



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:19 AM UTC

PDB ID : 3MI0 / pdb_00003mi0
Title : Crystal Structure of Mycobacterium Tuberculosis Proteasome at 2.2 Å
Authors : Li, D.; Li, H.
Deposited on : 2010-04-09
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

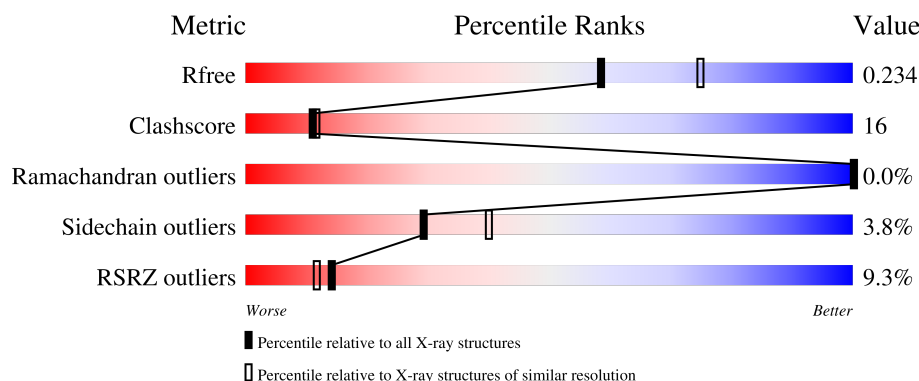
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.



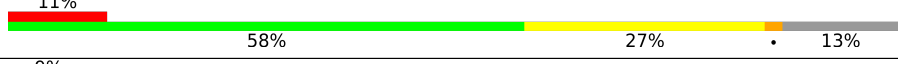
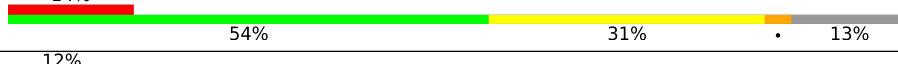
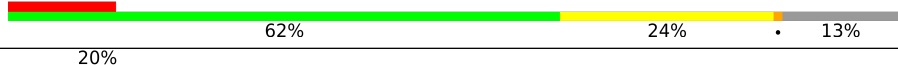
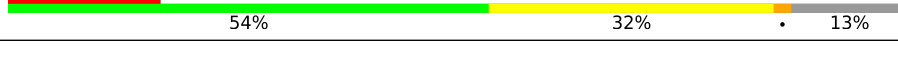
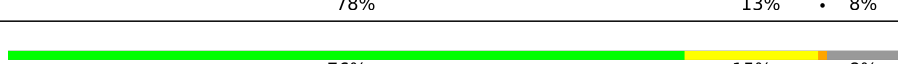
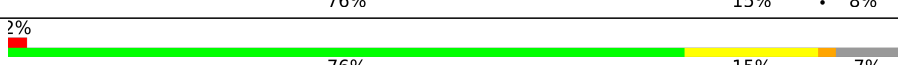
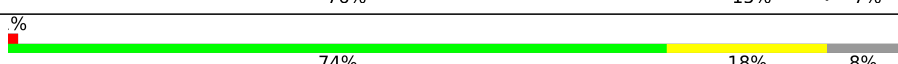
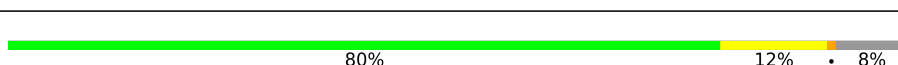
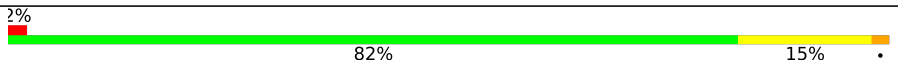
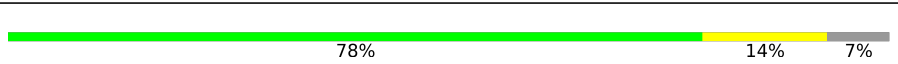
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 ≥ 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	11% 62% 24% • 13%
1	A	248	19% 59% 24% • 13%
1	B	248	11% 59% 23% • 14%
1	D	248	38% 49% 35% • 14%
1	F	248	12% 59% 28% • 11%

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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
3	DMF	2	108	-	-	X	-
3	DMF	2	112	-	-	X	-
3	DMF	2	4	-	-	X	-
3	DMF	C	103	-	-	X	-
3	DMF	D	251	-	-	X	-
3	DMF	E	20	-	-	X	-
3	DMF	E	75	-	-	X	-
3	DMF	G	119	-	-	X	-
3	DMF	G	12	-	-	X	-
3	DMF	G	64	-	-	X	-
3	DMF	H	43	-	-	X	-
3	DMF	J	123	-	-	X	-
3	DMF	K	250	-	-	X	-
3	DMF	L	97	-	-	X	-
3	DMF	N	104	-	-	X	-
3	DMF	N	118	-	-	X	-
3	DMF	N	22	-	-	X	-
3	DMF	N	90	-	-	X	-
3	DMF	N	93	-	-	X	-
3	DMF	P	107	-	-	X	-
3	DMF	P	14	-	-	X	-
3	DMF	Q	250	-	-	X	-
3	DMF	R	59	-	-	X	-
3	DMF	T	113	-	-	X	-
3	DMF	U	250	-	-	X	-
3	DMF	V	116	-	-	X	-
3	DMF	V	120	-	-	X	-
3	DMF	V	27	-	-	X	-
3	DMF	V	32	-	-	X	-
3	DMF	V	42	-	-	X	-
3	DMF	V	83	-	-	X	-
3	DMF	W	250	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 50080 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1654	1035	303	313	3			
1	B	213	Total	C	N	O	S	0	0	0
			1643	1028	301	311	3			
1	D	214	Total	C	N	O	S	0	0	0
			1650	1033	302	312	3			
1	F	220	Total	C	N	O	S	0	0	0
			1699	1068	308	320	3			
1	I	216	Total	C	N	O	S	0	0	0
			1669	1048	304	314	3			
1	K	216	Total	C	N	O	S	0	0	0
			1666	1045	304	314	3			
1	M	216	Total	C	N	O	S	0	0	0
			1666	1045	304	314	3			
1	O	216	Total	C	N	O	S	0	0	0
			1666	1045	304	314	3			
1	Q	215	Total	C	N	O	S	0	0	0
			1658	1039	303	313	3			
1	S	216	Total	C	N	O	S	0	0	0
			1665	1044	304	314	3			
1	U	216	Total	C	N	O	S	0	0	0
			1662	1041	304	314	3			
1	W	216	Total	C	N	O	S	0	0	0
			1669	1048	304	314	3			
1	Y	216	Total	C	N	O	S	0	0	0
			1666	1045	304	314	3			
1	1	215	Total	C	N	O	S	0	0	0
			1658	1039	303	313	3			

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	E	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	G	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	H	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	J	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	L	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	N	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	P	222	Total	C	N	O	S	0	0	0
			1638	1027	282	324	5			
2	R	239	Total	C	N	O	S	0	0	0
			1767	1103	310	349	5			
2	T	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	V	239	Total	C	N	O	S	0	0	0
			1767	1103	310	349	5			
2	X	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	Z	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			
2	2	223	Total	C	N	O	S	0	0	0
			1642	1029	283	325	5			

There are 84 discrepancies between the modelled and reference sequences:

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

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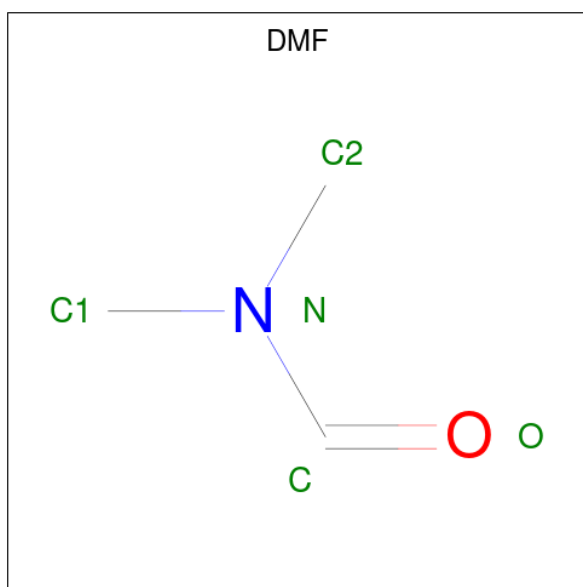
Chain	Residue	Modelled	Actual	Comment	Reference
G	535	HIS	-	expression tag	UNP O33245
G	536	HIS	-	expression tag	UNP O33245
G	537	HIS	-	expression tag	UNP O33245
G	538	HIS	-	expression tag	UNP O33245
G	539	HIS	-	expression tag	UNP O33245
G	540	HIS	-	expression tag	UNP O33245
H	535	HIS	-	expression tag	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	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	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	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	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
P	539	HIS	-	expression tag	UNP O33245
P	540	HIS	-	expression tag	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

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

- Molecule 3 is DIMETHYLFORMAMIDE (CCD ID: DMF) (formula: C₃H₇NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	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		
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		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	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	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	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		

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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	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	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	M	1	Total	C	N	O	0	0
			5	3	1	1		

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

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

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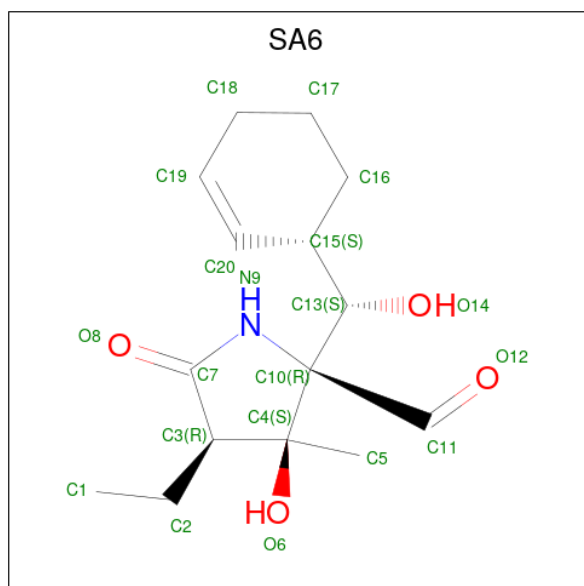
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	V	1	Total	C	N	O	0	0
			5	3	1	1		
3	V	1	Total	C	N	O	0	0
			5	3	1	1		
3	W	1	Total	C	N	O	0	0
			5	3	1	1		
3	W	1	Total	C	N	O	0	0
			5	3	1	1		
3	X	1	Total	C	N	O	0	0
			5	3	1	1		
3	X	1	Total	C	N	O	0	0
			5	3	1	1		
3	X	1	Total	C	N	O	0	0
			5	3	1	1		
3	X	1	Total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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		
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 (2R,3S,4R)-2-[(S)-(1S)-cyclohex-2-en-1-yl(hydroxy)methyl]-4-ethyl-3-hydroxy-3-methyl-5-oxopyrrolidine-2-carbaldehyde (CCD ID: SA6) (formula: C₁₅H₂₃NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			20	15	1	4		
4	E	1	Total	C	N	O	0	0
			20	15	1	4		
4	G	1	Total	C	N	O	0	0
			20	15	1	4		
4	H	1	Total	C	N	O	0	0
			20	15	1	4		
4	J	1	Total	C	N	O	0	0
			20	15	1	4		
4	L	1	Total	C	N	O	0	0
			20	15	1	4		
4	N	1	Total	C	N	O	0	0
			20	15	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	P	1	Total	C	N	O	0	0
			20	15	1	4		
4	R	1	Total	C	N	O	0	0
			20	15	1	4		
4	T	1	Total	C	N	O	0	0
			20	15	1	4		
4	V	1	Total	C	N	O	0	0
			20	15	1	4		
4	X	1	Total	C	N	O	0	0
			20	15	1	4		
4	Z	1	Total	C	N	O	0	0
			20	15	1	4		
4	2	1	Total	C	N	O	0	0
			20	15	1	4		

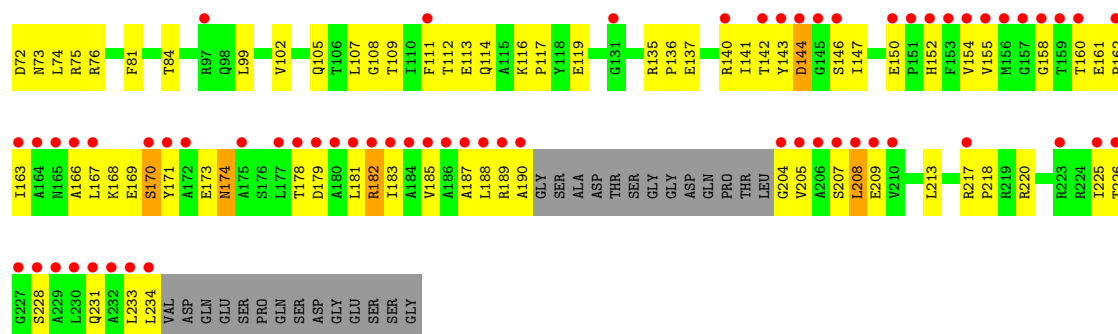
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	43	Total	O	0	0
			43	43		
5	B	41	Total	O	0	0
			41	41		
5	C	163	Total	O	0	0
			163	163		
5	D	40	Total	O	0	0
			40	40		
5	E	166	Total	O	0	0
			166	166		
5	F	58	Total	O	0	0
			58	58		
5	G	131	Total	O	0	0
			131	131		
5	H	148	Total	O	0	0
			148	148		
5	I	52	Total	O	0	0
			52	52		
5	J	142	Total	O	0	0
			142	142		
5	K	45	Total	O	0	0
			45	45		
5	L	153	Total	O	0	0
			153	153		

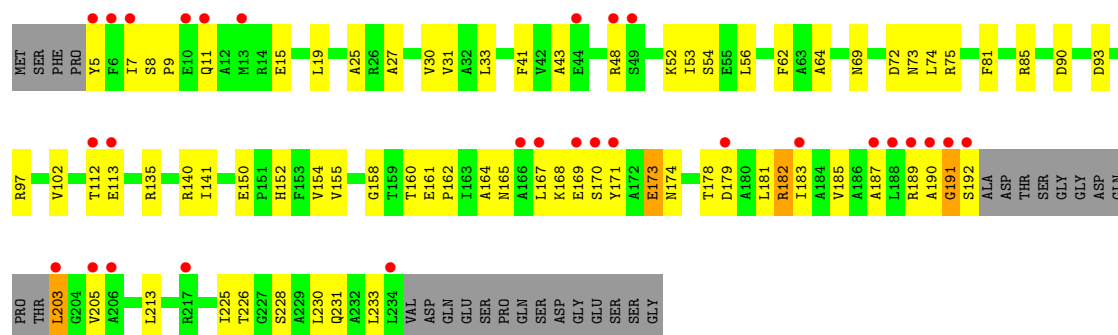
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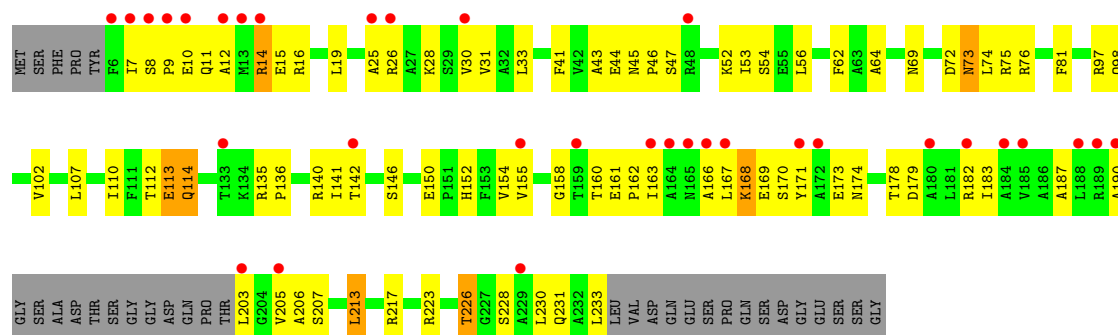
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	40	Total 40	O 40	0	0
5	N	154	Total 154	O 154	0	0
5	O	47	Total 47	O 47	0	0
5	P	139	Total 139	O 139	0	0
5	Q	38	Total 38	O 38	0	0
5	R	170	Total 170	O 170	0	0
5	S	42	Total 42	O 42	0	0
5	T	116	Total 116	O 116	0	0
5	U	49	Total 49	O 49	0	0
5	V	177	Total 177	O 177	0	0
5	W	35	Total 35	O 35	0	0
5	X	150	Total 150	O 150	0	0
5	Y	28	Total 28	O 28	0	0
5	Z	123	Total 123	O 123	0	0
5	1	47	Total 47	O 47	0	0
5	2	143	Total 143	O 143	0	0



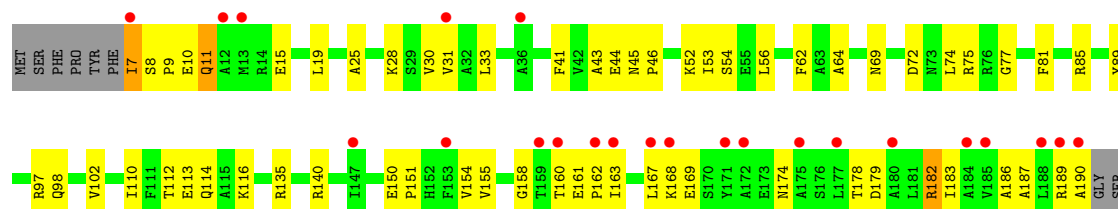
• Molecule 1: Proteasome subunit alpha

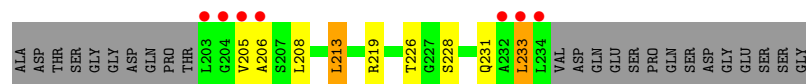


• Molecule 1: Proteasome subunit alpha

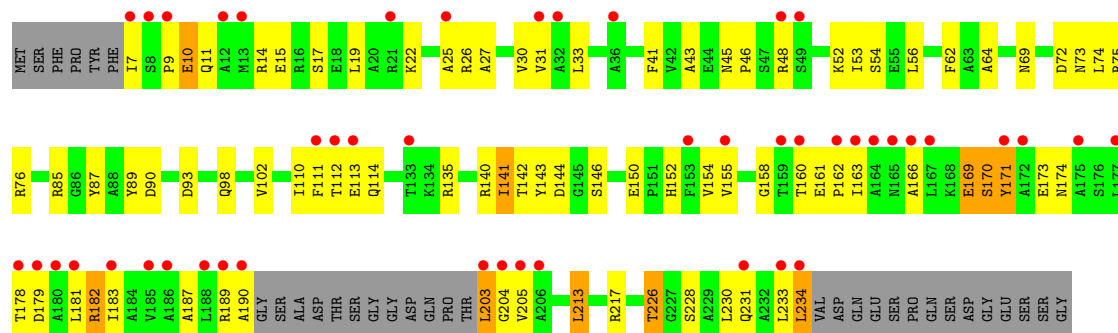


• Molecule 1: Proteasome subunit alpha

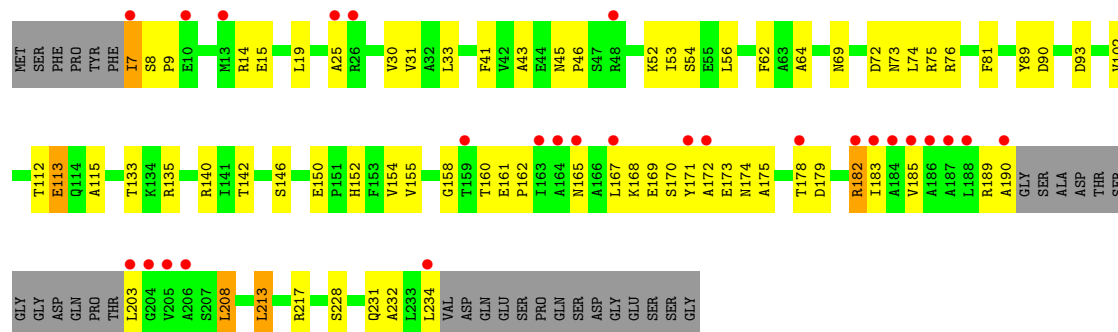




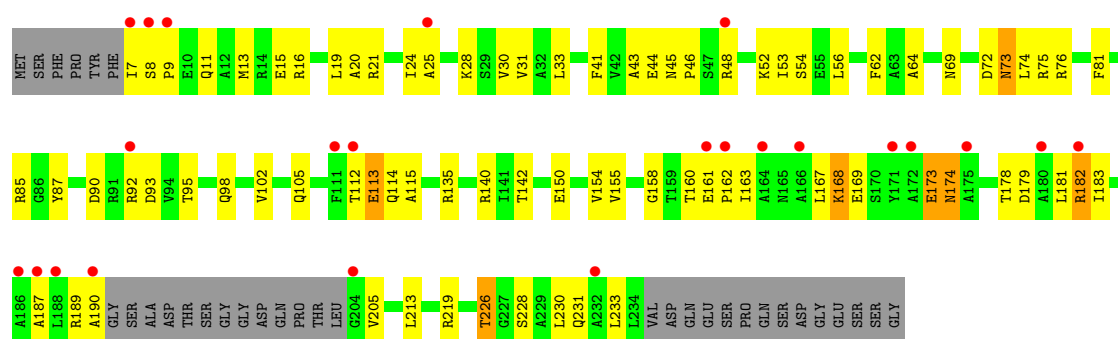
• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha

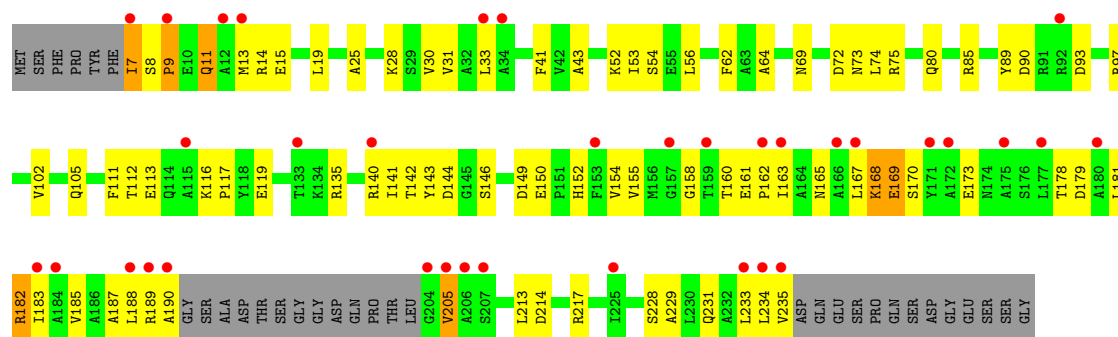


• Molecule 1: Proteasome subunit alpha

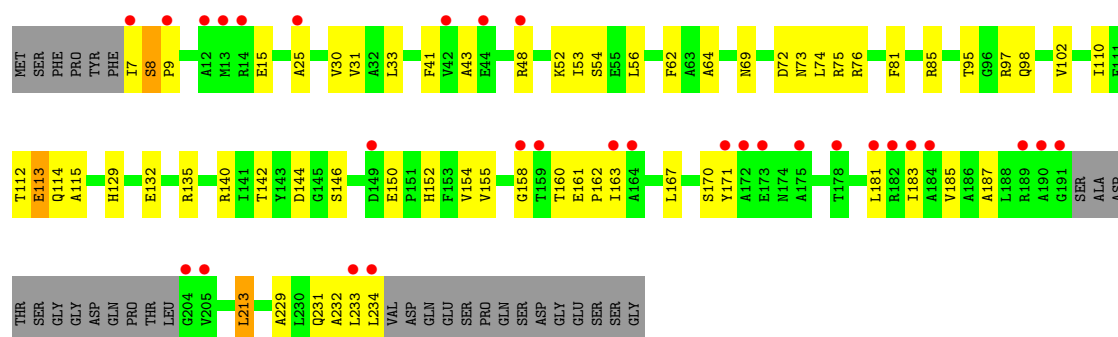


• Molecule 1: Proteasome subunit alpha

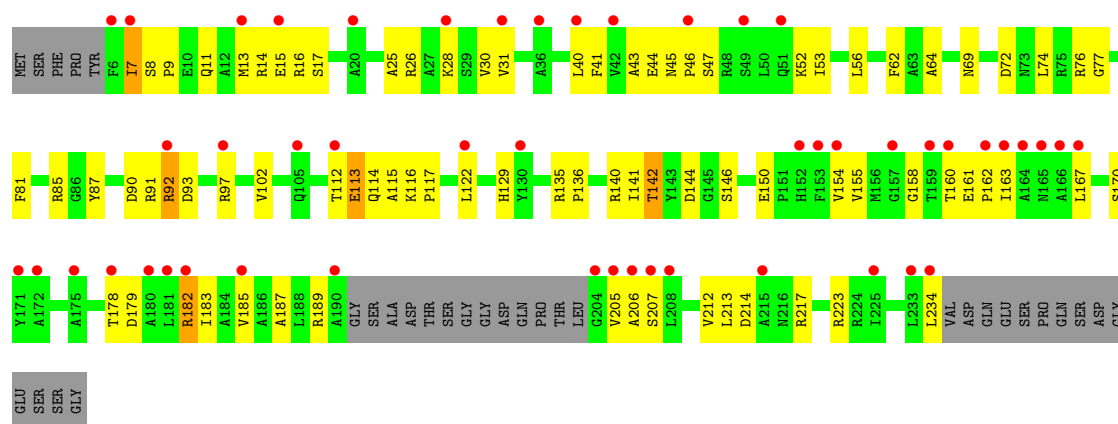




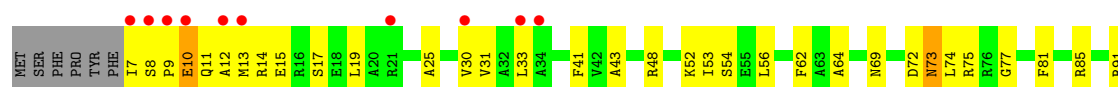
• Molecule 1: Proteasome subunit alpha

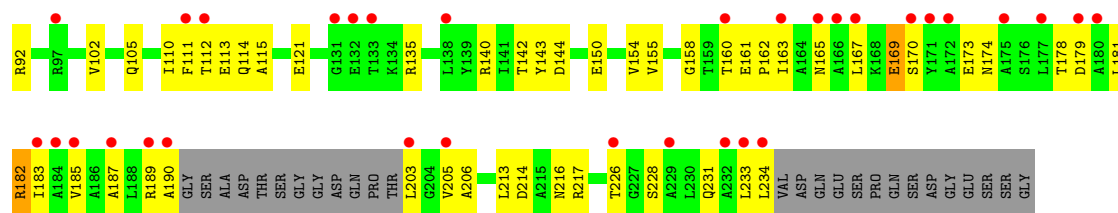


• Molecule 1: Proteasome subunit alpha

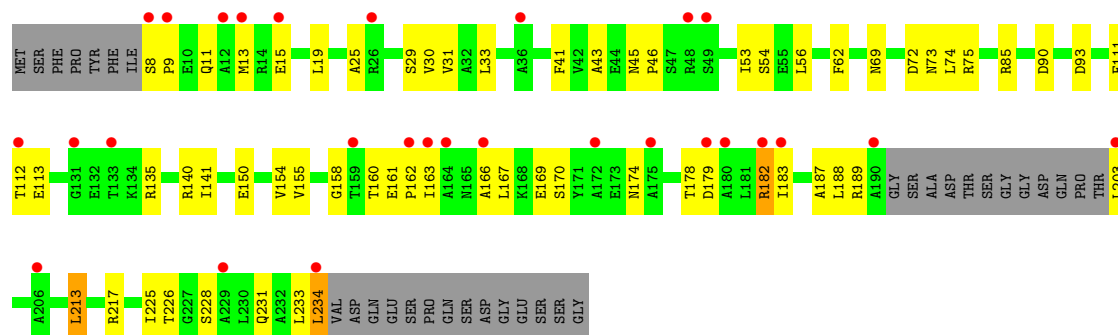


• Molecule 1: Proteasome subunit alpha

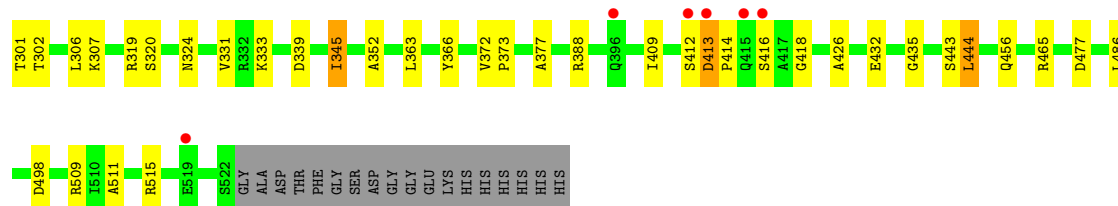
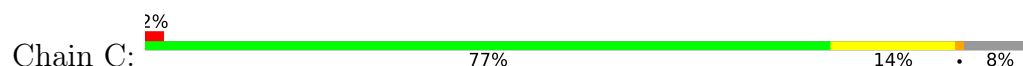




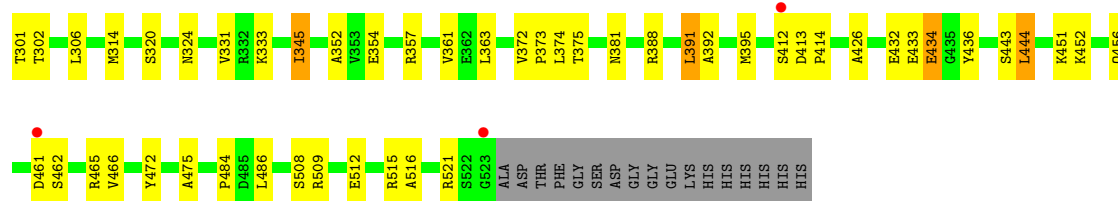
● Molecule 1: Proteasome subunit alpha



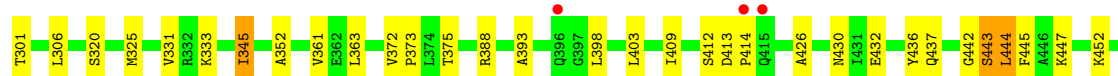
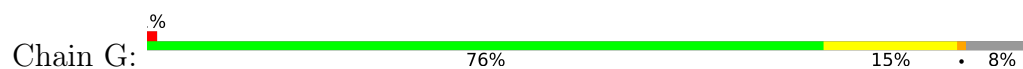
● Molecule 2: Proteasome subunit beta

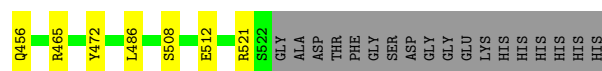


● Molecule 2: Proteasome subunit beta

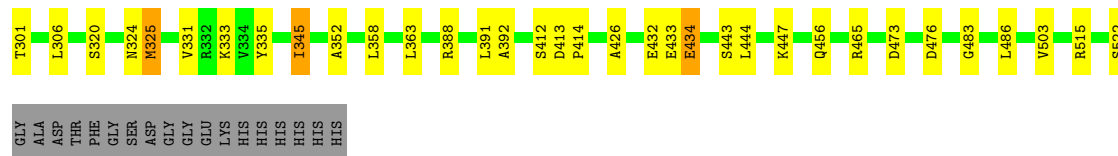
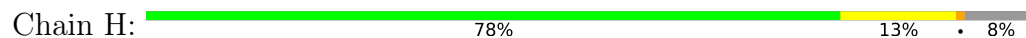


● Molecule 2: Proteasome subunit beta

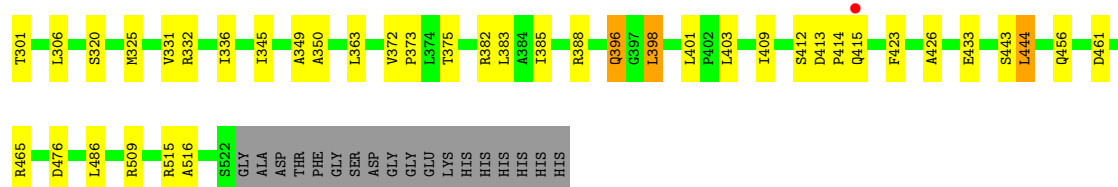




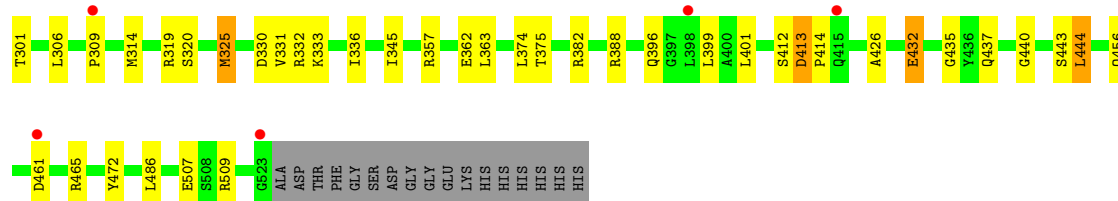
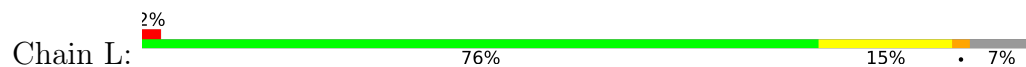
• Molecule 2: Proteasome subunit beta



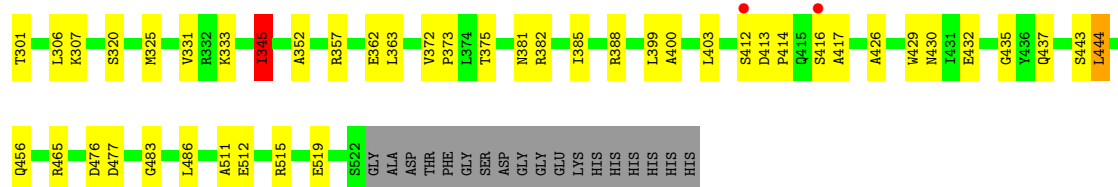
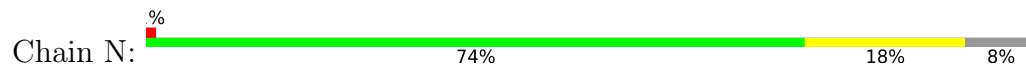
• Molecule 2: Proteasome subunit beta



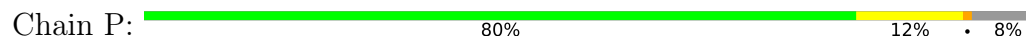
• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta



THR
PHE
GLY
SER
ASP
GLY
GLY
GLY
LYS
HIS
HIS
HIS
HIS
HIS

• Molecule 2: Proteasome subunit beta

Chain R:  2% 82% 15%

T301 L306 S320 G323 R324 V331 R332 T345 V351 R357 L363 K386 V387 R388 A394 L398 L399 L403 S412 D413 P414 A426 E433 Q442 S443 L444 F445 A446 K447 Q456 R465 D477 L486 I496 V505 R509

D525 D530 G531 G532 E533 K534 H535 H536 H537 H538 H539 HIS

• Molecule 2: Proteasome subunit beta

Chain T:  78% 14% 7%

T301 L306 M314 R319 S320 M325 V331 R332 V335 I336 I345 A349 A360 V361 E362 L363 R382 I385 R388 A392 L398 L403 S412 D413 P414 A426 A432 Q437 S443 L444 K452 L464 L486 R509

L513 G523 ASP THR PHE SER GLY GLY GLY LYS HIS HIS HIS HIS HIS HIS

• Molecule 2: Proteasome subunit beta

Chain V:  2% 82% 17%

T301 L306 M314 R319 S320 M325 V331 R332 K333 T345 E354 L363 A377 I380 N381 R382 R388 L391 A392 M395 L398 S412 D413 P414 A426 W429 W430 E433 E434 Q435 S443 L444 K451 Y472 D477 G483

L486 L496 D525 D530 G531 G532 E533 H538 H539 HIS

• Molecule 2: Proteasome subunit beta

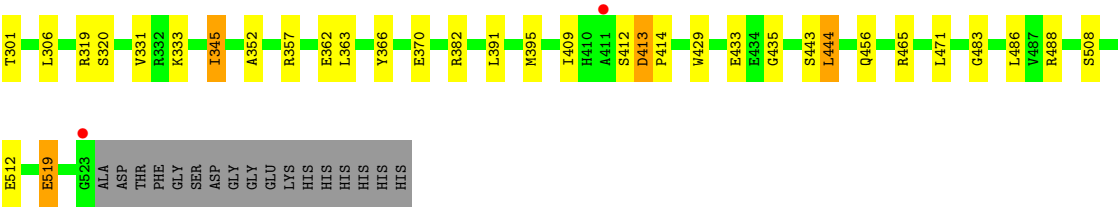
Chain X:  78% 15% 7%

T301 L306 M314 S320 V331 R332 I336 T345 A349 L358 E362 L363 Y366 E370 G371 V372 P373 R382 L383 A392 G397 I409 S412 D413 P414 Q415 W429 E434 Q435 S443 L444 K452 Q456 R465 D477

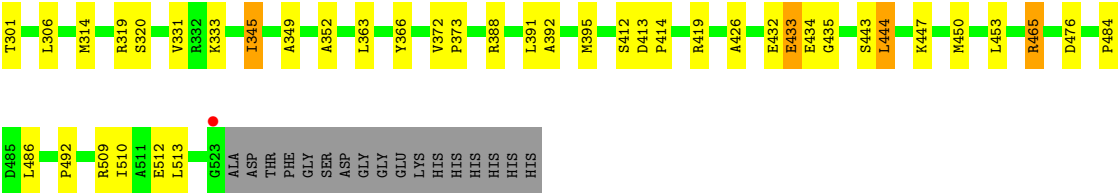
G483 L486 L496 E519 G523 ALA ASP THR PHE GLY SER ASP GLY GLY LYS HIS HIS HIS HIS HIS HIS

• Molecule 2: Proteasome subunit beta

Chain Z:  79% 12% 7%



● Molecule 2: Proteasome subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	170.37Å 118.44Å 195.25Å 90.00° 113.02° 90.00°	Depositor
Resolution (Å)	24.95 – 2.20 24.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.0 (24.95-2.20) 92.0 (24.95-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.11Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.234 0.205 , 0.234	Depositor DCC
R_{free} test set	18918 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	50080	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DMF, SA6

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	0.63	0/1683	0.99	3/2274 (0.1%)
1	A	0.58	0/1679	0.97	5/2268 (0.2%)
1	B	0.64	0/1668	0.99	4/2253 (0.2%)
1	D	0.55	0/1675	0.98	5/2263 (0.2%)
1	F	0.63	0/1726	1.00	4/2332 (0.2%)
1	I	0.62	0/1695	0.99	6/2290 (0.3%)
1	K	0.61	0/1691	0.99	6/2285 (0.3%)
1	M	0.61	0/1691	1.00	7/2285 (0.3%)
1	O	0.65	1/1691 (0.1%)	0.99	5/2285 (0.2%)
1	Q	0.58	0/1683	0.97	5/2274 (0.2%)
1	S	0.61	0/1690	1.00	4/2284 (0.2%)
1	U	0.60	0/1687	1.02	6/2279 (0.3%)
1	W	0.53	0/1695	0.96	2/2290 (0.1%)
1	Y	0.59	0/1691	1.04	6/2285 (0.3%)
2	2	0.83	2/1666 (0.1%)	1.05	6/2259 (0.3%)
2	C	0.89	0/1662	1.08	5/2254 (0.2%)
2	E	0.95	1/1666 (0.1%)	1.08	6/2259 (0.3%)
2	G	0.84	0/1662	1.05	5/2254 (0.2%)
2	H	0.90	2/1662 (0.1%)	1.06	4/2254 (0.2%)
2	J	0.89	0/1662	1.07	6/2254 (0.3%)
2	L	0.88	2/1666 (0.1%)	1.08	8/2259 (0.4%)
2	N	0.88	1/1662 (0.1%)	1.06	6/2254 (0.3%)
2	P	0.87	1/1662 (0.1%)	1.07	5/2254 (0.2%)
2	R	0.88	0/1797	1.09	7/2435 (0.3%)
2	T	0.85	2/1666 (0.1%)	1.06	6/2259 (0.3%)
2	V	0.88	1/1797 (0.1%)	1.05	6/2435 (0.2%)
2	X	0.83	1/1666 (0.1%)	1.07	6/2259 (0.3%)
2	Z	0.79	0/1666	1.03	5/2259 (0.2%)
All	All	0.75	14/47207 (0.0%)	1.03	149/63895 (0.2%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	314	MET	SD-CE	-8.32	1.58	1.79
1	O	7	ILE	C-N	7.92	1.44	1.33
2	L	325	MET	SD-CE	7.29	1.97	1.79
2	L	314	MET	SD-CE	-6.71	1.62	1.79
2	T	325	MET	SD-CE	6.42	1.95	1.79
2	N	325	MET	SD-CE	5.99	1.94	1.79
2	2	450	MET	SD-CE	5.71	1.93	1.79
2	X	314	MET	SD-CE	-5.58	1.65	1.79
2	H	325	MET	SD-CE	5.45	1.93	1.79
2	T	314	MET	SD-CE	-5.19	1.66	1.79
2	V	314	MET	SD-CE	-5.16	1.66	1.79
2	H	352	ALA	CA-CB	-5.12	1.45	1.53
2	P	325	MET	SD-CE	5.10	1.92	1.79
2	2	314	MET	SD-CE	-5.09	1.66	1.79

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	538	HIS	N-CA-C	-10.33	96.61	110.55
1	Y	169	GLU	N-CA-C	8.88	120.73	111.14
2	H	443	SER	N-CA-C	8.08	120.08	111.28
2	V	413	ASP	CA-C-N	7.83	128.25	119.32
2	V	413	ASP	C-N-CA	7.83	128.25	119.32
1	S	169	GLU	N-CA-C	7.62	119.67	111.36
2	E	413	ASP	CA-C-N	7.47	127.83	119.32
2	E	413	ASP	C-N-CA	7.47	127.83	119.32
2	T	413	ASP	CA-C-N	7.41	127.77	119.32
2	T	413	ASP	C-N-CA	7.41	127.77	119.32
2	2	413	ASP	CA-C-N	7.39	127.74	119.32
2	2	413	ASP	C-N-CA	7.39	127.74	119.32
2	G	413	ASP	CA-C-N	7.32	127.67	119.32
2	G	413	ASP	C-N-CA	7.32	127.67	119.32
2	X	413	ASP	CA-C-N	7.30	127.64	119.32
2	X	413	ASP	C-N-CA	7.30	127.64	119.32
2	P	413	ASP	CA-C-N	7.29	127.63	119.32
2	P	413	ASP	C-N-CA	7.29	127.63	119.32
1	M	170	SER	N-CA-C	7.28	119.29	111.36
2	H	413	ASP	CA-C-N	7.17	127.50	119.32
2	H	413	ASP	C-N-CA	7.17	127.50	119.32
2	R	413	ASP	CA-C-N	7.16	127.48	119.32
2	R	413	ASP	C-N-CA	7.16	127.48	119.32
2	C	413	ASP	CA-C-N	7.13	127.45	119.32
2	C	413	ASP	C-N-CA	7.13	127.45	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	413	ASP	CA-C-N	7.13	127.45	119.32
2	J	413	ASP	C-N-CA	7.13	127.45	119.32
2	L	413	ASP	CA-C-N	7.12	127.44	119.32
2	L	413	ASP	C-N-CA	7.12	127.44	119.32
2	N	413	ASP	CA-C-N	7.00	127.31	119.32
2	N	413	ASP	C-N-CA	7.00	127.31	119.32
2	Z	413	ASP	CA-C-N	7.00	127.30	119.32
2	Z	413	ASP	C-N-CA	7.00	127.30	119.32
1	Y	11	GLN	N-CA-C	-6.98	104.73	113.18
1	U	232	ALA	N-CA-C	6.97	118.53	111.07
1	Y	213	LEU	N-CA-C	-6.95	94.82	107.75
1	Q	72	ASP	N-CA-C	-6.87	103.88	111.36
1	F	72	ASP	N-CA-C	-6.76	103.98	111.82
2	N	443	SER	N-CA-C	6.63	118.51	111.28
2	X	383	LEU	N-CA-C	-6.61	104.00	111.14
2	V	443	SER	N-CA-C	6.59	118.46	111.28
1	I	213	LEU	N-CA-C	-6.53	95.60	107.75
1	I	72	ASP	N-CA-C	-6.53	104.25	111.82
1	K	213	LEU	N-CA-C	-6.53	95.61	107.75
1	K	116	LYS	CA-C-N	-6.46	113.64	120.03
1	K	116	LYS	C-N-CA	-6.46	113.64	120.03
1	B	72	ASP	N-CA-C	-6.43	104.35	111.36
1	O	72	ASP	N-CA-C	-6.42	104.36	111.36
1	S	168	LYS	N-CA-C	-6.41	104.29	111.28
1	U	72	ASP	N-CA-C	-6.36	104.43	111.36
2	X	349	ALA	N-CA-C	6.34	118.19	111.28
2	2	443	SER	N-CA-C	6.30	118.15	111.28
1	U	213	LEU	N-CA-C	-6.30	96.04	107.75
1	D	213	LEU	N-CA-C	-6.28	96.08	107.75
1	B	213	LEU	N-CA-C	-6.25	96.13	107.75
2	X	435	GLY	N-CA-C	6.23	122.34	114.25
1	M	72	ASP	N-CA-C	-6.22	104.58	111.36
1	Q	213	LEU	N-CA-C	-6.22	96.19	107.75
2	P	435	GLY	N-CA-C	6.18	122.28	114.25
1	M	213	LEU	N-CA-C	-6.16	96.29	107.75
1	W	213	LEU	N-CA-C	-6.13	96.34	107.75
1	A	213	LEU	N-CA-C	-6.13	96.34	107.75
1	O	213	LEU	N-CA-C	-6.13	96.34	107.75
1	F	213	LEU	N-CA-C	-6.10	97.20	107.99
1	S	72	ASP	N-CA-C	-6.09	104.72	111.36
1	1	213	LEU	N-CA-C	-6.08	96.44	107.75
1	F	27	ALA	N-CA-C	6.08	119.46	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	113	GLU	N-CA-C	6.07	120.82	113.41
2	Z	443	SER	N-CA-C	6.06	117.89	111.28
2	C	443	SER	N-CA-C	5.98	117.80	111.28
1	Y	72	ASP	N-CA-C	-5.92	104.91	111.36
1	D	11	GLN	N-CA-C	5.90	117.52	111.14
1	S	213	LEU	N-CA-C	-5.87	96.83	107.75
2	X	443	SER	N-CA-C	5.80	117.61	111.28
1	Q	168	LYS	N-CA-C	-5.78	105.33	112.38
2	E	443	SER	N-CA-C	5.72	117.51	111.28
1	1	72	ASP	N-CA-C	-5.71	105.19	111.82
2	P	443	SER	N-CA-C	5.67	118.23	111.71
2	L	336	ILE	N-CA-C	-5.65	100.18	108.54
1	M	171	TYR	N-CA-C	5.63	118.51	110.24
2	N	375	THR	N-CA-C	-5.61	103.12	110.53
1	D	168	LYS	N-CA-C	-5.60	105.54	112.38
2	E	462	SER	N-CA-C	-5.54	105.39	111.82
1	W	113	GLU	N-CA-C	5.54	120.31	113.50
1	A	72	ASP	N-CA-C	-5.49	105.45	111.82
2	R	399	LEU	N-CA-C	5.49	118.19	110.23
2	T	336	ILE	N-CA-C	-5.49	100.42	108.54
2	T	443	SER	N-CA-C	5.47	117.24	111.28
2	T	403	LEU	N-CA-C	-5.46	99.54	108.76
2	L	435	GLY	N-CA-C	5.45	121.33	114.25
2	E	375	THR	N-CA-C	-5.44	103.35	110.53
1	A	27	ALA	N-CA-C	5.43	118.13	110.14
2	E	391	LEU	N-CA-C	5.41	117.87	111.33
2	V	319	ARG	N-CA-C	5.40	118.74	110.20
1	F	226	THR	N-CA-C	5.40	116.48	108.86
1	I	168	LYS	N-CA-C	-5.40	104.84	111.75
1	1	29	SER	O-C-N	-5.39	116.90	123.10
2	P	336	ILE	N-CA-C	-5.39	99.99	108.23
1	K	72	ASP	N-CA-C	-5.37	105.51	111.36
1	Y	226	THR	N-CA-C	5.36	116.42	108.86
1	O	208	LEU	N-CA-C	5.35	117.95	109.50
1	D	72	ASP	N-CA-C	-5.34	105.62	111.82
1	K	168	LYS	N-CA-C	-5.34	105.87	112.38
2	J	375	THR	N-CA-C	-5.33	103.86	110.41
2	R	345	ILE	N-CA-C	5.32	116.38	108.46
1	B	226	THR	N-CA-C	5.31	116.35	108.86
1	Y	14	ARG	N-CA-C	5.31	116.88	111.14
2	2	435	GLY	N-CA-C	5.31	121.15	114.25
1	A	226	THR	N-CA-C	5.30	116.34	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	339	ASP	N-CA-C	5.27	117.78	111.71
2	L	319	ARG	N-CA-C	5.26	118.80	109.96
2	C	319	ARG	N-CA-C	5.26	118.79	109.96
1	I	14	ARG	N-CA-C	-5.25	105.24	110.97
2	R	443	SER	N-CA-C	5.25	117.75	111.71
2	G	375	THR	N-CA-C	-5.24	103.61	110.53
1	O	168	LYS	N-CA-C	-5.24	105.99	112.38
2	Z	319	ARG	N-CA-C	5.23	118.46	110.20
1	K	226	THR	N-CA-C	5.21	116.21	108.86
2	R	403	LEU	N-CA-C	-5.21	99.95	108.76
1	M	226	THR	N-CA-C	5.20	116.20	108.86
1	I	226	THR	N-CA-C	5.20	116.19	108.86
1	Q	113	GLU	N-CA-C	5.20	119.89	113.50
2	L	375	THR	N-CA-C	-5.20	103.67	110.53
2	H	345	ILE	N-CA-C	5.19	116.19	108.46
2	J	443	SER	N-CA-C	5.19	116.93	111.28
1	B	113	GLU	N-CA-C	5.18	119.87	113.50
1	M	27	ALA	N-CA-C	5.18	118.10	110.59
1	Q	226	THR	N-CA-C	5.18	116.16	108.86
1	I	113	GLU	N-CA-C	5.17	119.86	113.50
2	G	443	SER	N-CA-C	5.17	117.65	111.71
1	U	8	SER	CA-C-N	5.15	126.28	119.84
1	U	8	SER	C-N-CA	5.15	126.28	119.84
2	L	443	SER	N-CA-C	5.15	117.63	111.71
1	A	113	GLU	N-CA-C	5.11	119.78	113.50
2	2	319	ARG	N-CA-C	5.11	118.55	109.96
1	D	226	THR	N-CA-C	5.10	116.06	108.86
2	L	399	LEU	N-CA-C	5.10	117.70	110.10
2	J	403	LEU	N-CA-C	-5.09	100.15	108.76
2	G	403	LEU	N-CA-C	-5.09	100.60	108.90
1	M	204	GLY	N-CA-C	5.09	120.04	112.41
2	J	336	ILE	N-CA-C	-5.06	100.49	108.23
2	T	319	ARG	N-CA-C	5.05	118.45	109.96
2	N	345	ILE	N-CA-C	5.04	115.98	108.46
2	V	435	GLY	N-CA-C	5.03	120.68	114.69
2	V	391	LEU	N-CA-C	5.03	117.41	111.33
2	N	403	LEU	N-CA-C	-5.02	100.27	108.76
2	Z	435	GLY	N-CA-C	5.01	120.66	114.69
1	U	113	GLU	N-CA-C	5.00	119.66	113.50
2	2	349	ALA	N-CA-C	5.00	117.11	111.11

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	1658	0	1659	59	0
1	A	1654	0	1651	70	0
1	B	1643	0	1639	82	0
1	D	1650	0	1648	102	0
1	F	1699	0	1696	69	0
1	I	1669	0	1668	98	0
1	K	1666	0	1670	70	0
1	M	1666	0	1670	78	0
1	O	1666	0	1670	67	0
1	Q	1658	0	1659	84	0
1	S	1665	0	1668	90	0
1	U	1662	0	1662	52	0
1	W	1669	0	1668	71	0
1	Y	1666	0	1670	83	0
2	2	1642	0	1632	40	0
2	C	1638	0	1629	33	0
2	E	1642	0	1632	51	0
2	G	1638	0	1629	43	0
2	H	1638	0	1629	35	0
2	J	1638	0	1629	44	0
2	L	1642	0	1632	32	0
2	N	1638	0	1629	47	0
2	P	1638	0	1629	31	0
2	R	1767	0	1729	45	0
2	T	1642	0	1632	22	0
2	V	1767	0	1729	42	0
2	X	1642	0	1632	26	0
2	Z	1642	0	1632	25	0
3	1	5	0	7	0	0
3	2	40	0	56	28	0
3	A	10	0	14	1	0
3	B	10	0	14	2	0
3	C	35	0	49	16	0
3	D	25	0	35	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	30	0	42	16	0
3	F	15	0	21	1	0
3	G	45	0	63	31	0
3	H	30	0	42	12	0
3	I	10	0	14	2	0
3	J	15	0	21	7	0
3	K	20	0	28	11	0
3	L	20	0	28	5	0
3	M	20	0	28	0	0
3	N	25	0	35	26	0
3	O	15	0	21	1	0
3	P	40	0	56	14	0
3	Q	15	0	21	9	0
3	R	25	0	35	13	0
3	S	10	0	14	1	0
3	T	30	0	42	15	0
3	U	10	0	14	8	0
3	V	45	0	63	47	0
3	W	10	0	14	7	0
3	X	25	0	35	8	0
3	Y	15	0	21	4	0
3	Z	20	0	28	8	0
4	2	20	0	22	4	0
4	C	20	0	22	3	0
4	E	20	0	22	3	0
4	G	20	0	22	3	0
4	H	20	0	22	5	0
4	J	20	0	22	2	0
4	L	20	0	22	3	0
4	N	20	0	22	3	0
4	P	20	0	22	4	0
4	R	20	0	22	3	0
4	T	20	0	22	3	0
4	V	20	0	22	4	0
4	X	20	0	22	4	0
4	Z	20	0	22	3	0
5	1	47	0	0	1	0
5	2	143	0	0	7	0
5	A	43	0	0	4	0
5	B	41	0	0	6	0
5	C	163	0	0	10	0
5	D	40	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	166	0	0	9	0
5	F	58	0	0	4	0
5	G	131	0	0	2	0
5	H	148	0	0	7	0
5	I	52	0	0	9	0
5	J	142	0	0	10	0
5	K	45	0	0	5	0
5	L	153	0	0	12	0
5	M	40	0	0	4	0
5	N	154	0	0	6	0
5	O	47	0	0	4	0
5	P	139	0	0	6	0
5	Q	38	0	0	9	0
5	R	170	0	0	7	0
5	S	42	0	0	8	0
5	T	116	0	0	7	0
5	U	49	0	0	4	0
5	V	177	0	0	14	0
5	W	35	0	0	4	0
5	X	150	0	0	7	0
5	Y	28	0	0	6	0
5	Z	123	0	0	4	0
All	All	50080	0	47491	1555	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 16.

All (1555) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ILE:HG21	1:B:11:GLN:CG	1.63	1.27
1:F:7:ILE:CG2	1:F:11:GLN:HB3	1.65	1.27
1:A:80:GLN:HE21	1:A:80:GLN:C	1.45	1.24
3:R:92:DMF:H21	5:R:1869:HOH:O	1.30	1.23
1:O:9:PRO:HD2	1:U:15:GLU:CG	1.69	1.21
1:D:8:SER:HB3	1:D:9:PRO:CD	1.73	1.19
1:D:207:SER:O	1:D:208:LEU:HD23	1.41	1.17
3:N:90:DMF:C2	3:V:120:DMF:H11	1.73	1.17
1:Y:7:ILE:HG13	1:Y:8:SER:N	1.52	1.15
3:N:90:DMF:H22	3:V:120:DMF:H11	1.18	1.15
1:Y:13:MET:CE	1:Y:111:PHE:HE2	1.61	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:250:DMF:H23	3:V:27:DMF:H12	1.27	1.13
1:Y:7:ILE:HG13	1:Y:8:SER:H	0.96	1.13
1:B:7:ILE:CG2	1:B:11:GLN:HG2	1.78	1.12
2:Z:456:GLN:NE2	2:Z:465:ARG:HH22	1.48	1.11
2:N:432:GLU:OE1	3:N:104:DMF:H12	1.47	1.11
1:O:9:PRO:HD2	1:U:15:GLU:HG2	1.16	1.10
3:V:83:DMF:H11	5:V:1742:HOH:O	1.51	1.10
1:D:152:HIS:HB3	1:D:171:TYR:CE1	1.88	1.09
1:Y:13:MET:HE1	1:Y:111:PHE:HE2	1.11	1.09
1:Y:13:MET:HE1	1:Y:111:PHE:CE2	1.88	1.08
1:B:7:ILE:HG21	1:B:11:GLN:HG2	1.22	1.07
2:2:434:GLU:HB2	3:2:4:DMF:H23	1.35	1.06
3:G:12:DMF:H11	5:G:2627:HOH:O	1.53	1.06
2:E:461:ASP:HB2	5:E:1924:HOH:O	1.55	1.05
1:Q:7:ILE:CG2	1:Q:11:GLN:CB	2.35	1.05
1:I:203:LEU:HB3	1:I:207:SER:OG	1.57	1.05
1:D:174:ASN:N	1:D:174:ASN:HD22	1.55	1.03
3:U:250:DMF:H23	3:V:27:DMF:C1	1.89	1.02
2:P:452:LYS:HB3	3:P:33:DMF:H22	1.40	1.02
1:Q:7:ILE:CG2	1:Q:11:GLN:HB2	1.90	1.01
2:G:447:LYS:HD2	3:G:119:DMF:H23	1.43	1.01
1:D:8:SER:HB3	1:D:9:PRO:HD2	1.42	1.00
2:N:432:GLU:OE2	3:N:104:DMF:H23	1.62	0.99
1:Y:7:ILE:CG1	1:Y:8:SER:H	1.72	0.99
2:H:483:GLY:HA3	3:H:91:DMF:H22	1.44	0.99
1:K:15:GLU:HG2	1:M:9:PRO:HD2	1.42	0.99
3:N:90:DMF:H22	3:V:120:DMF:C1	1.92	0.98
1:D:8:SER:CB	1:D:9:PRO:HD3	1.94	0.97
3:N:22:DMF:HC	5:N:2569:HOH:O	1.64	0.97
1:B:7:ILE:N	1:B:7:ILE:HD12	1.78	0.97
2:N:429:TRP:CZ2	3:N:93:DMF:HC	1.98	0.97
1:A:161:GLU:HB2	1:A:162:PRO:HD3	1.47	0.97
3:C:103:DMF:H11	5:C:1438:HOH:O	1.64	0.97
5:P:223:HOH:O	3:V:82:DMF:HC	1.65	0.97
1:D:185:VAL:HG21	1:D:234:LEU:HD11	1.45	0.97
1:Q:7:ILE:HG22	1:Q:11:GLN:HB2	1.44	0.97
1:Q:161:GLU:HB2	1:Q:162:PRO:HD3	1.46	0.97
1:D:8:SER:CB	1:D:9:PRO:CD	2.40	0.96
1:I:15:GLU:HG3	1:S:9:PRO:HB2	1.47	0.96
1:S:161:GLU:HB2	1:S:162:PRO:HD3	1.48	0.96
3:N:90:DMF:C2	3:V:120:DMF:C1	2.43	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:161:GLU:HB2	1:W:162:PRO:HD3	1.48	0.95
1:Q:8:SER:HB3	1:Y:15:GLU:OE2	1.67	0.95
1:I:10:GLU:O	1:I:14:ARG:HG3	1.66	0.95
1:O:161:GLU:HB2	1:O:162:PRO:HD3	1.49	0.95
1:Q:7:ILE:CG2	1:Q:11:GLN:HB3	1.97	0.95
1:1:161:GLU:HB2	1:1:162:PRO:HD3	1.49	0.95
2:G:447:LYS:HD2	3:G:119:DMF:C2	1.95	0.95
2:T:362:GLU:OE2	2:T:382:ARG:HD3	1.67	0.94
1:M:161:GLU:HB2	1:M:162:PRO:HD3	1.48	0.94
1:U:161:GLU:HB2	1:U:162:PRO:HD3	1.49	0.94
2:E:456:GLN:HE21	2:E:465:ARG:NH2	1.66	0.94
1:K:161:GLU:HB2	1:K:162:PRO:HD3	1.49	0.94
1:Y:161:GLU:HB2	1:Y:162:PRO:HD3	1.49	0.94
1:D:161:GLU:HB2	1:D:162:PRO:HD3	1.48	0.94
1:F:9:PRO:HG2	1:M:15:GLU:HG3	1.48	0.94
1:F:7:ILE:HG22	1:F:11:GLN:HB3	1.46	0.93
1:B:7:ILE:CG2	1:B:11:GLN:CG	2.41	0.93
3:C:103:DMF:H13	2:H:447:LYS:NZ	1.83	0.93
1:B:161:GLU:HB2	1:B:162:PRO:HD3	1.51	0.93
2:E:456:GLN:HE21	2:E:465:ARG:HH21	1.12	0.93
1:A:166:ALA:O	1:A:169:GLU:HG2	1.68	0.93
1:F:161:GLU:HB2	1:F:162:PRO:HD3	1.49	0.93
2:E:436:TYR:CE1	3:E:75:DMF:H22	2.03	0.92
3:U:250:DMF:H12	3:V:27:DMF:H11	1.51	0.92
2:Z:456:GLN:HE21	2:Z:465:ARG:NH2	1.67	0.92
1:I:161:GLU:HB2	1:I:162:PRO:HD3	1.50	0.91
2:J:515:ARG:HH22	2:R:539:HIS:HB2	1.35	0.91
1:D:15:GLU:HG3	1:K:9:PRO:HG2	1.51	0.91
1:F:7:ILE:CG2	1:F:11:GLN:CB	2.49	0.90
1:I:44:GLU:HG3	1:I:203:LEU:HD21	1.52	0.90
2:N:307:LYS:HD2	2:V:530:ASP:OD1	1.70	0.90
3:W:250:DMF:H23	3:X:16:DMF:H23	1.51	0.90
2:2:434:GLU:CB	3:2:4:DMF:H23	2.00	0.90
1:D:8:SER:HB3	1:D:9:PRO:HD3	1.50	0.90
2:P:472:TYR:CE1	3:P:14:DMF:H12	2.07	0.90
2:Z:456:GLN:HE21	2:Z:465:ARG:HH22	0.94	0.90
2:G:445:PHE:CD2	3:G:64:DMF:H12	2.07	0.89
1:K:7:ILE:HG23	1:K:11:GLN:HB3	1.54	0.89
2:N:362:GLU:OE2	2:N:382:ARG:HD3	1.71	0.89
1:F:7:ILE:HG21	1:F:11:GLN:HB3	1.52	0.89
1:O:9:PRO:CD	1:U:15:GLU:HG2	2.01	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:30:VAL:HG13	1:W:43:ALA:HB2	1.55	0.89
2:G:447:LYS:CD	3:G:119:DMF:H23	2.03	0.89
1:Y:7:ILE:CG1	1:Y:8:SER:N	2.30	0.89
1:A:182:ARG:HH12	1:A:234:LEU:C	1.79	0.89
3:G:111:DMF:HC	5:2:807:HOH:O	1.73	0.89
1:A:80:GLN:C	1:A:80:GLN:NE2	2.30	0.89
2:R:325:MET:HE1	2:Z:444:LEU:HD11	1.56	0.88
1:B:15:GLU:HG3	1:I:9:PRO:HG2	1.55	0.88
2:H:456:GLN:NE2	2:H:465:ARG:HH21	1.72	0.88
1:D:225:ILE:HA	5:D:2295:HOH:O	1.72	0.87
1:S:152:HIS:HE1	1:S:173:GLU:OE2	1.56	0.87
1:K:186:ALA:O	1:K:189:ARG:HG2	1.75	0.87
1:B:233:LEU:HD12	1:B:233:LEU:N	1.89	0.86
2:E:456:GLN:NE2	2:E:465:ARG:HH21	1.74	0.86
1:O:9:PRO:HD2	1:U:15:GLU:HG3	1.56	0.86
1:Y:13:MET:CE	1:Y:111:PHE:CE2	2.50	0.86
2:2:465:ARG:HG3	2:2:465:ARG:HH11	1.37	0.86
2:R:456:GLN:HE21	2:R:465:ARG:HH21	1.24	0.86
1:B:7:ILE:CG2	1:B:11:GLN:HB3	2.05	0.86
2:J:456:GLN:NE2	2:J:465:ARG:HH21	1.73	0.86
3:T:113:DMF:H11	3:2:112:DMF:O	1.76	0.86
2:J:515:ARG:NH2	2:R:539:HIS:HB2	1.91	0.85
1:B:206:ALA:O	1:B:207:SER:OG	1.93	0.85
1:D:170:SER:HB2	1:D:183:ILE:HG23	1.56	0.85
2:J:515:ARG:NH1	2:R:539:HIS:H	1.74	0.85
1:1:30:VAL:HG13	1:1:43:ALA:HB2	1.58	0.85
2:E:381:ASN:HB2	3:E:53:DMF:H13	1.58	0.85
2:E:521:ARG:HD3	3:E:100:DMF:H12	1.58	0.85
2:N:456:GLN:HE21	2:N:465:ARG:HH21	1.18	0.85
1:O:189:ARG:CG	1:O:203:LEU:CD2	2.55	0.84
2:N:456:GLN:NE2	2:N:465:ARG:HH21	1.75	0.84
2:P:456:GLN:NE2	2:P:465:ARG:HH21	1.74	0.84
2:H:456:GLN:HE21	2:H:465:ARG:HH21	1.23	0.84
5:L:1466:HOH:O	3:P:33:DMF:HC	1.77	0.84
3:U:250:DMF:C2	3:V:27:DMF:C1	2.55	0.84
1:I:203:LEU:HB3	1:I:207:SER:HG	1.36	0.84
1:Y:25:ALA:O	1:Y:158:GLY:HA2	1.77	0.84
2:C:456:GLN:NE2	2:C:465:ARG:HH21	1.75	0.84
3:E:20:DMF:H21	5:E:2349:HOH:O	1.78	0.84
1:M:230:LEU:O	1:M:234:LEU:HD22	1.78	0.83
3:T:113:DMF:H11	3:2:112:DMF:C	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:163:ILE:HG23	1:U:187:ALA:O	1.79	0.83
3:V:83:DMF:H13	3:2:4:DMF:HC	1.58	0.83
1:B:15:GLU:CG	1:I:9:PRO:HG2	2.08	0.83
1:Y:10:GLU:OE1	1:Y:10:GLU:HA	1.79	0.83
1:D:13:MET:HE3	1:Q:19:LEU:HD11	1.60	0.83
1:B:7:ILE:CG2	1:B:11:GLN:CB	2.56	0.82
1:D:182:ARG:HD2	1:D:234:LEU:HD23	1.60	0.82
2:P:452:LYS:HB3	3:P:33:DMF:C2	2.07	0.82
1:D:152:HIS:HB3	1:D:171:TYR:CZ	2.13	0.82
1:S:142:THR:OG1	1:S:146:SER:HB2	1.80	0.82
1:A:27:ALA:HB1	5:A:1907:HOH:O	1.78	0.82
3:V:83:DMF:C1	3:2:4:DMF:HC	2.09	0.82
1:D:109:THR:N	3:D:251:DMF:H22	1.95	0.82
1:I:102:VAL:HG12	3:I:250:DMF:H12	1.62	0.82
1:Q:7:ILE:HG23	1:Q:11:GLN:CB	2.10	0.82
1:Q:226:THR:HG22	5:Q:959:HOH:O	1.79	0.81
1:Q:13:MET:HG3	1:Y:19:LEU:HD11	1.61	0.81
1:D:25:ALA:O	1:D:158:GLY:HA2	1.81	0.81
2:C:456:GLN:HE21	2:C:465:ARG:HH21	1.27	0.81
1:I:217:ARG:NH1	1:I:223:ARG:HD3	1.94	0.81
2:G:447:LYS:CD	3:G:119:DMF:C2	2.58	0.80
1:I:15:GLU:HG2	1:S:9:PRO:HD2	1.64	0.80
2:E:472:TYR:CE1	3:E:20:DMF:H12	2.16	0.80
2:P:444:LEU:HB3	5:P:926:HOH:O	1.80	0.80
2:R:445:PHE:CD2	3:R:59:DMF:H12	2.16	0.79
2:R:456:GLN:NE2	2:R:465:ARG:HH21	1.80	0.79
3:W:250:DMF:C2	5:X:2517:HOH:O	2.30	0.79
2:E:521:ARG:HD3	3:E:100:DMF:C1	2.13	0.79
2:C:301:THR:N	4:C:300:SA6:HO6	1.80	0.79
2:L:432:GLU:HG3	5:L:2512:HOH:O	1.82	0.79
1:I:25:ALA:O	1:I:158:GLY:HA2	1.82	0.79
1:B:7:ILE:HG22	1:B:11:GLN:HB3	1.61	0.79
2:X:496:ILE:HG21	3:X:40:DMF:H13	1.63	0.79
2:N:432:GLU:OE1	3:N:104:DMF:C1	2.29	0.79
1:B:7:ILE:HG21	1:B:11:GLN:CB	2.13	0.78
2:J:396:GLN:OE1	2:J:396:GLN:HA	1.80	0.78
3:C:103:DMF:C	3:H:43:DMF:H22	2.13	0.78
2:E:324:ASN:HB2	5:E:2164:HOH:O	1.82	0.78
1:B:15:GLU:HG2	1:I:9:PRO:HD2	1.64	0.78
3:C:103:DMF:H13	2:H:447:LYS:HZ1	1.46	0.78
2:N:430:ASN:HB2	5:N:2370:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLU:HB3	1:B:9:PRO:HG2	1.66	0.78
2:L:362:GLU:OE2	2:L:382:ARG:HD3	1.84	0.77
1:S:152:HIS:CE1	1:S:173:GLU:OE2	2.37	0.77
2:N:388:ARG:HD3	2:N:426:ALA:O	1.84	0.77
2:G:430:ASN:ND2	3:G:98:DMF:C	2.48	0.77
1:S:15:GLU:HG3	1:I:9:PRO:HD2	1.65	0.77
1:W:74:LEU:HD23	1:W:122:LEU:HD11	1.66	0.77
2:J:456:GLN:HE21	2:J:465:ARG:HH21	1.29	0.77
1:D:173:GLU:HB3	1:D:174:ASN:ND2	1.99	0.77
2:T:335:TYR:HB3	3:T:29:DMF:H13	1.66	0.77
2:G:456:GLN:NE2	2:G:465:ARG:HH21	1.83	0.77
1:A:230:LEU:O	1:A:234:LEU:HD22	1.84	0.77
1:B:22:LYS:HD2	1:I:10:GLU:OE2	1.84	0.77
1:Q:181:LEU:HD23	1:Q:233:LEU:HB3	1.66	0.77
2:2:509:ARG:HH12	3:2:52:DMF:C	1.97	0.77
2:T:362:GLU:OE2	2:T:382:ARG:CD	2.32	0.76
2:E:456:GLN:NE2	2:E:465:ARG:NH2	2.30	0.76
1:W:142:THR:OG1	1:W:146:SER:HB2	1.86	0.76
1:I:110:ILE:HG23	1:I:114:GLN:HG3	1.68	0.76
1:S:15:GLU:CD	1:I:8:SER:HB3	2.10	0.76
1:M:231:GLN:O	1:M:234:LEU:HD23	1.84	0.76
2:E:508:SER:OG	3:E:73:DMF:H13	1.86	0.75
1:D:207:SER:O	1:D:208:LEU:CD2	2.30	0.75
2:L:362:GLU:OE2	2:L:382:ARG:CD	2.35	0.75
1:O:189:ARG:CG	1:O:203:LEU:HD21	2.16	0.75
1:O:189:ARG:HG3	1:O:203:LEU:CD2	2.17	0.75
2:P:456:GLN:HE21	2:P:465:ARG:HH21	1.32	0.75
2:Z:483:GLY:HA3	3:Z:18:DMF:H22	1.67	0.75
2:V:429:TRP:CH2	3:V:42:DMF:H13	2.22	0.74
2:N:477:ASP:OD1	3:N:118:DMF:H12	1.88	0.74
2:V:483:GLY:HA3	3:V:116:DMF:H23	1.69	0.74
1:Y:30:VAL:HG13	1:Y:43:ALA:HB2	1.69	0.74
2:G:361:VAL:HG12	3:G:62:DMF:HC	1.70	0.74
3:U:250:DMF:C1	3:V:27:DMF:H11	2.17	0.74
1:Y:10:GLU:CD	1:Y:10:GLU:O	2.30	0.74
1:I:97:ARG:CZ	5:I:2433:HOH:O	2.36	0.74
1:M:87:TYR:O	2:N:357:ARG:NH1	2.20	0.74
2:P:456:GLN:HE21	2:P:465:ARG:NH2	1.86	0.74
1:Y:181:LEU:HD23	1:Y:233:LEU:HG	1.69	0.73
2:C:388:ARG:HD3	2:C:426:ALA:O	1.88	0.73
2:J:456:GLN:HE21	2:J:465:ARG:NH2	1.85	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:7:ILE:HD11	1:W:8:SER:HB2	1.70	0.73
5:Q:2679:HOH:O	3:Z:54:DMF:C	2.36	0.73
1:D:209:GLU:HA	5:D:2415:HOH:O	1.89	0.73
1:D:217:ARG:HG2	1:D:220:ARG:O	1.88	0.73
1:F:7:ILE:HG21	1:F:11:GLN:CB	2.14	0.73
1:M:25:ALA:O	1:M:158:GLY:HA2	1.88	0.73
2:T:326:ILE:O	3:T:115:DMF:H21	1.88	0.73
2:E:434:GLU:HB3	3:E:75:DMF:H21	1.70	0.73
1:F:170:SER:OG	1:F:183:ILE:HG23	1.88	0.73
3:W:250:DMF:H22	5:X:2517:HOH:O	1.89	0.73
1:F:7:ILE:HG21	1:F:11:GLN:CG	2.19	0.73
2:H:335:TYR:CE1	3:H:66:DMF:HC	2.24	0.73
2:H:456:GLN:HE21	2:H:465:ARG:NH2	1.86	0.73
2:J:388:ARG:HD3	2:J:426:ALA:O	1.88	0.73
1:D:30:VAL:HG13	1:D:43:ALA:HB2	1.70	0.72
1:B:7:ILE:HG22	1:B:11:GLN:CB	2.18	0.72
2:N:362:GLU:OE2	2:N:382:ARG:CD	2.36	0.72
1:B:41:PHE:HB3	1:B:53:ILE:HD13	1.70	0.72
1:D:173:GLU:C	1:D:174:ASN:HD22	1.97	0.72
2:T:301:THR:N	4:T:300:SA6:HO6	1.88	0.72
1:B:223:ARG:HG2	5:B:2211:HOH:O	1.90	0.72
1:A:182:ARG:NH1	1:A:234:LEU:C	2.47	0.72
2:E:357:ARG:HA	3:E:28:DMF:HC	1.71	0.72
5:Q:2679:HOH:O	3:Z:54:DMF:HC	1.87	0.72
2:N:456:GLN:HE21	2:N:465:ARG:NH2	1.87	0.72
1:Y:10:GLU:OE1	1:Y:10:GLU:CA	2.37	0.72
1:I:203:LEU:HD23	1:I:207:SER:HB2	1.70	0.72
1:Q:13:MET:SD	3:Q:250:DMF:C1	2.78	0.72
1:K:25:ALA:O	1:K:158:GLY:HA2	1.89	0.72
1:S:30:VAL:HG13	1:S:43:ALA:HB2	1.72	0.72
1:W:185:VAL:HG12	1:W:189:ARG:NH2	2.03	0.72
2:C:456:GLN:HE21	2:C:465:ARG:NH2	1.87	0.71
1:D:8:SER:OG	1:D:9:PRO:HD3	1.89	0.71
1:Q:25:ALA:O	1:Q:158:GLY:HA2	1.90	0.71
1:I:15:GLU:CG	1:S:9:PRO:HB2	2.20	0.71
1:Q:7:ILE:HG22	1:Q:8:SER:N	2.04	0.71
1:S:97:ARG:NH2	5:S:1917:HOH:O	2.23	0.71
2:X:301:THR:N	4:X:300:SA6:HO6	1.88	0.71
1:W:25:ALA:O	1:W:158:GLY:HA2	1.89	0.71
1:D:174:ASN:N	1:D:174:ASN:ND2	2.30	0.71
1:K:30:VAL:HG13	1:K:43:ALA:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:8:SER:H	1:S:11:GLN:HB2	1.55	0.71
1:Y:214:ASP:OD1	1:Y:216:ASN:N	2.22	0.71
3:K:250:DMF:H11	5:L:1474:HOH:O	1.91	0.71
2:V:388:ARG:HD3	2:V:426:ALA:O	1.90	0.71
1:O:30:VAL:HG13	1:O:43:ALA:HB2	1.73	0.71
3:T:113:DMF:C1	3:2:112:DMF:O	2.39	0.71
1:U:30:VAL:HG13	1:U:43:ALA:HB2	1.72	0.71
2:H:335:TYR:CE1	3:H:66:DMF:C	2.74	0.71
1:M:189:ARG:NH1	1:M:203:LEU:N	2.38	0.71
2:2:331:VAL:HG11	4:2:300:SA6:H19	1.73	0.70
2:T:388:ARG:HD3	2:T:426:ALA:O	1.90	0.70
2:V:434:GLU:HB2	3:V:32:DMF:C2	2.21	0.70
1:A:163:ILE:HG23	1:A:187:ALA:C	2.17	0.70
1:D:105:GLN:HB2	5:D:1313:HOH:O	1.91	0.70
1:F:25:ALA:O	1:F:158:GLY:HA2	1.92	0.70
2:E:484:PRO:HD2	5:E:2667:HOH:O	1.90	0.70
2:J:465:ARG:HD2	3:J:123:DMF:HC	1.74	0.70
3:V:83:DMF:H22	2:2:447:LYS:NZ	2.07	0.70
1:Y:121:GLU:HG3	5:Y:2504:HOH:O	1.91	0.70
1:B:105:GLN:HB2	5:B:1751:HOH:O	1.92	0.70
1:U:41:PHE:HB3	1:U:53:ILE:HD13	1.73	0.70
2:Z:409:ILE:HG12	5:Z:1615:HOH:O	1.91	0.70
1:B:7:ILE:HG21	1:B:11:GLN:HG3	1.70	0.70
2:R:386:MET:HE2	5:R:2543:HOH:O	1.91	0.70
1:Y:92:ARG:NH1	5:Y:1747:HOH:O	2.24	0.70
1:A:25:ALA:O	1:A:158:GLY:HA2	1.91	0.69
1:F:9:PRO:CG	1:M:15:GLU:HG3	2.20	0.69
1:B:19:LEU:HD23	1:B:19:LEU:O	1.91	0.69
1:A:15:GLU:HB3	1:B:9:PRO:CG	2.21	0.69
1:M:41:PHE:HB3	1:M:53:ILE:HD13	1.74	0.69
1:Q:7:ILE:HG21	1:Q:11:GLN:HB3	1.74	0.69
1:1:189:ARG:HH12	1:1:203:LEU:N	1.89	0.69
2:E:466:VAL:HG23	5:E:2061:HOH:O	1.93	0.69
1:Q:21:ARG:HD2	5:Q:2238:HOH:O	1.93	0.69
1:A:30:VAL:HG13	1:A:43:ALA:HB2	1.75	0.69
1:D:8:SER:HB2	1:Q:7:ILE:HG13	1.72	0.69
1:W:28:LYS:HD2	1:W:44:GLU:CD	2.16	0.69
2:Z:519:GLU:HG3	5:Z:1992:HOH:O	1.92	0.69
1:B:30:VAL:HG13	1:B:43:ALA:HB2	1.73	0.69
1:B:233:LEU:HD12	1:B:233:LEU:H	1.57	0.69
1:I:226:THR:HG22	5:I:691:HOH:O	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:332:ARG:HD3	5:R:1572:HOH:O	1.92	0.69
1:1:11:GLN:HE21	1:1:11:GLN:HA	1.58	0.69
1:1:170:SER:HB2	1:1:183:ILE:HG23	1.73	0.69
2:E:301:THR:N	4:E:300:SA6:HO6	1.91	0.69
2:G:388:ARG:HD3	2:G:426:ALA:O	1.93	0.69
1:I:30:VAL:HG13	1:I:43:ALA:HB2	1.75	0.69
2:J:398:LEU:HD12	2:J:398:LEU:N	2.08	0.69
1:U:110:ILE:HG23	1:U:114:GLN:NE2	2.08	0.69
2:Z:456:GLN:NE2	2:Z:465:ARG:NH2	2.30	0.68
1:M:31:VAL:HG12	1:M:155:VAL:HG22	1.75	0.68
1:A:182:ARG:NH1	1:A:234:LEU:HA	2.08	0.68
1:Q:31:VAL:HG12	1:Q:155:VAL:HG22	1.75	0.68
1:W:77:GLY:HA3	3:W:249:DMF:H12	1.75	0.68
1:W:185:VAL:CG1	1:W:189:ARG:NH2	2.57	0.68
2:N:301:THR:N	4:N:300:SA6:HO6	1.92	0.68
2:R:445:PHE:CD2	3:R:59:DMF:C1	2.76	0.68
1:Y:31:VAL:HG12	1:Y:155:VAL:HG22	1.75	0.68
1:1:31:VAL:HG12	1:1:155:VAL:HG22	1.75	0.68
1:D:152:HIS:CG	1:D:171:TYR:CZ	2.82	0.68
1:K:41:PHE:HB3	1:K:53:ILE:HD13	1.74	0.68
1:K:114:GLN:OE1	3:K:252:DMF:C1	2.41	0.68
2:P:447:LYS:HD2	3:P:107:DMF:H23	1.76	0.68
2:X:331:VAL:HG11	4:X:300:SA6:H19	1.76	0.68
1:D:182:ARG:HD2	1:D:234:LEU:CD2	2.22	0.68
1:W:31:VAL:HG12	1:W:155:VAL:HG22	1.75	0.68
1:A:163:ILE:CG2	1:A:187:ALA:HB1	2.24	0.68
2:E:388:ARG:HD3	2:E:426:ALA:O	1.94	0.68
2:J:456:GLN:NE2	2:J:465:ARG:NH2	2.42	0.68
1:W:41:PHE:HB3	1:W:53:ILE:HD13	1.76	0.68
3:C:103:DMF:C1	2:H:447:LYS:NZ	2.57	0.67
1:Q:7:ILE:HG23	1:Q:11:GLN:HB3	1.71	0.67
2:X:456:GLN:NE2	2:X:465:ARG:HH21	1.92	0.67
1:F:30:VAL:HG13	1:F:43:ALA:HB2	1.76	0.67
1:Y:41:PHE:HB3	1:Y:53:ILE:HD13	1.77	0.67
1:F:8:SER:HB2	1:M:15:GLU:HG2	1.77	0.67
1:K:97:ARG:NH1	5:K:1987:HOH:O	2.28	0.67
2:P:456:GLN:NE2	2:P:465:ARG:NH2	2.42	0.67
2:X:456:GLN:HE21	2:X:465:ARG:HH21	1.41	0.67
1:O:173:GLU:HG2	1:O:174:ASN:OD1	1.94	0.67
2:R:456:GLN:HE21	2:R:465:ARG:NH2	1.91	0.67
1:U:142:THR:OG1	1:U:146:SER:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:388:ARG:HD3	2:H:426:ALA:O	1.95	0.67
1:U:9:PRO:HG2	1:1:15:GLU:HG3	1.76	0.67
1:Y:165:ASN:O	1:Y:169:GLU:HG2	1.95	0.67
1:K:7:ILE:CG1	1:K:11:GLN:HG2	2.25	0.67
1:S:31:VAL:HG12	1:S:155:VAL:HG22	1.75	0.67
1:D:11:GLN:O	1:D:15:GLU:HB2	1.94	0.66
3:K:250:DMF:C1	5:L:1474:HOH:O	2.43	0.66
1:D:31:VAL:HG12	1:D:155:VAL:HG22	1.76	0.66
2:L:461:ASP:OD1	2:L:509:ARG:NH1	2.28	0.66
2:R:388:ARG:HD3	2:R:426:ALA:O	1.93	0.66
1:A:185:VAL:O	1:A:189:ARG:HG3	1.94	0.66
2:V:434:GLU:HB2	3:V:32:DMF:H22	1.76	0.66
5:D:980:HOH:O	1:K:112:THR:HG21	1.96	0.66
2:Z:429:TRP:CH2	3:Z:54:DMF:H22	2.31	0.66
1:I:15:GLU:HG2	1:S:9:PRO:CD	2.26	0.66
1:O:189:ARG:HG3	1:O:203:LEU:HD21	1.75	0.66
1:Q:41:PHE:HB3	1:Q:53:ILE:HD13	1.76	0.66
1:U:31:VAL:HG12	1:U:155:VAL:HG22	1.75	0.66
2:G:472:TYR:CE1	3:G:12:DMF:H22	2.30	0.66
2:H:515:ARG:HD2	5:H:542:HOH:O	1.94	0.66
1:K:219:ARG:CZ	3:K:250:DMF:H21	2.25	0.66
1:I:47:SER:HB2	5:S:1142:HOH:O	1.96	0.66
2:V:331:VAL:HG11	4:V:300:SA6:H19	1.76	0.66
2:L:331:VAL:HG11	4:L:300:SA6:H19	1.76	0.66
2:P:331:VAL:HG11	4:P:300:SA6:H19	1.78	0.66
2:P:388:ARG:HD3	2:P:426:ALA:O	1.96	0.66
3:U:250:DMF:C2	3:V:27:DMF:H12	2.12	0.66
1:O:25:ALA:O	1:O:158:GLY:HA2	1.96	0.65
1:O:189:ARG:HG2	1:O:203:LEU:CD2	2.26	0.65
1:S:8:SER:O	1:S:11:GLN:N	2.29	0.65
1:B:15:GLU:CG	1:I:9:PRO:HD2	2.25	0.65
1:B:226:THR:HB	5:B:1186:HOH:O	1.96	0.65
1:K:102:VAL:CG2	3:K:251:DMF:HC	2.26	0.65
1:M:141:ILE:N	1:M:141:ILE:HD12	2.11	0.65
1:B:7:ILE:HG22	1:B:8:SER:H	1.60	0.65
2:P:472:TYR:CD1	3:P:14:DMF:H12	2.31	0.65
2:G:445:PHE:CD2	3:G:64:DMF:C1	2.78	0.65
1:O:189:ARG:HG2	1:O:203:LEU:HD21	1.78	0.65
1:1:41:PHE:HB3	1:1:53:ILE:HD13	1.79	0.65
2:H:301:THR:N	4:H:300:SA6:HO6	1.95	0.65
1:M:30:VAL:HG13	1:M:43:ALA:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:436:TYR:O	3:G:119:DMF:H13	1.97	0.65
1:M:111:PHE:CE1	1:M:143:TYR:CE1	2.85	0.65
1:S:31:VAL:HB	5:S:2352:HOH:O	1.96	0.65
1:S:15:GLU:CG	1:1:9:PRO:HD2	2.26	0.65
1:S:165:ASN:O	1:S:169:GLU:HG2	1.97	0.65
1:U:9:PRO:HD2	1:1:15:GLU:HG2	1.77	0.65
1:F:97:ARG:HG2	5:F:2227:HOH:O	1.97	0.65
2:L:465:ARG:HD2	5:L:155:HOH:O	1.97	0.64
1:S:85:ARG:HD3	1:S:89:TYR:CD2	2.33	0.64
1:W:223:ARG:CD	5:W:1767:HOH:O	2.45	0.64
1:D:41:PHE:HB3	1:D:53:ILE:HD13	1.79	0.64
1:U:25:ALA:O	1:U:158:GLY:HA2	1.97	0.64
1:A:163:ILE:HG23	1:A:187:ALA:HB1	1.80	0.64
2:H:335:TYR:CD1	3:H:66:DMF:HC	2.33	0.64
1:Q:30:VAL:HG13	1:Q:43:ALA:HB2	1.79	0.64
3:V:116:DMF:C	5:V:2127:HOH:O	2.45	0.64
2:X:320:SER:HB3	2:X:331:VAL:HG21	1.80	0.64
1:A:9:PRO:HD2	1:O:15:GLU:HG2	1.79	0.64
2:N:432:GLU:CD	3:N:104:DMF:H12	2.21	0.64
1:U:97:ARG:NH2	5:U:1445:HOH:O	2.30	0.64
2:E:331:VAL:HG11	4:E:300:SA6:H19	1.79	0.64
2:Z:301:THR:N	4:Z:300:SA6:HO6	1.94	0.64
1:I:8:SER:O	1:I:11:GLN:N	2.30	0.64
2:V:538:HIS:HD2	5:V:1790:HOH:O	1.79	0.64
1:W:223:ARG:HD2	5:W:1767:HOH:O	1.98	0.64
1:B:97:ARG:NH2	5:B:2179:HOH:O	2.30	0.64
2:T:432:GLU:HG3	2:T:437:GLN:HB2	1.79	0.64
1:Y:48:ARG:NH1	5:Y:2550:HOH:O	2.30	0.64
1:B:170:SER:HB3	1:B:183:ILE:HG23	1.80	0.63
1:M:111:PHE:CE1	1:M:143:TYR:CD1	2.86	0.63
1:I:97:ARG:NH2	5:I:1706:HOH:O	2.30	0.63
1:S:41:PHE:HB3	1:S:53:ILE:HD13	1.80	0.63
1:1:112:THR:HG22	1:1:113:GLU:OE2	1.98	0.63
3:C:103:DMF:C1	2:H:447:LYS:HZ1	2.09	0.63
3:N:118:DMF:H22	3:V:32:DMF:C	2.29	0.63
1:Y:181:LEU:HD22	1:Y:233:LEU:HD23	1.79	0.63
2:H:447:LYS:HD2	3:H:43:DMF:H21	1.80	0.63
1:O:41:PHE:HB3	1:O:53:ILE:HD13	1.79	0.63
1:F:41:PHE:HB3	1:F:53:ILE:HD13	1.80	0.63
2:G:301:THR:N	4:G:300:SA6:HO6	1.97	0.63
1:K:7:ILE:HG12	1:K:11:GLN:HG2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:382:ARG:NH2	2:N:385:ILE:HD13	2.13	0.63
1:O:14:ARG:HH11	1:O:14:ARG:HB3	1.62	0.63
2:H:483:GLY:HA3	3:H:91:DMF:C2	2.24	0.63
1:S:15:GLU:HB3	1:I:9:PRO:HG2	1.80	0.63
3:U:250:DMF:N	3:V:27:DMF:C1	2.61	0.63
1:F:31:VAL:HG12	1:F:155:VAL:HG22	1.79	0.63
2:2:301:THR:N	4:2:300:SA6:HO6	1.96	0.63
2:2:388:ARG:HD3	2:2:426:ALA:O	1.99	0.63
2:N:429:TRP:CZ2	3:N:93:DMF:C	2.78	0.62
1:S:25:ALA:O	1:S:158:GLY:HA2	1.99	0.62
1:D:152:HIS:CB	1:D:171:TYR:CZ	2.81	0.62
2:N:331:VAL:HG11	4:N:300:SA6:H19	1.79	0.62
2:J:516:ALA:HB3	3:J:123:DMF:H12	1.79	0.62
2:L:401:LEU:HD12	3:L:97:DMF:H12	1.82	0.62
1:S:7:ILE:HG22	1:S:11:GLN:HB3	1.82	0.62
1:Q:7:ILE:CG2	1:Q:8:SER:N	2.63	0.62
2:G:456:GLN:NE2	2:G:465:ARG:NH2	2.47	0.62
2:H:331:VAL:HG11	4:H:300:SA6:H19	1.80	0.62
1:A:31:VAL:HG12	1:A:155:VAL:HG22	1.79	0.62
1:I:25:ALA:O	1:I:158:GLY:HA2	1.99	0.62
1:S:185:VAL:O	1:S:189:ARG:HG3	2.00	0.62
3:W:250:DMF:H23	3:X:16:DMF:C2	2.27	0.62
1:A:80:GLN:NE2	1:A:80:GLN:O	2.30	0.62
2:G:331:VAL:HG11	4:G:300:SA6:H19	1.82	0.62
2:G:456:GLN:HE21	2:G:465:ARG:NH2	1.98	0.62
1:B:15:GLU:HG3	1:I:9:PRO:CG	2.28	0.62
2:J:320:SER:HB3	2:J:331:VAL:HG21	1.82	0.62
3:K:250:DMF:H13	5:K:1480:HOH:O	1.99	0.62
3:N:90:DMF:H21	3:V:120:DMF:H11	1.78	0.62
2:R:444:LEU:H	3:R:59:DMF:C	2.12	0.62
2:C:331:VAL:HG11	4:C:300:SA6:H19	1.82	0.61
2:G:442:GLY:C	3:G:64:DMF:H11	2.24	0.61
2:2:419:ARG:HD3	3:2:108:DMF:HC	1.82	0.61
1:M:163:ILE:HG23	1:M:187:ALA:O	2.00	0.61
1:B:31:VAL:HG12	1:B:155:VAL:HG22	1.82	0.61
1:Y:52:LYS:HG2	3:Y:251:DMF:HC	1.83	0.61
2:Z:508:SER:O	2:Z:512:GLU:HG3	2.01	0.61
2:N:345:ILE:HB	2:N:352:ALA:HB1	1.83	0.61
2:Z:357:ARG:HD3	5:Z:2331:HOH:O	2.00	0.61
1:I:31:VAL:HG12	1:I:155:VAL:HG22	1.82	0.61
1:O:31:VAL:HG12	1:O:155:VAL:HG22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:9:PRO:CG	1:1:15:GLU:HG3	2.30	0.61
1:I:19:LEU:HD21	1:S:13:MET:HE2	1.81	0.61
1:K:31:VAL:HG12	1:K:155:VAL:HG22	1.81	0.61
1:Q:95:THR:OG1	1:Q:98:GLN:HG3	1.99	0.61
2:R:301:THR:N	4:R:300:SA6:HO6	1.98	0.61
1:B:173:GLU:HG3	1:B:174:ASN:ND2	2.16	0.61
1:F:9:PRO:HD2	1:M:15:GLU:CG	2.31	0.61
1:O:76:ARG:HD3	5:O:1434:HOH:O	2.00	0.61
1:B:18:GLU:OE1	1:B:21:ARG:NH2	2.30	0.61
1:B:25:ALA:O	1:B:158:GLY:HA2	2.00	0.61
2:C:320:SER:HB3	2:C:331:VAL:HG21	1.82	0.61
1:D:181:LEU:HD23	1:D:233:LEU:HB3	1.82	0.60
1:M:203:LEU:N	1:M:203:LEU:HD23	2.16	0.60
2:T:331:VAL:HG11	4:T:300:SA6:H19	1.83	0.60
2:2:320:SER:HB3	2:2:331:VAL:HG21	1.83	0.60
1:A:41:PHE:HB3	1:A:53:ILE:HD13	1.83	0.60
2:P:472:TYR:CZ	3:P:14:DMF:H12	2.36	0.60
1:S:169:GLU:HA	1:S:169:GLU:OE1	2.01	0.60
1:Y:185:VAL:O	1:Y:189:ARG:HG3	2.01	0.60
2:L:388:ARG:NH1	5:L:2158:HOH:O	2.29	0.60
2:2:434:GLU:HB2	3:2:4:DMF:C2	2.21	0.60
1:A:80:GLN:NE2	5:A:1422:HOH:O	2.30	0.60
2:E:515:ARG:NH1	5:E:2580:HOH:O	2.35	0.60
2:2:366:TYR:CD1	3:2:87:DMF:HC	2.36	0.60
1:A:182:ARG:NH1	1:A:234:LEU:CA	2.64	0.60
2:Z:320:SER:HB3	2:Z:331:VAL:HG21	1.84	0.60
1:A:77:GLY:HA3	3:A:249:DMF:C	2.32	0.60
3:R:95:DMF:HC	5:R:267:HOH:O	2.00	0.60
1:S:15:GLU:OE1	1:1:8:SER:HB3	2.00	0.60
1:M:112:THR:HG22	1:M:113:GLU:OE2	2.02	0.60
2:R:320:SER:HB3	2:R:331:VAL:HG21	1.82	0.60
1:S:205:VAL:O	1:S:205:VAL:CG2	2.50	0.60
1:Y:163:ILE:HG23	1:Y:187:ALA:O	2.02	0.60
1:I:142:THR:OG1	1:I:146:SER:HB2	2.02	0.60
2:V:398:LEU:HD12	2:V:398:LEU:N	2.16	0.60
2:2:366:TYR:HD1	3:2:87:DMF:HC	1.65	0.60
1:D:112:THR:HG22	1:D:113:GLU:OE2	2.02	0.60
2:H:456:GLN:NE2	2:H:465:ARG:NH2	2.46	0.60
2:J:301:THR:N	4:J:300:SA6:HO6	1.99	0.60
1:Q:11:GLN:O	1:Q:15:GLU:HG2	2.02	0.60
2:V:354:GLU:HG2	3:2:101:DMF:H22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:182:ARG:NH1	1:Y:234:LEU:O	2.35	0.60
1:F:112:THR:HG22	1:F:113:GLU:OE2	2.02	0.59
1:I:11:GLN:O	1:I:15:GLU:HB2	2.02	0.59
2:J:398:LEU:N	2:J:398:LEU:CD1	2.65	0.59
1:K:178:THR:HG22	1:K:182:ARG:HE	1.67	0.59
1:Q:7:ILE:HG23	1:Q:11:GLN:OE1	2.01	0.59
2:V:381:ASN:HB2	3:V:42:DMF:H21	1.84	0.59
1:Y:112:THR:HG22	1:Y:113:GLU:OE2	2.01	0.59
1:O:14:ARG:HB3	1:O:14:ARG:NH1	2.17	0.59
2:P:436:TYR:CE1	3:P:107:DMF:H22	2.36	0.59
1:Q:8:SER:N	1:Q:11:GLN:OE1	2.29	0.59
1:U:112:THR:HG22	1:U:113:GLU:OE2	2.02	0.59
1:B:112:THR:HG22	1:B:113:GLU:OE2	2.01	0.59
1:F:181:LEU:O	1:F:185:VAL:HG23	2.02	0.59
1:I:76:ARG:HD3	5:I:339:HOH:O	2.02	0.59
3:N:22:DMF:H13	5:N:674:HOH:O	2.02	0.59
1:A:9:PRO:HB2	1:O:15:GLU:HG3	1.84	0.59
1:I:41:PHE:HB3	1:I:53:ILE:HD13	1.83	0.59
1:W:112:THR:HG22	1:W:113:GLU:OE2	2.02	0.59
1:D:15:GLU:HG3	1:K:9:PRO:CG	2.30	0.59
1:D:136:PRO:O	1:Q:48:ARG:NH2	2.35	0.59
1:K:102:VAL:HG23	3:K:251:DMF:HC	1.85	0.59
1:M:231:GLN:HA	1:M:234:LEU:HD21	1.83	0.59
1:A:112:THR:HG22	1:A:113:GLU:OE2	2.02	0.59
1:I:163:ILE:HG23	1:I:187:ALA:O	2.03	0.59
1:A:161:GLU:HB2	1:A:162:PRO:CD	2.29	0.59
1:S:112:THR:HG22	1:S:113:GLU:OE2	2.02	0.59
2:P:476:ASP:OD1	3:P:14:DMF:H22	2.03	0.59
2:G:320:SER:HB3	2:G:331:VAL:HG21	1.85	0.58
1:W:142:THR:HG1	1:W:146:SER:HB2	1.68	0.58
1:S:161:GLU:HB2	1:S:162:PRO:CD	2.30	0.58
1:A:112:THR:HG22	1:O:115:ALA:HB3	1.85	0.58
1:I:112:THR:HG22	1:I:113:GLU:OE2	2.03	0.58
1:M:10:GLU:HG3	1:M:11:GLN:N	2.18	0.58
2:P:436:TYR:CE1	3:P:107:DMF:C2	2.87	0.58
1:Q:178:THR:HG22	1:Q:182:ARG:HE	1.67	0.58
1:D:8:SER:O	1:D:11:GLN:HB3	2.04	0.58
1:W:161:GLU:HB2	1:W:162:PRO:CD	2.31	0.58
1:W:163:ILE:HG23	1:W:187:ALA:O	2.03	0.58
5:X:2666:HOH:O	3:Z:94:DMF:H11	2.04	0.58
2:E:516:ALA:HB3	5:E:1124:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:362:GLU:OE2	2:L:382:ARG:HD2	2.03	0.58
2:P:320:SER:HB3	2:P:331:VAL:HG21	1.85	0.58
1:A:16:ARG:NH2	1:A:114:GLN:O	2.31	0.58
1:B:178:THR:HG22	1:B:182:ARG:HE	1.69	0.58
1:I:152:HIS:HB3	1:I:171:TYR:CE2	2.39	0.58
1:S:178:THR:HG22	1:S:182:ARG:HE	1.69	0.58
2:E:509:ARG:NH1	2:E:512:GLU:OE1	2.37	0.58
1:K:7:ILE:HG13	1:K:11:GLN:HE21	1.69	0.58
1:U:110:ILE:HG23	1:U:114:GLN:HE21	1.68	0.58
2:C:412:SER:O	2:C:414:PRO:HD3	2.04	0.58
2:Z:488:ARG:NE	3:Z:94:DMF:H22	2.19	0.58
1:I:173:GLU:O	1:I:174:ASN:HB2	2.04	0.57
1:K:112:THR:HG22	1:K:113:GLU:OE2	2.03	0.57
1:M:170:SER:HB2	1:M:183:ILE:HG23	1.85	0.57
1:W:223:ARG:HG2	5:W:2456:HOH:O	2.04	0.57
2:X:456:GLN:HE21	2:X:465:ARG:NH2	2.02	0.57
2:H:391:LEU:HB3	5:H:2626:HOH:O	2.05	0.57
1:I:223:ARG:HG2	5:I:1626:HOH:O	2.02	0.57
2:J:331:VAL:HG11	4:J:300:SA6:H19	1.86	0.57
1:K:114:GLN:OE1	3:K:252:DMF:H11	2.03	0.57
2:R:388:ARG:NH1	5:R:2204:HOH:O	2.36	0.57
3:C:69:DMF:H11	5:C:557:HOH:O	2.04	0.57
1:O:102:VAL:HG12	3:O:250:DMF:H22	1.86	0.57
1:S:85:ARG:HD3	1:S:89:TYR:HD2	1.68	0.57
1:W:76:ARG:NH1	2:X:370:GLU:OE2	2.37	0.57
2:L:401:LEU:HD12	3:L:97:DMF:C1	2.34	0.57
1:S:149:ASP:CB	5:S:1142:HOH:O	2.52	0.57
1:A:163:ILE:HG12	1:A:187:ALA:O	2.05	0.57
2:H:320:SER:HB3	2:H:331:VAL:HG21	1.85	0.57
2:J:465:ARG:NH1	5:J:1886:HOH:O	2.35	0.57
1:M:178:THR:HG22	1:M:182:ARG:HE	1.68	0.57
1:Q:161:GLU:HB2	1:Q:162:PRO:CD	2.29	0.57
1:D:189:ARG:N	5:D:2659:HOH:O	2.35	0.57
2:N:477:ASP:OD1	3:N:118:DMF:C1	2.51	0.57
1:D:84:THR:OG1	3:D:253:DMF:HC	2.05	0.57
1:K:15:GLU:HG2	1:M:9:PRO:CD	2.25	0.57
1:K:110:ILE:HA	1:K:114:GLN:HG3	1.85	0.57
2:V:301:THR:N	4:V:300:SA6:HO6	2.02	0.57
1:Y:214:ASP:OD1	1:Y:214:ASP:C	2.46	0.57
2:H:412:SER:O	2:H:414:PRO:HD3	2.05	0.57
1:O:165:ASN:O	1:O:169:GLU:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:112:THR:HG22	1:Q:113:GLU:OE2	2.05	0.57
3:T:84:DMF:C1	5:T:2221:HOH:O	2.52	0.57
1:B:155:VAL:HG12	1:B:160:THR:HG22	1.86	0.57
2:N:320:SER:HB3	2:N:331:VAL:HG21	1.87	0.57
2:E:509:ARG:CA	3:E:73:DMF:H12	2.34	0.57
1:F:19:LEU:C	1:F:19:LEU:HD23	2.30	0.57
1:M:155:VAL:HG12	1:M:160:THR:HG22	1.87	0.57
1:O:112:THR:HG22	1:O:113:GLU:OE2	2.05	0.57
1:S:155:VAL:HG12	1:S:160:THR:HG22	1.87	0.57
1:D:170:SER:CB	1:D:183:ILE:HG23	2.31	0.56
2:T:332:ARG:HB3	5:T:2540:HOH:O	2.05	0.56
1:A:170:SER:O	1:A:183:ILE:HD13	2.05	0.56
1:D:161:GLU:HB2	1:D:162:PRO:CD	2.30	0.56
2:J:412:SER:O	2:J:414:PRO:HD3	2.04	0.56
1:Q:163:ILE:HG23	1:Q:187:ALA:O	2.05	0.56
2:R:331:VAL:HG11	4:R:300:SA6:H19	1.87	0.56
1:Y:161:GLU:HB2	1:Y:162:PRO:CD	2.31	0.56
1:Y:205:VAL:HG23	1:Y:206:ALA:N	2.20	0.56
1:D:178:THR:HG22	1:D:182:ARG:HE	1.71	0.56
1:F:9:PRO:HD2	1:M:15:GLU:HG2	1.88	0.56
3:H:117:DMF:HC	5:H:555:HOH:O	2.06	0.56
1:I:7:ILE:HB	1:I:11:GLN:HB3	1.87	0.56
2:P:412:SER:O	2:P:414:PRO:HD3	2.05	0.56
2:T:432:GLU:CD	2:T:437:GLN:HE21	2.14	0.56
1:W:92:ARG:HD3	1:W:129:HIS:CE1	2.40	0.56
2:2:465:ARG:HG3	2:2:465:ARG:NH1	2.14	0.56
2:2:509:ARG:NH1	3:2:52:DMF:O	2.29	0.56
1:F:7:ILE:HG23	1:F:11:GLN:CD	2.30	0.56
1:O:178:THR:HG22	1:O:182:ARG:HE	1.70	0.56
2:P:301:THR:N	4:P:300:SA6:HO6	2.02	0.56
1:Q:102:VAL:CG1	3:Q:249:DMF:H13	2.35	0.56
1:S:15:GLU:CB	1:I:9:PRO:HG2	2.36	0.56
1:Y:169:GLU:OE1	1:Y:169:GLU:HA	2.05	0.56
1:1:189:ARG:NH1	1:1:203:LEU:N	2.53	0.56
1:Q:76:ARG:HD3	5:Q:1459:HOH:O	2.03	0.56
1:F:102:VAL:HG12	3:F:250:DMF:H12	1.88	0.56
3:N:118:DMF:H22	3:V:32:DMF:HC	1.88	0.56
1:K:43:ALA:O	1:K:208:LEU:HD22	2.05	0.56
1:1:163:ILE:HG23	1:1:187:ALA:O	2.05	0.56
1:B:15:GLU:HG2	1:I:9:PRO:CD	2.32	0.56
3:G:24:DMF:H13	2:2:453:LEU:HD23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:412:SER:O	2:L:414:PRO:HD3	2.06	0.56
2:N:416:SER:HB2	5:V:2273:HOH:O	2.06	0.56
1:W:178:THR:HG22	1:W:182:ARG:HE	1.69	0.56
2:C:456:GLN:NE2	2:C:465:ARG:NH2	2.48	0.56
1:D:173:GLU:C	1:D:174:ASN:ND2	2.63	0.56
2:G:508:SER:O	2:G:512:GLU:HG3	2.06	0.56
1:M:7:ILE:O	1:M:9:PRO:HD3	2.07	0.56
2:T:452:LYS:HB3	3:T:102:DMF:H22	1.86	0.56
2:G:412:SER:O	2:G:414:PRO:HD3	2.05	0.55
1:K:163:ILE:HG23	1:K:187:ALA:O	2.06	0.55
2:L:332:ARG:HD3	5:L:1905:HOH:O	2.06	0.55
1:S:189:ARG:O	1:S:190:ALA:C	2.48	0.55
2:2:465:ARG:HH11	2:2:465:ARG:CG	2.12	0.55
1:A:8:SER:O	1:A:11:GLN:N	2.40	0.55
1:F:7:ILE:HG22	1:F:8:SER:N	2.21	0.55
1:W:15:GLU:HG3	1:Y:9:PRO:HG2	1.87	0.55
1:1:178:THR:HG22	1:1:182:ARG:HE	1.70	0.55
1:I:19:LEU:HD11	1:S:13:MET:HG3	1.88	0.55
1:M:226:THR:HB	5:M:2302:HOH:O	2.07	0.55
1:U:231:GLN:O	1:U:234:LEU:HB2	2.05	0.55
1:1:11:GLN:HA	1:1:11:GLN:NE2	2.22	0.55
1:Y:9:PRO:O	1:Y:12:ALA:HB3	2.06	0.55
1:1:226:THR:HG22	5:1:2558:HOH:O	2.07	0.55
1:D:163:ILE:HG23	1:D:187:ALA:O	2.07	0.55
2:N:412:SER:O	2:N:414:PRO:HD3	2.06	0.55
1:U:48:ARG:NE	5:U:2461:HOH:O	2.39	0.55
2:V:538:HIS:CD2	5:V:1790:HOH:O	2.54	0.55
2:J:433:GLU:OE1	2:J:433:GLU:HA	2.05	0.55
1:M:189:ARG:O	1:M:190:ALA:C	2.47	0.55
1:O:189:ARG:HG3	1:O:203:LEU:HD23	1.89	0.55
1:S:229:ALA:O	1:S:233:LEU:HD13	2.07	0.55
2:T:320:SER:HB3	2:T:331:VAL:HG21	1.87	0.55
1:Q:54:SER:CB	1:Q:75:ARG:HD2	2.37	0.55
2:V:320:SER:HB3	2:V:331:VAL:HG21	1.89	0.55
3:V:83:DMF:C1	5:V:1742:HOH:O	2.29	0.55
1:B:7:ILE:N	1:B:7:ILE:CD1	2.51	0.55
2:E:434:GLU:HG2	3:E:75:DMF:H23	1.89	0.55
2:V:430:ASN:ND2	3:V:82:DMF:C	2.70	0.55
1:A:54:SER:CB	1:A:75:ARG:HD2	2.37	0.55
1:M:161:GLU:HB2	1:M:162:PRO:CD	2.31	0.55
1:M:173:GLU:O	1:M:174:ASN:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:472:TYR:O	3:P:14:DMF:H13	2.07	0.55
1:D:108:GLY:C	3:D:251:DMF:C2	2.80	0.55
1:F:7:ILE:CG2	1:F:11:GLN:CG	2.85	0.55
1:B:15:GLU:CG	1:I:9:PRO:CG	2.82	0.54
1:D:150:GLU:HG3	1:D:154:VAL:HG22	1.89	0.54
1:I:15:GLU:HG2	1:S:9:PRO:CG	2.37	0.54
1:B:174:ASN:N	1:B:174:ASN:HD22	2.04	0.54
2:E:461:ASP:OD2	2:E:509:ARG:NH2	2.37	0.54
2:V:444:LEU:HB2	5:V:1225:HOH:O	2.06	0.54
1:B:54:SER:CB	1:B:75:ARG:HD2	2.36	0.54
2:R:412:SER:O	2:R:414:PRO:HD3	2.06	0.54
1:S:163:ILE:HG23	1:S:187:ALA:O	2.06	0.54
1:I:161:GLU:HB2	1:I:162:PRO:CD	2.32	0.54
1:O:161:GLU:HB2	1:O:162:PRO:CD	2.31	0.54
1:A:80:GLN:HE21	1:A:81:PHE:N	2.00	0.54
1:B:150:GLU:HG3	1:B:154:VAL:HG22	1.90	0.54
1:M:111:PHE:CD1	1:M:143:TYR:HD1	2.25	0.54
1:Y:178:THR:HG22	1:Y:182:ARG:HE	1.72	0.54
1:F:97:ARG:CZ	5:F:2227:HOH:O	2.55	0.54
1:F:178:THR:HG22	1:F:182:ARG:HE	1.71	0.54
1:U:144:ASP:CG	1:U:146:SER:HG	2.14	0.54
1:U:181:LEU:O	1:U:185:VAL:HG23	2.07	0.54
2:Z:412:SER:O	2:Z:414:PRO:HD3	2.07	0.54
1:O:152:HIS:HB3	1:O:171:TYR:CE2	2.43	0.54
3:T:102:DMF:H13	2:X:452:LYS:HB3	1.88	0.54
2:R:525:ASP:OD1	2:R:538:HIS:HE1	1.90	0.54
1:U:150:GLU:HG3	1:U:154:VAL:HG22	1.89	0.54
1:A:186:ALA:HA	1:A:189:ARG:HD3	1.89	0.54
2:E:333:LYS:HG2	4:E:300:SA6:H18	1.90	0.54
2:E:509:ARG:HA	3:E:73:DMF:H12	1.89	0.54
2:V:354:GLU:OE2	3:2:101:DMF:H13	2.08	0.54
2:2:465:ARG:HG2	2:2:513:LEU:HD22	1.89	0.54
2:E:320:SER:HB3	2:E:331:VAL:HG21	1.90	0.54
2:R:509:ARG:NH2	3:R:80:DMF:H11	2.23	0.54
1:M:19:LEU:O	1:M:19:LEU:HD23	2.08	0.53
2:N:417:ALA:HA	5:N:2031:HOH:O	2.08	0.53
3:U:250:DMF:N	3:V:27:DMF:H11	2.23	0.53
2:V:412:SER:O	2:V:414:PRO:HD3	2.07	0.53
1:W:170:SER:OG	1:W:183:ILE:HG23	2.08	0.53
1:F:48:ARG:HH12	1:W:135:ARG:HB3	1.73	0.53
1:F:164:ALA:O	1:F:168:LYS:HG3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:445:PHE:H	3:G:64:DMF:C1	2.21	0.53
2:G:452:LYS:HD2	3:G:24:DMF:H11	1.90	0.53
2:H:522:SER:HB2	5:L:2277:HOH:O	2.08	0.53
1:Q:13:MET:HG2	3:Q:250:DMF:H11	1.90	0.53
2:2:433:GLU:OE1	3:2:108:DMF:H22	2.07	0.53
1:D:8:SER:HB2	1:Q:7:ILE:CG1	2.38	0.53
1:I:114:GLN:NE2	5:I:2530:HOH:O	2.30	0.53
1:Q:205:VAL:HG22	1:Q:230:LEU:HG	1.89	0.53
1:S:54:SER:CB	1:S:75:ARG:HD2	2.38	0.53
2:X:412:SER:O	2:X:414:PRO:HD3	2.09	0.53
1:1:19:LEU:C	1:1:19:LEU:HD23	2.32	0.53
1:1:54:SER:CB	1:1:75:ARG:HD2	2.38	0.53
1:B:141:ILE:N	1:B:141:ILE:HD12	2.23	0.53
2:G:445:PHE:CE2	3:G:64:DMF:H12	2.42	0.53
5:J:594:HOH:O	1:S:85:ARG:CG	2.56	0.53
1:O:142:THR:OG1	1:O:146:SER:HB2	2.09	0.53
1:U:155:VAL:HG12	1:U:160:THR:HG22	1.90	0.53
2:V:472:TYR:CZ	3:V:116:DMF:H13	2.43	0.53
1:Y:181:LEU:CD2	1:Y:233:LEU:HG	2.36	0.53
1:A:15:GLU:HG3	1:B:9:PRO:HD2	1.91	0.53
1:F:54:SER:CB	1:F:75:ARG:HD2	2.38	0.53
2:L:301:THR:N	4:L:300:SA6:HO6	2.07	0.53
2:V:496:ILE:HG21	3:V:39:DMF:H23	1.90	0.53
1:A:150:GLU:HG3	1:A:154:VAL:HG22	1.91	0.53
1:B:74:LEU:HD12	3:B:249:DMF:H13	1.90	0.53
1:D:111:PHE:CE1	1:D:143:TYR:HD1	2.26	0.53
1:D:111:PHE:CE1	1:D:143:TYR:CD1	2.97	0.53
2:J:409:ILE:HG12	5:J:1416:HOH:O	2.09	0.53
2:V:380:ILE:HB	3:V:42:DMF:H23	1.90	0.53
1:W:155:VAL:HG12	1:W:160:THR:HG22	1.90	0.53
1:Y:91:ARG:HD2	3:Y:249:DMF:H11	1.91	0.53
1:B:174:ASN:ND2	1:B:174:ASN:N	2.54	0.53
1:B:181:LEU:HD23	1:B:233:LEU:HB2	1.91	0.53
1:K:155:VAL:HG12	1:K:160:THR:HG22	1.91	0.53
1:B:110:ILE:HG23	1:B:114:GLN:OE1	2.09	0.53
1:I:203:LEU:N	1:I:203:LEU:HD12	2.24	0.53
1:M:54:SER:CB	1:M:75:ARG:HD2	2.38	0.53
3:N:90:DMF:H21	3:V:120:DMF:HC	1.89	0.53
1:Y:150:GLU:HG3	1:Y:154:VAL:HG22	1.91	0.53
2:C:498:ASP:OD2	3:C:38:DMF:H12	2.08	0.53
1:I:150:GLU:HG3	1:I:154:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:52:LYS:NZ	5:Q:1538:HOH:O	2.36	0.53
1:W:141:ILE:HD12	1:W:141:ILE:N	2.23	0.53
1:A:112:THR:CG2	1:O:115:ALA:HB3	2.38	0.53
2:C:366:TYR:HD1	3:C:63:DMF:HC	1.74	0.53
2:P:515:ARG:NH2	5:P:1195:HOH:O	2.40	0.53
1:Q:219:ARG:NH2	3:Q:251:DMF:H22	2.23	0.53
1:S:150:GLU:HG3	1:S:154:VAL:HG22	1.91	0.53
1:Y:13:MET:HE3	1:Y:13:MET:HA	1.91	0.53
1:D:16:ARG:NH1	1:D:117:PRO:HD3	2.25	0.52
1:D:137:GLU:HG2	1:Q:48:ARG:NH2	2.24	0.52
2:E:472:TYR:CD1	3:E:20:DMF:H12	2.43	0.52
1:M:179:ASP:O	1:M:183:ILE:HG13	2.09	0.52
1:M:231:GLN:HA	1:M:234:LEU:CD2	2.38	0.52
1:S:19:LEU:C	1:S:19:LEU:HD23	2.35	0.52
1:U:140:ARG:NH1	1:U:154:VAL:HG13	2.24	0.52
1:U:170:SER:OG	1:U:183:ILE:HG23	2.08	0.52
1:B:161:GLU:HB2	1:B:162:PRO:CD	2.32	0.52
2:T:412:SER:O	2:T:414:PRO:HD3	2.09	0.52
1:F:7:ILE:CD1	1:W:8:SER:HB2	2.39	0.52
1:F:191:GLY:O	1:F:192:SER:HB2	2.09	0.52
2:L:388:ARG:HD3	2:L:426:ALA:O	2.08	0.52
1:O:9:PRO:CD	1:U:15:GLU:CG	2.64	0.52
1:Q:9:PRO:HD2	1:Y:15:GLU:HG3	1.91	0.52
2:R:445:PHE:CE2	3:R:59:DMF:H12	2.45	0.52
2:V:306:LEU:HD12	2:V:306:LEU:C	2.34	0.52
2:E:412:SER:O	2:E:414:PRO:HD3	2.09	0.52
1:F:225:ILE:HG21	1:F:233:LEU:HD12	1.91	0.52
1:K:54:SER:CB	1:K:75:ARG:HD2	2.39	0.52
1:Q:173:GLU:O	1:Q:174:ASN:HB2	2.08	0.52
1:W:150:GLU:HG3	1:W:154:VAL:HG22	1.91	0.52
1:Y:54:SER:CB	1:Y:75:ARG:HD2	2.39	0.52
1:I:155:VAL:HG12	1:I:160:THR:HG22	1.91	0.52
1:F:155:VAL:HG12	1:F:160:THR:HG22	1.91	0.52
1:M:150:GLU:HG3	1:M:154:VAL:HG22	1.91	0.52
1:Q:90:ASP:HB3	1:Q:93:ASP:OD2	2.09	0.52
2:J:461:ASP:OD1	2:J:509:ARG:NH2	2.40	0.52
1:O:89:TYR:CD1	2:V:382:ARG:HD3	2.45	0.52
1:F:7:ILE:CG2	1:F:11:GLN:CD	2.83	0.52
1:M:152:HIS:HB3	1:M:171:TYR:CE2	2.45	0.52
1:U:54:SER:CB	1:U:75:ARG:HD2	2.40	0.52
1:I:155:VAL:HG12	1:I:160:THR:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:15:GLU:OE2	1:M:10:GLU:HB3	2.10	0.52
1:O:54:SER:CB	1:O:75:ARG:HD2	2.39	0.52
1:1:8:SER:O	1:1:11:GLN:N	2.36	0.52
1:B:170:SER:CB	1:B:183:ILE:HG23	2.40	0.52
2:J:465:ARG:HD2	3:J:123:DMF:H11	1.91	0.52
2:J:476:ASP:OD1	3:J:45:DMF:HC	2.10	0.52
1:K:7:ILE:CG1	1:K:11:GLN:HE21	2.23	0.52
1:K:114:GLN:OE1	3:K:252:DMF:H13	2.08	0.52
2:T:335:TYR:CB	3:T:29:DMF:H13	2.37	0.52
1:A:87:TYR:CZ	2:H:358:LEU:HD13	2.45	0.51
2:V:434:GLU:HB2	3:V:32:DMF:H21	1.92	0.51
1:W:214:ASP:HB3	1:W:217:ARG:HG2	1.91	0.51
2:X:306:LEU:C	2:X:306:LEU:HD12	2.34	0.51
1:Y:135:ARG:NH1	1:Y:135:ARG:HB2	2.25	0.51
1:1:182:ARG:NH1	1:1:234:LEU:O	2.42	0.51
3:C:103:DMF:O	3:H:43:DMF:H22	2.10	0.51
1:D:179:ASP:O	1:D:183:ILE:HG13	2.10	0.51
1:S:141:ILE:HD12	1:S:141:ILE:N	2.25	0.51
1:W:87:TYR:CZ	2:X:358:LEU:HD13	2.45	0.51
1:1:150:GLU:HG3	1:1:154:VAL:HG22	1.92	0.51
1:B:8:SER:HB2	1:B:9:PRO:HD2	1.92	0.51
2:J:509:ARG:NH1	2:J:509:ARG:HG2	2.26	0.51
1:M:98:GLN:O	1:M:102:VAL:HG23	2.10	0.51
1:S:149:ASP:HB2	5:S:1142:HOH:O	2.11	0.51
1:W:97:ARG:NH2	5:W:1773:HOH:O	2.23	0.51
1:D:140:ARG:NH1	1:D:154:VAL:HG13	2.24	0.51
1:I:7:ILE:HB	1:I:11:GLN:CB	2.41	0.51
1:K:150:GLU:HG3	1:K:154:VAL:HG22	1.92	0.51
2:L:440:GLY:HA2	3:L:97:DMF:HC	1.92	0.51
2:T:349:ALA:HA	4:T:300:SA6:H17A	1.92	0.51
1:W:185:VAL:CG1	1:W:189:ARG:HH21	2.22	0.51
2:C:345:ILE:HB	2:C:352:ALA:HB1	1.91	0.51
3:C:103:DMF:H13	2:H:447:LYS:HZ2	1.69	0.51
1:D:144:ASP:OD2	1:D:146:SER:CB	2.59	0.51
1:F:187:ALA:O	1:F:190:ALA:HB3	2.11	0.51
2:J:465:ARG:HD2	3:J:123:DMF:C	2.39	0.51
1:K:44:GLU:HA	1:K:208:LEU:HD23	1.93	0.51
1:Q:16:ARG:NE	3:Q:250:DMF:H22	2.24	0.51
1:Q:155:VAL:HG12	1:Q:160:THR:HG22	1.91	0.51
1:S:8:SER:H	1:S:11:GLN:CB	2.21	0.51
3:V:116:DMF:HC	5:V:2127:HOH:O	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LEU:O	1:A:185:VAL:HG23	2.11	0.51
1:F:150:GLU:HG3	1:F:154:VAL:HG22	1.93	0.51
1:Q:102:VAL:HG12	3:Q:249:DMF:H13	1.92	0.51
1:Y:77:GLY:HA3	3:Y:250:DMF:H23	1.93	0.51
1:A:56:LEU:HG	1:A:62:PHE:HB2	1.92	0.51
1:F:152:HIS:HB3	1:F:171:TYR:CE2	2.46	0.51
1:K:140:ARG:NH1	1:K:154:VAL:HG13	2.26	0.51
1:M:111:PHE:CE1	1:M:143:TYR:HE1	2.28	0.51
1:Q:87:TYR:O	2:R:357:ARG:NH1	2.42	0.51
1:Y:105:GLN:HB2	5:Y:1882:HOH:O	2.09	0.51
1:A:182:ARG:HH11	1:A:234:LEU:HA	1.74	0.51
1:I:8:SER:O	1:I:12:ALA:N	2.39	0.51
1:D:155:VAL:HG12	1:D:160:THR:HG22	1.92	0.51
2:G:306:LEU:C	2:G:306:LEU:HD12	2.36	0.51
5:O:2444:HOH:O	3:V:42:DMF:C	2.59	0.51
1:S:179:ASP:O	1:S:183:ILE:HG13	2.11	0.51
2:V:332:ARG:HD3	5:V:2665:HOH:O	2.11	0.51
2:C:511:ALA:O	2:C:515:ARG:HG3	2.11	0.51
1:I:140:ARG:NH1	1:I:154:VAL:HG13	2.26	0.51
2:J:332:ARG:HD3	5:J:545:HOH:O	2.10	0.51
2:L:432:GLU:HG2	2:L:437:GLN:HB2	1.93	0.51
3:P:2:DMF:C	5:P:791:HOH:O	2.59	0.51
1:U:9:PRO:HD2	1:I:15:GLU:CG	2.40	0.51
1:Y:155:VAL:HG12	1:Y:160:THR:HG22	1.93	0.51
1:B:233:LEU:N	1:B:233:LEU:CD1	2.63	0.50
1:F:165:ASN:O	1:F:169:GLU:HG2	2.11	0.50
2:G:447:LYS:HD3	3:G:119:DMF:H23	1.87	0.50
1:K:135:ARG:NH1	1:K:135:ARG:HB2	2.26	0.50
1:U:167:LEU:HG	1:U:187:ALA:CB	2.42	0.50
1:I:54:SER:CB	1:I:75:ARG:HD2	2.41	0.50
2:J:515:ARG:NH1	2:R:539:HIS:N	2.54	0.50
1:O:155:VAL:HG12	1:O:160:THR:HG22	1.93	0.50
1:Q:174:ASN:N	1:Q:174:ASN:HD22	2.10	0.50
1:B:19:LEU:HD23	1:B:19:LEU:C	2.36	0.50
1:Q:13:MET:CG	1:Y:19:LEU:HD11	2.39	0.50
2:R:306:LEU:C	2:R:306:LEU:HD12	2.36	0.50
1:S:140:ARG:NH1	1:S:154:VAL:HG13	2.25	0.50
1:W:135:ARG:NH1	1:W:135:ARG:HB2	2.27	0.50
1:A:54:SER:HB2	5:A:2123:HOH:O	2.11	0.50
1:A:163:ILE:HG23	1:A:187:ALA:O	2.11	0.50
1:M:166:ALA:O	1:M:170:SER:OG	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:525:ASP:OD2	2:V:538:HIS:HE1	1.94	0.50
1:W:179:ASP:O	1:W:183:ILE:HG13	2.10	0.50
2:2:465:ARG:NH1	2:2:465:ARG:CG	2.74	0.50
1:O:172:ALA:O	1:O:175:ALA:HB2	2.12	0.50
1:O:189:ARG:O	1:O:190:ALA:C	2.55	0.50
3:V:83:DMF:H11	3:2:4:DMF:HC	1.92	0.50
1:W:116:LYS:NZ	1:W:117:PRO:O	2.45	0.50
1:1:56:LEU:HG	1:1:62:PHE:HB2	1.93	0.50
1:B:140:ARG:NH1	1:B:154:VAL:HG13	2.26	0.50
2:X:336:ILE:O	3:X:16:DMF:H13	2.11	0.50
1:Y:179:ASP:O	1:Y:183:ILE:HG13	2.11	0.50
1:D:144:ASP:OD2	1:D:146:SER:OG	2.30	0.50
1:F:48:ARG:NH2	1:W:136:PRO:O	2.45	0.50
1:S:116:LYS:NZ	1:S:119:GLU:OE2	2.37	0.50
2:V:477:ASP:OD2	5:V:2199:HOH:O	2.20	0.50
1:W:11:GLN:HG2	1:W:14:ARG:NH2	2.27	0.50
1:K:161:GLU:HB2	1:K:162:PRO:CD	2.31	0.50
1:M:135:ARG:NH1	1:M:135:ARG:HB2	2.27	0.50
1:Y:56:LEU:HG	1:Y:62:PHE:HB2	1.93	0.50
2:C:509:ARG:HG2	5:C:2378:HOH:O	2.10	0.49
2:H:333:LYS:HG2	4:H:300:SA6:H18	1.94	0.49
1:I:141:ILE:HD12	1:I:141:ILE:N	2.27	0.49
1:K:102:VAL:HG22	3:K:251:DMF:HC	1.92	0.49
1:Q:7:ILE:CG2	1:Q:8:SER:H	2.24	0.49
1:D:54:SER:CB	1:D:75:ARG:HD2	2.42	0.49
1:F:165:ASN:HA	1:F:168:LYS:HD2	1.95	0.49
1:F:173:GLU:O	1:F:174:ASN:HB2	2.11	0.49
2:H:324:ASN:HB2	5:H:2206:HOH:O	2.11	0.49
1:Y:10:GLU:OE1	1:Y:10:GLU:O	2.30	0.49
1:Y:140:ARG:NH1	1:Y:154:VAL:HG13	2.27	0.49
1:A:140:ARG:NH1	1:A:154:VAL:HG13	2.27	0.49
1:A:155:VAL:HG12	1:A:160:THR:HG22	1.94	0.49
1:B:16:ARG:NH2	1:B:114:GLN:O	2.29	0.49
2:G:430:ASN:HD22	3:G:98:DMF:C	2.23	0.49
1:I:233:LEU:HD12	1:I:233:LEU:N	2.27	0.49
1:U:33:LEU:HD12	1:U:33:LEU:O	2.13	0.49
1:W:91:ARG:NH1	3:W:250:DMF:HC	2.27	0.49
1:W:144:ASP:OD1	1:W:146:SER:OG	2.30	0.49
1:1:225:ILE:HG21	1:1:233:LEU:HD12	1.94	0.49
2:C:413:ASP:HB3	5:C:2547:HOH:O	2.12	0.49
3:V:83:DMF:H23	5:V:2660:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:ARG:HB2	1:D:135:ARG:NH1	2.27	0.49
1:W:140:ARG:NH1	1:W:154:VAL:HG13	2.28	0.49
1:A:163:ILE:HG22	1:A:187:ALA:HB1	1.93	0.49
1:M:183:ILE:HD11	5:M:2226:HOH:O	2.12	0.49
2:G:445:PHE:H	3:G:64:DMF:H13	1.77	0.49
1:M:56:LEU:HG	1:M:62:PHE:HB2	1.95	0.49
1:Q:150:GLU:HG3	1:Q:154:VAL:HG22	1.93	0.49
1:U:144:ASP:OD1	1:U:146:SER:OG	2.30	0.49
3:V:116:DMF:C	5:V:1032:HOH:O	2.60	0.49
1:Y:85:ARG:NH2	5:Y:1296:HOH:O	2.39	0.49
1:D:204:GLY:O	1:D:208:LEU:HG	2.12	0.49
2:E:465:ARG:NH2	5:E:2061:HOH:O	2.45	0.49
1:F:185:VAL:O	1:F:189:ARG:HB2	2.11	0.49
2:L:374:LEU:HD21	1:M:89:TYR:CD1	2.48	0.49
1:Q:16:ARG:CD	3:Q:250:DMF:H22	2.42	0.49
2:R:443:SER:N	3:R:59:DMF:HC	2.28	0.49
2:2:412:SER:O	2:2:414:PRO:HD3	2.13	0.49
2:H:392:ALA:N	5:H:2626:HOH:O	2.36	0.49
1:I:56:LEU:HG	1:I:62:PHE:HB2	1.94	0.49
2:P:333:LYS:HG2	4:P:300:SA6:H18	1.95	0.49
2:R:456:GLN:NE2	2:R:465:ARG:NH2	2.56	0.49
1:W:114:GLN:O	1:W:115:ALA:C	2.56	0.49
1:Y:167:LEU:HG	1:Y:187:ALA:CB	2.43	0.49
1:D:142:THR:OG1	1:D:144:ASP:OD2	2.30	0.49
1:S:56:LEU:HG	1:S:62:PHE:HB2	1.95	0.49
1:Y:181:LEU:HD22	1:Y:233:LEU:CD2	2.42	0.49
2:2:432:GLU:OE2	2:2:434:GLU:HB2	2.13	0.49
2:H:306:LEU:HD12	2:H:306:LEU:C	2.38	0.48
1:K:167:LEU:HG	1:K:187:ALA:CB	2.43	0.48
1:Q:135:ARG:HB2	1:Q:135:ARG:NH1	2.28	0.48
1:S:14:ARG:HG2	1:S:14:ARG:HH21	1.79	0.48
1:Y:142:THR:OG1	1:Y:144:ASP:OD1	2.30	0.48
1:B:15:GLU:CG	1:I:9:PRO:CD	2.90	0.48
1:B:56:LEU:HG	1:B:62:PHE:HB2	1.94	0.48
1:D:144:ASP:OD1	1:D:146:SER:OG	2.30	0.48
2:E:433:GLU:HG3	2:L:330:ASP:CG	2.39	0.48
1:I:179:ASP:O	1:I:183:ILE:HG13	2.13	0.48
2:L:472:TYR:CZ	3:L:81:DMF:H11	2.48	0.48
1:Q:33:LEU:HD12	1:Q:33:LEU:O	2.13	0.48
3:T:113:DMF:C1	3:2:112:DMF:C	2.86	0.48
1:Y:110:ILE:HG23	1:Y:114:GLN:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:444:LEU:HD21	2:L:325:MET:SD	2.54	0.48
1:M:140:ARG:NH1	1:M:154:VAL:HG13	2.28	0.48
2:N:382:ARG:NH2	2:N:385:ILE:CD1	2.77	0.48
1:O:150:GLU:HG3	1:O:154:VAL:HG22	1.95	0.48
1:Q:167:LEU:HG	1:Q:187:ALA:CB	2.43	0.48
1:S:15:GLU:OE1	1:1:8:SER:CB	2.60	0.48
2:X:429:TRP:CH2	3:X:41:DMF:H12	2.47	0.48
2:Z:331:VAL:HG11	4:Z:300:SA6:H19	1.95	0.48
1:1:140:ARG:NH1	1:1:154:VAL:HG13	2.28	0.48
2:E:436:TYR:CZ	3:E:75:DMF:H22	2.47	0.48
2:G:432:GLU:CD	3:G:119:DMF:H11	2.37	0.48
2:J:515:ARG:HH12	2:R:539:HIS:H	1.56	0.48
2:N:515:ARG:O	2:N:519:GLU:HG3	2.14	0.48
1:Q:140:ARG:NH1	1:Q:154:VAL:HG13	2.28	0.48
3:Z:18:DMF:H13	5:Z:932:HOH:O	2.12	0.48
2:2:345:ILE:HB	2:2:352:ALA:HB1	1.95	0.48
1:B:142:THR:OG1	1:B:146:SER:HB2	2.13	0.48
2:C:416:SER:HB2	2:R:533:GLU:HB2	1.94	0.48
1:D:170:SER:HB2	1:D:183:ILE:CG2	2.35	0.48
2:G:444:LEU:H	3:G:64:DMF:C	2.27	0.48
1:M:111:PHE:CE1	1:M:143:TYR:HD1	2.30	0.48
1:M:152:HIS:HB3	1:M:171:TYR:CZ	2.48	0.48
2:N:483:GLY:HA3	3:N:22:DMF:H22	1.95	0.48
1:Q:19:LEU:C	1:Q:19:LEU:HD23	2.38	0.48
2:2:392:ALA:HA	2:2:395:MET:HE3	1.96	0.48
1:F:7:ILE:HG23	1:F:11:GLN:OE1	2.12	0.48
2:R:442:GLY:C	3:R:59:DMF:H11	2.39	0.48
3:T:102:DMF:H11	2:X:452:LYS:O	2.13	0.48
1:U:152:HIS:HB3	1:U:171:TYR:CE2	2.48	0.48
3:V:83:DMF:H22	2:2:447:LYS:CE	2.42	0.48
1:Y:19:LEU:C	1:Y:19:LEU:HD23	2.37	0.48
2:C:306:LEU:HD12	2:C:306:LEU:C	2.37	0.48
3:C:38:DMF:H21	5:C:1447:HOH:O	2.13	0.48
1:F:81:PHE:CZ	1:F:102:VAL:HG21	2.49	0.48
1:K:15:GLU:CG	1:M:9:PRO:HD2	2.31	0.48
2:2:333:LYS:HG2	4:2:300:SA6:H18	1.94	0.48
1:F:97:ARG:NH2	5:F:2383:HOH:O	2.46	0.48
1:F:161:GLU:HB2	1:F:162:PRO:CD	2.32	0.48
1:S:15:GLU:OE2	1:1:8:SER:HB3	2.13	0.48
1:S:149:ASP:HB3	5:S:1142:HOH:O	2.13	0.48
1:1:19:LEU:HD23	1:1:19:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:90:ASP:HB3	1:O:93:ASP:OD2	2.13	0.48
1:U:229:ALA:O	1:U:233:LEU:HD13	2.14	0.48
1:1:167:LEU:HG	1:1:187:ALA:CB	2.43	0.48
1:B:135:ARG:HB2	1:B:135:ARG:NH1	2.29	0.48
1:D:56:LEU:HG	1:D:62:PHE:HB2	1.95	0.48
1:F:135:ARG:NH1	1:F:135:ARG:HB2	2.29	0.48
1:S:205:VAL:O	1:S:205:VAL:HG22	2.13	0.48
2:T:382:ARG:NH2	2:T:385:ILE:HD13	2.28	0.48
2:Z:306:LEU:C	2:Z:306:LEU:HD12	2.39	0.48
1:1:135:ARG:HB2	1:1:135:ARG:NH1	2.29	0.48
2:E:452:LYS:NZ	2:H:473:ASP:OD2	2.46	0.47
1:M:11:GLN:HG2	1:M:14:ARG:HH22	1.79	0.47
1:M:144:ASP:OD1	1:M:146:SER:OG	2.30	0.47
2:P:508:SER:O	2:P:512:GLU:HG3	2.14	0.47
1:Q:233:LEU:N	1:Q:233:LEU:HD22	2.29	0.47
1:A:135:ARG:NH1	1:A:135:ARG:HB2	2.29	0.47
1:Q:13:MET:HG3	1:Y:19:LEU:CD1	2.38	0.47
1:Y:228:SER:O	1:Y:231:GLN:HB3	2.14	0.47
1:A:170:SER:OG	1:A:183:ILE:HG23	2.14	0.47
2:H:392:ALA:HB3	5:H:7:HOH:O	2.12	0.47
1:K:167:LEU:C	1:K:169:GLU:N	2.70	0.47
1:O:135:ARG:NH1	1:O:135:ARG:HB2	2.29	0.47
1:O:167:LEU:C	1:O:169:GLU:N	2.70	0.47
2:R:445:PHE:H	3:R:59:DMF:C1	2.27	0.47
1:S:33:LEU:HD12	1:S:33:LEU:O	2.14	0.47
1:A:163:ILE:HG23	1:A:187:ALA:CB	2.43	0.47
2:G:437:GLN:NE2	3:G:119:DMF:H12	2.29	0.47
1:K:179:ASP:O	1:K:183:ILE:HG13	2.15	0.47
2:P:351:VAL:HG21	2:P:398:LEU:HB3	1.95	0.47
2:V:398:LEU:N	2:V:398:LEU:CD1	2.78	0.47
1:1:161:GLU:HB2	1:1:162:PRO:CD	2.31	0.47
1:A:226:THR:HG22	5:A:1272:HOH:O	2.15	0.47
1:B:7:ILE:HG23	1:B:11:GLN:HG2	1.88	0.47
1:D:116:LYS:NZ	1:D:119:GLU:OE2	2.47	0.47
1:I:228:SER:O	1:I:231:GLN:HB3	2.15	0.47
2:X:477:ASP:HB3	3:2:112:DMF:H11	1.97	0.47
1:1:166:ALA:O	1:1:170:SER:OG	2.22	0.47
1:B:15:GLU:HG2	1:I:9:PRO:HG2	1.94	0.47
1:F:56:LEU:HG	1:F:62:PHE:HB2	1.96	0.47
1:O:33:LEU:O	1:O:33:LEU:HD12	2.14	0.47
1:S:144:ASP:OD1	1:S:146:SER:OG	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:333:LYS:HG2	4:X:300:SA6:H18	1.95	0.47
1:B:179:ASP:O	1:B:183:ILE:HG13	2.14	0.47
2:C:372:VAL:HG23	2:C:373:PRO:HD2	1.97	0.47
1:F:7:ILE:HG21	1:F:11:GLN:HG2	1.97	0.47
1:I:135:ARG:HB2	1:I:135:ARG:NH1	2.30	0.47
1:O:140:ARG:NH1	1:O:154:VAL:HG13	2.29	0.47
1:U:135:ARG:HB2	1:U:135:ARG:NH1	2.29	0.47
4:V:300:SA6:O6	4:V:300:SA6:H1B	2.15	0.47
1:Y:17:SER:OG	1:Y:143:TYR:OH	2.30	0.47
1:Y:17:SER:HG	1:Y:143:TYR:HH	1.57	0.47
2:2:484:PRO:HD2	5:2:2503:HOH:O	2.15	0.47
1:I:167:LEU:O	1:I:168:LYS:C	2.57	0.47
2:2:388:ARG:NH1	5:2:2358:HOH:O	2.46	0.47
1:F:15:GLU:HG2	1:W:9:PRO:HG2	1.96	0.47
1:O:19:LEU:C	1:O:19:LEU:HD23	2.40	0.47
1:O:179:ASP:O	1:O:183:ILE:HG13	2.15	0.47
1:S:52:LYS:HE2	1:S:64:ALA:O	2.15	0.47
1:S:80:GLN:NE2	5:S:2220:HOH:O	2.48	0.47
1:S:102:VAL:HG12	3:S:249:DMF:H12	1.97	0.47
1:D:8:SER:HG	1:D:9:PRO:HD3	1.80	0.47
1:S:169:GLU:OE1	1:S:169:GLU:CA	2.62	0.47
1:S:228:SER:O	1:S:231:GLN:HB3	2.15	0.47
2:V:477:ASP:CG	3:V:120:DMF:H23	2.40	0.47
2:C:498:ASP:OD2	3:C:38:DMF:C1	2.63	0.46
1:D:167:LEU:HG	1:D:187:ALA:CB	2.45	0.46
1:K:33:LEU:HD12	1:K:33:LEU:O	2.14	0.46
1:S:135:ARG:HB2	1:S:135:ARG:NH1	2.30	0.46
1:U:231:GLN:HA	1:U:234:LEU:HD12	1.97	0.46
2:X:331:VAL:HG11	4:X:300:SA6:C19	2.43	0.46
2:C:333:LYS:HG2	4:C:300:SA6:H18	1.97	0.46
2:C:416:SER:CB	2:R:533:GLU:HB2	2.45	0.46
2:G:432:GLU:OE1	3:G:119:DMF:H11	2.14	0.46
1:K:228:SER:O	1:K:231:GLN:HB3	2.15	0.46
1:O:8:SER:O	1:O:9:PRO:C	2.59	0.46
1:Q:20:ALA:O	1:Q:24:ILE:HG13	2.15	0.46
1:U:161:GLU:HB2	1:U:162:PRO:CD	2.31	0.46
1:O:19:LEU:HD23	1:O:19:LEU:O	2.16	0.46
1:U:8:SER:HA	1:U:9:PRO:HD2	1.71	0.46
2:V:377:ALA:O	3:V:42:DMF:H23	2.16	0.46
2:C:301:THR:HG22	2:C:302:THR:N	2.30	0.46
1:D:108:GLY:C	3:D:251:DMF:H22	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:LEU:HD12	1:F:33:LEU:O	2.15	0.46
1:I:167:LEU:HG	1:I:187:ALA:CB	2.45	0.46
2:J:382:ARG:NH2	2:J:385:ILE:CD1	2.79	0.46
2:L:320:SER:HB3	2:L:331:VAL:HG21	1.96	0.46
1:Q:142:THR:HA	5:Q:2537:HOH:O	2.16	0.46
1:D:109:THR:N	3:D:251:DMF:C2	2.75	0.46
2:N:306:LEU:C	2:N:306:LEU:HD12	2.40	0.46
2:N:333:LYS:HG2	4:N:300:SA6:H18	1.98	0.46
1:O:189:ARG:CG	1:O:203:LEU:HD23	2.41	0.46
1:S:11:GLN:OE1	1:S:14:ARG:HD3	2.15	0.46
1:S:178:THR:CG2	1:S:182:ARG:HE	2.28	0.46
2:V:483:GLY:HA3	3:V:116:DMF:C2	2.43	0.46
1:W:26:ARG:O	1:W:26:ARG:CG	2.64	0.46
1:W:90:ASP:HB3	1:W:93:ASP:OD2	2.15	0.46
3:X:15:DMF:C1	5:X:1898:HOH:O	2.63	0.46
1:Y:110:ILE:HG23	1:Y:114:GLN:HE21	1.80	0.46
1:A:9:PRO:CD	1:O:15:GLU:HG2	2.46	0.46
1:D:15:GLU:HG2	1:K:9:PRO:HD2	1.97	0.46
1:D:16:ARG:NH2	1:D:114:GLN:O	2.40	0.46
3:G:12:DMF:C1	5:V:723:HOH:O	2.63	0.46
1:I:170:SER:O	1:I:183:ILE:HD13	2.16	0.46
2:J:382:ARG:NH2	2:J:385:ILE:HD13	2.31	0.46
2:J:415:GLN:NE2	5:J:1604:HOH:O	2.47	0.46
1:O:133:THR:HA	5:O:1191:HOH:O	2.15	0.46
2:R:477:ASP:OD2	5:R:2581:HOH:O	2.20	0.46
1:W:56:LEU:HG	1:W:62:PHE:HB2	1.98	0.46
1:A:167:LEU:HD23	1:A:167:LEU:HA	1.82	0.46
2:H:432:GLU:OE2	2:H:434:GLU:HG3	2.16	0.46
2:J:516:ALA:O	3:J:123:DMF:H23	2.14	0.46
2:L:309:PRO:HB2	5:L:1576:HOH:O	2.14	0.46
1:I:179:ASP:O	1:I:183:ILE:HG13	2.16	0.46
2:G:521:ARG:HB3	3:G:70:DMF:H11	1.97	0.46
1:M:142:THR:OG1	1:M:144:ASP:OD2	2.30	0.46
1:Q:167:LEU:C	1:Q:169:GLU:N	2.71	0.46
2:T:360:ALA:CB	3:T:29:DMF:H23	2.46	0.46
1:U:56:LEU:HG	1:U:62:PHE:HB2	1.98	0.46
1:I:8:SER:O	1:I:11:GLN:HB3	2.15	0.46
1:B:15:GLU:CD	1:I:8:SER:HB3	2.41	0.46
1:D:33:LEU:HD12	1:D:33:LEU:O	2.16	0.46
1:D:109:THR:OG1	3:D:251:DMF:H13	2.15	0.46
1:D:111:PHE:CD1	1:D:143:TYR:HD1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:233:LEU:HD11	5:I:1562:HOH:O	2.16	0.46
3:N:90:DMF:C2	3:V:120:DMF:H12	2.43	0.46
2:X:409:ILE:HG12	5:X:2539:HOH:O	2.15	0.46
2:Z:391:LEU:O	2:Z:395:MET:HG3	2.15	0.46
1:B:226:THR:HG22	5:B:1667:HOH:O	2.16	0.46
1:I:19:LEU:CD2	1:S:13:MET:HE2	2.46	0.46
1:K:178:THR:CG2	1:K:182:ARG:HE	2.28	0.46
1:W:185:VAL:HG12	1:W:189:ARG:HH21	1.79	0.46
1:Y:33:LEU:HD12	1:Y:33:LEU:O	2.16	0.46
1:Y:170:SER:OG	1:Y:183:ILE:HG23	2.15	0.46
1:Y:178:THR:CG2	1:Y:182:ARG:HE	2.29	0.46
1:A:230:LEU:O	1:A:234:LEU:CD2	2.60	0.45
1:B:178:THR:CG2	1:B:182:ARG:HE	2.29	0.45
1:D:76:ARG:HD3	5:D:546:HOH:O	2.16	0.45
1:D:167:LEU:C	1:D:169:GLU:N	2.70	0.45
1:I:162:PRO:HB3	1:I:190:ALA:O	2.16	0.45
1:O:203:LEU:N	1:O:203:LEU:HD22	2.31	0.45
2:C:444:LEU:HD21	2:J:325:MET:SD	2.56	0.45
3:V:83:DMF:H22	2:2:447:LYS:HZ1	1.81	0.45
1:D:107:LEU:HD12	1:D:141:ILE:CG2	2.47	0.45
1:I:170:SER:HB2	1:I:183:ILE:HG23	1.99	0.45
2:Z:333:LYS:HG2	4:Z:300:SA6:H18	1.98	0.45
2:2:306:LEU:HD12	2:2:306:LEU:C	2.41	0.45
1:F:19:LEU:HD23	1:F:19:LEU:O	2.16	0.45
1:F:167:LEU:O	1:F:168:LYS:C	2.57	0.45
1:I:228:SER:O	1:I:231:GLN:HB3	2.16	0.45
2:C:307:LYS:HE3	2:C:418:GLY:O	2.16	0.45
2:G:333:LYS:HG2	4:G:300:SA6:H18	1.98	0.45
1:M:52:LYS:HE2	1:M:64:ALA:O	2.17	0.45
1:W:52:LYS:HE2	1:W:64:ALA:O	2.17	0.45
3:2:108:DMF:C1	5:2:1666:HOH:O	2.65	0.45
3:C:88:DMF:O	2:R:447:LYS:NZ	2.46	0.45
1:D:9:PRO:HD2	1:Q:15:GLU:HG3	1.98	0.45
1:D:144:ASP:CG	1:D:146:SER:OG	2.60	0.45
1:F:179:ASP:O	1:F:183:ILE:HG13	2.17	0.45
2:L:333:LYS:HG2	4:L:300:SA6:H18	1.98	0.45
2:L:456:GLN:NE2	2:L:465:ARG:HH22	2.14	0.45
1:M:178:THR:CG2	1:M:182:ARG:HE	2.30	0.45
3:T:84:DMF:H13	5:T:2221:HOH:O	2.15	0.45
1:W:16:ARG:NH1	1:W:117:PRO:HD3	2.31	0.45
1:Y:121:GLU:CG	5:Y:2504:HOH:O	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:461:ASP:CG	2:E:509:ARG:HH21	2.23	0.45
1:M:33:LEU:HD12	1:M:33:LEU:O	2.16	0.45
1:S:19:LEU:HD23	1:S:19:LEU:O	2.17	0.45
1:S:142:THR:HG1	1:S:146:SER:HB2	1.81	0.45
1:I:102:VAL:CG1	3:I:250:DMF:H12	2.41	0.45
2:J:306:LEU:HD12	2:J:306:LEU:C	2.41	0.45
1:M:110:ILE:HA	1:M:114:GLN:HG3	1.98	0.45
2:N:399:LEU:HD12	2:N:400:ALA:N	2.32	0.45
2:N:432:GLU:CD	2:N:437:GLN:HE21	2.25	0.45
1:O:56:LEU:HG	1:O:62:PHE:HB2	1.98	0.45
1:O:76:ARG:NH1	5:O:1434:HOH:O	2.35	0.45
1:W:77:GLY:HA3	3:W:249:DMF:C1	2.44	0.45
1:W:81:PHE:CZ	1:W:102:VAL:HG21	2.52	0.45
1:Y:169:GLU:OE1	1:Y:169:GLU:CA	2.63	0.45
1:F:141:ILE:HD12	1:F:141:ILE:N	2.32	0.45
1:I:178:THR:CG2	1:I:182:ARG:NH2	2.80	0.45
1:M:17:SER:OG	1:M:143:TYR:OH	2.23	0.45
1:M:228:SER:O	1:M:231:GLN:HB3	2.16	0.45
1:Q:8:SER:O	1:Q:11:GLN:N	2.48	0.45
1:Q:13:MET:SD	3:Q:250:DMF:H12	2.54	0.45
2:X:362:GLU:OE2	2:X:382:ARG:NE	2.49	0.45
1:1:178:THR:CG2	1:1:182:ARG:HE	2.30	0.45
1:D:207:SER:C	1:D:208:LEU:HD23	2.30	0.45
1:F:85:ARG:NH2	5:F:1784:HOH:O	2.49	0.45
2:N:372:VAL:HG23	2:N:373:PRO:HD2	1.99	0.45
1:O:178:THR:CG2	1:O:182:ARG:HE	2.30	0.45
2:R:534:LYS:NZ	3:R:92:DMF:O	2.50	0.45
1:W:72:ASP:O	1:W:76:ARG:HG3	2.17	0.45
1:1:13:MET:HE3	1:1:111:PHE:HE2	1.82	0.45
2:C:307:LYS:HD3	2:R:530:ASP:OD1	2.17	0.44
2:E:451:LYS:NZ	2:H:476:ASP:OD2	2.37	0.44
2:N:456:GLN:NE2	2:N:465:ARG:NH2	2.51	0.44
1:A:8:SER:O	1:A:11:GLN:HB3	2.18	0.44
1:F:228:SER:O	1:F:231:GLN:HB3	2.17	0.44
1:K:44:GLU:HA	1:K:208:LEU:CD2	2.47	0.44
1:K:151:PRO:HD2	5:K:1959:HOH:O	2.17	0.44
2:L:396:GLN:OE1	2:L:396:GLN:HA	2.16	0.44
1:S:111:PHE:CE1	1:S:143:TYR:CE1	3.05	0.44
1:1:45:ASN:HA	1:1:46:PRO:HD2	1.90	0.44
1:B:74:LEU:HA	3:B:249:DMF:H12	1.99	0.44
2:C:432:GLU:HB3	5:C:1566:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:301:THR:HG22	2:E:302:THR:N	2.32	0.44
1:O:232:ALA:C	1:O:234:LEU:H	2.24	0.44
2:T:392:ALA:HB3	5:T:1471:HOH:O	2.17	0.44
1:U:85:ARG:NH2	5:U:2357:HOH:O	2.50	0.44
2:X:392:ALA:HB3	5:X:1744:HOH:O	2.16	0.44
2:R:444:LEU:H	3:R:59:DMF:HC	1.82	0.44
1:S:214:ASP:OD1	1:S:214:ASP:C	2.61	0.44
1:S:234:LEU:O	1:S:235:VAL:HG13	2.17	0.44
2:V:392:ALA:HA	2:V:395:MET:CE	2.48	0.44
1:B:24:ILE:HD11	1:B:120:VAL:O	2.17	0.44
1:D:19:LEU:HD23	1:D:19:LEU:C	2.43	0.44
1:D:52:LYS:HE2	1:D:64:ALA:O	2.18	0.44
1:D:166:ALA:O	1:D:170:SER:OG	2.32	0.44
2:E:374:LEU:HD21	1:K:89:TYR:CD1	2.52	0.44
1:M:213:LEU:HD23	1:M:213:LEU:HA	1.89	0.44
2:N:381:ASN:HB2	3:N:93:DMF:H21	1.99	0.44
1:Q:167:LEU:O	1:Q:168:LYS:C	2.59	0.44
1:S:167:LEU:HG	1:S:187:ALA:HB1	1.98	0.44
1:U:167:LEU:HG	1:U:187:ALA:HB1	1.99	0.44
2:X:372:VAL:HG23	2:X:373:PRO:HD2	1.99	0.44
2:2:391:LEU:HG	2:2:395:MET:HE2	2.00	0.44
1:I:81:PHE:CZ	1:I:102:VAL:HG21	2.53	0.44
1:A:186:ALA:HA	1:A:189:ARG:CD	2.47	0.44
1:O:52:LYS:HE2	1:O:64:ALA:O	2.17	0.44
2:2:419:ARG:NH1	3:2:108:DMF:HC	2.33	0.44
2:E:392:ALA:HA	2:E:395:MET:CE	2.48	0.44
1:I:8:SER:H	1:I:11:GLN:HB2	1.83	0.44
1:I:56:LEU:HD23	1:I:56:LEU:HA	1.85	0.44
2:J:444:LEU:HB3	5:J:764:HOH:O	2.17	0.44
2:V:325:MET:SD	2:2:444:LEU:HD21	2.57	0.44
1:D:228:SER:O	1:D:231:GLN:HB3	2.17	0.44
1:I:16:ARG:NH2	1:I:114:GLN:O	2.37	0.44
2:R:351:VAL:HG21	2:R:398:LEU:O	2.18	0.44
1:U:114:GLN:O	1:U:115:ALA:C	2.60	0.44
2:2:434:GLU:HB3	3:2:4:DMF:H23	1.94	0.44
1:D:189:ARG:CG	5:D:2659:HOH:O	2.65	0.43
1:F:7:ILE:CG2	1:F:8:SER:N	2.81	0.43
1:F:203:LEU:HD23	1:F:203:LEU:HA	1.89	0.43
2:G:443:SER:N	3:G:64:DMF:HC	2.32	0.43
2:J:372:VAL:HG23	2:J:373:PRO:HD2	1.99	0.43
1:K:189:ARG:O	1:K:190:ALA:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:48:ARG:NH2	5:M:2620:HOH:O	2.44	0.43
2:N:416:SER:CB	2:V:533:GLU:HB2	2.48	0.43
1:O:170:SER:OG	1:O:183:ILE:HG23	2.18	0.43
1:D:99:LEU:HD13	1:D:99:LEU:HA	1.91	0.43
2:L:507:GLU:OE2	5:L:72:HOH:O	2.21	0.43
2:N:429:TRP:CE2	3:N:93:DMF:HC	2.49	0.43
1:Q:52:LYS:HE2	1:Q:64:ALA:O	2.18	0.43
1:Y:10:GLU:CD	1:Y:10:GLU:C	2.78	0.43
1:A:213:LEU:HD23	1:A:213:LEU:HA	1.88	0.43
1:B:213:LEU:HD23	1:B:213:LEU:HA	1.88	0.43
1:F:205:VAL:HG22	1:F:230:LEU:HG	1.99	0.43
2:G:472:TYR:CZ	3:G:12:DMF:H22	2.53	0.43
2:J:396:GLN:OE1	2:J:396:GLN:CA	2.61	0.43
1:S:116:LYS:HG2	1:S:117:PRO:O	2.18	0.43
2:V:354:GLU:CD	3:2:101:DMF:H13	2.42	0.43
1:B:110:ILE:HG12	1:B:114:GLN:OE1	2.18	0.43
2:E:345:ILE:HD12	2:E:352:ALA:O	2.18	0.43
1:I:26:ARG:CG	1:I:26:ARG:O	2.65	0.43
1:K:19:LEU:HD23	1:K:19:LEU:C	2.43	0.43
2:N:416:SER:C	5:N:2031:HOH:O	2.61	0.43
2:V:380:ILE:HG22	3:V:42:DMF:H22	1.99	0.43
1:W:7:ILE:HG12	1:W:8:SER:N	2.31	0.43
1:W:142:THR:OG1	1:W:144:ASP:OD2	2.30	0.43
1:A:228:SER:O	1:A:231:GLN:HB3	2.18	0.43
1:D:144:ASP:CG	1:D:146:SER:HG	2.26	0.43
1:F:52:LYS:HE2	1:F:64:ALA:O	2.18	0.43
1:I:33:LEU:HD12	1:I:33:LEU:O	2.19	0.43
1:K:7:ILE:HG23	1:K:8:SER:N	2.32	0.43
2:N:435:GLY:HA2	2:V:530:ASP:OD1	2.19	0.43
1:O:45:ASN:HA	1:O:46:PRO:HD2	1.88	0.43
1:Q:13:MET:SD	3:Q:250:DMF:H11	2.57	0.43
1:Q:228:SER:O	1:Q:231:GLN:HB3	2.18	0.43
1:S:11:GLN:OE1	1:S:11:GLN:HA	2.19	0.43
1:S:217:ARG:HG3	1:S:217:ARG:HH11	1.83	0.43
1:U:81:PHE:CZ	1:U:102:VAL:HG21	2.54	0.43
1:W:135:ARG:CB	1:W:135:ARG:HH11	2.32	0.43
2:2:372:VAL:HG23	2:2:373:PRO:HD2	2.01	0.43
2:E:475:ALA:HB3	3:E:20:DMF:H11	2.00	0.43
1:M:152:HIS:CG	1:M:171:TYR:CE2	3.07	0.43
2:R:394:ALA:HB1	2:R:399:LEU:HB2	2.01	0.43
1:Y:135:ARG:CB	1:Y:135:ARG:HH11	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:388:ARG:NH1	5:E:2197:HOH:O	2.48	0.43
1:K:135:ARG:CB	1:K:135:ARG:HH11	2.32	0.43
2:L:306:LEU:C	2:L:306:LEU:HD12	2.44	0.43
1:O:213:LEU:HD23	1:O:213:LEU:HA	1.86	0.43
1:S:8:SER:N	1:S:11:GLN:HB2	2.29	0.43
1:S:181:LEU:HD23	1:S:233:LEU:HB3	2.00	0.43
1:I:85:ARG:HD3	1:I:85:ARG:HA	1.87	0.43
1:A:52:LYS:HE2	1:A:64:ALA:O	2.18	0.43
2:E:391:LEU:HG	2:E:395:MET:HE2	2.00	0.43
1:I:52:LYS:HE2	1:I:64:ALA:O	2.18	0.43
1:I:73:ASN:ND2	1:S:105:GLN:OE1	2.52	0.43
2:L:456:GLN:HE22	2:L:465:ARG:HH22	1.67	0.43
1:B:33:LEU:HD12	1:B:33:LEU:O	2.19	0.43
1:I:178:THR:HG21	1:I:182:ARG:NH2	2.33	0.43
1:I:213:LEU:HD23	1:I:213:LEU:HA	1.87	0.43
1:D:19:LEU:HD23	1:D:19:LEU:O	2.19	0.43
1:D:178:THR:CG2	1:D:182:ARG:HE	2.31	0.43
1:D:188:LEU:HB3	5:D:2659:HOH:O	2.18	0.43
1:F:178:THR:CG2	1:F:182:ARG:HE	2.31	0.43
4:H:300:SA6:O6	4:H:300:SA6:H1B	2.19	0.43
1:K:77:GLY:HA3	3:K:249:DMF:C	2.48	0.43
1:Q:81:PHE:CZ	1:Q:102:VAL:HG21	2.54	0.43
1:W:13:MET:O	1:W:17:SER:HB2	2.19	0.43
1:Y:217:ARG:HG3	1:Y:217:ARG:HH11	1.84	0.43
1:A:19:LEU:C	1:A:19:LEU:HD23	2.44	0.42
1:B:97:ARG:NH2	5:B:1679:HOH:O	2.51	0.42
1:D:56:LEU:HD23	1:D:56:LEU:HA	1.86	0.42
1:I:162:PRO:CB	1:I:190:ALA:O	2.67	0.42
5:J:1118:HOH:O	2:R:536:HIS:HE1	2.02	0.42
1:K:56:LEU:HG	1:K:62:PHE:HB2	2.00	0.42
2:P:436:TYR:CE1	3:P:107:DMF:H21	2.52	0.42
2:R:323:GLY:N	5:R:2674:HOH:O	2.47	0.42
1:S:111:PHE:CE1	1:S:143:TYR:HE1	2.37	0.42
3:T:84:DMF:H11	5:T:2221:HOH:O	2.16	0.42
1:W:45:ASN:OD1	1:W:46:PRO:HD2	2.19	0.42
1:W:46:PRO:HA	1:W:207:SER:HA	2.01	0.42
1:Y:135:ARG:NH1	1:Y:135:ARG:CB	2.82	0.42
1:I:33:LEU:HD12	1:I:33:LEU:O	2.19	0.42
2:2:509:ARG:HG2	5:2:2190:HOH:O	2.19	0.42
1:B:230:LEU:O	1:B:230:LEU:HD12	2.18	0.42
2:C:377:ALA:O	3:C:47:DMF:H12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:477:ASP:OD1	3:C:88:DMF:H23	2.19	0.42
2:E:372:VAL:HG23	2:E:373:PRO:HD2	2.01	0.42
1:F:140:ARG:NH1	1:F:154:VAL:HG13	2.35	0.42
2:G:345:ILE:HB	2:G:352:ALA:HB1	2.00	0.42
5:J:594:HOH:O	1:S:85:ARG:HD2	2.19	0.42
1:M:45:ASN:HA	1:M:46:PRO:HD2	1.91	0.42
1:M:169:GLU:OE1	1:M:169:GLU:CA	2.66	0.42
1:S:90:ASP:HB3	1:S:93:ASP:OD2	2.19	0.42
1:W:170:SER:O	1:W:183:ILE:HD13	2.19	0.42
1:Y:174:ASN:HD22	1:Y:174:ASN:HA	1.64	0.42
1:Y:205:VAL:CG2	1:Y:206:ALA:N	2.81	0.42
2:N:511:ALA:O	2:N:515:ARG:HG3	2.19	0.42
1:Q:178:THR:CG2	1:Q:182:ARG:HE	2.31	0.42
1:U:52:LYS:HE2	1:U:64:ALA:O	2.19	0.42
1:W:205:VAL:HG23	1:W:206:ALA:N	2.35	0.42
1:I:45:ASN:HA	1:I:46:PRO:HD2	1.90	0.42
1:K:233:LEU:HD12	1:K:233:LEU:HA	1.93	0.42
1:M:142:THR:OG1	1:M:146:SER:HB2	2.20	0.42
1:O:81:PHE:CZ	1:O:102:VAL:HG21	2.54	0.42
2:G:447:LYS:HD3	3:G:119:DMF:C2	2.44	0.42
1:I:8:SER:N	1:I:11:GLN:HB2	2.34	0.42
1:W:178:THR:CG2	1:W:182:ARG:HE	2.31	0.42
2:Z:471:LEU:HD23	2:Z:471:LEU:HA	1.91	0.42
1:B:229:ALA:O	1:B:233:LEU:CD1	2.68	0.42
3:H:71:DMF:H21	5:P:1400:HOH:O	2.18	0.42
2:J:415:GLN:HG2	5:J:1219:HOH:O	2.18	0.42
1:K:28:LYS:HD2	1:K:44:GLU:OE2	2.20	0.42
1:K:81:PHE:CZ	1:K:102:VAL:HG21	2.54	0.42
1:M:90:ASP:HB3	1:M:93:ASP:OD2	2.20	0.42
1:O:228:SER:O	1:O:231:GLN:HB3	2.20	0.42
1:S:28:LYS:HG2	5:S:1910:HOH:O	2.19	0.42
1:W:135:ARG:NH1	1:W:135:ARG:CB	2.83	0.42
1:Y:52:LYS:CG	3:Y:251:DMF:HC	2.47	0.42
2:Z:366:TYR:CZ	2:Z:370:GLU:HG3	2.55	0.42
3:H:117:DMF:C	5:H:555:HOH:O	2.66	0.42
1:I:44:GLU:HG3	1:I:203:LEU:CD2	2.37	0.42
1:K:19:LEU:HD23	1:K:19:LEU:O	2.19	0.42
1:M:135:ARG:CB	1:M:135:ARG:HH11	2.32	0.42
1:W:11:GLN:O	1:W:14:ARG:HB3	2.19	0.42
1:W:182:ARG:NH2	1:W:234:LEU:O	2.52	0.42
1:Y:19:LEU:HD23	1:Y:19:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:52:LYS:HE2	1:Y:64:ALA:O	2.20	0.42
2:Z:362:GLU:OE2	2:Z:382:ARG:NE	2.47	0.42
1:A:142:THR:OG1	1:A:146:SER:HB2	2.20	0.42
1:A:188:LEU:HD12	1:A:188:LEU:HA	1.84	0.42
2:C:435:GLY:HA2	2:R:530:ASP:OD1	2.20	0.42
2:G:393:ALA:HB1	2:G:398:LEU:HD12	2.01	0.42
1:I:233:LEU:CD1	5:I:1562:HOH:O	2.67	0.42
2:N:432:GLU:OE2	3:N:104:DMF:C2	2.52	0.42
2:X:444:LEU:HB2	5:X:2327:HOH:O	2.19	0.42
1:B:45:ASN:HA	1:B:46:PRO:HD2	1.89	0.42
1:K:135:ARG:NH1	1:K:135:ARG:CB	2.83	0.42
1:Q:45:ASN:HA	1:Q:46:PRO:HD2	1.91	0.42
2:R:306:LEU:HD12	2:R:306:LEU:O	2.20	0.42
1:A:8:SER:OG	1:A:11:GLN:HB2	2.19	0.42
1:D:144:ASP:OD2	1:D:146:SER:HB2	2.19	0.42
2:E:381:ASN:HB2	3:E:53:DMF:C1	2.39	0.42
2:G:447:LYS:CD	3:G:119:DMF:H22	2.46	0.42
1:M:85:ARG:HD3	1:M:85:ARG:HA	1.90	0.42
1:M:217:ARG:HG3	1:M:217:ARG:HH11	1.85	0.42
1:B:135:ARG:HH11	1:B:135:ARG:CB	2.33	0.41
2:C:324:ASN:HB2	5:C:1419:HOH:O	2.19	0.41
2:G:444:LEU:HB2	3:G:64:DMF:H13	2.02	0.41
1:I:98:GLN:O	1:I:102:VAL:HG23	2.19	0.41
2:J:349:ALA:O	2:J:350:ALA:C	2.63	0.41
1:K:45:ASN:HA	1:K:46:PRO:HD2	1.88	0.41
2:T:362:GLU:OE2	2:T:382:ARG:HD2	2.18	0.41
5:T:1568:HOH:O	3:2:112:DMF:H21	2.18	0.41
1:U:161:GLU:CB	1:U:162:PRO:HD3	2.34	0.41
2:V:486:LEU:HB2	5:V:553:HOH:O	2.20	0.41
1:I:8:SER:O	1:I:9:PRO:C	2.62	0.41
3:2:108:DMF:H11	5:2:1666:HOH:O	2.20	0.41
1:D:162:PRO:HB3	1:D:190:ALA:O	2.20	0.41
1:F:52:LYS:HE2	1:F:52:LYS:HB3	1.91	0.41
2:L:444:LEU:HB2	5:L:45:HOH:O	2.19	0.41
2:N:430:ASN:ND2	3:N:104:DMF:C	2.83	0.41
2:N:430:ASN:ND2	3:N:104:DMF:N	2.68	0.41
1:Q:8:SER:HG	1:Q:11:GLN:CD	2.27	0.41
1:Q:56:LEU:HG	1:Q:62:PHE:HB2	2.01	0.41
1:Q:90:ASP:O	1:Q:93:ASP:HB2	2.20	0.41
1:Q:92:ARG:NH1	5:Q:1250:HOH:O	2.54	0.41
1:S:8:SER:OG	1:S:11:GLN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:233:LEU:HD12	1:S:233:LEU:N	2.36	0.41
5:T:548:HOH:O	3:Z:94:DMF:H13	2.20	0.41
2:X:366:TYR:CZ	2:X:370:GLU:HG3	2.55	0.41
1:Y:81:PHE:CZ	1:Y:102:VAL:HG21	2.55	0.41
1:Y:181:LEU:O	1:Y:185:VAL:HG23	2.20	0.41
2:G:325:MET:SD	2:N:444:LEU:HD21	2.60	0.41
1:I:19:LEU:HD23	1:I:19:LEU:C	2.44	0.41
2:J:461:ASP:OD1	2:J:509:ARG:NE	2.51	0.41
1:M:230:LEU:O	1:M:234:LEU:CD2	2.57	0.41
1:S:167:LEU:O	1:S:168:LYS:C	2.63	0.41
2:2:331:VAL:HG11	4:2:300:SA6:C19	2.47	0.41
1:D:81:PHE:CZ	1:D:102:VAL:HG21	2.56	0.41
2:E:301:THR:CG2	2:E:302:THR:N	2.84	0.41
1:F:225:ILE:HG21	1:F:233:LEU:CD1	2.50	0.41
2:H:325:MET:SD	2:P:444:LEU:HD21	2.61	0.41
1:I:166:ALA:O	1:I:170:SER:OG	2.36	0.41
1:I:205:VAL:HG12	1:I:230:LEU:HG	2.01	0.41
1:K:52:LYS:HE2	1:K:52:LYS:HB3	1.91	0.41
2:L:357:ARG:HD3	5:L:1243:HOH:O	2.21	0.41
1:M:22:LYS:HB3	1:M:26:ARG:HH21	1.85	0.41
1:O:203:LEU:CB	1:O:208:LEU:HD11	2.50	0.41
1:Q:85:ARG:HG2	5:Q:2261:HOH:O	2.20	0.41
3:V:83:DMF:H13	3:2:4:DMF:C	2.40	0.41
1:W:45:ASN:O	1:W:207:SER:C	2.64	0.41
1:W:46:PRO:CD	1:W:47:SER:H	2.33	0.41
2:X:434:GLU:CD	3:X:15:DMF:H22	2.46	0.41
1:1:217:ARG:HH11	1:1:217:ARG:HG3	1.86	0.41
2:2:465:ARG:NH1	5:2:2328:HOH:O	2.37	0.41
1:B:135:ARG:NH1	1:B:135:ARG:CB	2.84	0.41
1:B:217:ARG:HH11	1:B:217:ARG:HG3	1.86	0.41
2:E:306:LEU:HD12	2:E:306:LEU:C	2.45	0.41
1:K:85:ARG:NH2	5:K:2534:HOH:O	2.44	0.41
2:L:413:ASP:HA	2:L:414:PRO:HD3	1.88	0.41
2:P:447:LYS:CD	3:P:107:DMF:H23	2.49	0.41
2:R:496:ILE:HG13	2:R:505:VAL:CG2	2.50	0.41
1:S:15:GLU:CD	1:1:9:PRO:HD2	2.46	0.41
1:W:85:ARG:HD3	1:W:85:ARG:HA	1.86	0.41
2:Z:413:ASP:HA	2:Z:414:PRO:HD3	1.89	0.41
2:C:409:ILE:HG23	5:C:2502:HOH:O	2.20	0.41
2:G:409:ILE:HG12	5:G:2516:HOH:O	2.20	0.41
1:I:19:LEU:HD11	1:S:13:MET:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:383:LEU:HD23	2:J:423:PHE:CZ	2.56	0.41
2:J:516:ALA:CB	3:J:123:DMF:H12	2.46	0.41
2:P:413:ASP:HA	2:P:414:PRO:HD3	1.90	0.41
1:I:90:ASP:HB3	1:I:93:ASP:OD2	2.20	0.41
2:H:447:LYS:HD2	3:H:43:DMF:C2	2.47	0.41
1:I:167:LEU:C	1:I:169:GLU:N	2.73	0.41
2:J:401:LEU:HD13	5:J:2229:HOH:O	2.20	0.41
2:L:440:GLY:HA2	3:L:97:DMF:C	2.51	0.41
1:U:76:ARG:HD3	5:U:2597:HOH:O	2.20	0.41
1:U:213:LEU:HD23	1:U:213:LEU:HA	1.90	0.41
2:V:429:TRP:CZ3	3:V:42:DMF:H13	2.56	0.41
2:Z:345:ILE:HD12	2:Z:352:ALA:O	2.21	0.41
1:I:135:ARG:HH11	1:I:135:ARG:CB	2.34	0.41
2:2:492:PRO:O	2:2:510:ILE:HD13	2.20	0.41
2:G:372:VAL:HG23	2:G:373:PRO:HD2	2.03	0.41
2:H:331:VAL:HG11	4:H:300:SA6:C19	2.49	0.41
1:M:135:ARG:NH1	1:M:135:ARG:CB	2.83	0.41
1:O:56:LEU:HD23	1:O:56:LEU:HA	1.86	0.41
1:O:135:ARG:CB	1:O:135:ARG:HH11	2.34	0.41
1:Q:28:LYS:HD2	1:Q:44:GLU:OE2	2.21	0.41
1:W:40:LEU:HD12	1:W:212:VAL:HG12	2.03	0.41
1:W:40:LEU:CD1	1:W:212:VAL:HG12	2.50	0.41
2:X:483:GLY:HA3	3:X:122:DMF:H12	2.02	0.41
2:Z:345:ILE:HB	2:Z:352:ALA:HB1	2.02	0.41
1:B:52:LYS:HE2	1:B:64:ALA:O	2.21	0.41
1:B:206:ALA:O	1:B:207:SER:CB	2.63	0.41
1:D:15:GLU:CG	1:K:9:PRO:CG	2.98	0.41
1:D:217:ARG:HG3	1:D:218:PRO:HD2	2.03	0.41
1:I:107:LEU:HD23	1:I:107:LEU:HA	1.93	0.41
1:I:213:LEU:HD23	1:I:213:LEU:HA	1.84	0.41
1:I:217:ARG:HH12	1:I:223:ARG:HD3	1.82	0.41
1:M:10:GLU:CD	1:M:14:ARG:NH1	2.79	0.41
1:O:7:ILE:CG2	1:O:8:SER:N	2.84	0.41
2:P:331:VAL:HG11	4:P:300:SA6:C19	2.49	0.41
1:Q:179:ASP:O	1:Q:183:ILE:HG13	2.21	0.41
1:Q:189:ARG:O	1:Q:190:ALA:C	2.63	0.41
2:T:306:LEU:HD12	2:T:306:LEU:C	2.46	0.41
1:U:135:ARG:CB	1:U:135:ARG:HH11	2.34	0.41
2:V:333:LYS:HG2	4:V:300:SA6:H18	2.03	0.41
1:Y:56:LEU:HD23	1:Y:56:LEU:HA	1.83	0.41
1:I:167:LEU:C	1:I:169:GLU:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:476:ASP:OD1	3:2:49:DMF:H11	2.21	0.41
1:A:141:ILE:HD12	1:A:141:ILE:N	2.36	0.41
2:C:465:ARG:CD	5:C:1693:HOH:O	2.69	0.41
1:D:107:LEU:HD12	1:D:141:ILE:HG22	2.02	0.41
1:D:135:ARG:NH1	1:D:135:ARG:CB	2.84	0.41
1:K:85:ARG:HD2	5:K:254:HOH:O	2.20	0.41
1:K:98:GLN:O	1:K:102:VAL:HG23	2.21	0.41
3:N:22:DMF:C	5:N:2569:HOH:O	2.44	0.41
2:P:345:ILE:HB	2:P:352:ALA:HB1	2.03	0.41
2:R:444:LEU:HB2	3:R:59:DMF:N	2.35	0.41
1:U:129:HIS:O	1:U:132:GLU:HB3	2.21	0.41
1:U:135:ARG:NH1	1:U:135:ARG:CB	2.84	0.41
1:Y:189:ARG:O	1:Y:190:ALA:C	2.64	0.41
1:A:33:LEU:HD12	1:A:33:LEU:O	2.21	0.40
1:D:105:GLN:OE1	1:Q:73:ASN:ND2	2.53	0.40
1:D:135:ARG:CB	1:D:135:ARG:HH11	2.33	0.40
1:I:28:LYS:HD2	1:I:44:GLU:OE2	2.21	0.40
1:I:205:VAL:HG23	1:I:206:ALA:N	2.35	0.40
1:K:205:VAL:HG23	1:K:206:ALA:N	2.36	0.40
1:M:114:GLN:HE21	1:M:114:GLN:HB3	1.59	0.40
2:N:307:LYS:HD2	2:V:530:ASP:CG	2.40	0.40
1:Q:135:ARG:HH11	1:Q:135:ARG:CB	2.34	0.40
1:S:163:ILE:HD13	1:S:188:LEU:HD12	2.03	0.40
2:T:464:LEU:HG	2:T:513:LEU:CD1	2.50	0.40
1:U:95:THR:OG1	1:U:98:GLN:HG3	2.21	0.40
1:I:135:ARG:NH1	1:I:135:ARG:CB	2.85	0.40
1:A:233:LEU:N	1:A:233:LEU:HD12	2.36	0.40
2:C:465:ARG:HD2	5:C:1693:HOH:O	2.20	0.40
1:F:90:ASP:HB3	1:F:93:ASP:OD2	2.20	0.40
1:I:217:ARG:NH1	1:I:223:ARG:CD	2.77	0.40
2:J:515:ARG:HH12	2:R:539:HIS:N	2.16	0.40
1:M:181:LEU:HD23	1:M:233:LEU:HB3	2.03	0.40
1:O:217:ARG:HG3	1:O:217:ARG:HH11	1.86	0.40
1:Y:114:GLN:O	1:Y:115:ALA:C	2.64	0.40
1:I:141:ILE:N	1:I:141:ILE:HD12	2.36	0.40
1:A:135:ARG:CB	1:A:135:ARG:HH11	2.34	0.40
1:A:217:ARG:HG3	1:A:217:ARG:HH11	1.86	0.40
3:D:253:DMF:H13	2:E:361:VAL:HG11	2.02	0.40
1:K:56:LEU:HD23	1:K:56:LEU:HA	1.82	0.40
1:K:167:LEU:C	1:K:169:GLU:H	2.30	0.40
1:M:76:ARG:HD3	5:M:1491:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:362:GLU:OE2	2:N:382:ARG:HD2	2.20	0.40
2:P:415:GLN:NE2	5:P:2154:HOH:O	2.43	0.40
1:Q:105:GLN:OE1	1:Y:73:ASN:ND2	2.55	0.40
1:U:233:LEU:HD12	1:U:233:LEU:N	2.36	0.40
1:W:45:ASN:N	1:W:207:SER:O	2.54	0.40
1:1:163:ILE:HD13	1:1:188:LEU:HD12	2.02	0.40
1:A:11:GLN:O	1:A:12:ALA:C	2.63	0.40
1:D:52:LYS:HE2	1:D:52:LYS:HB3	1.89	0.40
2:E:432:GLU:OE2	2:E:434:GLU:HB2	2.21	0.40
1:F:8:SER:HB2	1:F:9:PRO:HD2	2.03	0.40
2:N:476:ASP:OD2	2:V:451:LYS:NZ	2.48	0.40
1:O:135:ARG:NH1	1:O:135:ARG:CB	2.85	0.40
4:R:300:SA6:H1B	4:R:300:SA6:O6	2.21	0.40
2:T:413:ASP:HA	2:T:414:PRO:HD3	1.89	0.40
3:T:113:DMF:H12	3:2:112:DMF:H21	2.03	0.40
1:W:167:LEU:HG	1:W:187:ALA:HB1	2.02	0.40
1:A:98:GLN:O	1:A:102:VAL:HG23	2.21	0.40
2:E:392:ALA:HA	2:E:395:MET:HE3	2.04	0.40
1:I:52:LYS:HE2	1:I:52:LYS:HB3	1.90	0.40
1:I:97:ARG:NE	5:I:2433:HOH:O	2.52	0.40
1:I:233:LEU:HD12	1:I:233:LEU:H	1.87	0.40
1:K:52:LYS:HE2	1:K:64:ALA:O	2.22	0.40
1:K:213:LEU:HA	1:K:213:LEU:HD23	1.86	0.40
1:M:182:ARG:NH1	1:M:234:LEU:O	2.55	0.40
1:Q:16:ARG:NH2	1:Q:115:ALA:O	2.54	0.40
1:S:85:ARG:CD	1:S:89:TYR:CD2	3.04	0.40
1:1:11:GLN:HE21	1:1:11:GLN:CA	2.26	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%)	199 (94%)	12 (6%)	0	100	100
1	A	211/248 (85%)	203 (96%)	8 (4%)	0	100	100
1	B	209/248 (84%)	201 (96%)	8 (4%)	0	100	100
1	D	210/248 (85%)	201 (96%)	9 (4%)	0	100	100
1	F	216/248 (87%)	209 (97%)	6 (3%)	1 (0%)	24	27
1	I	212/248 (86%)	201 (95%)	11 (5%)	0	100	100
1	K	212/248 (86%)	202 (95%)	10 (5%)	0	100	100
1	M	212/248 (86%)	201 (95%)	11 (5%)	0	100	100
1	O	212/248 (86%)	199 (94%)	13 (6%)	0	100	100
1	Q	211/248 (85%)	198 (94%)	13 (6%)	0	100	100
1	S	212/248 (86%)	203 (96%)	9 (4%)	0	100	100
1	U	212/248 (86%)	200 (94%)	12 (6%)	0	100	100
1	W	212/248 (86%)	199 (94%)	13 (6%)	0	100	100
1	Y	212/248 (86%)	202 (95%)	10 (5%)	0	100	100
2	2	221/240 (92%)	220 (100%)	1 (0%)	0	100	100
2	C	220/240 (92%)	219 (100%)	1 (0%)	0	100	100
2	E	221/240 (92%)	219 (99%)	2 (1%)	0	100	100
2	G	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	H	220/240 (92%)	219 (100%)	1 (0%)	0	100	100
2	J	220/240 (92%)	219 (100%)	1 (0%)	0	100	100
2	L	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
2	N	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	P	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	R	237/240 (99%)	236 (100%)	1 (0%)	0	100	100
2	T	221/240 (92%)	220 (100%)	1 (0%)	0	100	100
2	V	237/240 (99%)	234 (99%)	3 (1%)	0	100	100
2	X	221/240 (92%)	219 (99%)	2 (1%)	0	100	100
2	Z	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
All	All	6084/6832 (89%)	5913 (97%)	170 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	191	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	165/192 (86%)	159 (96%)	6 (4%)	31	42
1	A	164/192 (85%)	155 (94%)	9 (6%)	19	24
1	B	163/192 (85%)	154 (94%)	9 (6%)	19	24
1	D	164/192 (85%)	153 (93%)	11 (7%)	15	17
1	F	169/192 (88%)	162 (96%)	7 (4%)	27	37
1	I	166/192 (86%)	161 (97%)	5 (3%)	36	49
1	K	166/192 (86%)	158 (95%)	8 (5%)	23	30
1	M	166/192 (86%)	156 (94%)	10 (6%)	17	21
1	O	166/192 (86%)	161 (97%)	5 (3%)	36	49
1	Q	165/192 (86%)	158 (96%)	7 (4%)	26	36
1	S	166/192 (86%)	157 (95%)	9 (5%)	20	25
1	U	165/192 (86%)	161 (98%)	4 (2%)	43	58
1	W	166/192 (86%)	161 (97%)	5 (3%)	36	49
1	Y	166/192 (86%)	159 (96%)	7 (4%)	26	36
2	2	165/178 (93%)	158 (96%)	7 (4%)	26	36
2	C	165/178 (93%)	161 (98%)	4 (2%)	43	58
2	E	165/178 (93%)	159 (96%)	6 (4%)	31	42
2	G	165/178 (93%)	161 (98%)	4 (2%)	43	58
2	H	165/178 (93%)	158 (96%)	7 (4%)	26	36
2	J	165/178 (93%)	159 (96%)	6 (4%)	31	42
2	L	165/178 (93%)	160 (97%)	5 (3%)	36	49
2	N	165/178 (93%)	160 (97%)	5 (3%)	36	49
2	P	165/178 (93%)	161 (98%)	4 (2%)	43	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	177/178 (99%)	170 (96%)	7 (4%)	28	38
2	T	165/178 (93%)	159 (96%)	6 (4%)	31	42
2	V	177/178 (99%)	172 (97%)	5 (3%)	38	52
2	X	165/178 (93%)	160 (97%)	5 (3%)	36	49
2	Z	165/178 (93%)	159 (96%)	6 (4%)	31	42
All	All	4651/5180 (90%)	4472 (96%)	179 (4%)	29	40

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

Mol	Chain	Res	Type
1	A	9	PRO
1	A	69	ASN
1	A	73	ASN
1	A	74	LEU
1	A	80	GLN
1	A	173	GLU
1	A	182	ARG
1	A	188	LEU
1	A	234	LEU
1	B	7	ILE
1	B	14	ARG
1	B	21	ARG
1	B	69	ASN
1	B	73	ASN
1	B	74	LEU
1	B	174	ASN
1	B	182	ARG
1	B	233	LEU
2	C	345	ILE
2	C	363	LEU
2	C	444	LEU
2	C	486	LEU
1	D	10	GLU
1	D	69	ASN
1	D	73	ASN
1	D	74	LEU
1	D	144	ASP
1	D	147	ILE
1	D	170	SER
1	D	174	ASN

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Mol	Chain	Res	Type
1	D	182	ARG
1	D	205	VAL
1	D	208	LEU
2	E	345	ILE
2	E	354	GLU
2	E	363	LEU
2	E	434	GLU
2	E	444	LEU
2	E	486	LEU
1	F	5	TYR
1	F	69	ASN
1	F	73	ASN
1	F	74	LEU
1	F	173	GLU
1	F	182	ARG
1	F	203	LEU
2	G	345	ILE
2	G	363	LEU
2	G	444	LEU
2	G	486	LEU
2	H	345	ILE
2	H	363	LEU
2	H	433	GLU
2	H	434	GLU
2	H	444	LEU
2	H	486	LEU
2	H	503	VAL
1	I	69	ASN
1	I	73	ASN
1	I	74	LEU
1	I	114	GLN
1	I	136	PRO
2	J	345	ILE
2	J	363	LEU
2	J	396	GLN
2	J	398	LEU
2	J	444	LEU
2	J	486	LEU
1	K	7	ILE
1	K	10	GLU
1	K	11	GLN
1	K	69	ASN

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Mol	Chain	Res	Type
1	K	74	LEU
1	K	174	ASN
1	K	182	ARG
1	K	233	LEU
2	L	345	ILE
2	L	363	LEU
2	L	432	GLU
2	L	444	LEU
2	L	486	LEU
1	M	10	GLU
1	M	69	ASN
1	M	73	ASN
1	M	74	LEU
1	M	141	ILE
1	M	169	GLU
1	M	182	ARG
1	M	203	LEU
1	M	205	VAL
1	M	234	LEU
2	N	345	ILE
2	N	363	LEU
2	N	444	LEU
2	N	486	LEU
2	N	512	GLU
1	O	69	ASN
1	O	73	ASN
1	O	74	LEU
1	O	182	ARG
1	O	185	VAL
2	P	345	ILE
2	P	363	LEU
2	P	444	LEU
2	P	486	LEU
1	Q	69	ASN
1	Q	73	ASN
1	Q	74	LEU
1	Q	114	GLN
1	Q	173	GLU
1	Q	174	ASN
1	Q	182	ARG
2	R	345	ILE
2	R	363	LEU

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Mol	Chain	Res	Type
2	R	412	SER
2	R	433	GLU
2	R	444	LEU
2	R	486	LEU
2	R	538	HIS
1	S	7	ILE
1	S	9	PRO
1	S	11	GLN
1	S	69	ASN
1	S	73	ASN
1	S	74	LEU
1	S	170	SER
1	S	182	ARG
1	S	205	VAL
2	T	345	ILE
2	T	363	LEU
2	T	398	LEU
2	T	444	LEU
2	T	486	LEU
2	T	509	ARG
1	U	7	ILE
1	U	69	ASN
1	U	73	ASN
1	U	74	LEU
2	V	345	ILE
2	V	363	LEU
2	V	433	GLU
2	V	444	LEU
2	V	486	LEU
1	W	7	ILE
1	W	69	ASN
1	W	92	ARG
1	W	142	THR
1	W	182	ARG
2	X	345	ILE
2	X	363	LEU
2	X	444	LEU
2	X	486	LEU
2	X	519	GLU
1	Y	10	GLU
1	Y	69	ASN
1	Y	73	ASN

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Mol	Chain	Res	Type
1	Y	74	LEU
1	Y	173	GLU
1	Y	182	ARG
1	Y	203	LEU
2	Z	345	ILE
2	Z	363	LEU
2	Z	433	GLU
2	Z	444	LEU
2	Z	486	LEU
2	Z	519	GLU
1	1	69	ASN
1	1	73	ASN
1	1	74	LEU
1	1	174	ASN
1	1	182	ARG
1	1	234	LEU
2	2	345	ILE
2	2	363	LEU
2	2	433	GLU
2	2	444	LEU
2	2	465	ARG
2	2	486	LEU
2	2	512	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	80	GLN
1	A	101	ASN
1	A	114	GLN
1	A	129	HIS
1	B	69	ASN
1	B	80	GLN
1	B	101	ASN
1	B	174	ASN
2	C	456	GLN
1	D	69	ASN
1	D	73	ASN
1	D	80	GLN
1	D	98	GLN
1	D	114	GLN

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Mol	Chain	Res	Type
1	D	152	HIS
1	D	174	ASN
2	E	430	ASN
2	E	456	GLN
1	F	69	ASN
1	F	73	ASN
1	F	80	GLN
1	F	101	ASN
1	F	114	GLN
2	G	410	HIS
2	G	430	ASN
2	G	456	GLN
2	H	410	HIS
2	H	456	GLN
1	I	69	ASN
1	I	73	ASN
1	I	80	GLN
1	I	101	ASN
1	I	114	GLN
2	J	322	GLN
2	J	410	HIS
2	J	456	GLN
1	K	11	GLN
1	K	69	ASN
1	K	80	GLN
1	K	101	ASN
1	K	165	ASN
2	L	456	GLN
1	M	11	GLN
1	M	69	ASN
1	M	80	GLN
1	M	114	GLN
2	N	430	ASN
2	N	456	GLN
1	O	69	ASN
1	O	80	GLN
1	O	101	ASN
1	O	114	GLN
2	P	456	GLN
1	Q	69	ASN
1	Q	73	ASN
1	Q	80	GLN

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Mol	Chain	Res	Type
1	Q	174	ASN
2	R	410	HIS
2	R	456	GLN
2	R	536	HIS
2	R	538	HIS
2	R	539	HIS
1	S	69	ASN
1	S	73	ASN
1	S	80	GLN
1	S	114	GLN
1	S	152	HIS
2	T	456	GLN
1	U	69	ASN
1	U	80	GLN
1	U	101	ASN
1	U	114	GLN
1	U	129	HIS
1	U	231	GLN
2	V	430	ASN
2	V	456	GLN
2	V	538	HIS
1	W	69	ASN
1	W	80	GLN
1	W	114	GLN
1	W	129	HIS
2	X	410	HIS
2	X	456	GLN
1	Y	69	ASN
1	Y	73	ASN
1	Y	80	GLN
1	Y	101	ASN
1	Y	114	GLN
1	Y	174	ASN
2	Z	430	ASN
2	Z	456	GLN
1	1	11	GLN
1	1	69	ASN
1	1	80	GLN
1	1	101	ASN
1	1	114	GLN
2	2	456	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

137 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	J	45	-	4,4,4	0.30	0	4,4,4	0.33	0
3	DMF	N	90	-	4,4,4	0.31	0	4,4,4	0.47	0
3	DMF	L	81	-	4,4,4	0.30	0	4,4,4	0.35	0
3	DMF	Q	250	-	4,4,4	0.27	0	4,4,4	0.55	0
4	SA6	X	300	2	16,21,21	3.04	8 (50%)	21,32,32	1.66	2 (9%)
3	DMF	E	28	-	4,4,4	0.30	0	4,4,4	0.22	0
3	DMF	F	250	-	4,4,4	0.30	0	4,4,4	0.37	0
3	DMF	H	71	-	4,4,4	0.52	0	4,4,4	0.39	0
3	DMF	A	249	-	4,4,4	0.60	0	4,4,4	0.28	0
3	DMF	G	64	-	4,4,4	0.32	0	4,4,4	0.39	0
3	DMF	H	117	-	4,4,4	0.42	0	4,4,4	0.82	0
3	DMF	V	39	-	4,4,4	0.33	0	4,4,4	0.39	0
3	DMF	W	250	-	4,4,4	0.30	0	4,4,4	0.46	0
3	DMF	D	253	-	4,4,4	0.27	0	4,4,4	0.34	0
3	DMF	X	122	-	4,4,4	0.31	0	4,4,4	0.36	0
3	DMF	E	100	-	4,4,4	0.31	0	4,4,4	0.48	0
3	DMF	C	103	-	4,4,4	0.32	0	4,4,4	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DMF	E	75	-	4,4,4	0.28	0	4,4,4	0.43	0
3	DMF	Y	250	-	4,4,4	0.68	0	4,4,4	0.33	0
3	DMF	G	111	-	4,4,4	0.25	0	4,4,4	0.36	0
3	DMF	P	2	-	4,4,4	0.28	0	4,4,4	0.55	0
3	DMF	F	251	-	4,4,4	0.21	0	4,4,4	0.41	0
3	DMF	P	33	-	4,4,4	0.29	0	4,4,4	0.26	0
3	DMF	N	104	-	4,4,4	0.35	0	4,4,4	0.42	0
3	DMF	P	60	-	4,4,4	0.29	0	4,4,4	0.41	0
3	DMF	X	15	-	4,4,4	0.32	0	4,4,4	0.48	0
3	DMF	R	95	-	4,4,4	0.35	0	4,4,4	0.40	0
3	DMF	N	93	-	4,4,4	0.33	0	4,4,4	0.41	0
3	DMF	K	251	-	4,4,4	0.32	0	4,4,4	0.17	0
3	DMF	Z	94	-	4,4,4	0.27	0	4,4,4	0.40	0
3	DMF	I	249	-	4,4,4	0.32	0	4,4,4	0.41	0
3	DMF	R	80	-	4,4,4	0.30	0	4,4,4	0.39	0
3	DMF	E	20	-	4,4,4	0.31	0	4,4,4	0.46	0
3	DMF	K	252	-	4,4,4	0.28	0	4,4,4	0.38	0
3	DMF	G	77	-	4,4,4	0.45	0	4,4,4	0.43	0
3	DMF	M	249	-	4,4,4	0.31	0	4,4,4	0.45	0
3	DMF	Z	114	-	4,4,4	0.34	0	4,4,4	0.47	0
3	DMF	2	4	-	4,4,4	0.32	0	4,4,4	0.48	0
4	SA6	E	300	2	16,21,21	2.81	7 (43%)	21,32,32	1.79	5 (23%)
3	DMF	V	109	-	4,4,4	0.23	0	4,4,4	0.32	0
3	DMF	T	29	-	4,4,4	0.30	0	4,4,4	0.41	0
3	DMF	G	119	-	4,4,4	0.28	0	4,4,4	0.37	0
3	DMF	C	38	-	4,4,4	0.18	0	4,4,4	0.53	0
3	DMF	Q	251	-	4,4,4	0.32	0	4,4,4	0.36	0
3	DMF	P	14	-	4,4,4	0.28	0	4,4,4	0.43	0
3	DMF	J	110	-	4,4,4	0.34	0	4,4,4	0.61	0
3	DMF	N	118	-	4,4,4	0.38	0	4,4,4	0.68	0
3	DMF	K	249	-	4,4,4	0.29	0	4,4,4	0.41	0
3	DMF	D	250	-	4,4,4	0.34	0	4,4,4	0.41	0
4	SA6	2	300	2	16,21,21	2.48	4 (25%)	21,32,32	1.83	6 (28%)
3	DMF	M	252	-	4,4,4	0.33	0	4,4,4	0.39	0
4	SA6	N	300	2	16,21,21	2.77	6 (37%)	21,32,32	1.74	5 (23%)
3	DMF	O	249	-	4,4,4	0.26	0	4,4,4	0.53	0
3	DMF	2	87	-	4,4,4	0.30	0	4,4,4	0.45	0
3	DMF	O	251	-	4,4,4	0.41	0	4,4,4	0.81	0
3	DMF	X	16	-	4,4,4	0.29	0	4,4,4	0.41	0
3	DMF	R	59	-	4,4,4	0.32	0	4,4,4	0.42	0
3	DMF	R	89	-	4,4,4	0.41	0	4,4,4	0.70	0
3	DMF	G	12	-	4,4,4	0.30	0	4,4,4	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SA6	G	300	2	16,21,21	3.07	7 (43%)	21,32,32	1.53	3 (14%)
4	SA6	Z	300	2	16,21,21	3.30	10 (62%)	21,32,32	1.52	1 (4%)
4	SA6	J	300	2	16,21,21	3.04	8 (50%)	21,32,32	1.51	3 (14%)
3	DMF	U	249	-	4,4,4	0.29	0	4,4,4	0.35	0
3	DMF	E	53	-	4,4,4	0.30	0	4,4,4	0.41	0
3	DMF	V	82	-	4,4,4	0.35	0	4,4,4	0.43	0
3	DMF	G	62	-	4,4,4	0.31	0	4,4,4	0.43	0
3	DMF	Z	18	-	4,4,4	0.24	0	4,4,4	0.44	0
3	DMF	H	66	-	4,4,4	0.31	0	4,4,4	0.44	0
3	DMF	F	249	-	4,4,4	0.28	0	4,4,4	0.39	0
3	DMF	T	115	-	4,4,4	0.32	0	4,4,4	0.51	0
3	DMF	Z	54	-	4,4,4	0.35	0	4,4,4	0.49	0
3	DMF	W	249	-	4,4,4	0.31	0	4,4,4	0.43	0
3	DMF	X	41	-	4,4,4	0.56	0	4,4,4	0.36	0
3	DMF	B	250	-	4,4,4	0.30	0	4,4,4	0.36	0
3	DMF	L	97	-	4,4,4	0.30	0	4,4,4	0.45	0
4	SA6	L	300	2	16,21,21	3.09	7 (43%)	21,32,32	1.90	6 (28%)
3	DMF	P	86	-	4,4,4	0.30	0	4,4,4	0.42	0
3	DMF	T	102	-	4,4,4	0.16	0	4,4,4	0.13	0
3	DMF	2	52	-	4,4,4	0.33	0	4,4,4	0.44	0
4	SA6	R	300	2	16,21,21	3.73	7 (43%)	21,32,32	1.77	5 (23%)
3	DMF	R	92	-	4,4,4	0.30	0	4,4,4	0.42	0
3	DMF	V	42	-	4,4,4	0.30	0	4,4,4	0.49	0
3	DMF	1	249	-	4,4,4	0.30	0	4,4,4	0.39	0
3	DMF	S	249	-	4,4,4	0.29	0	4,4,4	0.38	0
3	DMF	C	63	-	4,4,4	0.29	0	4,4,4	0.53	0
3	DMF	T	84	-	4,4,4	0.08	0	4,4,4	0.15	0
3	DMF	V	32	-	4,4,4	0.31	0	4,4,4	0.49	0
3	DMF	N	22	-	4,4,4	0.32	0	4,4,4	0.37	0
3	DMF	V	83	-	4,4,4	0.24	0	4,4,4	0.44	0
3	DMF	C	69	-	4,4,4	0.29	0	4,4,4	0.47	0
3	DMF	P	56	-	4,4,4	0.31	0	4,4,4	0.46	0
3	DMF	C	88	-	4,4,4	0.33	0	4,4,4	0.51	0
3	DMF	V	27	-	4,4,4	0.30	0	4,4,4	0.36	0
4	SA6	T	300	2	16,21,21	3.23	8 (50%)	21,32,32	1.81	4 (19%)
3	DMF	C	121	-	4,4,4	0.31	0	4,4,4	0.45	0
3	DMF	T	113	-	4,4,4	0.25	0	4,4,4	0.44	0
3	DMF	Y	249	-	4,4,4	0.32	0	4,4,4	0.44	0
4	SA6	V	300	2	16,21,21	3.11	10 (62%)	21,32,32	1.41	2 (9%)
3	DMF	H	72	-	4,4,4	0.33	0	4,4,4	0.42	0
3	DMF	J	123	-	4,4,4	0.31	0	4,4,4	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DMF	V	120	-	4,4,4	0.35	0	4,4,4	0.46	0
4	SA6	C	300	2	16,21,21	2.89	6 (37%)	21,32,32	1.93	6 (28%)
3	DMF	P	51	-	4,4,4	0.26	0	4,4,4	0.37	0
3	DMF	U	250	-	4,4,4	0.71	0	4,4,4	0.34	0
3	DMF	2	101	-	4,4,4	0.34	0	4,4,4	0.43	0
3	DMF	L	36	-	4,4,4	0.33	0	4,4,4	0.48	0
3	DMF	I	250	-	4,4,4	0.28	0	4,4,4	0.35	0
3	DMF	H	91	-	4,4,4	0.29	0	4,4,4	0.47	0
3	DMF	D	249	-	4,4,4	0.60	0	4,4,4	0.37	0
3	DMF	Q	249	-	4,4,4	0.31	0	4,4,4	0.42	0
3	DMF	H	43	-	4,4,4	0.37	0	4,4,4	0.75	0
3	DMF	M	250	-	4,4,4	0.32	0	4,4,4	0.37	0
4	SA6	P	300	2	16,21,21	2.82	6 (37%)	21,32,32	1.71	4 (19%)
3	DMF	Y	251	-	4,4,4	0.31	0	4,4,4	0.43	0
3	DMF	2	57	-	4,4,4	0.31	0	4,4,4	0.34	0
3	DMF	D	251	-	4,4,4	0.31	0	4,4,4	0.43	0
3	DMF	2	49	-	4,4,4	0.25	0	4,4,4	0.51	0
3	DMF	S	250	-	4,4,4	0.70	0	4,4,4	0.37	0
3	DMF	E	73	-	4,4,4	0.29	0	4,4,4	0.45	0
3	DMF	V	116	-	4,4,4	0.45	0	4,4,4	1.07	0
3	DMF	C	47	-	4,4,4	0.57	0	4,4,4	0.24	0
4	SA6	H	300	2	16,21,21	3.09	7 (43%)	21,32,32	1.58	4 (19%)
3	DMF	D	252	-	4,4,4	0.30	0	4,4,4	0.40	0
3	DMF	2	108	-	4,4,4	0.32	0	4,4,4	0.46	0
3	DMF	G	98	-	4,4,4	0.32	0	4,4,4	0.43	0
3	DMF	O	250	-	4,4,4	0.35	0	4,4,4	0.40	0
3	DMF	G	70	-	4,4,4	0.73	0	4,4,4	0.30	0
3	DMF	K	250	-	4,4,4	0.28	0	4,4,4	0.35	0
3	DMF	M	251	-	4,4,4	0.32	0	4,4,4	0.34	0
3	DMF	P	107	-	4,4,4	0.23	0	4,4,4	0.46	0
3	DMF	2	112	-	4,4,4	0.19	0	4,4,4	0.40	0
3	DMF	L	50	-	4,4,4	0.24	0	4,4,4	0.30	0
3	DMF	X	40	-	4,4,4	0.32	0	4,4,4	0.42	0
3	DMF	B	249	-	4,4,4	0.29	0	4,4,4	0.43	0
3	DMF	G	24	-	4,4,4	0.31	0	4,4,4	0.42	0
3	DMF	T	10	-	4,4,4	0.35	0	4,4,4	0.53	0
3	DMF	A	250	-	4,4,4	0.48	0	4,4,4	0.53	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	J	45	-	-	0/2/2/2	-
3	DMF	N	90	-	-	2/2/2/2	-
3	DMF	L	81	-	-	0/2/2/2	-
3	DMF	Q	250	-	-	2/2/2/2	-
4	SA6	X	300	2	-	0/6/47/47	0/2/2/2
3	DMF	E	28	-	-	2/2/2/2	-
3	DMF	F	250	-	-	2/2/2/2	-
3	DMF	H	71	-	-	0/2/2/2	-
3	DMF	A	249	-	-	0/2/2/2	-
3	DMF	G	64	-	-	2/2/2/2	-
3	DMF	H	117	-	-	2/2/2/2	-
3	DMF	V	39	-	-	2/2/2/2	-
3	DMF	W	250	-	-	2/2/2/2	-
3	DMF	D	253	-	-	2/2/2/2	-
3	DMF	X	122	-	-	0/2/2/2	-
3	DMF	E	100	-	-	2/2/2/2	-
3	DMF	C	103	-	-	2/2/2/2	-
3	DMF	E	75	-	-	2/2/2/2	-
3	DMF	Y	250	-	-	0/2/2/2	-
3	DMF	G	111	-	-	2/2/2/2	-
3	DMF	P	2	-	-	2/2/2/2	-
3	DMF	F	251	-	-	2/2/2/2	-
3	DMF	P	33	-	-	1/2/2/2	-
3	DMF	N	104	-	-	1/2/2/2	-
3	DMF	P	60	-	-	2/2/2/2	-
3	DMF	X	15	-	-	2/2/2/2	-
3	DMF	R	95	-	-	2/2/2/2	-
3	DMF	N	93	-	-	2/2/2/2	-
3	DMF	K	251	-	-	2/2/2/2	-
3	DMF	Z	94	-	-	2/2/2/2	-
3	DMF	I	249	-	-	2/2/2/2	-
3	DMF	R	80	-	-	2/2/2/2	-
3	DMF	E	20	-	-	2/2/2/2	-
3	DMF	K	252	-	-	2/2/2/2	-
3	DMF	G	77	-	-	0/2/2/2	-
3	DMF	M	249	-	-	0/2/2/2	-
3	DMF	Z	114	-	-	0/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	2	4	-	-	0/2/2/2	-
4	SA6	E	300	2	-	1/6/47/47	0/2/2/2
3	DMF	V	109	-	-	0/2/2/2	-
3	DMF	T	29	-	-	2/2/2/2	-
3	DMF	G	119	-	-	2/2/2/2	-
3	DMF	C	38	-	-	2/2/2/2	-
3	DMF	Q	251	-	-	2/2/2/2	-
3	DMF	P	14	-	-	2/2/2/2	-
3	DMF	J	110	-	-	2/2/2/2	-
3	DMF	N	118	-	-	2/2/2/2	-
3	DMF	K	249	-	-	1/2/2/2	-
3	DMF	D	250	-	-	2/2/2/2	-
4	SA6	2	300	2	-	0/6/47/47	0/2/2/2
3	DMF	M	252	-	-	2/2/2/2	-
4	SA6	N	300	2	-	1/6/47/47	0/2/2/2
3	DMF	O	249	-	-	2/2/2/2	-
3	DMF	2	87	-	-	2/2/2/2	-
3	DMF	O	251	-	-	2/2/2/2	-
3	DMF	X	16	-	-	2/2/2/2	-
3	DMF	R	59	-	-	0/2/2/2	-
3	DMF	R	89	-	-	0/2/2/2	-
3	DMF	G	12	-	-	2/2/2/2	-
4	SA6	G	300	2	-	1/6/47/47	0/2/2/2
4	SA6	Z	300	2	-	0/6/47/47	0/2/2/2
4	SA6	J	300	2	-	0/6/47/47	0/2/2/2
3	DMF	U	249	-	-	2/2/2/2	-
3	DMF	E	53	-	-	0/2/2/2	-
3	DMF	V	82	-	-	0/2/2/2	-
3	DMF	G	62	-	-	2/2/2/2	-
3	DMF	Z	18	-	-	2/2/2/2	-
3	DMF	H	66	-	-	2/2/2/2	-
3	DMF	F	249	-	-	0/2/2/2	-
3	DMF	T	115	-	-	2/2/2/2	-
3	DMF	Z	54	-	-	2/2/2/2	-
3	DMF	W	249	-	-	2/2/2/2	-
3	DMF	X	41	-	-	0/2/2/2	-
3	DMF	B	250	-	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	L	97	-	-	2/2/2/2	-
4	SA6	L	300	2	-	2/6/47/47	0/2/2/2
3	DMF	P	86	-	-	2/2/2/2	-
3	DMF	T	102	-	-	0/2/2/2	-
3	DMF	2	52	-	-	2/2/2/2	-
4	SA6	R	300	2	-	0/6/47/47	0/2/2/2
3	DMF	R	92	-	-	0/2/2/2	-
3	DMF	V	42	-	-	2/2/2/2	-
3	DMF	1	249	-	-	0/2/2/2	-
3	DMF	S	249	-	-	2/2/2/2	-
3	DMF	C	63	-	-	2/2/2/2	-
3	DMF	T	84	-	-	2/2/2/2	-
3	DMF	V	32	-	-	2/2/2/2	-
3	DMF	N	22	-	-	2/2/2/2	-
3	DMF	V	83	-	-	0/2/2/2	-
3	DMF	C	69	-	-	2/2/2/2	-
3	DMF	P	56	-	-	2/2/2/2	-
3	DMF	C	88	-	-	2/2/2/2	-
3	DMF	V	27	-	-	2/2/2/2	-
4	SA6	T	300	2	-	0/6/47/47	0/2/2/2
3	DMF	C	121	-	-	2/2/2/2	-
3	DMF	T	113	-	-	2/2/2/2	-
3	DMF	Y	249	-	-	2/2/2/2	-
4	SA6	V	300	2	-	0/6/47/47	0/2/2/2
3	DMF	H	72	-	-	2/2/2/2	-
3	DMF	J	123	-	-	0/2/2/2	-
3	DMF	V	120	-	-	2/2/2/2	-
4	SA6	C	300	2	-	1/6/47/47	0/2/2/2
3	DMF	P	51	-	-	2/2/2/2	-
3	DMF	U	250	-	-	0/2/2/2	-
3	DMF	2	101	-	-	2/2/2/2	-
3	DMF	L	36	-	-	2/2/2/2	-
3	DMF	I	250	-	-	0/2/2/2	-
3	DMF	H	91	-	-	2/2/2/2	-
3	DMF	D	249	-	-	0/2/2/2	-
3	DMF	Q	249	-	-	0/2/2/2	-
3	DMF	H	43	-	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	M	250	-	-	2/2/2/2	-
4	SA6	P	300	2	-	0/6/47/47	0/2/2/2
3	DMF	Y	251	-	-	2/2/2/2	-
3	DMF	2	57	-	-	0/2/2/2	-
3	DMF	D	251	-	-	2/2/2/2	-
3	DMF	2	49	-	-	0/2/2/2	-
3	DMF	S	250	-	-	0/2/2/2	-
3	DMF	E	73	-	-	2/2/2/2	-
3	DMF	V	116	-	-	0/2/2/2	-
3	DMF	C	47	-	-	0/2/2/2	-
4	SA6	H	300	2	-	0/6/47/47	0/2/2/2
3	DMF	D	252	-	-	2/2/2/2	-
3	DMF	2	108	-	-	0/2/2/2	-
3	DMF	G	98	-	-	0/2/2/2	-
3	DMF	O	250	-	-	0/2/2/2	-
3	DMF	G	70	-	-	0/2/2/2	-
3	DMF	K	250	-	-	2/2/2/2	-
3	DMF	M	251	-	-	2/2/2/2	-
3	DMF	P	107	-	-	2/2/2/2	-
3	DMF	2	112	-	-	2/2/2/2	-
3	DMF	L	50	-	-	0/2/2/2	-
3	DMF	X	40	-	-	0/2/2/2	-
3	DMF	B	249	-	-	0/2/2/2	-
3	DMF	G	24	-	-	0/2/2/2	-
3	DMF	T	10	-	-	2/2/2/2	-
3	DMF	A	250	-	-	0/2/2/2	-

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	300	SA6	C5-C4	8.58	1.62	1.52
4	T	300	SA6	C5-C4	8.00	1.61	1.52
4	Z	300	SA6	C5-C4	7.61	1.61	1.52
4	H	300	SA6	C5-C4	7.40	1.61	1.52
4	L	300	SA6	C5-C4	7.32	1.61	1.52
4	X	300	SA6	C5-C4	6.73	1.60	1.52
4	N	300	SA6	C5-C4	6.45	1.60	1.52
4	J	300	SA6	C15-C13	6.40	1.64	1.54
4	V	300	SA6	C16-C15	6.38	1.66	1.54
4	G	300	SA6	C16-C15	6.21	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	300	SA6	C5-C4	6.16	1.59	1.52
4	Z	300	SA6	C16-C15	6.12	1.65	1.54
4	L	300	SA6	C16-C15	6.06	1.65	1.54
4	R	300	SA6	C2-C3	6.01	1.63	1.53
4	P	300	SA6	C5-C4	6.01	1.59	1.52
4	R	300	SA6	C16-C15	5.94	1.65	1.54
4	C	300	SA6	C16-C15	5.92	1.65	1.54
4	J	300	SA6	C16-C15	5.78	1.65	1.54
4	E	300	SA6	C5-C4	5.69	1.59	1.52
4	P	300	SA6	C16-C15	5.61	1.64	1.54
4	V	300	SA6	C5-C4	5.59	1.59	1.52
4	T	300	SA6	C16-C15	5.58	1.64	1.54
4	X	300	SA6	C16-C15	5.43	1.64	1.54
4	2	300	SA6	C5-C4	5.32	1.58	1.52
4	C	300	SA6	C2-C3	5.28	1.62	1.53
4	2	300	SA6	C16-C15	5.19	1.63	1.54
4	G	300	SA6	C15-C13	5.16	1.62	1.54
4	E	300	SA6	C16-C15	5.13	1.63	1.54
4	N	300	SA6	C16-C15	5.02	1.63	1.54
4	J	300	SA6	C5-C4	4.99	1.58	1.52
4	R	300	SA6	C7-N9	-4.89	1.29	1.34
4	C	300	SA6	C5-C4	4.86	1.58	1.52
4	R	300	SA6	C15-C13	4.84	1.62	1.54
4	H	300	SA6	C15-C13	4.64	1.61	1.54
4	T	300	SA6	C15-C13	4.63	1.61	1.54
4	H	300	SA6	C16-C15	4.61	1.62	1.54
4	X	300	SA6	C2-C3	4.60	1.61	1.53
4	L	300	SA6	C7-N9	-4.15	1.29	1.34
4	H	300	SA6	C2-C3	4.15	1.60	1.53
4	E	300	SA6	C15-C13	4.14	1.61	1.54
4	P	300	SA6	C15-C13	4.09	1.61	1.54
4	G	300	SA6	C2-C3	4.03	1.60	1.53
4	V	300	SA6	C15-C20	3.91	1.57	1.50
4	C	300	SA6	C15-C13	3.88	1.60	1.54
4	2	300	SA6	C15-C13	3.88	1.60	1.54
4	N	300	SA6	C15-C13	3.82	1.60	1.54
4	Z	300	SA6	C15-C13	3.74	1.60	1.54
4	V	300	SA6	C15-C13	3.72	1.60	1.54
4	N	300	SA6	C2-C3	3.71	1.59	1.53
4	E	300	SA6	C2-C3	3.68	1.59	1.53
4	V	300	SA6	C2-C3	3.66	1.59	1.53
4	C	300	SA6	C7-N9	-3.62	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Z	300	SA6	C2-C3	3.62	1.59	1.53
4	J	300	SA6	O14-C13	3.52	1.49	1.42
4	P	300	SA6	C2-C3	3.52	1.59	1.53
4	X	300	SA6	C15-C13	3.51	1.60	1.54
4	V	300	SA6	O14-C13	3.47	1.49	1.42
4	X	300	SA6	C15-C20	3.43	1.56	1.50
4	L	300	SA6	C15-C13	3.35	1.59	1.54
4	Z	300	SA6	C7-N9	-3.34	1.30	1.34
4	G	300	SA6	C15-C20	3.24	1.55	1.50
4	E	300	SA6	O6-C4	3.21	1.48	1.43
4	T	300	SA6	C15-C20	3.20	1.55	1.50
4	T	300	SA6	O6-C4	3.20	1.48	1.43
4	P	300	SA6	C15-C20	3.16	1.55	1.50
4	X	300	SA6	O6-C4	3.15	1.48	1.43
4	E	300	SA6	C3-C7	3.11	1.56	1.52
4	Z	300	SA6	C15-C20	3.08	1.55	1.50
4	T	300	SA6	C2-C3	3.05	1.58	1.53
4	J	300	SA6	O6-C4	2.93	1.48	1.43
4	R	300	SA6	O14-C13	2.92	1.48	1.42
4	H	300	SA6	C7-N9	-2.90	1.31	1.34
4	Z	300	SA6	O14-C13	2.87	1.48	1.42
4	2	300	SA6	C2-C3	2.84	1.58	1.53
4	L	300	SA6	C15-C20	2.81	1.55	1.50
4	J	300	SA6	C20-C19	2.81	1.39	1.32
4	N	300	SA6	O14-C13	2.79	1.48	1.42
4	J	300	SA6	C2-C3	2.78	1.58	1.53
4	L	300	SA6	C2-C3	2.76	1.58	1.53
4	H	300	SA6	O14-C13	2.73	1.48	1.42
4	V	300	SA6	O6-C4	2.64	1.47	1.43
4	P	300	SA6	C20-C19	2.53	1.38	1.32
4	X	300	SA6	O14-C13	2.45	1.47	1.42
4	V	300	SA6	C18-C19	2.43	1.57	1.48
4	J	300	SA6	C15-C20	2.40	1.54	1.50
4	G	300	SA6	O6-C4	2.38	1.47	1.43
4	Z	300	SA6	C20-C19	2.36	1.38	1.32
4	C	300	SA6	C3-C7	2.36	1.55	1.52
4	G	300	SA6	C20-C19	2.34	1.38	1.32
4	T	300	SA6	C7-N9	-2.33	1.32	1.34
4	X	300	SA6	C20-C19	2.32	1.38	1.32
4	N	300	SA6	C3-C7	2.30	1.55	1.52
4	Z	300	SA6	O6-C4	2.30	1.47	1.43
4	L	300	SA6	O6-C4	2.28	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Z	300	SA6	C3-C7	2.24	1.55	1.52
4	E	300	SA6	C20-C19	2.23	1.37	1.32
4	R	300	SA6	C15-C20	2.18	1.54	1.50
4	H	300	SA6	O6-C4	2.12	1.47	1.43
4	T	300	SA6	C20-C19	2.06	1.37	1.32
4	V	300	SA6	C20-C19	2.03	1.37	1.32
4	V	300	SA6	C3-C7	2.00	1.55	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	300	SA6	C4-C3-C7	-5.24	99.79	104.23
4	T	300	SA6	C4-C3-C7	-5.06	99.95	104.23
4	R	300	SA6	C4-C3-C7	-4.61	100.32	104.23
4	C	300	SA6	C4-C3-C7	-4.60	100.34	104.23
4	P	300	SA6	C4-C3-C7	-4.58	100.35	104.23
4	Z	300	SA6	C4-C3-C7	-4.13	100.73	104.23
4	N	300	SA6	C4-C3-C7	-4.10	100.76	104.23
4	2	300	SA6	C4-C3-C7	-4.05	100.80	104.23
4	L	300	SA6	C10-C13-C15	4.01	119.12	114.09
4	V	300	SA6	C4-C3-C7	-3.98	100.85	104.23
4	E	300	SA6	C4-C3-C7	-3.96	100.87	104.23
4	H	300	SA6	C4-C3-C7	-3.90	100.92	104.23
4	J	300	SA6	C4-C3-C7	-3.74	101.06	104.23
4	T	300	SA6	C10-C13-C15	3.71	118.75	114.09
4	L	300	SA6	C4-C3-C7	-3.70	101.10	104.23
4	E	300	SA6	C10-C13-C15	3.59	118.60	114.09
4	2	300	SA6	C10-C13-C15	3.42	118.39	114.09
4	G	300	SA6	C4-C3-C7	-3.35	101.39	104.23
4	C	300	SA6	C10-C13-C15	3.22	118.13	114.09
4	L	300	SA6	O14-C13-C15	-3.08	103.04	109.98
4	L	300	SA6	C2-C3-C4	2.95	120.12	115.56
4	E	300	SA6	C1-C2-C3	2.91	120.78	113.61
4	N	300	SA6	C2-C3-C4	2.91	120.06	115.56
4	P	300	SA6	C10-C13-C15	2.86	117.68	114.09
4	N	300	SA6	C1-C2-C3	2.82	120.56	113.61
4	2	300	SA6	C2-C3-C4	2.81	119.92	115.56
4	G	300	SA6	C10-C13-C15	2.79	117.59	114.09
4	R	300	SA6	C10-C13-C15	2.60	117.35	114.09
4	L	300	SA6	C1-C2-C3	2.59	119.99	113.61
4	2	300	SA6	O14-C13-C15	-2.59	104.14	109.98
4	C	300	SA6	O14-C13-C15	-2.55	104.23	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	300	SA6	C10-C13-C15	2.54	117.28	114.09
4	T	300	SA6	O14-C13-C15	-2.54	104.25	109.98
4	G	300	SA6	C1-C2-C3	2.53	119.85	113.61
4	C	300	SA6	C2-C3-C4	2.52	119.46	115.56
4	C	300	SA6	C1-C2-C3	2.52	119.81	113.61
4	P	300	SA6	O8-C7-C3	-2.47	123.52	126.15
4	X	300	SA6	C1-C2-C3	2.45	119.64	113.61
4	J	300	SA6	C10-C13-C15	2.44	117.15	114.09
4	E	300	SA6	C2-C3-C4	2.35	119.20	115.56
4	2	300	SA6	C1-C2-C3	2.35	119.41	113.61
4	R	300	SA6	C1-C2-C3	2.33	119.36	113.61
4	C	300	SA6	O6-C4-C5	-2.30	102.51	108.11
4	R	300	SA6	C16-C15-C13	2.23	118.75	113.36
4	T	300	SA6	O8-C7-C3	-2.23	123.78	126.15
4	2	300	SA6	O8-C7-C3	-2.22	123.79	126.15
4	V	300	SA6	O8-C7-C3	-2.21	123.80	126.15
4	P	300	SA6	C1-C2-C3	2.20	119.04	113.61
4	H	300	SA6	O6-C4-C5	-2.17	102.84	108.11
4	J	300	SA6	O8-C7-C3	-2.16	123.85	126.15
4	H	300	SA6	O14-C13-C15	-2.11	105.22	109.98
4	L	300	SA6	O6-C4-C5	-2.11	102.97	108.11
4	R	300	SA6	O14-C13-C15	-2.11	105.22	109.98
4	N	300	SA6	C10-C13-C15	2.04	116.65	114.09
4	N	300	SA6	C16-C15-C13	2.02	118.24	113.36
4	E	300	SA6	O6-C4-C5	-2.01	103.21	108.11

There are no chirality outliers.

All (169) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	300	SA6	C1-C2-C3-C4
4	E	300	SA6	C1-C2-C3-C4
4	G	300	SA6	C1-C2-C3-C4
4	L	300	SA6	C1-C2-C3-C4
4	N	300	SA6	C1-C2-C3-C4
3	E	73	DMF	O-C-N-C1
3	L	36	DMF	O-C-N-C2
3	K	250	DMF	O-C-N-C1
3	L	36	DMF	O-C-N-C1
3	E	73	DMF	O-C-N-C2
3	K	250	DMF	O-C-N-C2
3	C	63	DMF	O-C-N-C1

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Mol	Chain	Res	Type	Atoms
3	T	84	DMF	O-C-N-C1
3	T	84	DMF	O-C-N-C2
3	T	115	DMF	O-C-N-C1
3	C	63	DMF	O-C-N-C2
3	N	93	DMF	O-C-N-C1
3	N	93	DMF	O-C-N-C2
3	P	86	DMF	O-C-N-C1
3	C	121	DMF	O-C-N-C1
3	C	121	DMF	O-C-N-C2
3	D	250	DMF	O-C-N-C1
3	D	250	DMF	O-C-N-C2
3	K	251	DMF	O-C-N-C2
3	K	252	DMF	O-C-N-C1
3	P	86	DMF	O-C-N-C2
3	2	112	DMF	O-C-N-C1
3	K	251	DMF	O-C-N-C1
3	E	75	DMF	O-C-N-C1
3	T	115	DMF	O-C-N-C2
3	M	251	DMF	O-C-N-C1
3	R	80	DMF	O-C-N-C1
3	Z	18	DMF	O-C-N-C1
3	2	112	DMF	O-C-N-C2
3	E	75	DMF	O-C-N-C2
3	H	117	DMF	O-C-N-C1
3	M	251	DMF	O-C-N-C2
3	Z	18	DMF	O-C-N-C2
3	P	60	DMF	O-C-N-C1
3	2	101	DMF	O-C-N-C1
3	H	43	DMF	O-C-N-C1
3	K	252	DMF	O-C-N-C2
3	Q	250	DMF	O-C-N-C1
3	C	88	DMF	O-C-N-C1
3	R	80	DMF	O-C-N-C2
3	E	28	DMF	O-C-N-C1
3	G	119	DMF	O-C-N-C1
3	H	117	DMF	O-C-N-C2
3	J	110	DMF	O-C-N-C1
3	P	60	DMF	O-C-N-C2
3	T	113	DMF	O-C-N-C1
3	N	90	DMF	O-C-N-C1
3	P	51	DMF	O-C-N-C1
3	S	249	DMF	O-C-N-C1

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Mol	Chain	Res	Type	Atoms
3	C	88	DMF	O-C-N-C2
3	2	101	DMF	O-C-N-C2
3	G	12	DMF	O-C-N-C1
3	E	28	DMF	O-C-N-C2
3	N	22	DMF	O-C-N-C1
3	P	51	DMF	O-C-N-C2
3	V	32	DMF	O-C-N-C1
3	T	113	DMF	O-C-N-C2
3	V	120	DMF	O-C-N-C1
3	G	119	DMF	O-C-N-C2
3	S	249	DMF	O-C-N-C2
3	H	43	DMF	O-C-N-C2
3	Q	250	DMF	O-C-N-C2
3	X	16	DMF	O-C-N-C1
3	H	91	DMF	O-C-N-C1
3	O	251	DMF	O-C-N-C1
3	N	90	DMF	O-C-N-C2
3	J	110	DMF	O-C-N-C2
3	C	38	DMF	O-C-N-C2
3	N	22	DMF	O-C-N-C2
3	M	252	DMF	O-C-N-C1
3	V	32	DMF	O-C-N-C2
3	B	250	DMF	O-C-N-C1
3	T	10	DMF	O-C-N-C1
3	G	12	DMF	O-C-N-C2
3	M	250	DMF	O-C-N-C1
3	V	120	DMF	O-C-N-C2
3	C	38	DMF	O-C-N-C1
3	H	91	DMF	O-C-N-C2
3	X	16	DMF	O-C-N-C2
3	O	251	DMF	O-C-N-C2
3	Z	54	DMF	O-C-N-C1
3	Y	249	DMF	O-C-N-C1
3	T	29	DMF	O-C-N-C1
3	U	249	DMF	O-C-N-C1
3	H	66	DMF	O-C-N-C1
3	F	251	DMF	O-C-N-C1
3	2	87	DMF	O-C-N-C1
3	C	103	DMF	O-C-N-C1
3	2	52	DMF	O-C-N-C1
3	B	250	DMF	O-C-N-C2
3	G	62	DMF	O-C-N-C1

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Mol	Chain	Res	Type	Atoms
3	M	252	DMF	O-C-N-C2
3	D	251	DMF	O-C-N-C1
3	E	100	DMF	O-C-N-C1
3	M	250	DMF	O-C-N-C2
3	T	10	DMF	O-C-N-C2
3	Q	251	DMF	O-C-N-C1
3	L	97	DMF	O-C-N-C1
3	V	27	DMF	O-C-N-C1
3	X	15	DMF	O-C-N-C1
3	Z	54	DMF	O-C-N-C2
3	Y	249	DMF	O-C-N-C2
3	U	249	DMF	O-C-N-C2
3	T	29	DMF	O-C-N-C2
3	I	249	DMF	O-C-N-C1
3	P	56	DMF	O-C-N-C1
3	F	251	DMF	O-C-N-C2
3	P	14	DMF	O-C-N-C1
3	H	66	DMF	O-C-N-C2
3	2	87	DMF	O-C-N-C2
3	C	103	DMF	O-C-N-C2
3	D	252	DMF	O-C-N-C1
3	W	250	DMF	O-C-N-C1
3	F	250	DMF	O-C-N-C1
3	2	52	DMF	O-C-N-C2
3	Q	251	DMF	O-C-N-C2
3	D	251	DMF	O-C-N-C2
3	G	62	DMF	O-C-N-C2
3	E	100	DMF	O-C-N-C2
3	L	97	DMF	O-C-N-C2
3	V	27	DMF	O-C-N-C2
3	X	15	DMF	O-C-N-C2
3	P	56	DMF	O-C-N-C2
3	I	249	DMF	O-C-N-C2
3	G	64	DMF	O-C-N-C1
3	R	95	DMF	O-C-N-C1
3	D	252	DMF	O-C-N-C2
3	P	14	DMF	O-C-N-C2
3	O	249	DMF	O-C-N-C2
3	P	2	DMF	O-C-N-C1
3	G	111	DMF	O-C-N-C1
3	W	250	DMF	O-C-N-C2
3	F	250	DMF	O-C-N-C2

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Mol	Chain	Res	Type	Atoms
3	V	39	DMF	O-C-N-C1
3	C	69	DMF	O-C-N-C1
3	D	253	DMF	O-C-N-C1
4	L	300	SA6	C1-C2-C3-C7
3	V	42	DMF	O-C-N-C1
3	E	20	DMF	O-C-N-C1
3	G	64	DMF	O-C-N-C2
3	W	249	DMF	O-C-N-C1
3	R	95	DMF	O-C-N-C2
3	G	111	DMF	O-C-N-C2
3	V	39	DMF	O-C-N-C2
3	P	2	DMF	O-C-N-C2
3	C	69	DMF	O-C-N-C2
3	P	107	DMF	O-C-N-C1
3	D	253	DMF	O-C-N-C2
3	V	42	DMF	O-C-N-C2
3	E	20	DMF	O-C-N-C2
3	N	118	DMF	O-C-N-C2
3	Z	94	DMF	O-C-N-C1
3	N	118	DMF	O-C-N-C1
3	W	249	DMF	O-C-N-C2
3	P	107	DMF	O-C-N-C2
3	Y	251	DMF	O-C-N-C1
3	O	249	DMF	O-C-N-C1
3	H	72	DMF	O-C-N-C1
3	Z	94	DMF	O-C-N-C2
3	P	33	DMF	O-C-N-C1
3	K	249	DMF	O-C-N-C1
3	N	104	DMF	O-C-N-C1
3	Y	251	DMF	O-C-N-C2
3	H	72	DMF	O-C-N-C2

There are no ring outliers.

105 monomers are involved in 317 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	45	DMF	1	0
3	N	90	DMF	7	0
3	L	81	DMF	1	0
3	Q	250	DMF	6	0
4	X	300	SA6	4	0
3	E	28	DMF	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	250	DMF	1	0
3	H	71	DMF	1	0
3	A	249	DMF	1	0
3	G	64	DMF	9	0
3	H	117	DMF	2	0
3	V	39	DMF	1	0
3	W	250	DMF	5	0
3	D	253	DMF	2	0
3	X	122	DMF	1	0
3	E	100	DMF	2	0
3	C	103	DMF	8	0
3	E	75	DMF	4	0
3	Y	250	DMF	1	0
3	G	111	DMF	1	0
3	P	2	DMF	1	0
3	P	33	DMF	3	0
3	N	104	DMF	7	0
3	X	15	DMF	2	0
3	R	95	DMF	1	0
3	N	93	DMF	4	0
3	K	251	DMF	3	0
3	Z	94	DMF	3	0
3	R	80	DMF	1	0
3	E	20	DMF	4	0
3	K	252	DMF	3	0
3	2	4	DMF	8	0
4	E	300	SA6	3	0
3	T	29	DMF	3	0
3	G	119	DMF	11	0
3	C	38	DMF	3	0
3	Q	251	DMF	1	0
3	P	14	DMF	5	0
3	N	118	DMF	4	0
3	K	249	DMF	1	0
4	2	300	SA6	4	0
4	N	300	SA6	3	0
3	2	87	DMF	2	0
3	X	16	DMF	3	0
3	R	59	DMF	9	0
3	G	12	DMF	4	0
4	G	300	SA6	3	0
4	Z	300	SA6	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	300	SA6	2	0
3	E	53	DMF	2	0
3	V	82	DMF	2	0
3	G	62	DMF	1	0
3	Z	18	DMF	2	0
3	H	66	DMF	3	0
3	T	115	DMF	1	0
3	Z	54	DMF	3	0
3	W	249	DMF	2	0
3	X	41	DMF	1	0
3	L	97	DMF	4	0
4	L	300	SA6	3	0
3	T	102	DMF	3	0
3	2	52	DMF	2	0
4	R	300	SA6	3	0
3	R	92	DMF	2	0
3	V	42	DMF	7	0
3	S	249	DMF	1	0
3	C	63	DMF	1	0
3	T	84	DMF	3	0
3	V	32	DMF	5	0
3	N	22	DMF	4	0
3	V	83	DMF	10	0
3	C	69	DMF	1	0
3	C	88	DMF	2	0
3	V	27	DMF	8	0
4	T	300	SA6	3	0
3	T	113	DMF	5	0
3	Y	249	DMF	1	0
4	V	300	SA6	4	0
3	J	123	DMF	6	0
3	V	120	DMF	8	0
4	C	300	SA6	3	0
3	U	250	DMF	8	0
3	2	101	DMF	3	0
3	I	250	DMF	2	0
3	H	91	DMF	2	0
3	Q	249	DMF	2	0
3	H	43	DMF	4	0
4	P	300	SA6	4	0
3	Y	251	DMF	2	0
3	D	251	DMF	5	0

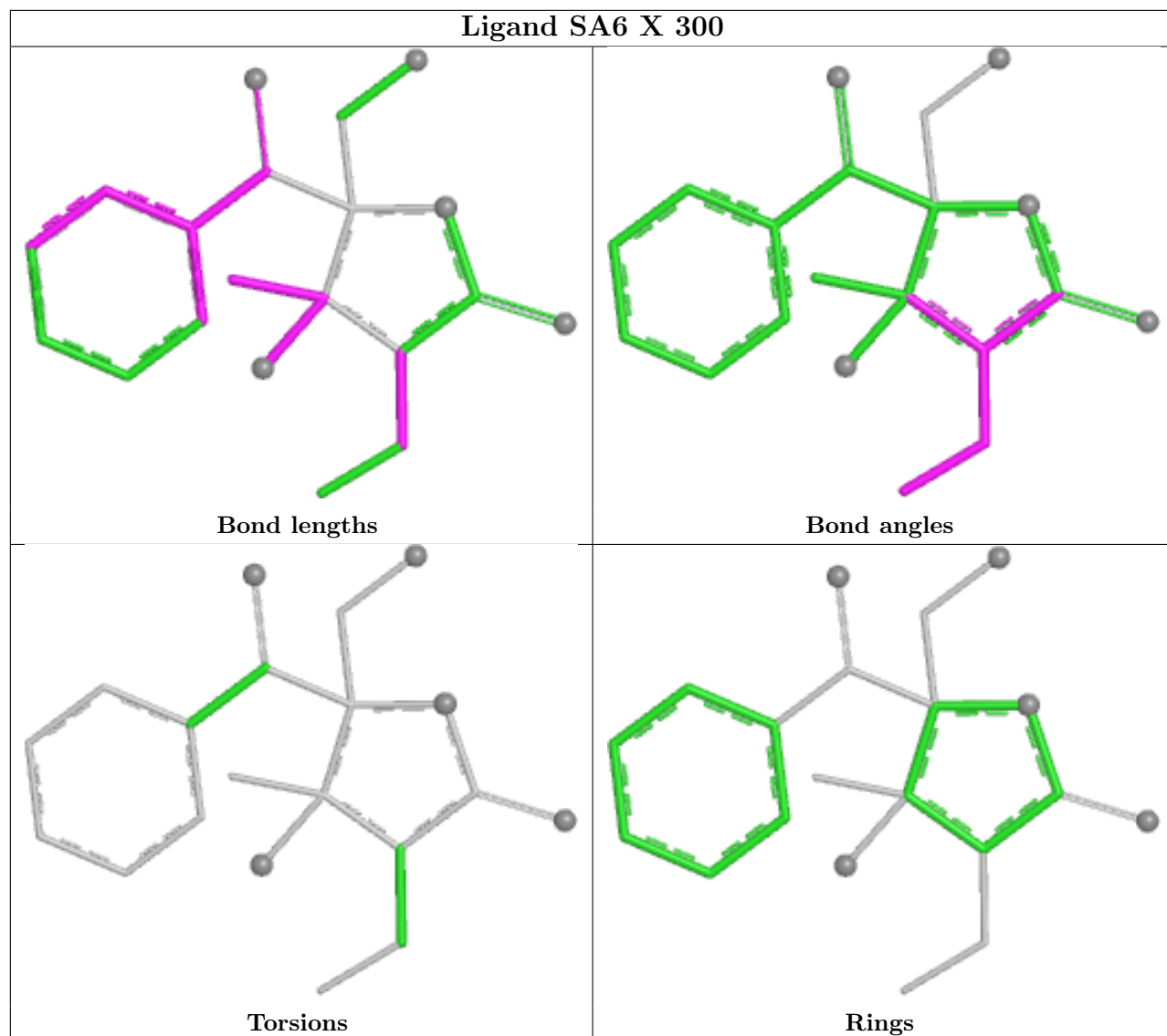
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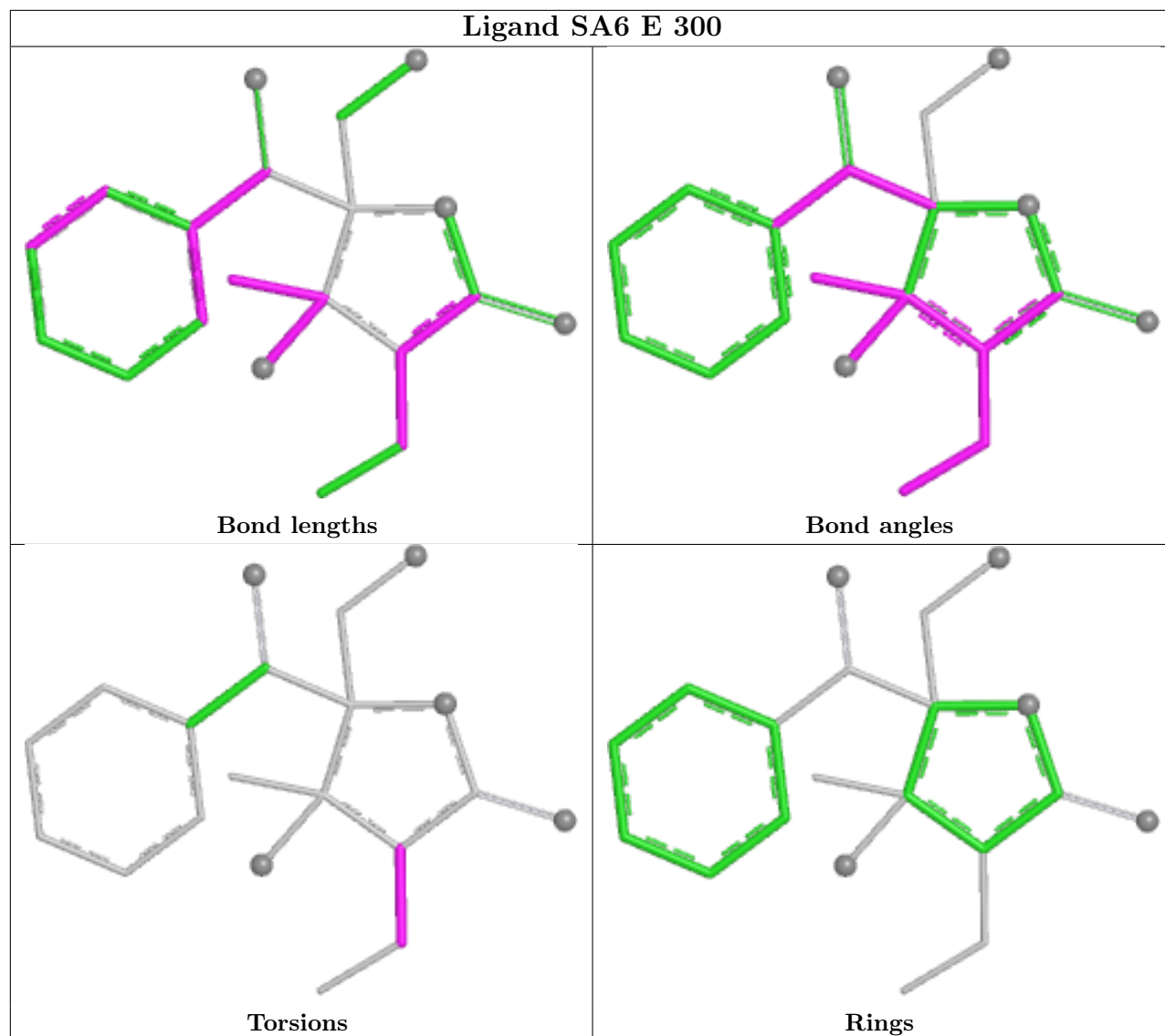
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	2	49	DMF	1	0
3	E	73	DMF	3	0
3	V	116	DMF	6	0
3	C	47	DMF	1	0
4	H	300	SA6	5	0
3	2	108	DMF	5	0
3	G	98	DMF	2	0
3	O	250	DMF	1	0
3	G	70	DMF	1	0
3	K	250	DMF	4	0
3	P	107	DMF	5	0
3	2	112	DMF	7	0
3	X	40	DMF	1	0
3	B	249	DMF	2	0
3	G	24	DMF	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

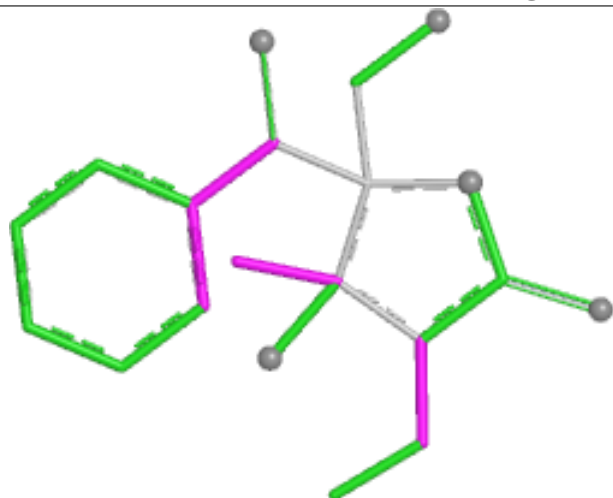
Ligand SA6 X 300



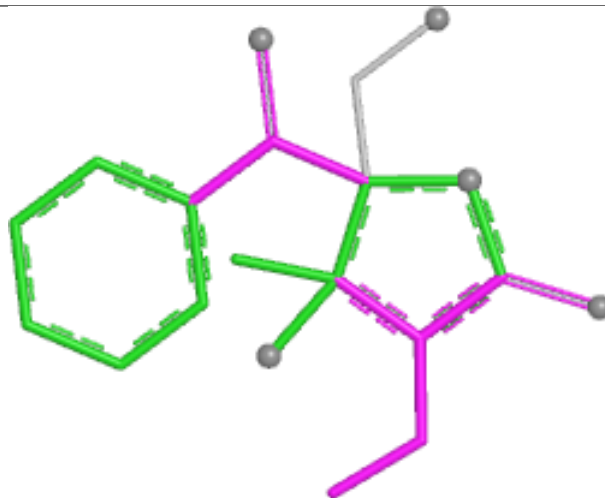
Ligand SA6 E 300



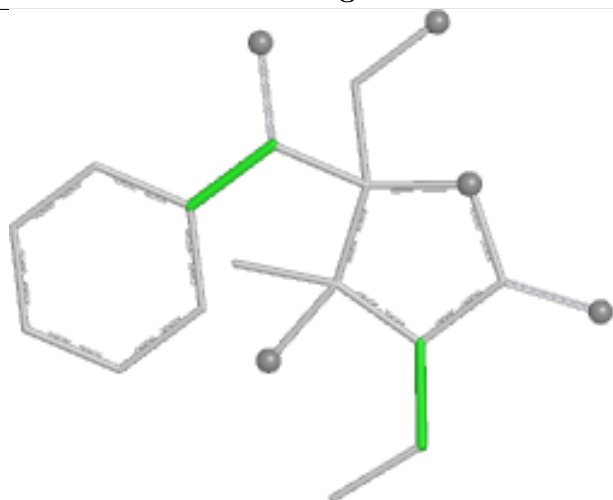
Ligand SA6 2 300



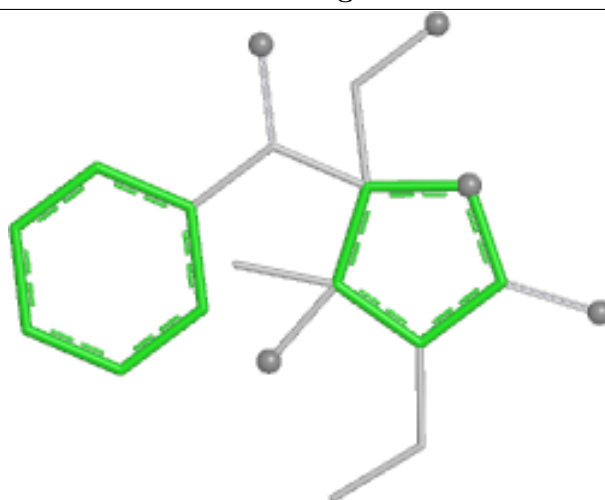
Bond lengths



Bond angles

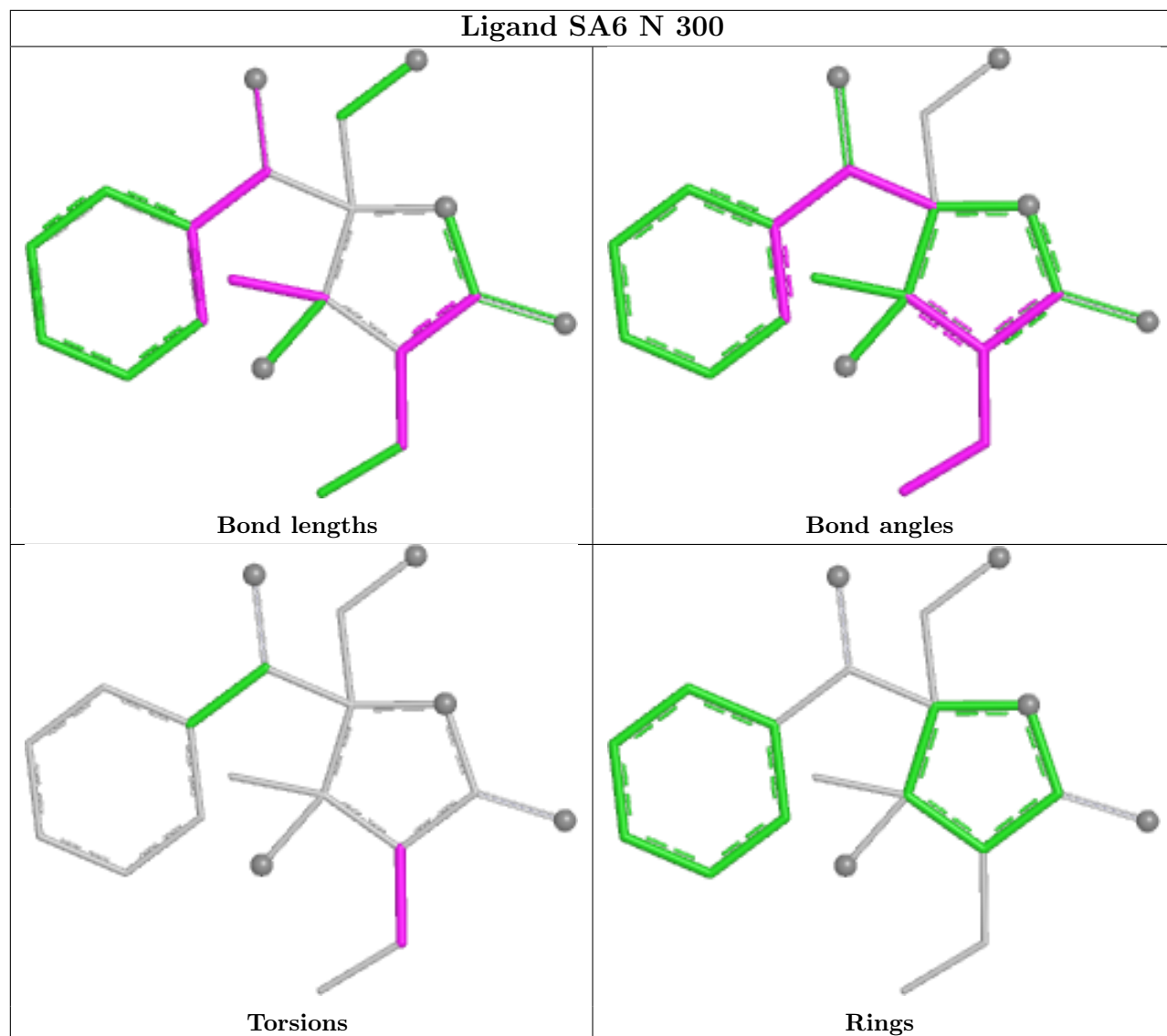


Torsions

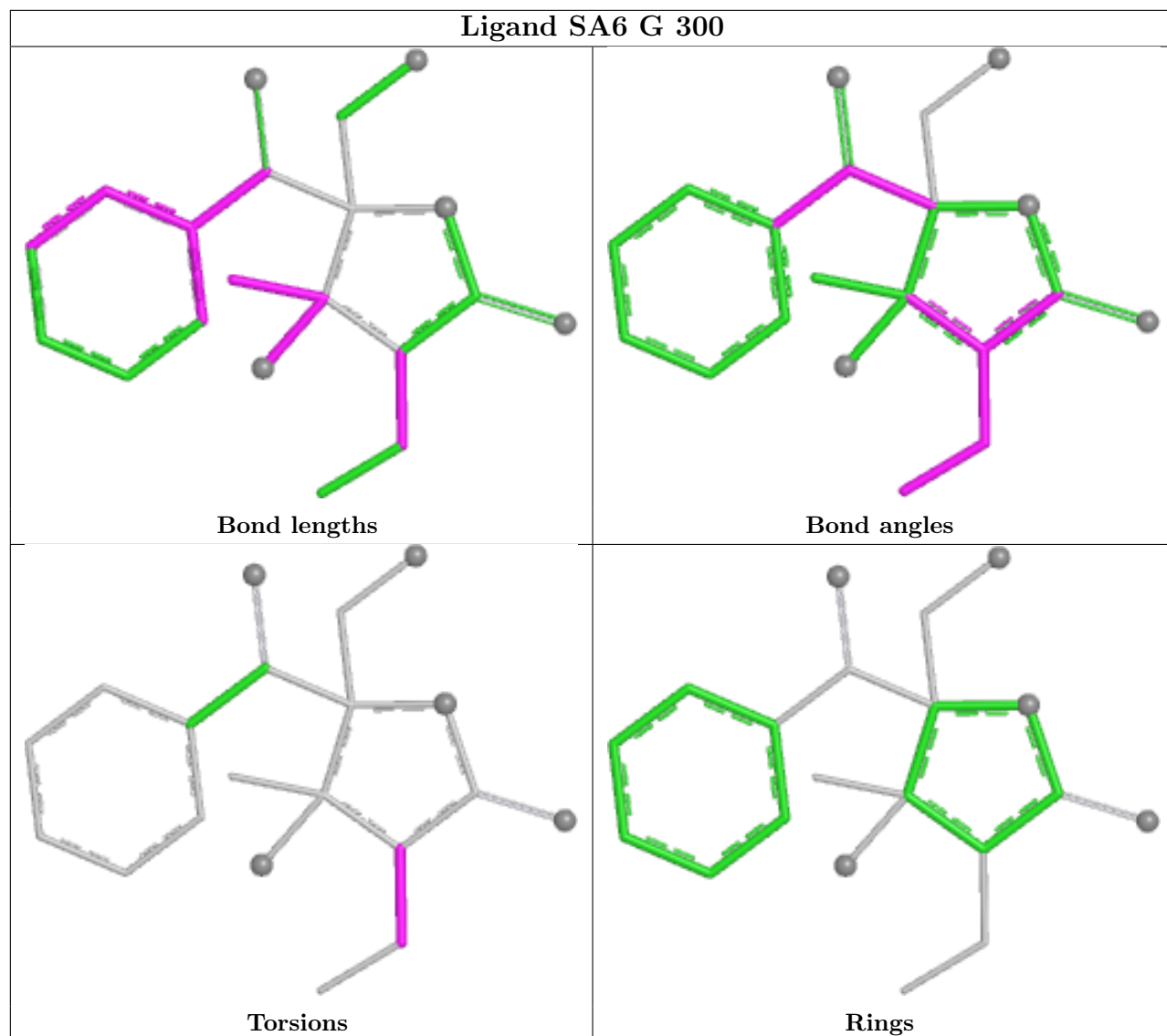


Rings

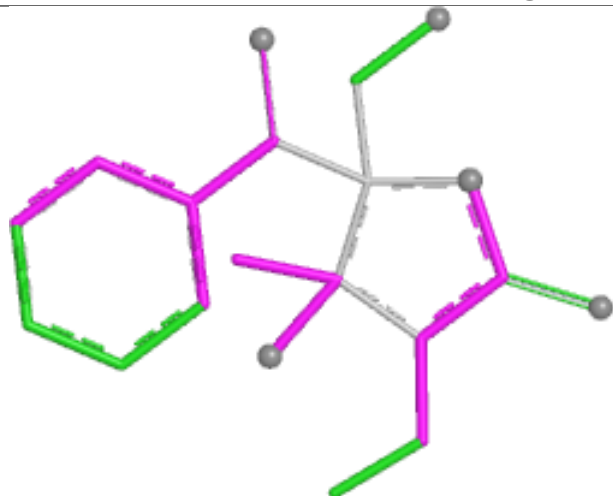
Ligand SA6 N 300



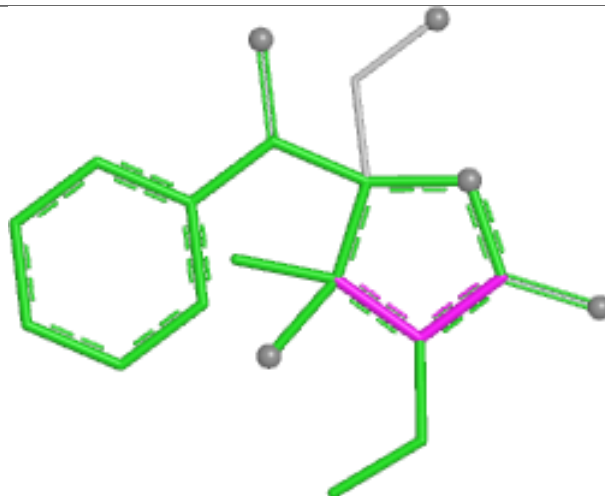
Ligand SA6 G 300



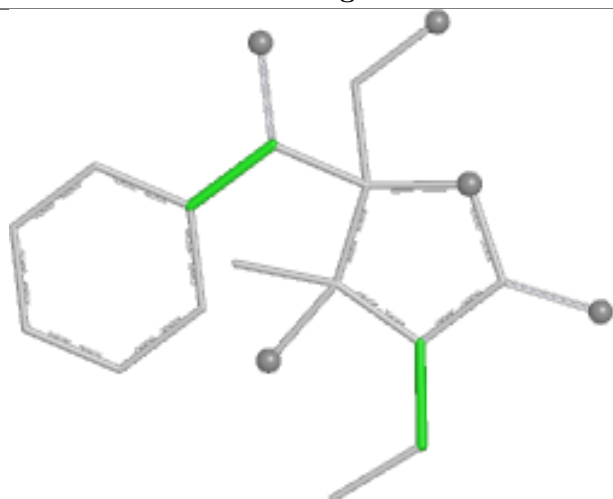
Ligand SA6 Z 300



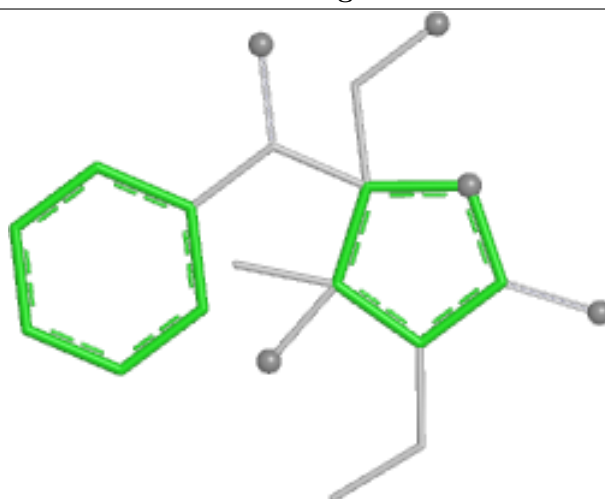
Bond lengths



Bond angles

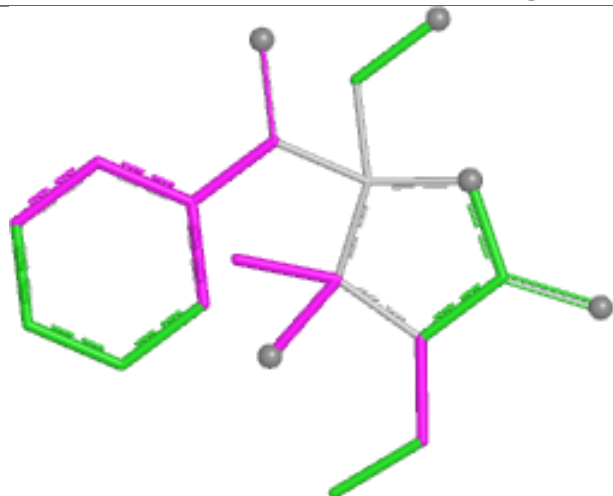


Torsions

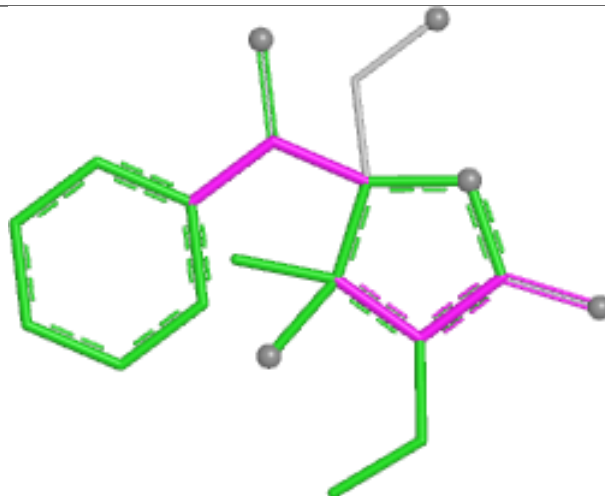


Rings

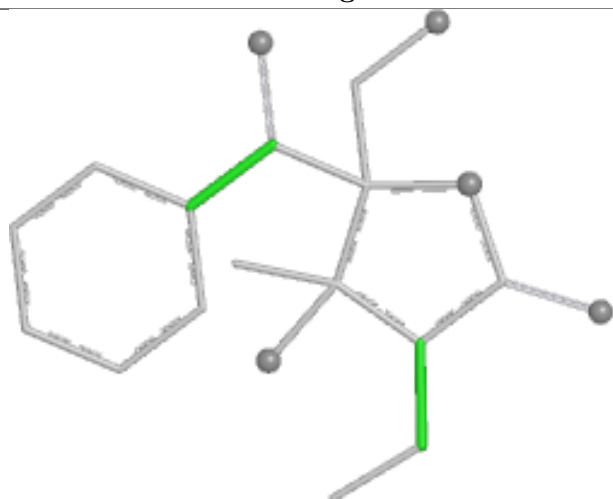
Ligand SA6 J 300



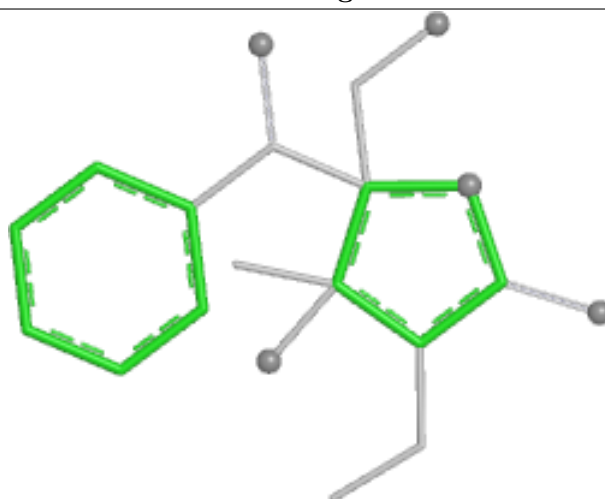
Bond lengths



Bond angles

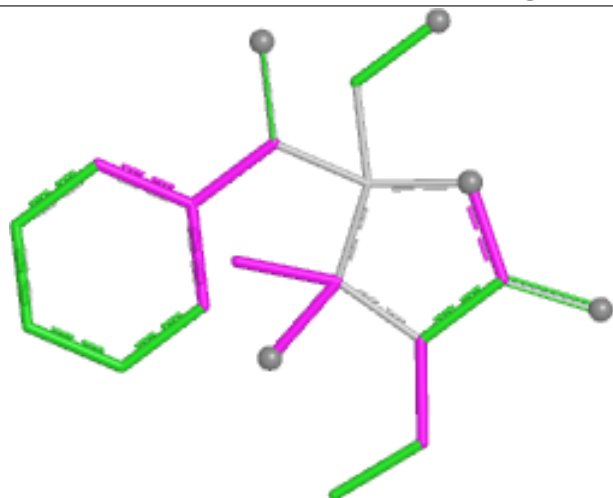


Torsions

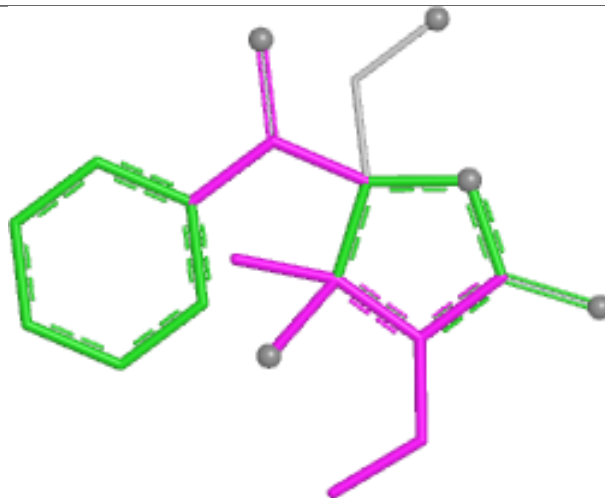


Rings

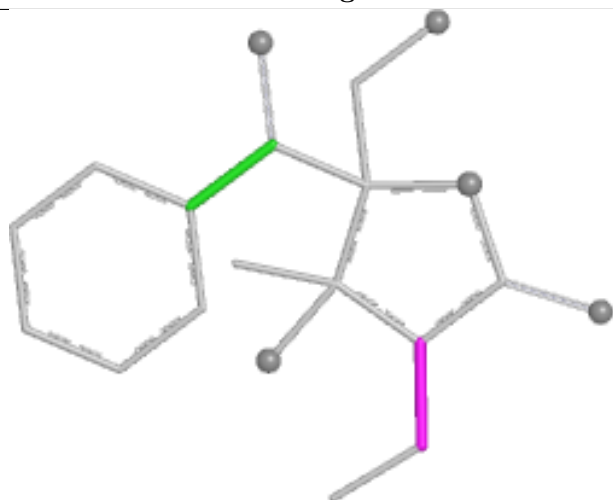
Ligand SA6 L 300



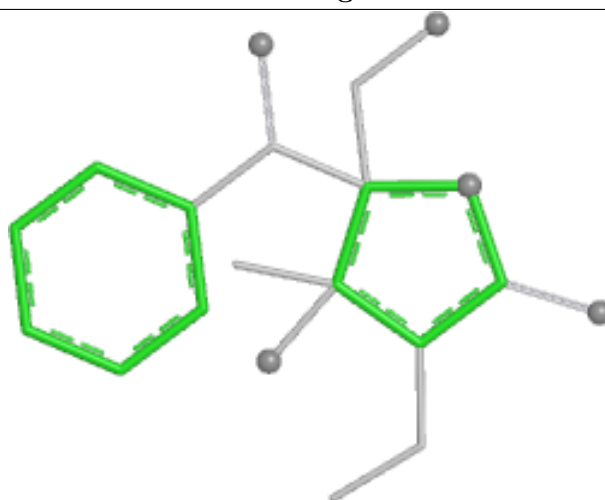
Bond lengths



Bond angles

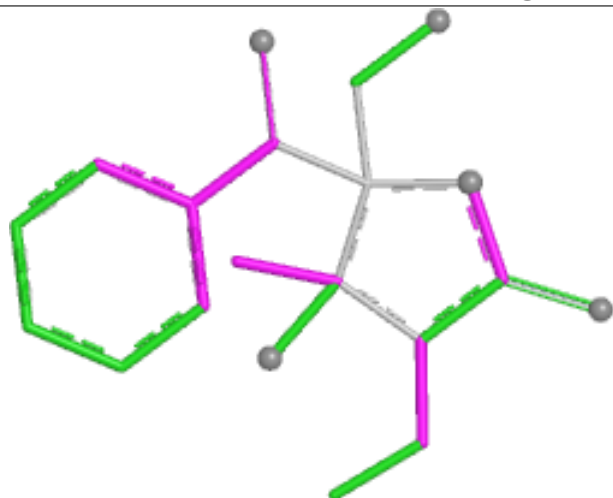


Torsions

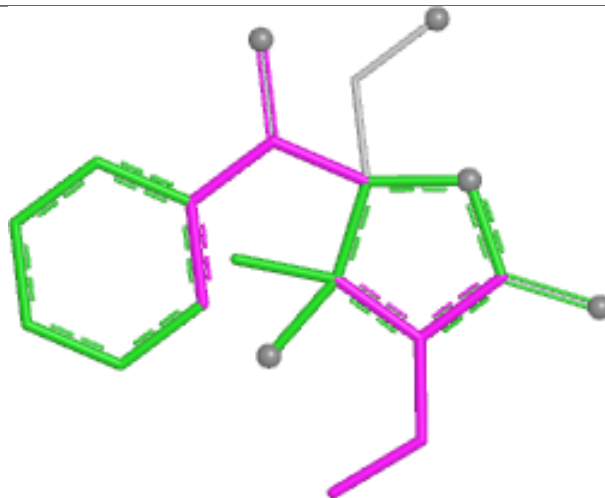


Rings

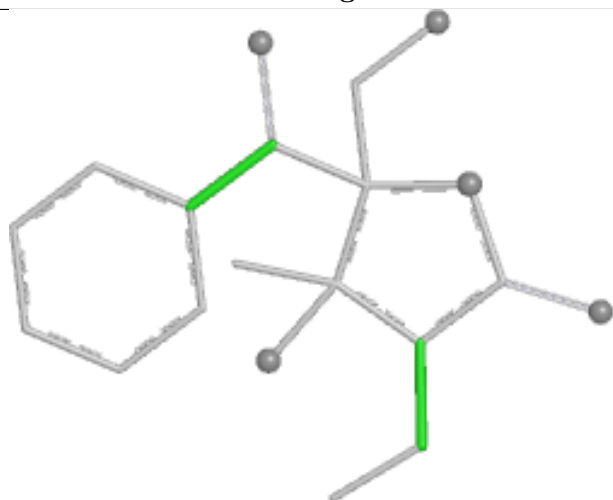
Ligand SA6 R 300



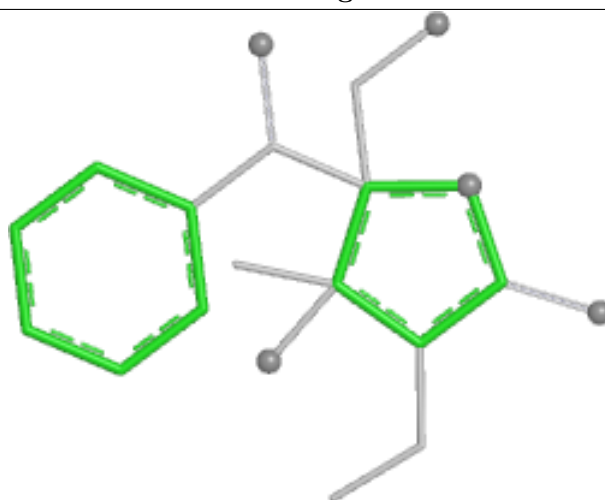
Bond lengths



Bond angles

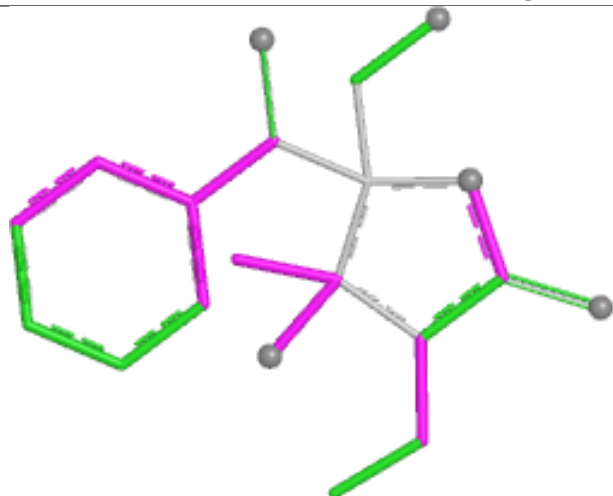


Torsions

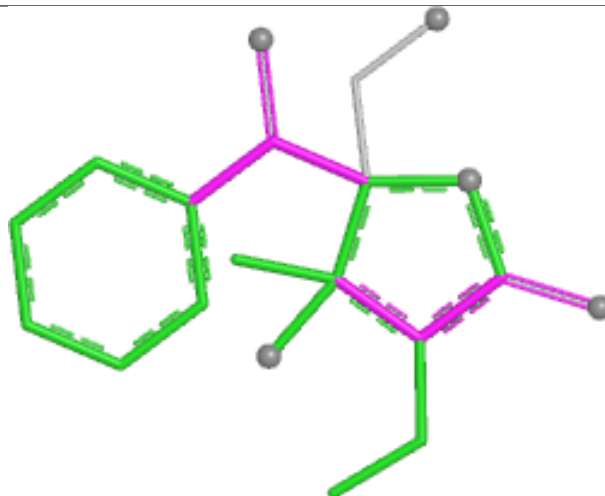


Rings

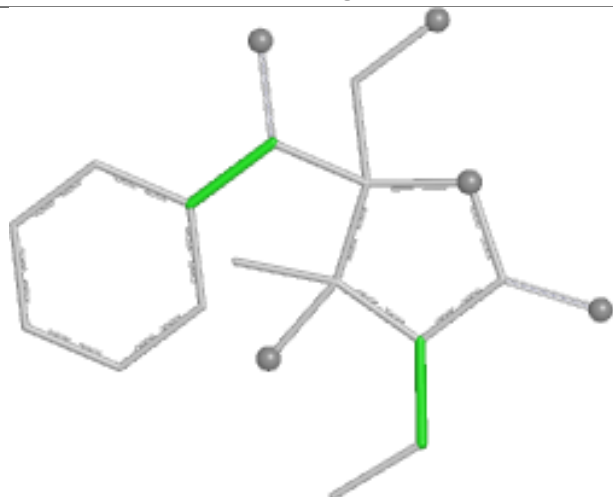
Ligand SA6 T 300



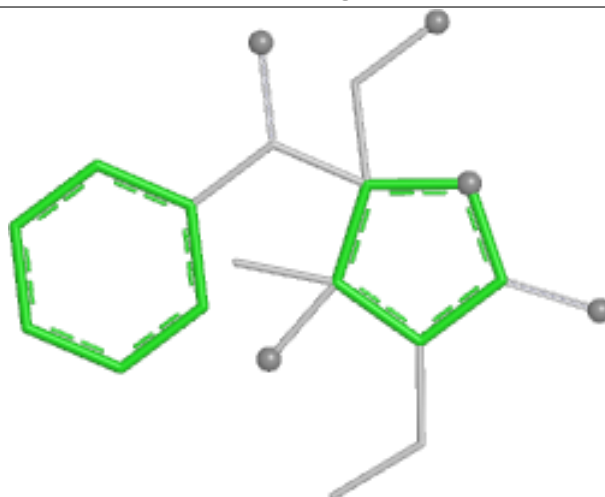
Bond lengths



Bond angles

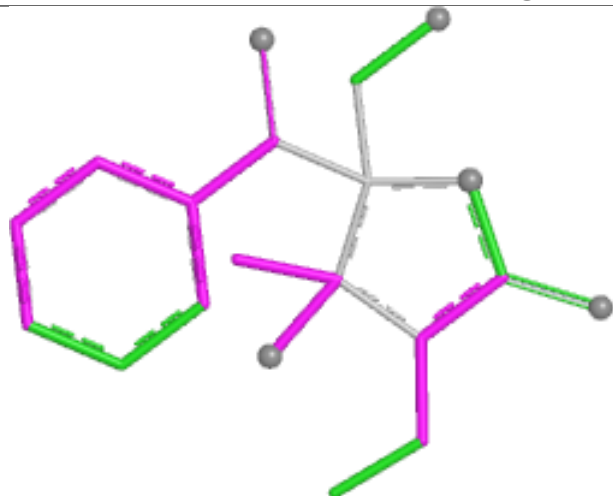


Torsions

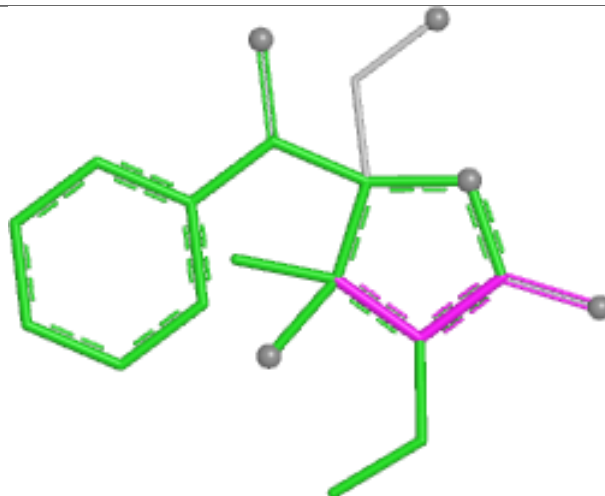


Rings

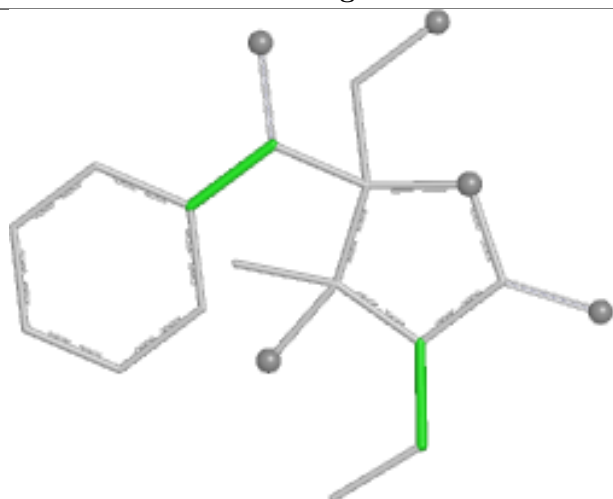
Ligand SA6 V 300



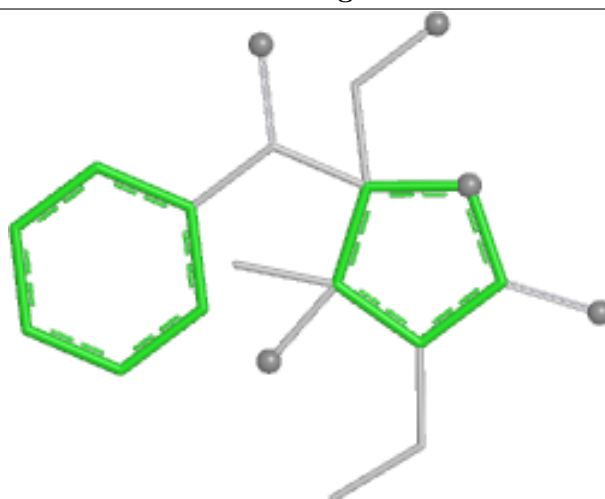
Bond lengths



Bond angles

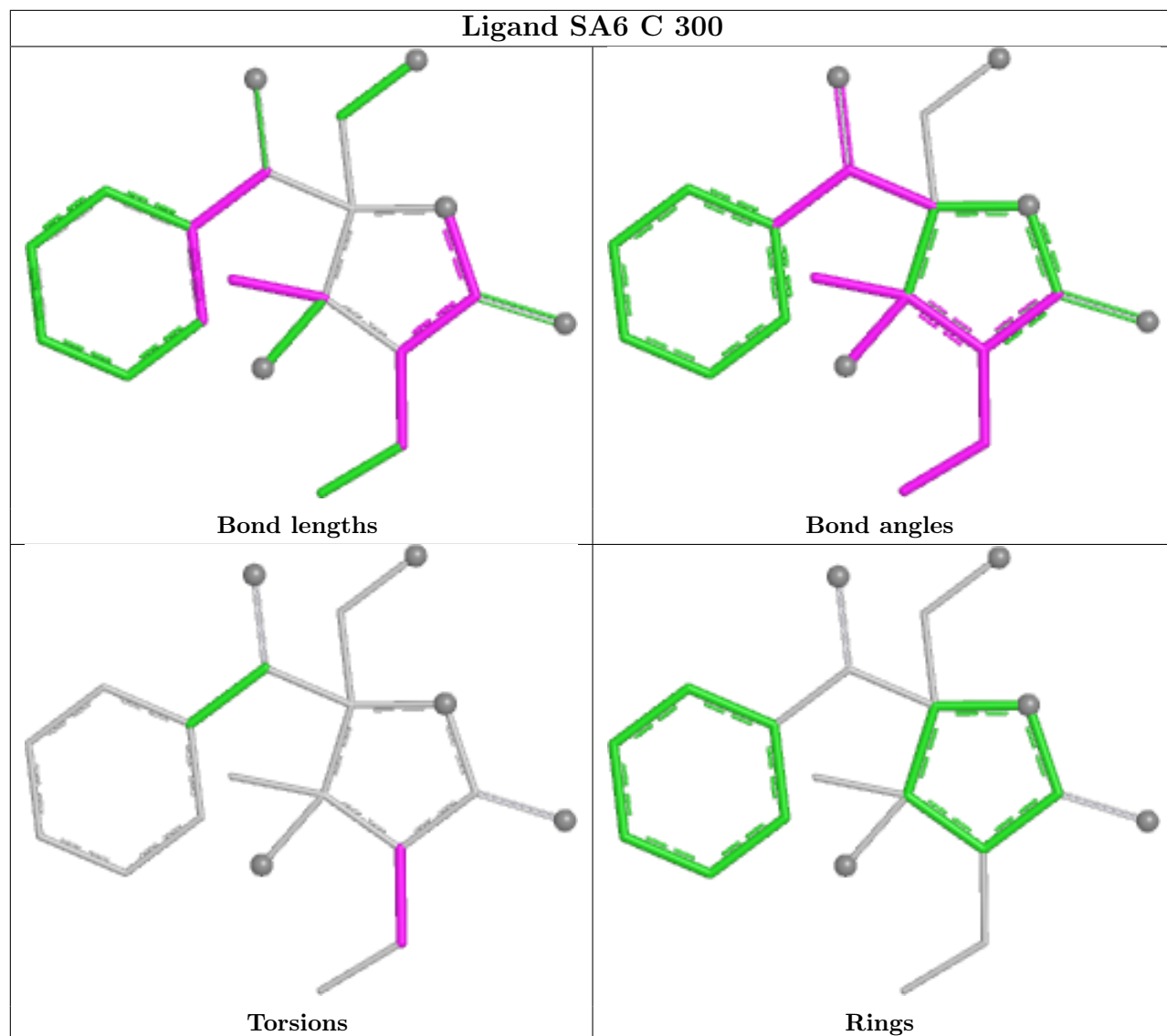


Torsions

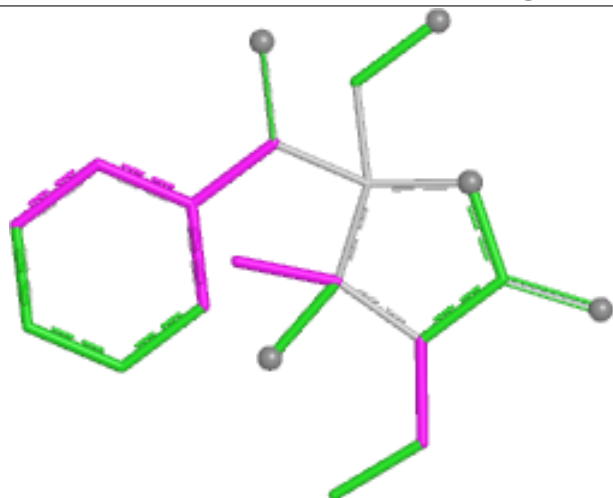


Rings

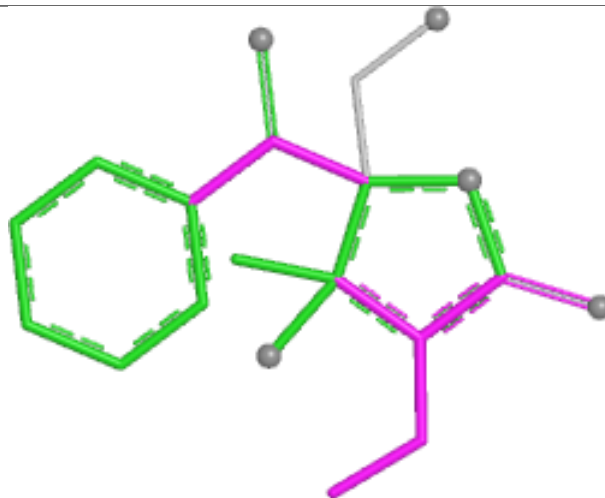
Ligand SA6 C 300



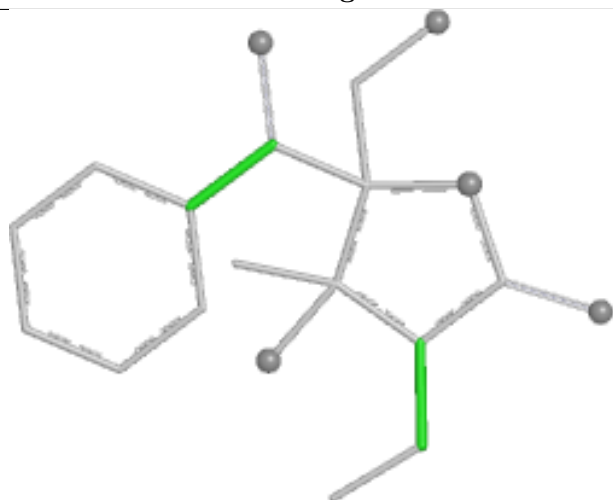
Ligand SA6 P 300



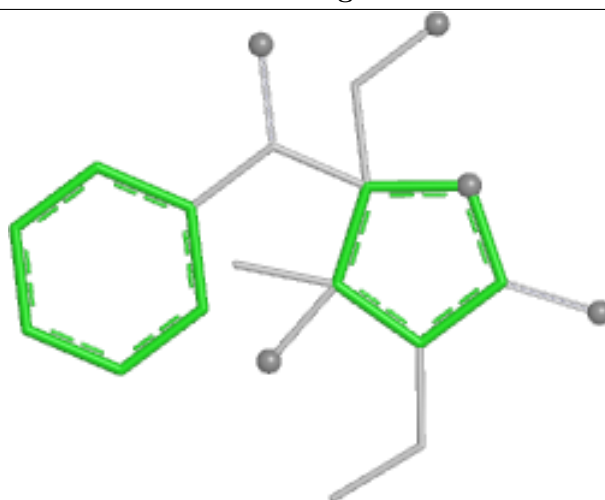
Bond lengths



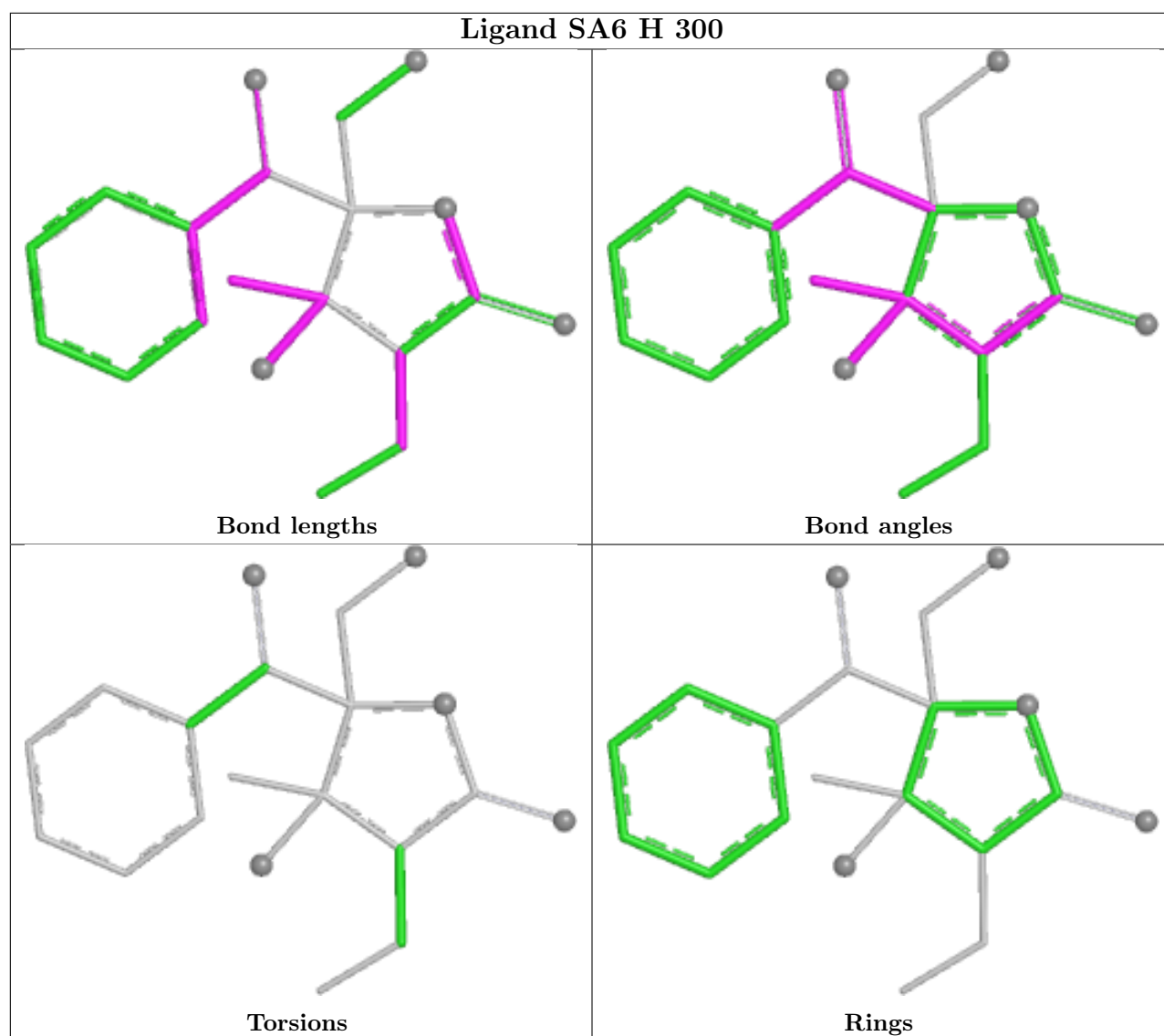
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	215/248 (86%)	0.82	28 (13%) 7 5	19, 48, 88, 109	0
1	A	215/248 (86%)	1.05	46 (21%) 2 2	20, 54, 91, 107	0
1	B	213/248 (85%)	0.84	28 (13%) 7 5	20, 49, 88, 106	0
1	D	214/248 (86%)	1.76	93 (43%) 0 0	20, 65, 98, 110	0
1	F	220/248 (88%)	0.87	29 (13%) 7 5	17, 48, 86, 104	0
1	I	216/248 (87%)	0.96	33 (15%) 5 4	18, 52, 92, 108	0
1	K	216/248 (87%)	0.97	30 (13%) 6 5	21, 55, 92, 107	0
1	M	216/248 (87%)	1.11	47 (21%) 2 1	18, 53, 92, 104	0
1	O	216/248 (87%)	0.87	27 (12%) 8 6	17, 49, 87, 102	0
1	Q	215/248 (86%)	0.91	23 (10%) 11 8	22, 50, 86, 99	0
1	S	216/248 (87%)	1.05	35 (16%) 4 3	20, 56, 91, 104	0
1	U	216/248 (87%)	0.90	30 (13%) 6 5	16, 49, 86, 102	0
1	W	216/248 (87%)	1.37	49 (22%) 2 1	20, 63, 94, 107	0
1	Y	216/248 (87%)	1.22	42 (19%) 3 2	22, 58, 94, 123	0
2	2	223/240 (92%)	-0.39	1 (0%) 88 87	11, 21, 45, 65	0
2	C	222/240 (92%)	-0.39	6 (2%) 56 53	8, 20, 48, 79	0
2	E	223/240 (92%)	-0.41	3 (1%) 75 73	8, 20, 46, 63	0
2	G	222/240 (92%)	-0.34	3 (1%) 73 71	10, 23, 53, 75	0
2	H	222/240 (92%)	-0.38	0 100 100	9, 23, 50, 71	0
2	J	222/240 (92%)	-0.39	1 (0%) 87 85	9, 21, 49, 70	0
2	L	223/240 (92%)	-0.31	5 (2%) 62 59	8, 21, 46, 66	0
2	N	222/240 (92%)	-0.42	2 (0%) 81 79	8, 21, 47, 79	0
2	P	222/240 (92%)	-0.38	0 100 100	10, 23, 49, 73	0
2	R	239/240 (99%)	-0.39	5 (2%) 63 60	8, 20, 55, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	T	223/240 (92%)	-0.25	0 100 100	10, 24, 53, 72	0
2	V	239/240 (99%)	-0.38	5 (2%) 63 60	8, 20, 63, 91	0
2	X	223/240 (92%)	-0.32	3 (1%) 75 73	10, 24, 56, 73	0
2	Z	223/240 (92%)	-0.29	2 (0%) 81 79	11, 24, 52, 69	0
All	All	6168/6832 (90%)	0.33	576 (9%) 14 12	8, 33, 84, 123	0

All (576) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	GLY	6.8
1	Y	9	PRO	6.3
1	M	203	LEU	5.7
1	O	203	LEU	5.5
1	I	203	LEU	5.4
1	S	7	ILE	5.3
1	D	180	ALA	5.3
1	Y	190	ALA	5.1
1	D	233	LEU	5.0
1	D	159	THR	4.9
1	D	234	LEU	4.9
2	L	309	PRO	4.9
2	V	530	ASP	4.9
1	F	190	ALA	4.9
1	I	190	ALA	4.9
1	W	163	ILE	4.7
2	E	461	ASP	4.7
1	Y	203	LEU	4.7
1	B	7	ILE	4.6
1	Q	7	ILE	4.6
1	M	190	ALA	4.6
1	K	7	ILE	4.6
1	B	206	ALA	4.5
1	M	12	ALA	4.5
1	Q	190	ALA	4.5
2	R	530	ASP	4.4
1	M	167	LEU	4.4
1	D	153	PHE	4.4
1	F	192	SER	4.3
1	D	172	ALA	4.3
1	D	167	LEU	4.3
1	D	184	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	42	VAL	4.2
1	I	6	PHE	4.2
1	D	204	GLY	4.1
1	D	183	ILE	4.1
1	D	227	GLY	4.1
1	B	13	MET	4.1
1	Y	7	ILE	4.1
1	1	163	ILE	4.1
1	W	234	LEU	4.0
1	1	203	LEU	4.0
2	X	523	GLY	4.0
1	K	190	ALA	4.0
1	W	206	ALA	4.0
1	W	172	ALA	4.0
1	D	163	ILE	4.0
1	S	235	VAL	4.0
1	F	234	LEU	4.0
2	L	461	ASP	4.0
1	D	205	VAL	3.9
1	K	203	LEU	3.9
1	S	204	GLY	3.9
1	F	7	ILE	3.9
1	D	188	LEU	3.9
1	I	12	ALA	3.9
1	O	187	ALA	3.9
1	Y	172	ALA	3.9
1	K	204	GLY	3.9
1	D	190	ALA	3.8
1	B	190	ALA	3.8
1	U	190	ALA	3.8
1	W	204	GLY	3.8
1	O	172	ALA	3.8
1	M	7	ILE	3.8
1	K	189	ARG	3.7
1	A	172	ALA	3.7
1	Y	8	SER	3.7
1	A	190	ALA	3.7
1	1	190	ALA	3.7
1	Y	131	GLY	3.6
2	2	523	GLY	3.6
1	B	233	LEU	3.6
1	F	203	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	166	ALA	3.6
1	D	32	ALA	3.6
1	S	12	ALA	3.6
1	B	171	TYR	3.6
1	D	8	SER	3.6
1	I	7	ILE	3.6
1	D	12	ALA	3.6
1	Q	172	ALA	3.6
1	S	172	ALA	3.6
1	1	15	GLU	3.6
1	M	13	MET	3.6
1	W	233	LEU	3.6
1	Y	234	LEU	3.6
1	S	190	ALA	3.6
1	W	190	ALA	3.6
1	S	163	ILE	3.5
1	M	180	ALA	3.5
1	D	171	TYR	3.5
1	U	205	VAL	3.5
1	A	205	VAL	3.5
1	D	33	LEU	3.5
1	D	31	VAL	3.4
1	D	40	LEU	3.4
1	D	177	LEU	3.4
1	Y	171	TYR	3.4
1	D	155	VAL	3.4
1	U	234	LEU	3.4
2	C	416	SER	3.4
1	W	180	ALA	3.4
1	F	6	PHE	3.3
1	A	180	ALA	3.3
1	A	188	LEU	3.3
1	M	171	TYR	3.3
1	D	30	VAL	3.3
1	W	205	VAL	3.3
1	D	157	GLY	3.3
1	D	182	ARG	3.3
1	F	5	TYR	3.3
1	M	234	LEU	3.2
1	I	171	TYR	3.2
1	I	172	ALA	3.2
1	K	172	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	157	GLY	3.2
1	D	10	GLU	3.2
1	D	179	ASP	3.2
1	W	162	PRO	3.2
1	Y	163	ILE	3.2
1	O	7	ILE	3.2
1	D	158	GLY	3.1
1	D	165	ASN	3.1
1	Q	180	ALA	3.1
1	A	171	TYR	3.1
1	D	228	SER	3.1
1	A	163	ILE	3.1
1	U	7	ILE	3.1
1	F	191	GLY	3.1
1	Y	12	ALA	3.1
1	Y	175	ALA	3.1
1	D	181	LEU	3.1
1	W	208	LEU	3.1
1	U	171	TYR	3.1
1	W	130	TYR	3.1
1	1	159	THR	3.1
1	D	41	PHE	3.1
1	D	231	GLN	3.1
1	D	185	VAL	3.1
1	Y	13	MET	3.1
1	U	163	ILE	3.0
1	A	204	GLY	3.0
1	D	25	ALA	3.0
1	W	159	THR	3.0
1	B	175	ALA	3.0
1	1	12	ALA	3.0
1	S	188	LEU	3.0
1	W	167	LEU	3.0
1	I	13	MET	3.0
1	D	36	ALA	3.0
1	D	206	ALA	3.0
1	1	172	ALA	3.0
1	K	233	LEU	3.0
1	M	205	VAL	3.0
2	J	415	GLN	3.0
1	D	160	THR	3.0
1	S	162	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	Q	175	ALA	2.9
1	A	13	MET	2.9
1	Q	161	GLU	2.9
1	K	188	LEU	2.9
1	S	171	TYR	2.9
1	S	207	SER	2.9
1	M	9	PRO	2.9
1	A	175	ALA	2.9
1	D	232	ALA	2.9
1	M	32	ALA	2.9
1	M	233	LEU	2.9
1	W	6	PHE	2.9
1	U	173	GLU	2.9
1	W	157	GLY	2.9
1	W	165	ASN	2.9
1	Q	162	PRO	2.9
1	A	234	LEU	2.9
1	D	111	PHE	2.9
1	D	186	ALA	2.9
1	I	180	ALA	2.9
1	M	165	ASN	2.9
1	Q	204	GLY	2.8
1	I	189	ARG	2.8
1	D	230	LEU	2.8
1	S	167	LEU	2.8
1	Y	180	ALA	2.8
1	D	14	ARG	2.8
1	I	188	LEU	2.8
1	I	234	LEU	2.8
1	D	229	ALA	2.8
1	I	184	ALA	2.8
1	M	133	THR	2.8
1	M	163	ILE	2.8
1	I	112	THR	2.8
1	A	9	PRO	2.8
1	A	12	ALA	2.8
1	D	164	ALA	2.8
1	S	175	ALA	2.8
1	O	185	VAL	2.8
1	W	42	VAL	2.8
1	Q	48	ARG	2.8
1	U	189	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	159	THR	2.8
1	1	8	SER	2.8
1	O	10	GLU	2.8
1	K	177	LEU	2.8
1	A	164	ALA	2.8
2	N	416	SER	2.7
1	D	46	PRO	2.7
1	F	217	ARG	2.7
1	M	164	ALA	2.7
1	Y	187	ALA	2.7
1	D	152	HIS	2.7
1	O	205	VAL	2.7
1	D	225	ILE	2.7
2	R	531	GLY	2.7
2	V	531	GLY	2.7
1	D	207	SER	2.7
2	E	412	SER	2.7
1	D	9	PRO	2.7
1	D	189	ARG	2.7
1	S	34	ALA	2.7
2	G	415	GLN	2.7
1	D	226	THR	2.7
1	M	178	THR	2.7
1	U	204	GLY	2.7
1	1	13	MET	2.7
1	B	172	ALA	2.7
1	1	175	ALA	2.7
1	S	205	VAL	2.7
1	M	112	THR	2.7
1	O	159	THR	2.7
1	Q	9	PRO	2.7
1	1	9	PRO	2.7
1	I	182	ARG	2.7
1	W	13	MET	2.7
1	O	234	LEU	2.7
1	D	11	GLN	2.6
1	K	206	ALA	2.6
1	O	206	ALA	2.6
1	U	172	ALA	2.6
1	F	171	TYR	2.6
1	D	162	PRO	2.6
1	I	163	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	G	414	PRO	2.6
1	K	13	MET	2.6
1	K	234	LEU	2.6
1	U	181	LEU	2.6
1	D	43	ALA	2.6
1	D	166	ALA	2.6
1	F	166	ALA	2.6
1	M	111	PHE	2.6
1	1	179	ASP	2.6
1	W	97	ARG	2.6
1	I	185	VAL	2.6
1	B	170	SER	2.6
1	K	147	ILE	2.6
1	O	163	ILE	2.6
1	I	167	LEU	2.6
1	O	188	LEU	2.6
1	Y	167	LEU	2.6
1	Y	233	LEU	2.6
1	S	206	ALA	2.6
1	Y	229	ALA	2.6
1	A	144	ASP	2.6
1	D	143	TYR	2.6
2	V	532	GLY	2.6
1	B	49	SER	2.6
1	1	183	ILE	2.6
1	A	167	LEU	2.6
1	D	208	LEU	2.6
1	M	188	LEU	2.6
1	W	40	LEU	2.6
1	W	181	LEU	2.6
1	A	97	ARG	2.6
1	K	12	ALA	2.6
1	M	206	ALA	2.6
1	M	162	PRO	2.6
1	Y	160	THR	2.6
1	Y	205	VAL	2.6
1	D	170	SER	2.6
1	B	167	LEU	2.5
1	O	164	ALA	2.5
1	B	159	THR	2.5
1	D	154	VAL	2.5
1	D	210	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	205	VAL	2.5
1	Q	8	SER	2.5
1	A	44	GLU	2.5
1	B	44	GLU	2.5
1	A	182	ARG	2.5
1	O	13	MET	2.5
1	U	13	MET	2.5
1	M	36	ALA	2.5
1	Y	184	ALA	2.5
1	I	162	PRO	2.5
1	M	159	THR	2.5
1	M	185	VAL	2.5
1	Y	170	SER	2.5
1	B	147	ILE	2.5
1	B	173	GLU	2.5
1	Q	182	ARG	2.5
1	S	189	ARG	2.5
1	Y	189	ARG	2.5
1	S	234	LEU	2.5
1	B	232	ALA	2.5
1	D	34	ALA	2.5
1	O	190	ALA	2.5
1	U	25	ALA	2.5
1	U	175	ALA	2.5
1	W	20	ALA	2.5
1	A	131	GLY	2.5
1	S	9	PRO	2.5
1	I	133	THR	2.5
1	I	159	THR	2.5
1	D	140	ARG	2.5
1	U	182	ARG	2.5
1	W	154	VAL	2.5
1	A	181	LEU	2.5
1	I	166	ALA	2.5
1	I	180	ALA	2.5
1	K	175	ALA	2.5
1	M	186	ALA	2.5
1	I	10	GLU	2.4
1	W	160	THR	2.4
1	M	8	SER	2.4
1	W	185	VAL	2.4
1	K	171	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	206	ALA	2.4
1	D	44	GLU	2.4
1	D	131	GLY	2.4
1	I	26	ARG	2.4
1	1	166	ALA	2.4
1	U	158	GLY	2.4
2	X	397	GLY	2.4
1	M	183	ILE	2.4
1	W	31	VAL	2.4
1	S	33	LEU	2.4
1	U	149	ASP	2.4
1	O	204	GLY	2.4
1	Q	187	ALA	2.4
1	S	166	ALA	2.4
2	Z	523	GLY	2.4
1	1	49	SER	2.4
1	I	205	VAL	2.4
1	K	153	PHE	2.4
1	Y	30	VAL	2.4
2	R	535	HIS	2.4
1	W	105	GLN	2.4
1	A	25	ALA	2.4
1	A	184	ALA	2.4
1	A	206	ALA	2.4
1	K	180	ALA	2.4
1	M	166	ALA	2.4
1	O	186	ALA	2.4
1	U	191	GLY	2.4
1	A	33	LEU	2.4
1	A	189	ARG	2.4
1	D	21	ARG	2.4
1	W	182	ARG	2.4
1	M	204	GLY	2.3
1	I	25	ALA	2.3
1	M	25	ALA	2.3
1	Q	166	ALA	2.3
1	Y	34	ALA	2.3
1	D	178	THR	2.3
1	S	159	THR	2.3
1	Y	112	THR	2.3
1	D	146	SER	2.3
1	A	48	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	48	ARG	2.3
2	R	539	HIS	2.3
1	U	233	LEU	2.3
1	U	44	GLU	2.3
1	Y	132	GLU	2.3
1	M	179	ASP	2.3
1	S	157	GLY	2.3
2	L	523	GLY	2.3
1	K	36	ALA	2.3
1	K	184	ALA	2.3
1	Q	232	ALA	2.3
1	W	166	ALA	2.3
2	Z	411	ALA	2.3
1	A	49	SER	2.3
1	D	156	MET	2.3
1	D	53	ILE	2.3
1	F	11	GLN	2.3
2	L	398	LEU	2.3
1	D	145	GLY	2.3
1	D	27	ALA	2.3
1	Q	25	ALA	2.3
1	S	115	ALA	2.3
1	W	49	SER	2.3
2	N	412	SER	2.3
1	D	209	GLU	2.3
1	W	7	ILE	2.3
1	M	153	PHE	2.3
1	B	188	LEU	2.3
1	K	167	LEU	2.3
1	M	177	LEU	2.3
1	D	151	PRO	2.3
1	A	34	ALA	2.3
1	F	187	ALA	2.3
1	U	12	ALA	2.3
1	Y	97	ARG	2.3
1	A	159	THR	2.3
1	Y	226	THR	2.3
1	D	29	SER	2.3
1	M	49	SER	2.3
1	W	207	SER	2.3
1	D	150	GLU	2.3
1	F	169	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	188	LEU	2.2
1	Y	185	VAL	2.3
1	B	165	ASN	2.2
1	Y	179	ASP	2.2
1	S	13	MET	2.2
1	B	164	ALA	2.2
1	I	164	ALA	2.2
1	Q	171	TYR	2.2
1	S	184	ALA	2.2
1	I	142	THR	2.2
1	K	160	THR	2.2
1	W	171	TYR	2.2
1	B	163	ILE	2.2
1	K	163	ILE	2.2
1	O	183	ILE	2.2
1	S	183	ILE	2.2
1	K	31	VAL	2.2
1	Y	177	LEU	2.2
1	F	179	ASP	2.2
1	F	13	MET	2.2
1	B	191	GLY	2.2
2	E	523	GLY	2.2
1	A	173	GLU	2.2
2	C	519	GLU	2.2
1	D	175	ALA	2.2
1	S	180	ALA	2.2
1	1	164	ALA	2.2
1	1	206	ALA	2.2
1	F	49	SER	2.2
1	W	225	ILE	2.2
1	S	233	LEU	2.2
1	M	155	VAL	2.2
1	B	153	PHE	2.2
1	Y	111	PHE	2.2
1	D	97	ARG	2.2
1	S	140	ARG	2.2
1	I	9	PRO	2.2
1	U	9	PRO	2.2
1	F	10	GLU	2.2
1	M	113	GLU	2.2
1	A	43	ALA	2.2
1	B	180	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	172	ALA	2.2
1	O	184	ALA	2.2
1	D	49	SER	2.2
1	U	178	THR	2.2
1	A	143	TYR	2.2
1	O	171	TYR	2.2
1	Q	92	ARG	2.2
1	S	92	ARG	2.2
1	S	177	LEU	2.2
2	R	398	LEU	2.2
1	D	13	MET	2.2
1	O	165	ASN	2.2
2	C	413	ASP	2.2
1	W	152	HIS	2.2
1	A	207	SER	2.2
1	D	65	ALA	2.2
1	I	229	ALA	2.2
1	Q	112	THR	2.2
1	W	164	ALA	2.2
1	Y	166	ALA	2.2
1	1	229	ALA	2.2
2	C	412	SER	2.2
1	1	48	ARG	2.1
1	M	181	LEU	2.1
1	D	144	ASP	2.1
1	I	165	ASN	2.1
1	M	31	VAL	2.1
1	U	42	VAL	2.1
1	A	113	GLU	2.1
1	D	18	GLU	2.1
1	F	113	GLU	2.1
1	Q	111	PHE	2.1
1	W	15	GLU	2.1
1	W	153	PHE	2.1
1	B	152	HIS	2.1
1	A	232	ALA	2.1
1	D	47	SER	2.1
1	D	187	ALA	2.1
1	Q	186	ALA	2.1
1	D	217	ARG	2.1
1	M	21	ARG	2.1
1	O	26	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	182	ARG	2.1
1	1	26	ARG	2.1
1	1	182	ARG	2.1
1	F	167	LEU	2.1
1	Q	188	LEU	2.1
1	Y	33	LEU	2.1
1	A	169	GLU	2.1
1	Y	165	ASN	2.1
2	V	533	GLU	2.1
1	K	162	PRO	2.1
1	K	185	VAL	2.1
1	W	51	GLN	2.1
2	C	415	GLN	2.1
1	A	158	GLY	2.1
1	A	178	THR	2.1
1	D	48	ARG	2.1
1	D	142	THR	2.1
1	F	112	THR	2.1
1	O	25	ALA	2.1
1	U	184	ALA	2.1
1	Y	232	ALA	2.1
1	O	167	LEU	2.1
1	Y	183	ILE	2.1
1	M	231	GLN	2.1
2	G	396	GLN	2.1
2	L	415	GLN	2.1
2	X	415	GLN	2.1
1	1	131	GLY	2.1
1	M	160	THR	2.1
1	W	112	THR	2.1
1	W	178	THR	2.1
1	M	175	ALA	2.1
1	Q	164	ALA	2.1
1	W	36	ALA	2.1
1	1	36	ALA	2.1
1	Y	10	GLU	2.1
1	A	208	LEU	2.1
1	Y	138	LEU	2.1
1	F	183	ILE	2.1
2	C	396	GLN	2.1
1	A	151	PRO	2.1
1	F	205	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	153	PHE	2.1
1	D	223	ARG	2.1
1	K	168	LYS	2.0
1	B	8	SER	2.0
1	F	170	SER	2.0
1	O	178	THR	2.0
1	S	133	THR	2.0
1	U	159	THR	2.0
1	Y	133	THR	2.0
2	V	412	SER	2.0
1	A	187	ALA	2.0
1	B	169	GLU	2.0
1	K	232	ALA	2.0
1	U	164	ALA	2.0
1	W	215	ALA	2.0
1	B	231	GLN	2.0
1	U	183	ILE	2.0
1	A	46	PRO	2.0
1	W	46	PRO	2.0
1	A	31	VAL	2.0
1	D	39	VAL	2.0
1	I	14	ARG	2.0
1	I	30	VAL	2.0
1	I	48	ARG	2.0
1	I	155	VAL	2.0
1	M	189	ARG	2.0
1	O	48	ARG	2.0
1	W	92	ARG	2.0
1	W	28	LYS	2.0
1	F	44	GLU	2.0
1	I	8	SER	2.0
1	1	133	THR	2.0
1	W	175	ALA	2.0
1	W	122	LEU	2.0
1	F	48	ARG	2.0
1	F	189	ARG	2.0
1	S	225	ILE	2.0
1	U	14	ARG	2.0
1	U	48	ARG	2.0
1	Y	21	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DMF	D	253	5/5	0.54	0.32	20,20,20,20	0
3	DMF	O	251	5/5	0.54	0.26	20,20,20,20	0
3	DMF	K	251	5/5	0.62	0.29	63,63,64,64	0
3	DMF	2	57	5/5	0.63	0.24	54,56,57,57	0
3	DMF	V	39	5/5	0.64	0.23	60,60,61,61	0
3	DMF	E	28	5/5	0.66	0.28	61,61,63,64	0
3	DMF	H	66	5/5	0.66	0.25	69,69,69,70	0
3	DMF	M	251	5/5	0.67	0.27	64,64,66,66	0
3	DMF	K	252	5/5	0.68	0.22	80,81,82,82	0
3	DMF	2	112	5/5	0.68	0.36	20,20,20,20	0
3	DMF	J	45	5/5	0.69	0.23	41,43,45,46	0
3	DMF	Z	114	5/5	0.69	0.36	20,20,20,20	0
3	DMF	X	40	5/5	0.71	0.28	84,85,85,85	0
3	DMF	P	60	5/5	0.71	0.28	68,69,69,69	0
3	DMF	P	51	5/5	0.72	0.25	75,76,76,77	0
3	DMF	Y	251	5/5	0.72	0.35	20,20,20,20	0
3	DMF	H	117	5/5	0.72	0.28	20,20,20,20	0
3	DMF	2	52	5/5	0.72	0.28	77,77,78,78	0
3	DMF	U	249	5/5	0.72	0.22	40,40,44,45	0
3	DMF	P	33	5/5	0.72	0.23	65,66,66,66	0
3	DMF	N	104	5/5	0.73	0.34	20,20,20,20	0
3	DMF	T	102	5/5	0.73	0.28	20,20,20,20	0
3	DMF	V	82	5/5	0.73	0.25	45,47,47,48	0
3	DMF	J	110	5/5	0.74	0.30	20,20,20,20	0
3	DMF	L	36	5/5	0.74	0.22	41,42,43,43	0
3	DMF	Z	54	5/5	0.74	0.24	58,59,60,61	0
3	DMF	M	250	5/5	0.74	0.24	60,61,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DMF	R	95	5/5	0.74	0.29	20,20,20,20	0
3	DMF	V	120	5/5	0.74	0.29	20,20,20,20	0
3	DMF	W	249	5/5	0.74	0.23	69,70,71,72	0
3	DMF	C	121	5/5	0.75	0.23	20,20,20,20	0
3	DMF	2	49	5/5	0.75	0.26	57,57,57,58	0
3	DMF	G	62	5/5	0.75	0.26	72,73,73,74	0
3	DMF	T	10	5/5	0.75	0.27	71,72,72,74	0
3	DMF	C	103	5/5	0.75	0.31	20,20,20,20	0
3	DMF	G	24	5/5	0.76	0.24	65,67,68,68	0
3	DMF	2	108	5/5	0.76	0.32	20,20,20,20	0
3	DMF	J	123	5/5	0.76	0.31	20,20,20,20	0
3	DMF	P	86	5/5	0.77	0.31	20,20,20,20	0
3	DMF	X	122	5/5	0.77	0.23	20,20,20,20	0
3	DMF	N	93	5/5	0.77	0.26	20,20,20,20	0
3	DMF	Z	18	5/5	0.77	0.25	55,55,55,55	0
3	DMF	D	251	5/5	0.77	0.25	94,95,96,96	0
3	DMF	Z	94	5/5	0.77	0.33	20,20,20,20	0
3	DMF	G	98	5/5	0.78	0.30	20,20,20,20	0
3	DMF	G	111	5/5	0.78	0.28	20,20,20,20	0
3	DMF	T	113	5/5	0.78	0.34	20,20,20,20	0
3	DMF	G	119	5/5	0.78	0.33	20,20,20,20	0
3	DMF	D	250	5/5	0.78	0.22	61,63,64,65	0
3	DMF	H	72	5/5	0.78	0.31	20,20,20,20	0
3	DMF	L	81	5/5	0.78	0.25	59,60,61,62	0
3	DMF	C	63	5/5	0.78	0.24	58,59,59,60	0
3	DMF	D	249	5/5	0.78	0.17	53,53,53,54	0
3	DMF	S	250	5/5	0.78	0.20	59,59,60,61	0
3	DMF	K	250	5/5	0.79	0.25	77,78,79,79	0
3	DMF	B	249	5/5	0.79	0.20	50,51,51,53	0
3	DMF	C	88	5/5	0.79	0.34	20,20,20,20	0
3	DMF	R	59	5/5	0.80	0.29	54,55,57,57	0
3	DMF	R	89	5/5	0.80	0.29	20,20,20,20	0
3	DMF	L	50	5/5	0.80	0.23	55,56,57,57	0
3	DMF	T	29	5/5	0.81	0.23	76,76,76,76	0
3	DMF	H	91	5/5	0.81	0.29	20,20,20,20	0
3	DMF	G	70	5/5	0.81	0.21	37,38,41,41	0
3	DMF	T	115	5/5	0.81	0.28	20,20,20,20	0
3	DMF	M	249	5/5	0.81	0.17	46,47,48,48	0
3	DMF	E	53	5/5	0.81	0.20	56,57,58,59	0
3	DMF	Q	251	5/5	0.81	0.18	53,53,56,57	0
3	DMF	A	250	5/5	0.82	0.16	39,41,42,44	0
3	DMF	E	100	5/5	0.82	0.31	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DMF	D	252	5/5	0.82	0.25	20,20,20,20	0
3	DMF	P	2	5/5	0.82	0.25	62,62,64,64	0
3	DMF	N	22	5/5	0.82	0.14	44,45,49,50	0
3	DMF	G	77	5/5	0.83	0.18	49,50,50,51	0
3	DMF	E	73	5/5	0.83	0.45	120,120,121,121	0
3	DMF	Q	250	5/5	0.83	0.19	84,85,85,86	0
3	DMF	C	38	5/5	0.83	0.17	64,64,65,65	0
3	DMF	P	14	5/5	0.83	0.25	56,58,58,59	0
3	DMF	X	41	5/5	0.83	0.21	61,61,62,62	0
3	DMF	K	249	5/5	0.83	0.16	49,50,51,52	0
3	DMF	2	101	5/5	0.83	0.24	20,20,20,20	0
3	DMF	Y	250	5/5	0.83	0.13	42,42,44,44	0
3	DMF	F	249	5/5	0.83	0.30	90,91,91,91	0
3	DMF	E	75	5/5	0.84	0.20	64,64,64,65	0
3	DMF	I	250	5/5	0.84	0.17	41,41,42,42	0
3	DMF	C	47	5/5	0.84	0.21	61,62,62,62	0
3	DMF	H	43	5/5	0.84	0.27	82,82,83,83	0
3	DMF	R	80	5/5	0.84	0.20	74,75,76,76	0
3	DMF	V	42	5/5	0.84	0.27	58,58,59,61	0
3	DMF	F	250	5/5	0.85	0.18	56,56,58,59	0
3	DMF	G	64	5/5	0.85	0.26	66,68,68,69	0
3	DMF	F	251	5/5	0.85	0.20	54,54,55,55	0
3	DMF	B	250	5/5	0.85	0.20	53,53,55,55	0
3	DMF	P	107	5/5	0.85	0.26	20,20,20,20	0
3	DMF	X	16	5/5	0.85	0.24	86,86,86,86	0
3	DMF	I	249	5/5	0.85	0.14	40,42,42,43	0
3	DMF	X	15	5/5	0.86	0.20	66,67,68,70	0
3	DMF	H	71	5/5	0.86	0.17	54,55,55,56	0
3	DMF	P	56	5/5	0.86	0.18	59,60,60,61	0
3	DMF	2	4	5/5	0.86	0.21	62,62,62,62	0
3	DMF	V	83	5/5	0.86	0.18	58,59,60,62	0
3	DMF	V	109	5/5	0.86	0.31	20,20,20,20	0
3	DMF	Y	249	5/5	0.86	0.19	62,64,64,65	0
3	DMF	T	84	5/5	0.86	0.21	59,59,60,62	0
3	DMF	C	69	5/5	0.86	0.19	48,48,50,50	0
3	DMF	W	250	5/5	0.86	0.18	63,63,64,64	0
3	DMF	N	118	5/5	0.87	0.29	20,20,20,20	0
3	DMF	N	90	5/5	0.87	0.27	20,20,20,20	0
3	DMF	U	250	5/5	0.87	0.15	49,50,51,51	0
3	DMF	V	32	5/5	0.88	0.21	73,74,74,74	0
3	DMF	Q	249	5/5	0.88	0.16	48,48,49,49	0
3	DMF	R	92	5/5	0.88	0.25	20,20,20,20	0

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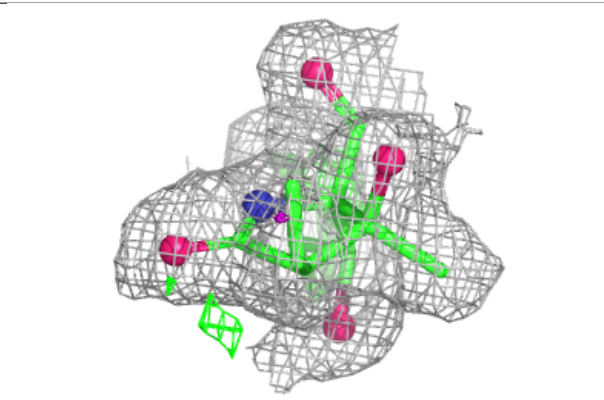
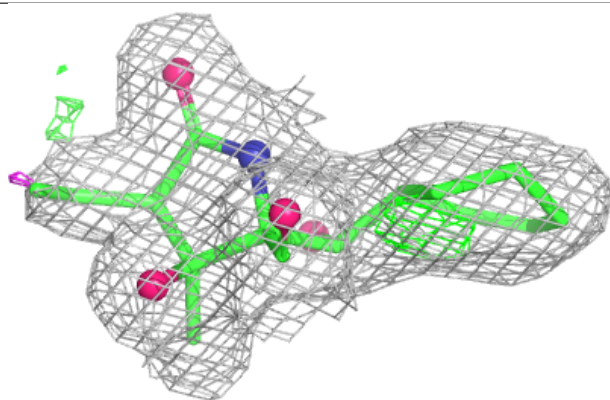
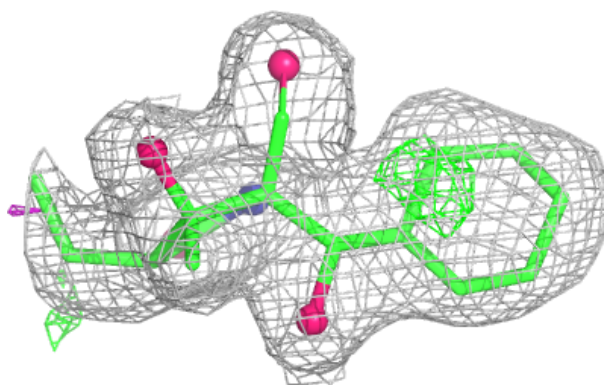
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DMF	V	27	5/5	0.88	0.22	63,63,64,64	0
3	DMF	S	249	5/5	0.89	0.15	54,54,55,56	0
3	DMF	L	97	5/5	0.89	0.21	20,20,20,20	0
3	DMF	V	116	5/5	0.89	0.23	20,20,20,20	0
3	DMF	G	12	5/5	0.89	0.21	60,61,62,63	0
3	DMF	2	87	5/5	0.89	0.26	20,20,20,20	0
3	DMF	O	250	5/5	0.89	0.14	44,45,46,48	0
3	DMF	M	252	5/5	0.89	0.20	20,20,20,20	0
3	DMF	1	249	5/5	0.89	0.12	45,47,48,49	0
3	DMF	A	249	5/5	0.90	0.14	44,44,44,44	0
3	DMF	O	249	5/5	0.90	0.15	39,40,41,41	0
3	DMF	E	20	5/5	0.92	0.23	76,77,77,78	0
4	SA6	H	300	20/20	0.92	0.08	16,21,23,24	0
4	SA6	L	300	20/20	0.93	0.08	16,19,26,27	0
4	SA6	E	300	20/20	0.94	0.07	12,18,21,24	0
4	SA6	N	300	20/20	0.94	0.07	13,18,23,26	0
4	SA6	V	300	20/20	0.94	0.07	15,17,21,22	0
4	SA6	2	300	20/20	0.94	0.08	17,20,28,29	0
4	SA6	R	300	20/20	0.95	0.07	12,21,24,31	0
4	SA6	T	300	20/20	0.95	0.07	17,22,28,29	0
4	SA6	G	300	20/20	0.95	0.07	11,19,22,24	0
4	SA6	X	300	20/20	0.95	0.06	15,17,23,25	0
4	SA6	Z	300	20/20	0.95	0.06	17,19,22,25	0
4	SA6	C	300	20/20	0.95	0.06	16,19,24,24	0
4	SA6	J	300	20/20	0.96	0.06	12,19,24,27	0
4	SA6	P	300	20/20	0.96	0.06	16,20,28,29	0

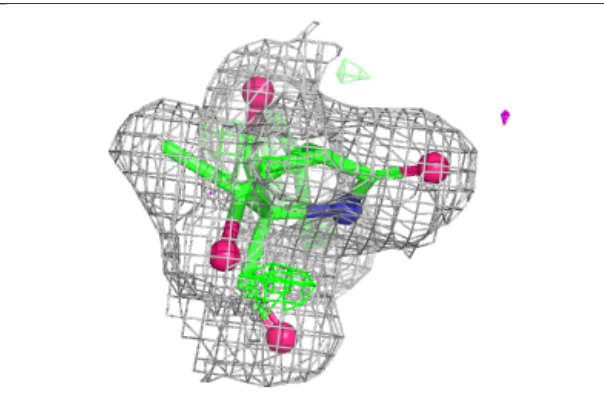
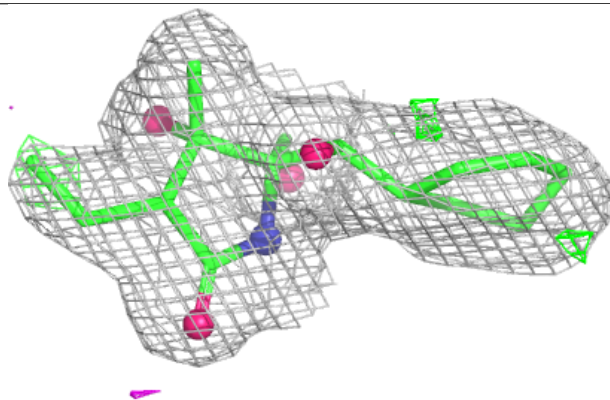
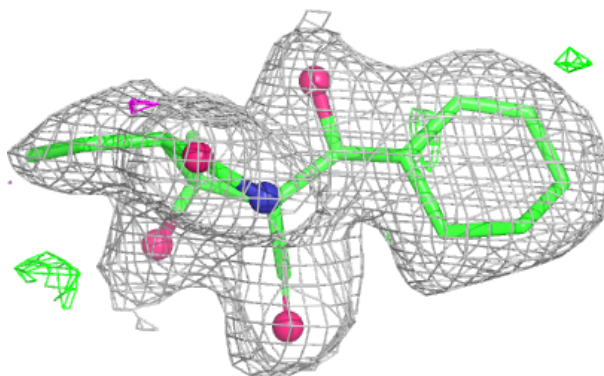
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SA6 H 300:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

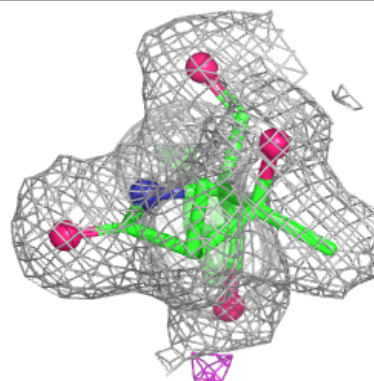
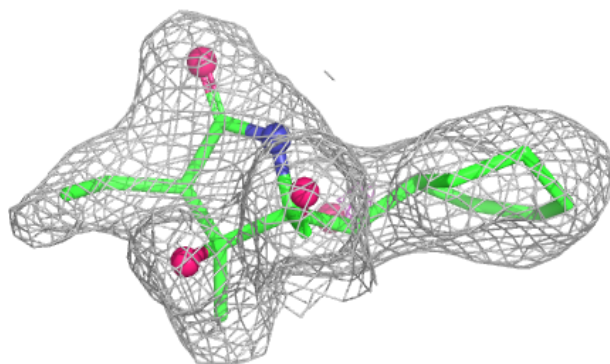
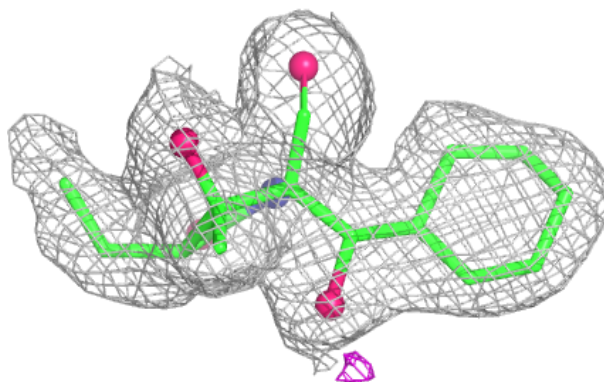
**Electron density around SA6 L 300:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

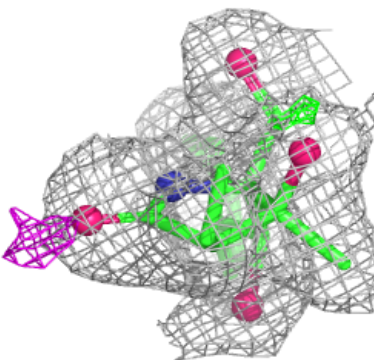
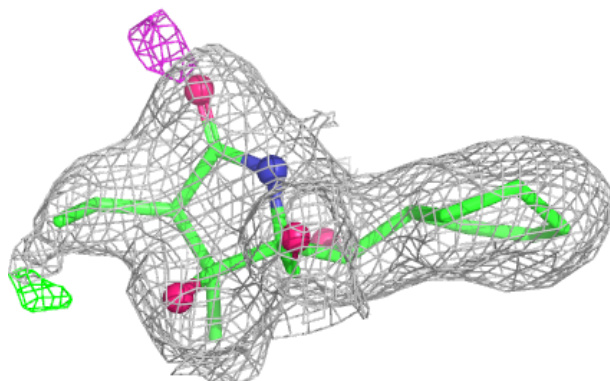
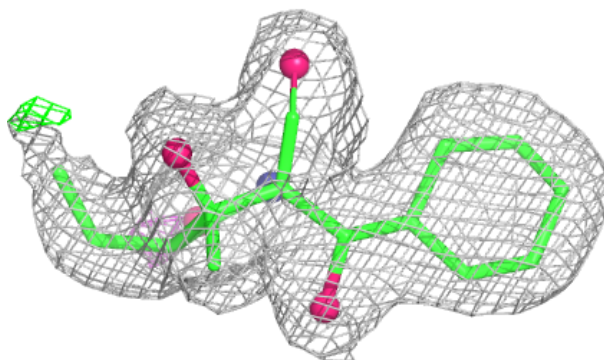


Electron density around SA6 E 300:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

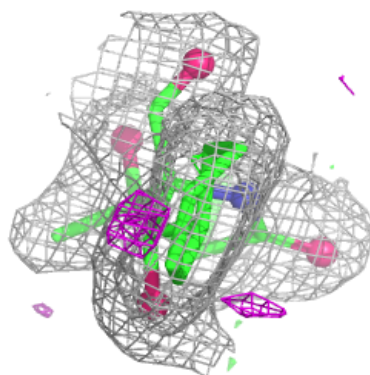
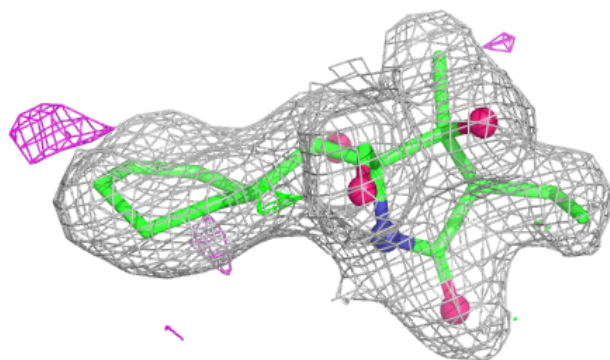
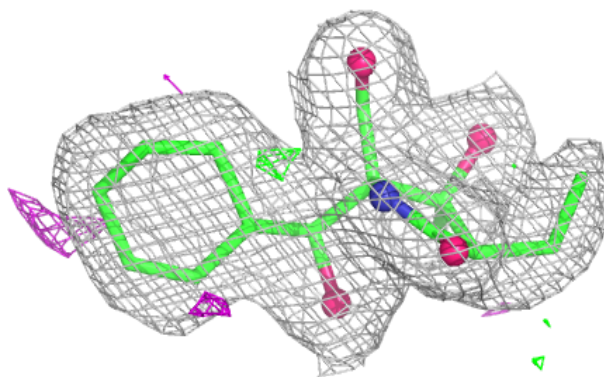
**Electron density around SA6 N 300:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

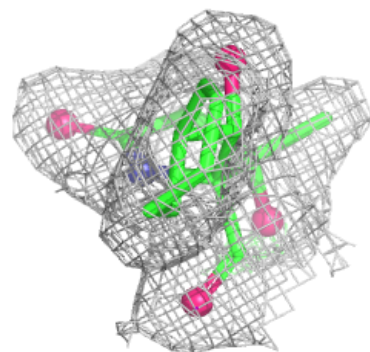
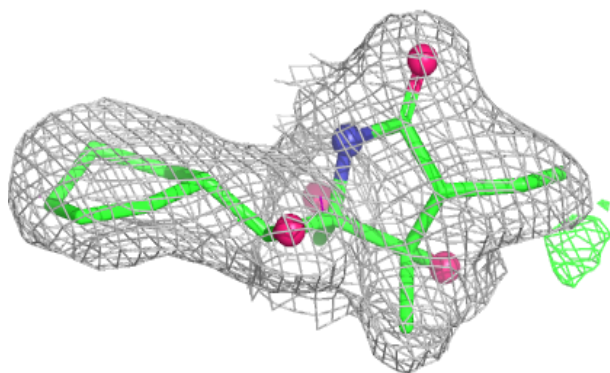
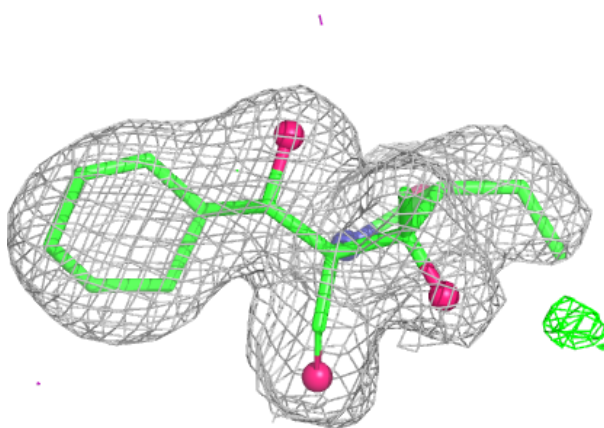


Electron density around SA6 V 300:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

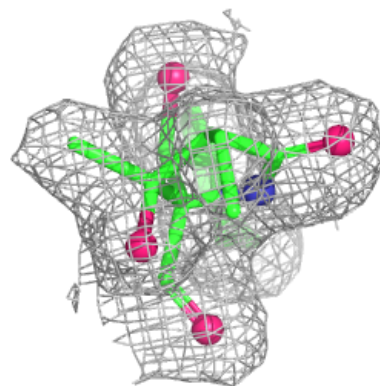
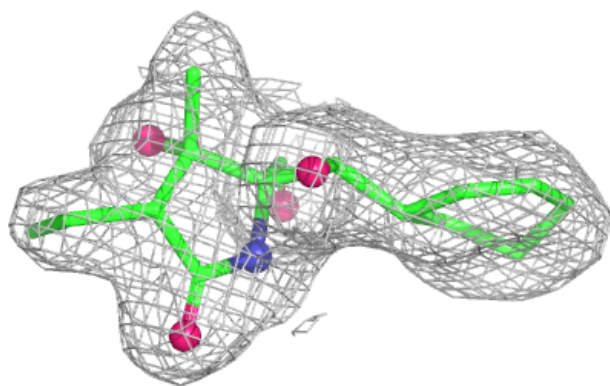
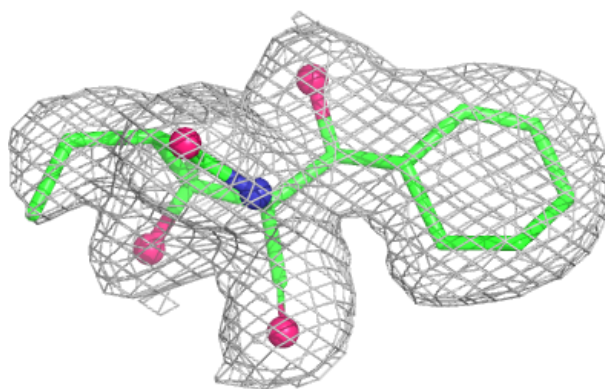
**Electron density around SA6 2 300:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

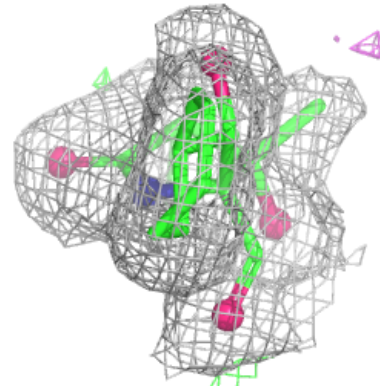
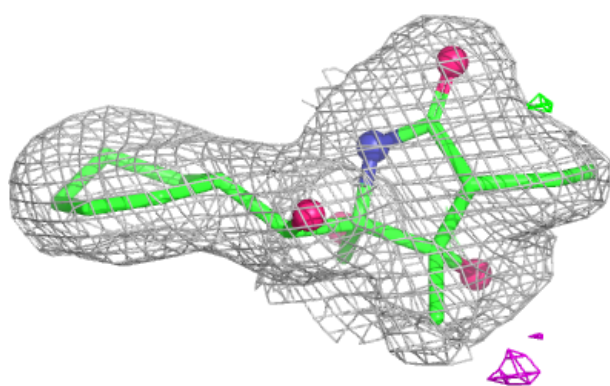
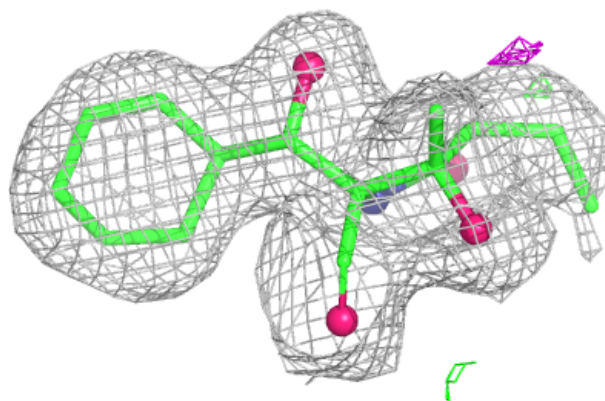


Electron density around SA6 R 300:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

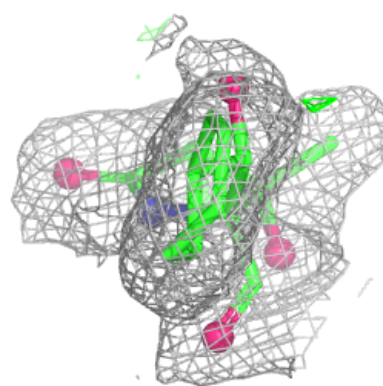
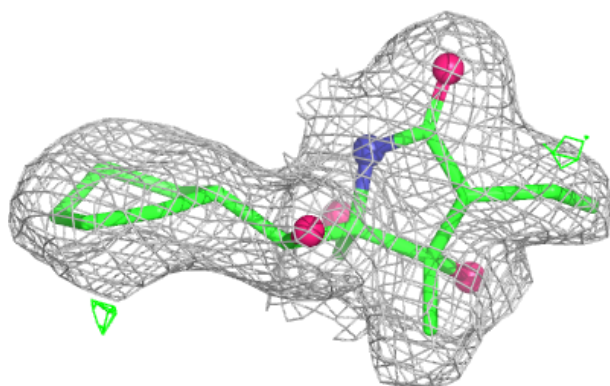
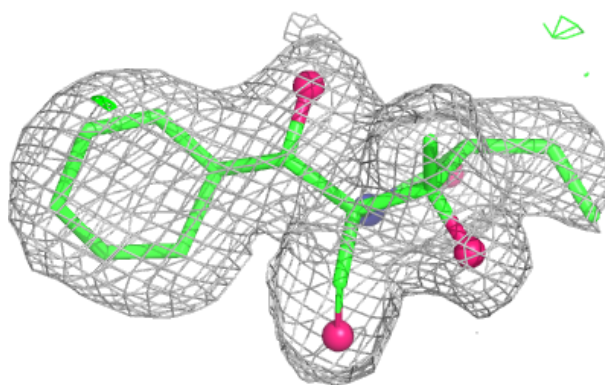
**Electron density around SA6 T 300:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

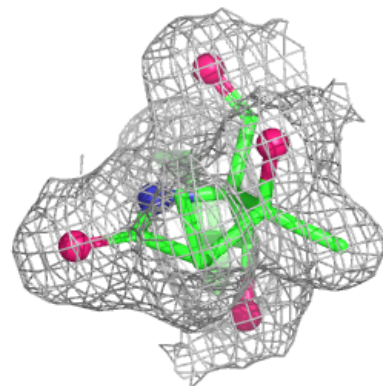
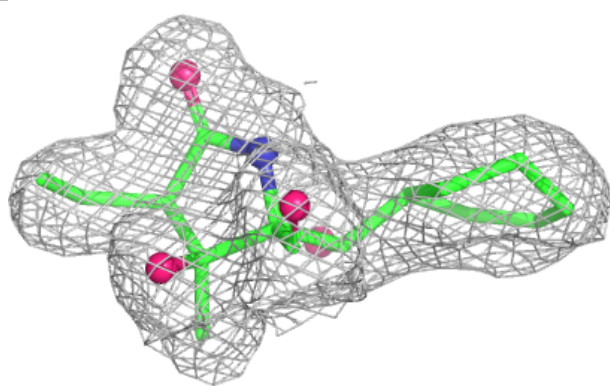
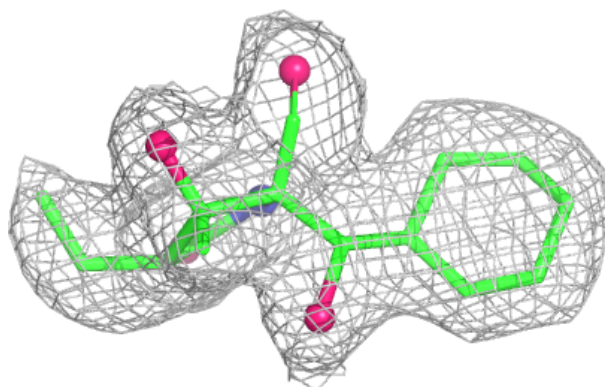


Electron density around SA6 G 300:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

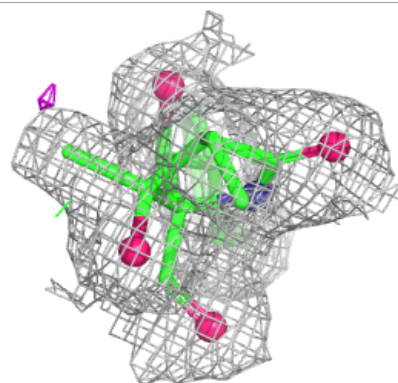
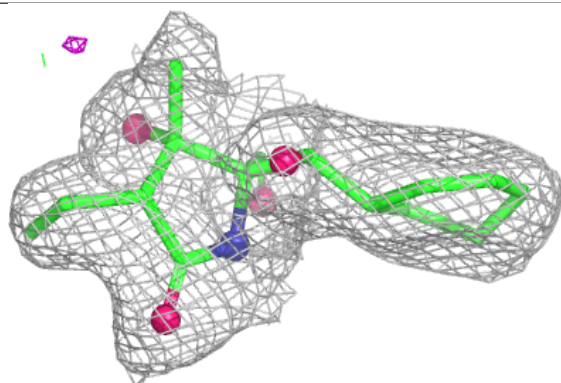
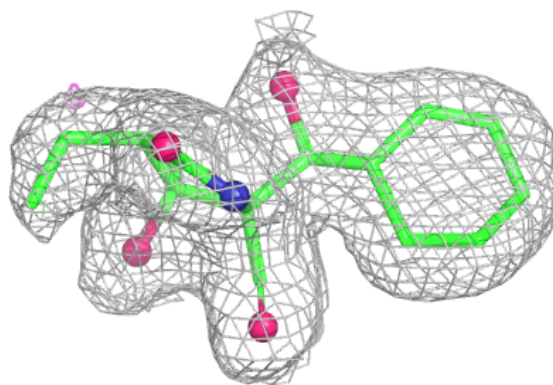
**Electron density around SA6 X 300:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

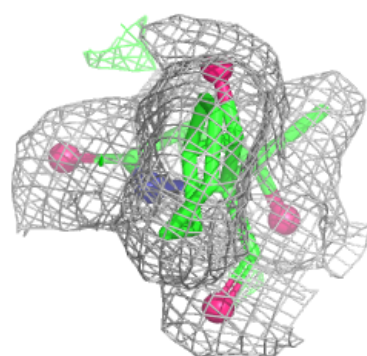
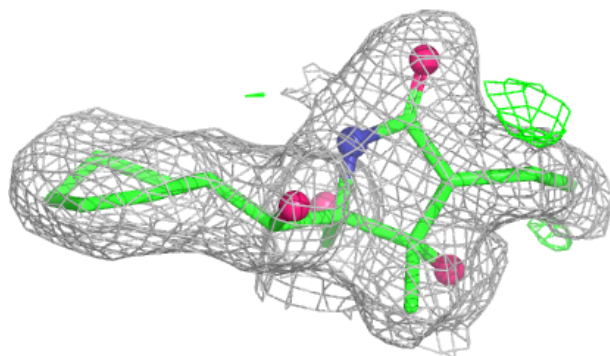
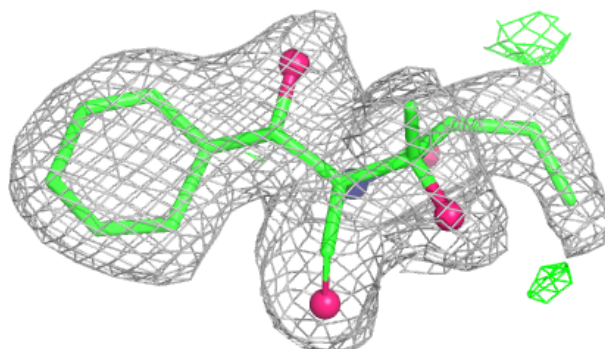


Electron density around SA6 Z 300:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

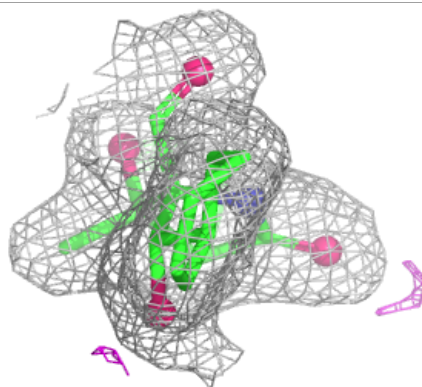
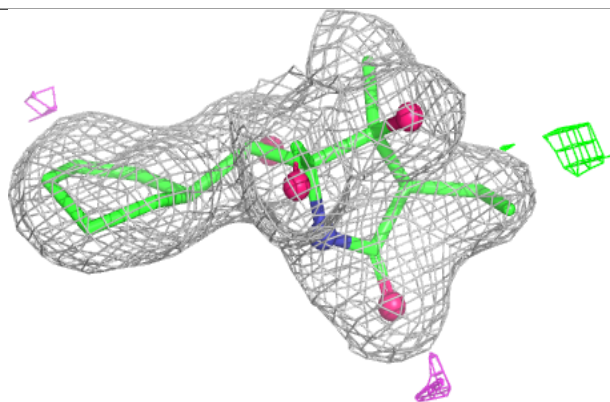
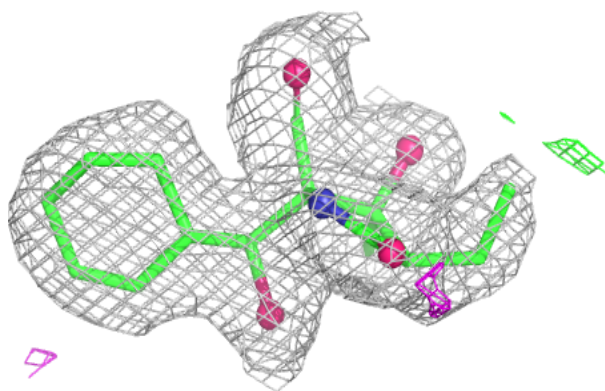
**Electron density around SA6 C 300:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

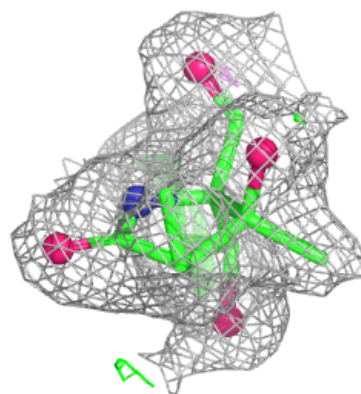
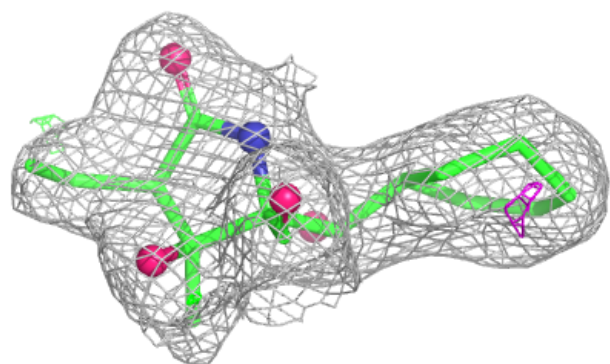
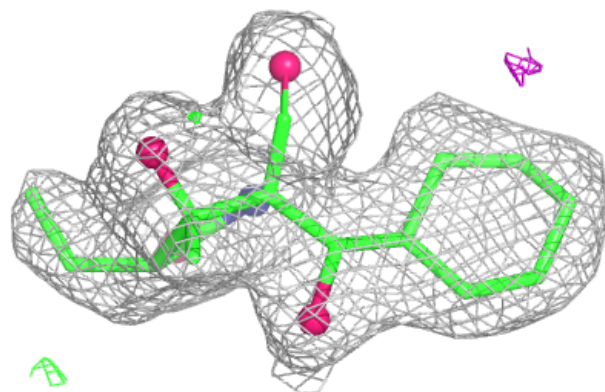


Electron density around SA6 J 300:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around SA6 P 300:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.