA	3.1
1	S	11	GLN	3.1
2	E	391	LEU	3.1
1	O	189	ARG	3.0
1	B	14	ARG	3.0
1	1	159	THR	3.0
1	Y	13	MET	3.0
1	K	131	GLY	3.0
1	1	160	THR	3.0
2	E	392	ALA	3.0
1	I	205	VAL	3.0
1	I	188	LEU	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	S	191	GLY	3.0
1	K	148	ALA	2.9
1	S	153	PHE	2.9
1	S	227	GLY	2.9
1	A	169	GLU	2.9
1	I	161	GLU	2.9
1	S	44	GLU	2.9
2	R	392	ALA	2.9
2	E	426	ALA	2.9
1	1	152	HIS	2.8
1	K	10	GLU	2.8
1	U	171	TYR	2.8
1	A	163	ILE	2.8
1	K	161	GLU	2.8
1	B	227	GLY	2.8
1	A	8	SER	2.8
1	1	205	VAL	2.8
1	I	206	ALA	2.8
1	B	10	GLU	2.8
2	T	412	SER	2.8
1	F	165	ASN	2.8
1	S	160	THR	2.8
2	C	416	SER	2.8
1	A	165	ASN	2.7
1	W	178	THR	2.7
1	S	36	ALA	2.7
1	K	203	LEU	2.7
2	X	426	ALA	2.7
1	O	153	PHE	2.7
1	Q	203	LEU	2.7
1	1	203	LEU	2.7
1	U	169	GLU	2.7
1	W	48	ARG	2.7
1	Q	36	ALA	2.7
1	K	147	ILE	2.7
2	L	391	LEU	2.7
1	W	135	ARG	2.7
1	M	11	GLN	2.7
1	A	133	THR	2.7
1	F	172	ALA	2.7
1	Q	204	GLY	2.7
1	W	165	ASN	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	1	11	GLN	2.6
1	S	169	GLU	2.6
1	Y	15	GLU	2.6
1	S	186	ALA	2.6
1	S	131	GLY	2.6
1	D	133	THR	2.6
1	B	173	GLU	2.6
1	Q	10	GLU	2.6
1	U	228	SER	2.6
1	D	229	ALA	2.6
1	Q	131	GLY	2.6
1	I	10	GLU	2.6
1	1	161	GLU	2.6
1	A	53	ILE	2.6
1	O	231	GLN	2.6
1	I	182	ARG	2.6
1	W	14	ARG	2.6
1	W	228	SER	2.6
1	F	10	GLU	2.6
1	Q	169	GLU	2.6
1	Y	172	ALA	2.5
1	W	162	PRO	2.5
1	I	26	ARG	2.5
1	S	135	ARG	2.5
1	S	10	GLU	2.5
1	S	161	GLU	2.5
1	U	173	GLU	2.5
1	I	189	ARG	2.5
1	B	228	SER	2.5
2	J	412	SER	2.5
1	K	206	ALA	2.5
1	S	231	GLN	2.5
1	1	48	ARG	2.5
1	W	231	GLN	2.5
1	A	232	ALA	2.5
1	K	130	TYR	2.5
1	K	188	LEU	2.5
1	S	15	GLU	2.5
1	W	15	GLU	2.5
2	C	412	SER	2.5
1	O	165	ASN	2.5
1	B	171	TYR	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	2	391	LEU	2.5
1	M	228	SER	2.5
1	Y	228	SER	2.5
1	D	179	ASP	2.5
1	B	161	GLU	2.5
1	A	203	LEU	2.4
1	1	231	GLN	2.4
2	J	399	LEU	2.4
2	P	391	LEU	2.4
1	S	28	LYS	2.4
1	F	133	THR	2.4
1	W	182	ARG	2.4
2	Z	392	ALA	2.4
1	A	31	VAL	2.4
1	A	171	TYR	2.4
1	U	131	GLY	2.4
1	W	26	ARG	2.4
1	W	46	PRO	2.4
2	C	392	ALA	2.4
1	1	228	SER	2.4
1	S	179	ASP	2.4
1	S	171	TYR	2.4
1	A	11	GLN	2.4
1	M	231	GLN	2.4
1	M	46	PRO	2.4
1	I	184	ALA	2.4
1	Y	161	GLU	2.4
1	S	182	ARG	2.4
1	I	204	GLY	2.4
1	A	173	GLU	2.4
2	C	425	ALA	2.4
1	Q	8	SER	2.4
1	Y	135	ARG	2.4
1	A	205	VAL	2.4
1	1	163	ILE	2.4
2	X	400	ALA	2.4
1	A	135	ARG	2.4
1	W	207	SER	2.4
1	W	233	LEU	2.4
1	Q	168	LYS	2.4
1	W	188	LEU	2.4
1	A	48	ARG	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	28	LYS	2.3
1	M	234	LEU	2.3
2	T	426	ALA	2.3
1	S	159	THR	2.3
2	P	399	LEU	2.3
1	I	135	ARG	2.3
1	B	152	HIS	2.3
1	W	12	ALA	2.3
1	D	205	VAL	2.3
1	I	15	GLU	2.3
2	V	392	ALA	2.3
1	Y	22	LYS	2.3
2	G	392	ALA	2.3
2	P	426	ALA	2.3
1	D	160	THR	2.3
1	K	149	ASP	2.3
1	M	44	GLU	2.3
1	O	10	GLU	2.3
1	O	48	ARG	2.3
2	2	425	ALA	2.3
1	U	233	LEU	2.3
1	S	12	ALA	2.2
1	K	135	ARG	2.2
1	M	161	GLU	2.2
1	Q	113	GLU	2.2
2	V	425	ALA	2.2
1	S	133	THR	2.2
1	D	37	GLY	2.2
2	V	389	GLY	2.2
1	F	162	PRO	2.2
1	Y	233	LEU	2.2
1	F	14	ARG	2.2
1	Y	207	SER	2.2
2	H	412	SER	2.2
1	F	161	GLU	2.2
2	P	392	ALA	2.2
1	M	179	ASP	2.2
2	J	391	LEU	2.2
2	C	391	LEU	2.2
1	D	21	ARG	2.1
1	I	191	GLY	2.1
1	U	227	GLY	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	161	GLU	2.1
1	D	234	LEU	2.1
1	D	49	SER	2.1
1	Y	149	ASP	2.1
1	B	190	ALA	2.1
1	K	31	VAL	2.1
1	K	165	ASN	2.1
1	K	189	ARG	2.1
1	Q	189	ARG	2.1
1	Y	189	ARG	2.1
1	1	135	ARG	2.1
1	W	23	GLY	2.1
2	V	391	LEU	2.1
2	2	412	SER	2.1
1	A	190	ALA	2.1
1	Y	168	LYS	2.1
1	I	133	THR	2.1
1	I	231	GLN	2.1
1	1	9	PRO	2.1
1	Y	111	PHE	2.1
1	S	233	LEU	2.1
1	K	152	HIS	2.1
1	A	130	TYR	2.1
1	S	27	ALA	2.1
1	A	162	PRO	2.1
1	S	165	ASN	2.1
1	Y	204	GLY	2.1
1	D	11	GLN	2.1
1	I	190	ALA	2.1
1	A	159	THR	2.1
1	1	178	THR	2.1
1	M	163	ILE	2.1
1	B	230	LEU	2.1
1	O	135	ARG	2.1
1	D	188	LEU	2.1
1	F	203	LEU	2.1
1	I	177	LEU	2.1
1	Y	19	LEU	2.1
1	1	172	ALA	2.0
1	A	188	LEU	2.0
1	O	173	GLU	2.0
1	K	204	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	O	131	GLY	2.0
1	A	182	ARG	2.0
1	A	180	ALA	2.0
1	M	12	ALA	2.0
1	D	152	HIS	2.0
1	Q	44	GLU	2.0
1	S	152	HIS	2.0
1	F	11	GLN	2.0
1	A	189	ARG	2.0
1	W	153	PHE	2.0
1	F	36	ALA	2.0
1	K	26	ARG	2.0
1	K	228	SER	2.0
1	A	177	LEU	2.0
1	W	203	LEU	2.0
2	P	401	LEU	2.0
1	D	130	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	OZT	R	301	9/10	0.87	0.19	23,29,35,38	0
2	OZT	V	301	9/10	0.90	0.15	23,30,35,36	0
2	OZT	C	301	9/10	0.91	0.15	19,28,34,37	0
2	OZT	2	301	9/10	0.91	0.16	23,30,34,35	0
2	OZT	P	301	9/10	0.92	0.15	25,29,34,39	0
2	OZT	J	301	9/10	0.92	0.16	24,30,34,38	0
2	OZT	L	301	9/10	0.92	0.13	25,29,34,35	0
2	OZT	X	301	9/10	0.92	0.14	28,31,35,36	0
2	OZT	N	301	9/10	0.92	0.13	23,28,35,38	0
2	OZT	E	301	9/10	0.94	0.13	25,31,33,36	0
2	OZT	H	301	9/10	0.94	0.12	24,30,33,33	0
2	OZT	Z	301	9/10	0.95	0.12	25,28,32,33	0
2	OZT	G	301	9/10	0.96	0.11	24,30,34,37	0
2	OZT	T	301	9/10	0.96	0.11	26,29,32,34	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	DMF	D	249	5/5	0.56	0.45	83,83,84,84	0
3	DMF	T	35	5/5	0.59	0.36	75,75,76,77	0
3	DMF	D	252	5/5	0.60	0.33	50,50,54,55	0
3	DMF	H	31	5/5	0.61	0.55	64,66,68,68	0
3	DMF	T	94	5/5	0.68	0.44	104,104,104,104	0
3	DMF	G	39	5/5	0.69	0.32	55,57,59,60	0
3	DMF	F	250	5/5	0.70	0.28	68,69,71,71	0
3	DMF	W	250	5/5	0.70	0.35	61,62,64,64	0
3	DMF	E	32	5/5	0.72	0.43	60,62,63,65	0
3	DMF	Q	250	5/5	0.73	0.32	69,70,70,71	0
3	DMF	B	251	5/5	0.74	0.27	61,64,64,64	0
3	DMF	2	58	5/5	0.74	0.38	60,62,64,64	0
3	DMF	G	20	5/5	0.75	0.35	46,50,51,53	0
3	DMF	S	250	5/5	0.75	0.28	48,49,51,51	0
3	DMF	S	249	5/5	0.76	0.33	63,64,65,66	0
3	DMF	C	48	5/5	0.76	0.31	68,69,70,70	0
3	DMF	C	43	5/5	0.77	0.25	57,57,59,59	0
3	DMF	N	99	5/5	0.78	0.25	50,52,53,54	0
3	DMF	R	54	5/5	0.78	0.32	46,48,49,51	0
3	DMF	J	82	5/5	0.79	0.30	50,52,54,57	0
3	DMF	2	66	5/5	0.79	0.33	69,70,70,71	0
3	DMF	N	36	5/5	0.80	0.31	50,53,54,57	0
3	DMF	G	96	5/5	0.80	0.29	79,80,80,81	0
3	DMF	V	65	5/5	0.80	0.28	60,60,61,61	0
3	DMF	D	251	5/5	0.81	0.27	51,53,54,56	0
3	DMF	O	250	5/5	0.81	0.32	59,60,60,61	0
3	DMF	A	250	5/5	0.81	0.25	52,54,56,59	0
3	DMF	E	95	5/5	0.82	0.26	46,49,51,55	0
3	DMF	B	250	5/5	0.82	0.19	39,39,43,45	0
3	DMF	P	61	5/5	0.83	0.28	58,59,61,62	0
3	DMF	K	250	5/5	0.83	0.29	59,61,62,63	0
3	DMF	X	67	5/5	0.83	0.25	58,59,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DMF	1	250	5/5	0.83	0.20	60,60,61,61	0
3	DMF	1	251	5/5	0.83	0.26	45,48,49,49	0
3	DMF	R	3	5/5	0.83	0.33	63,63,65,65	0
3	DMF	N	97	5/5	0.83	0.27	31,36,38,38	0
3	DMF	H	19	5/5	0.84	0.27	52,53,55,58	0
3	DMF	T	62	5/5	0.84	0.30	56,58,58,60	0
3	DMF	H	41	5/5	0.84	0.28	62,63,63,64	0
3	DMF	Z	27	5/5	0.84	0.34	57,62,64,65	0
3	DMF	Y	249	5/5	0.85	0.20	58,59,61,62	0
3	DMF	X	25	5/5	0.86	0.24	47,49,50,51	0
3	DMF	C	5	5/5	0.86	0.32	77,77,78,78	0
3	DMF	W	249	5/5	0.86	0.26	77,77,78,78	0
3	DMF	P	100	5/5	0.86	0.23	53,54,54,55	0
3	DMF	C	73	5/5	0.87	0.24	53,54,54,55	0
3	DMF	N	37	5/5	0.87	0.29	63,64,65,67	0
3	DMF	H	52	5/5	0.87	0.26	65,66,66,67	0
3	DMF	U	251	5/5	0.87	0.22	45,45,46,48	0
3	DMF	S	251	5/5	0.87	0.20	69,70,70,70	0
3	DMF	R	89	5/5	0.88	0.26	52,53,53,54	0
3	DMF	X	88	5/5	0.88	0.24	46,48,50,51	0
3	DMF	C	15	5/5	0.88	0.29	51,53,54,56	0
3	DMF	L	9	5/5	0.88	0.28	61,63,64,65	0
3	DMF	U	250	5/5	0.89	0.14	71,71,72,72	0
3	DMF	L	60	5/5	0.89	0.22	57,57,58,59	0
3	DMF	U	252	5/5	0.89	0.18	60,60,61,61	0
3	DMF	O	249	5/5	0.89	0.22	42,46,47,49	0
3	DMF	F	249	5/5	0.89	0.27	55,55,56,56	0
3	DMF	2	78	5/5	0.89	0.19	43,44,46,48	0
3	DMF	C	64	5/5	0.90	0.26	60,60,60,61	0
3	DMF	H	102	5/5	0.90	0.26	73,73,74,74	0
3	DMF	Z	69	5/5	0.90	0.28	69,70,71,71	0
3	DMF	N	21	5/5	0.90	0.26	75,76,76,76	0
3	DMF	E	70	5/5	0.90	0.26	77,77,78,78	0
3	DMF	R	68	5/5	0.90	0.23	53,56,57,57	0
3	DMF	E	83	5/5	0.90	0.24	64,65,65,66	0
3	DMF	P	74	5/5	0.90	0.29	72,73,74,74	0
3	DMF	D	250	5/5	0.91	0.24	67,67,67,68	0
3	DMF	Z	50	5/5	0.91	0.21	48,49,50,52	0
3	DMF	C	28	5/5	0.91	0.21	53,54,56,57	0
3	DMF	Z	71	5/5	0.91	0.26	52,52,54,56	0
3	DMF	Z	91	5/5	0.91	0.24	54,55,55,56	0
3	DMF	T	92	5/5	0.91	0.29	41,44,45,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DMF	P	85	5/5	0.91	0.23	52,53,54,54	0
3	DMF	B	249	5/5	0.91	0.22	49,52,53,55	0
3	DMF	C	17	5/5	0.91	0.17	37,38,41,42	0
3	DMF	P	23	5/5	0.91	0.30	60,60,61,63	0
3	DMF	I	249	5/5	0.92	0.19	42,43,44,45	0
3	DMF	I	250	5/5	0.92	0.16	48,51,51,52	0
3	DMF	1	249	5/5	0.92	0.19	56,57,58,59	0
3	DMF	V	16	5/5	0.92	0.23	48,50,51,52	0
3	DMF	H	14	5/5	0.92	0.24	63,63,64,64	0
3	DMF	V	90	5/5	0.92	0.20	66,66,68,71	0
3	DMF	M	250	5/5	0.92	0.19	35,37,37,38	0
3	DMF	N	2	5/5	0.92	0.23	44,45,48,50	0
3	DMF	G	1	5/5	0.93	0.24	38,42,43,46	0
3	DMF	Z	79	5/5	0.93	0.19	38,38,39,40	0
3	DMF	Q	249	5/5	0.93	0.21	52,52,53,54	0
3	DMF	N	24	5/5	0.93	0.15	41,42,44,46	0
3	DMF	H	53	5/5	0.93	0.21	63,64,65,65	0
3	DMF	J	6	5/5	0.93	0.22	53,54,55,57	0
3	DMF	V	86	5/5	0.93	0.23	44,44,45,48	0
3	DMF	E	44	5/5	0.93	0.19	42,44,46,46	0
3	DMF	K	249	5/5	0.93	0.17	37,40,41,41	0
3	DMF	A	249	5/5	0.94	0.15	54,55,55,56	0
3	DMF	U	249	5/5	0.94	0.23	46,47,48,49	0
3	DMF	T	46	5/5	0.94	0.18	45,46,47,48	0
3	DMF	M	249	5/5	0.95	0.17	43,43,44,46	0
3	DMF	L	4	5/5	0.95	0.13	47,47,47,48	0
3	DMF	E	55	5/5	0.96	0.16	41,41,42,42	0
3	DMF	J	59	5/5	0.96	0.15	65,65,66,66	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.