Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:11 AM GMT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

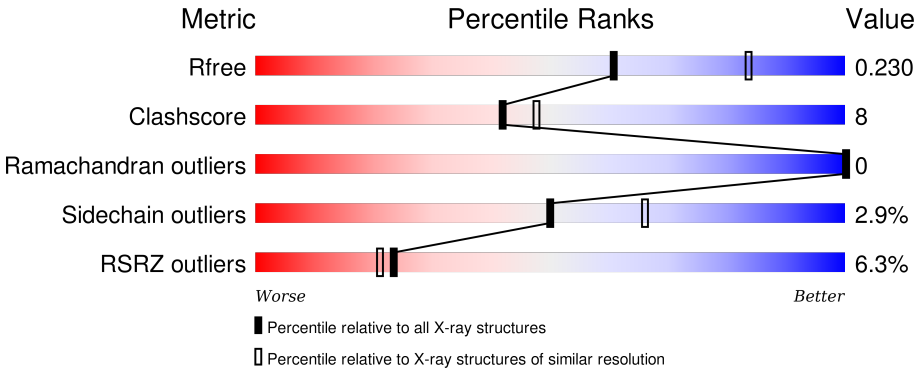
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1003 (2.46-2.42)
Clashscore	102246	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)
RSRZ outliers	91569	1005 (2.46-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	9% 75% 10% • 13%
1	A	248	15% 75% 11% 13%
1	B	248	8% 74% 12% • 14%
1	D	248	12% 71% 12% • 14%
1	F	248	6% 73% 14% • 13%

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Mol	Chain	Length	Quality of chain
1	I	248	8% 75% 12% 13%
1	K	248	10% 67% 18% 13%
1	M	248	6% 77% 9% 13%
1	O	248	8% 71% 16% 13%
1	Q	248	7% 71% 15% 12%
1	S	248	14% 75% 10% 13%
1	U	248	7% 70% 16% 13%
1	W	248	8% 73% 14% 13%
1	Y	248	15% 69% 15% 14%
2	2	240	2% 82% 8% 10%
2	C	240	3% 79% 10% 10%
2	E	240	2% 80% 10% 10%
2	G	240	80% 9% 10%
2	H	240	% 79% 10% 11%
2	J	240	% 81% 8% 10%
2	L	240	% 76% 14% 10%
2	N	240	% 80% 9% 11%
2	P	240	3% 78% 11% 10%
2	R	240	% 85% 8% 7%
2	T	240	2% 78% 12% 10%
2	V	240	2% 82% 10% 8%
2	X	240	2% 80% 10% 10%
2	Z	240	% 80% 8% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OZT	P	301	-	-	X	-
3	DMF	1	249	-	-	-	X
3	DMF	1	250	-	-	-	X
3	DMF	1	251	-	-	-	X
3	DMF	2	66	-	-	-	X
3	DMF	2	78	-	-	-	X
3	DMF	A	250	-	-	-	X
3	DMF	B	249	-	-	-	X
3	DMF	B	250	-	-	-	X
3	DMF	B	251	-	-	-	X
3	DMF	C	15	-	-	-	X
3	DMF	C	17	-	-	-	X
3	DMF	C	43	-	-	-	X
3	DMF	C	48	-	-	-	X
3	DMF	C	5	-	-	X	X
3	DMF	C	64	-	-	X	-
3	DMF	C	73	-	-	X	X
3	DMF	D	249	-	-	-	X
3	DMF	D	250	-	-	-	X
3	DMF	D	251	-	-	-	X
3	DMF	D	252	-	-	-	X
3	DMF	E	32	-	-	-	X
3	DMF	E	44	-	-	-	X
3	DMF	E	70	-	-	-	X
3	DMF	E	83	-	-	-	X
3	DMF	E	95	-	-	-	X
3	DMF	F	249	-	-	-	X
3	DMF	F	250	-	-	-	X
3	DMF	G	1	-	-	-	X
3	DMF	G	20	-	-	-	X
3	DMF	G	39	-	-	-	X
3	DMF	G	96	-	-	-	X
3	DMF	H	102	-	-	-	X
3	DMF	H	19	-	-	X	-
3	DMF	H	31	-	-	-	X
3	DMF	H	41	-	-	-	X
3	DMF	H	53	-	-	-	X
3	DMF	I	249	-	-	-	X
3	DMF	J	6	-	-	X	X
3	DMF	J	82	-	-	-	X
3	DMF	K	250	-	-	-	X
3	DMF	L	4	-	-	-	X
3	DMF	L	60	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DMF	L	9	-	-	-	X
3	DMF	M	249	-	-	-	X
3	DMF	M	250	-	-	-	X
3	DMF	N	21	-	-	-	X
3	DMF	N	24	-	-	-	X
3	DMF	N	36	-	-	-	X
3	DMF	N	37	-	-	-	X
3	DMF	N	97	-	-	-	X
3	DMF	N	99	-	-	-	X
3	DMF	O	249	-	-	-	X
3	DMF	O	250	-	-	X	X
3	DMF	P	100	-	-	-	X
3	DMF	P	74	-	-	-	X
3	DMF	Q	250	-	-	-	X
3	DMF	R	54	-	-	-	X
3	DMF	R	68	-	-	-	X
3	DMF	R	89	-	-	-	X
3	DMF	S	249	-	-	-	X
3	DMF	S	250	-	-	-	X
3	DMF	S	251	-	-	-	X
3	DMF	T	35	-	-	X	X
3	DMF	T	46	-	-	-	X
3	DMF	T	62	-	-	-	X
3	DMF	T	92	-	-	-	X
3	DMF	T	94	-	-	-	X
3	DMF	U	249	-	-	-	X
3	DMF	U	251	-	-	-	X
3	DMF	V	65	-	-	-	X
3	DMF	V	86	-	-	-	X
3	DMF	V	90	-	-	-	X
3	DMF	W	249	-	-	-	X
3	DMF	W	250	-	-	-	X
3	DMF	X	25	-	-	-	X
3	DMF	X	88	-	-	-	X
3	DMF	Y	249	-	-	-	X
3	DMF	Z	50	-	-	-	X
3	DMF	Z	71	-	-	-	X
3	DMF	Z	91	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 48540 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome (Alpha subunit) PrcA.

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

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

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

There are 98 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	301	OZT	-	INSERTION	UNP O33245
C	535	HIS	-	EXPRESSION TAG	UNP O33245
C	536	HIS	-	EXPRESSION TAG	UNP O33245
C	537	HIS	-	EXPRESSION TAG	UNP O33245
C	538	HIS	-	EXPRESSION TAG	UNP O33245
C	539	HIS	-	EXPRESSION TAG	UNP O33245
C	540	HIS	-	EXPRESSION TAG	UNP O33245
E	301	OZT	-	INSERTION	UNP O33245
E	535	HIS	-	EXPRESSION TAG	UNP O33245
E	536	HIS	-	EXPRESSION TAG	UNP O33245
E	537	HIS	-	EXPRESSION TAG	UNP O33245
E	538	HIS	-	EXPRESSION TAG	UNP O33245

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

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

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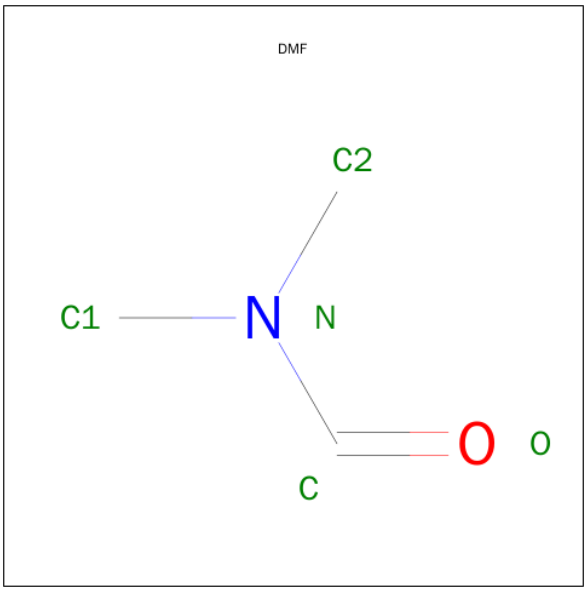
Chain	Residue	Modelled	Actual	Comment	Reference
2	539	HIS	-	EXPRESSION TAG	UNP O33245
2	540	HIS	-	EXPRESSION TAG	UNP O33245

- Molecule 3 is DIMETHYLFORMAMIDE (three-letter code: DMF) (formula: C_3H_7NO).



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

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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	N	1	Total	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	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	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	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		

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

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

- Molecule 4 is water.

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

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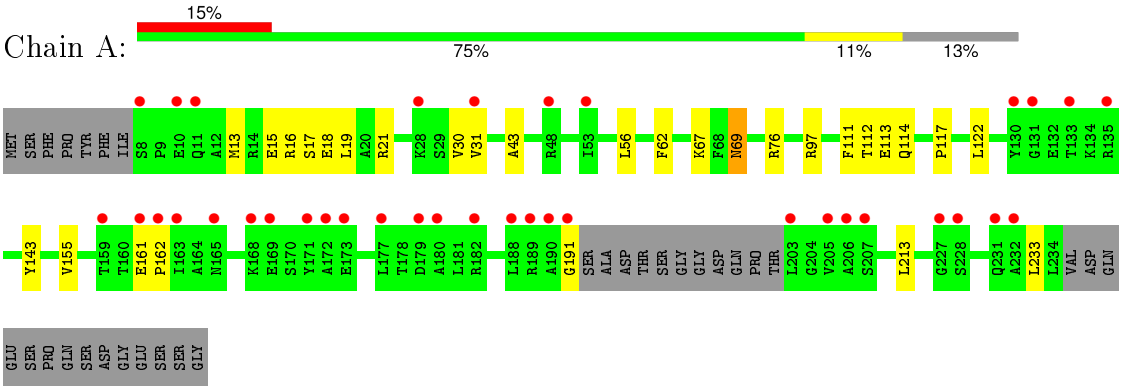
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	138	Total O 138 138	0	0
4	M	52	Total O 52 52	0	0
4	N	118	Total O 118 118	0	0
4	O	51	Total O 51 51	0	0
4	P	111	Total O 111 111	0	0
4	Q	41	Total O 41 41	0	0
4	R	141	Total O 141 141	0	0
4	S	31	Total O 31 31	0	0
4	T	112	Total O 112 112	0	0
4	U	43	Total O 43 43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

3 Residue-property plots (i)

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

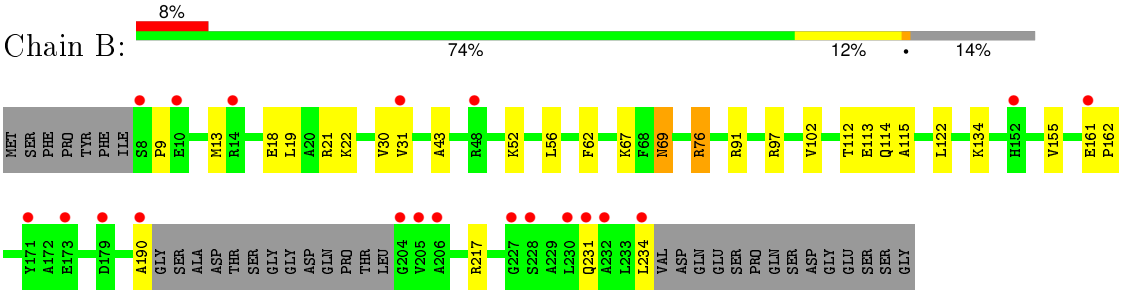
- Molecule 1: Proteasome (Alpha subunit) PrcA

Chain A:



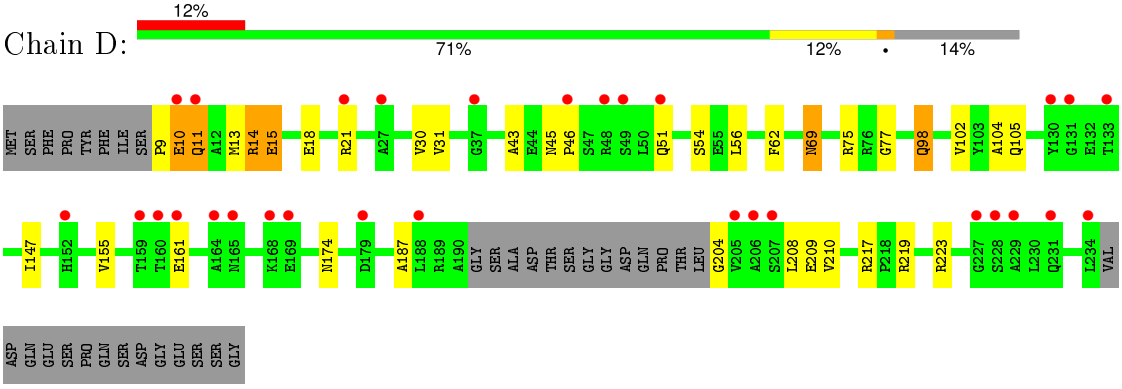
- Molecule 1: Proteasome (Alpha subunit) PrcA

Chain B:



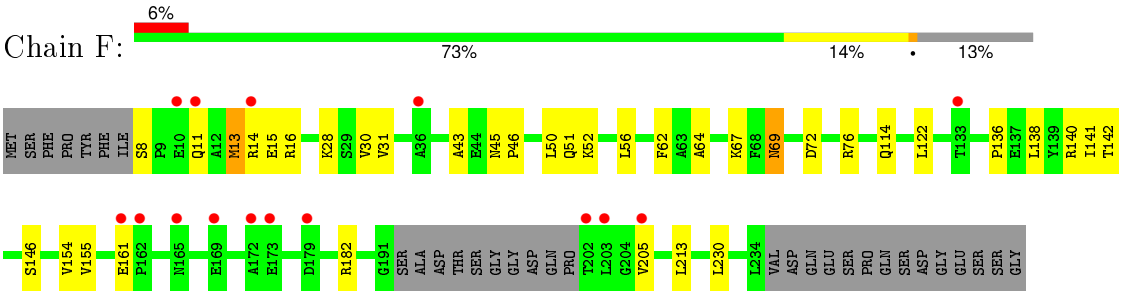
- Molecule 1: Proteasome (Alpha subunit) PrcA

Chain D:



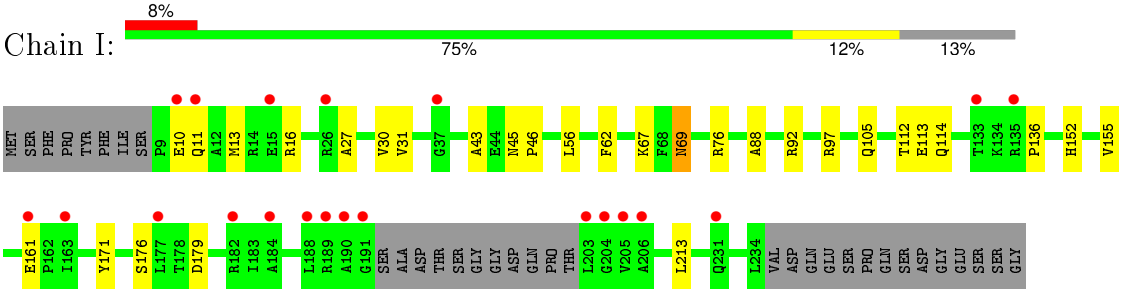
- Molecule 1: Proteasome (Alpha subunit) PrcA

Chain F:



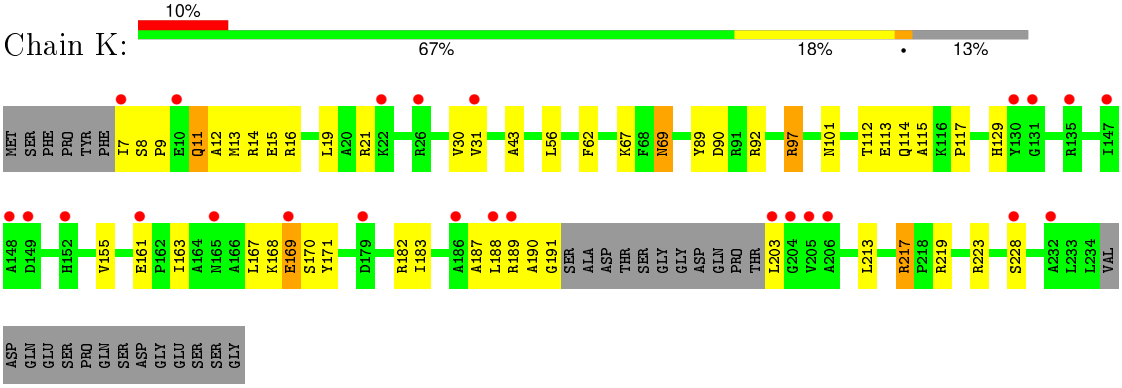
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain I:



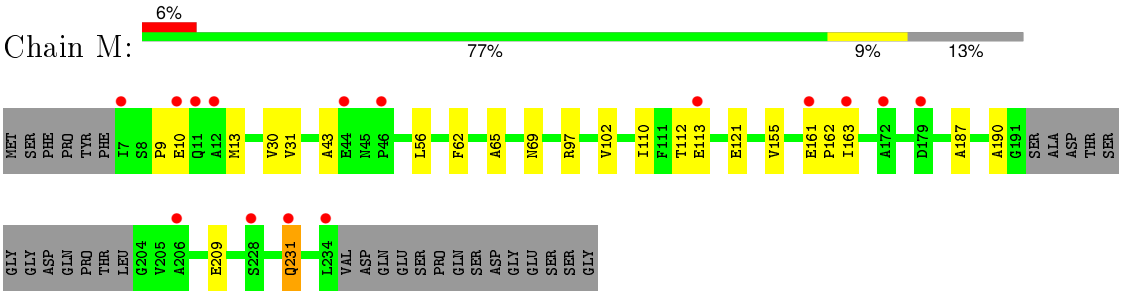
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain K:



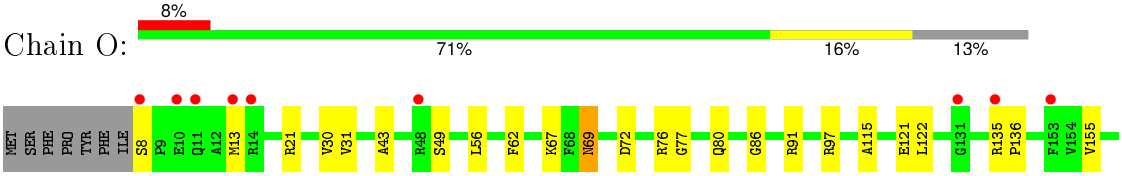
• Molecule 1: Proteasome (Alpha subunit) PrcA

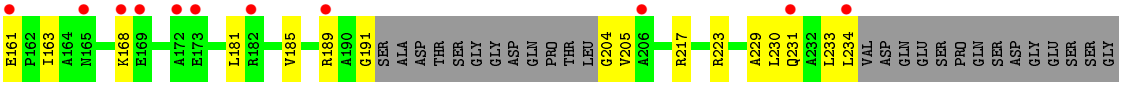
Chain M:



• Molecule 1: Proteasome (Alpha subunit) PrcA

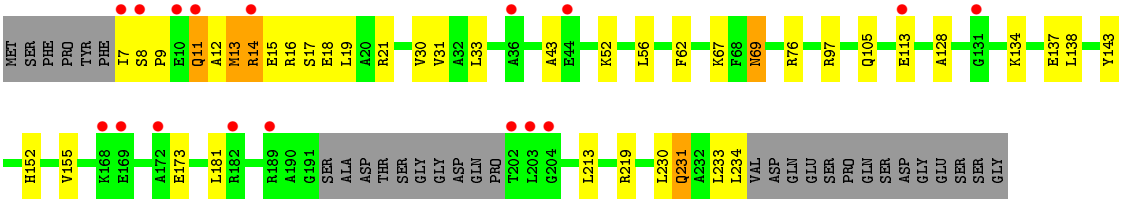
Chain O:





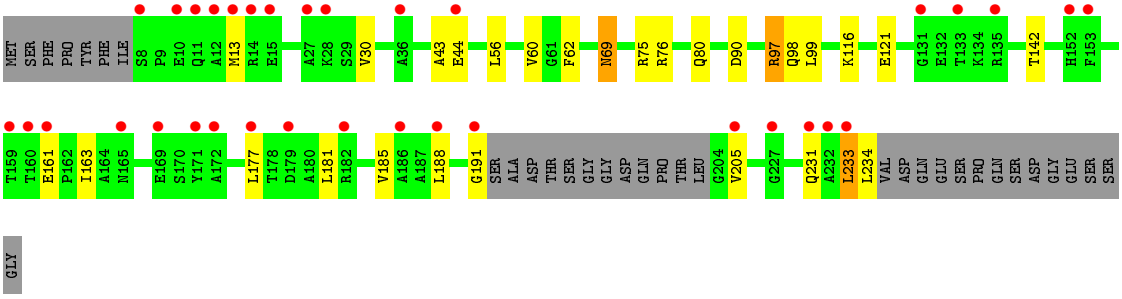
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain Q:



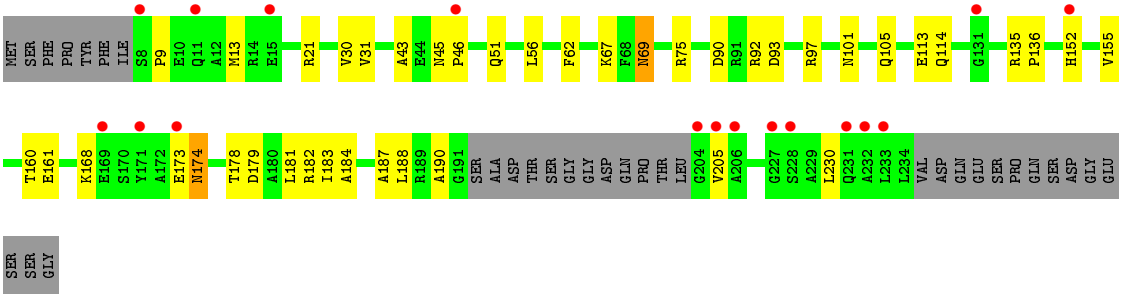
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain S:



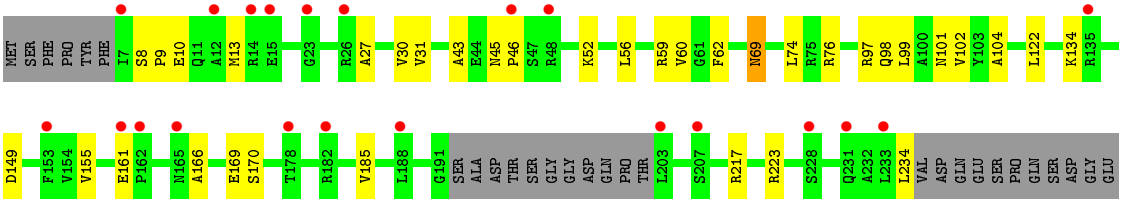
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain U:



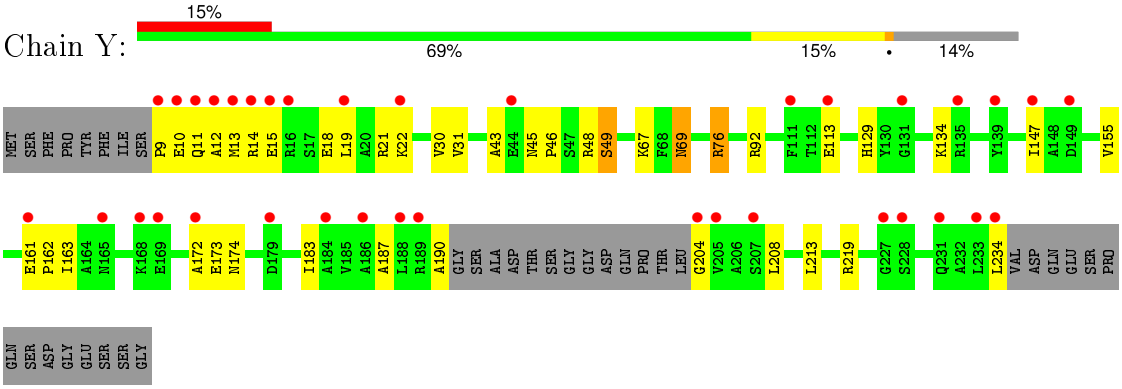
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain W:



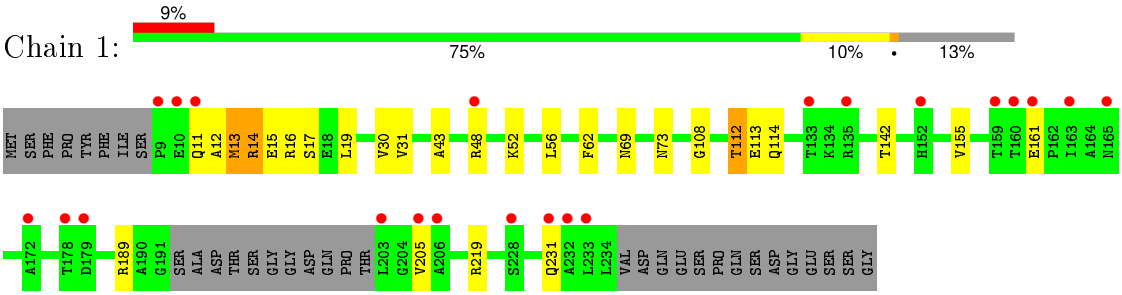
- Molecule 1: Proteasome (Alpha subunit) PrcA

Chain Y:



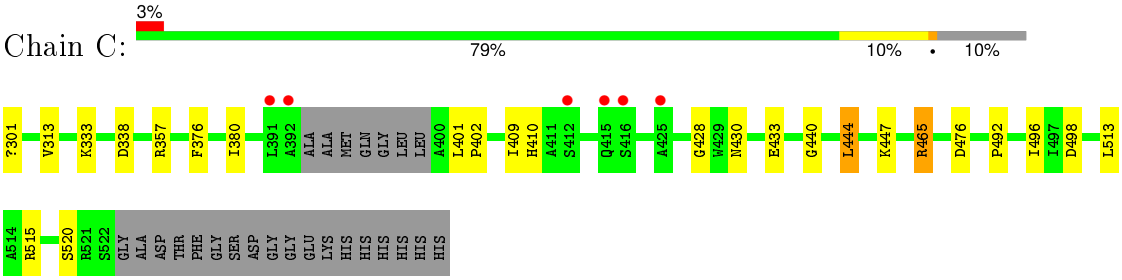
- Molecule 1: Proteasome (Alpha subunit) PrcA

Chain 1:



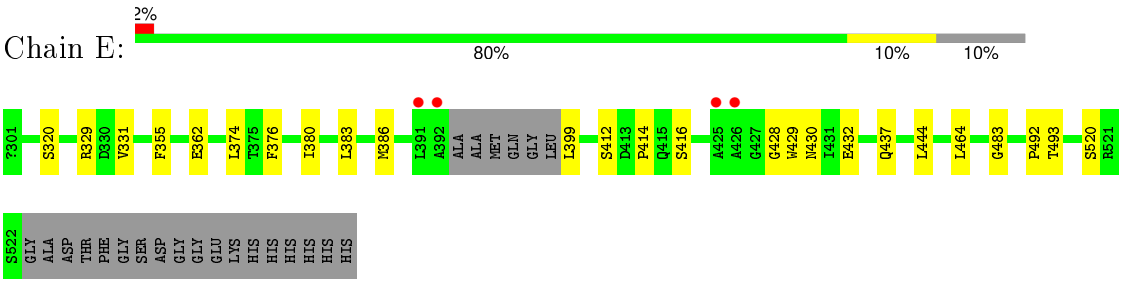
- Molecule 2: Proteasome (Beta subunit) PrcB

Chain C:



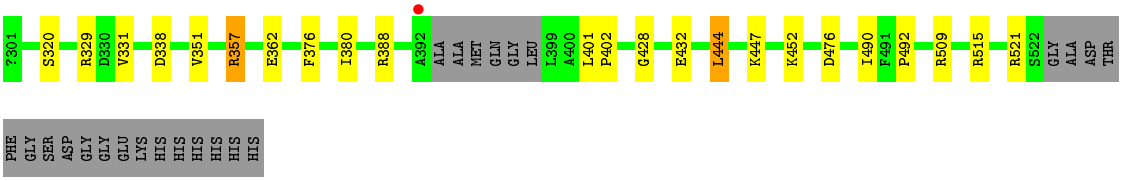
- Molecule 2: Proteasome (Beta subunit) PrcB

Chain E:

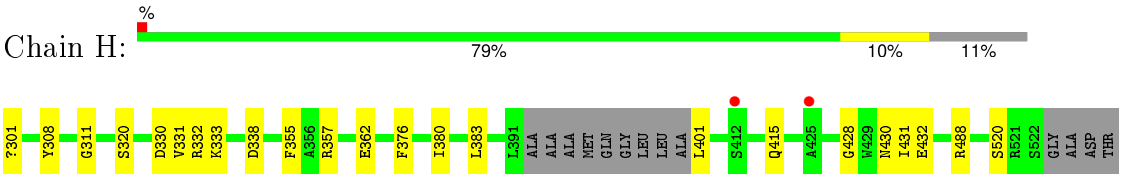


- Molecule 2: Proteasome (Beta subunit) PrcB

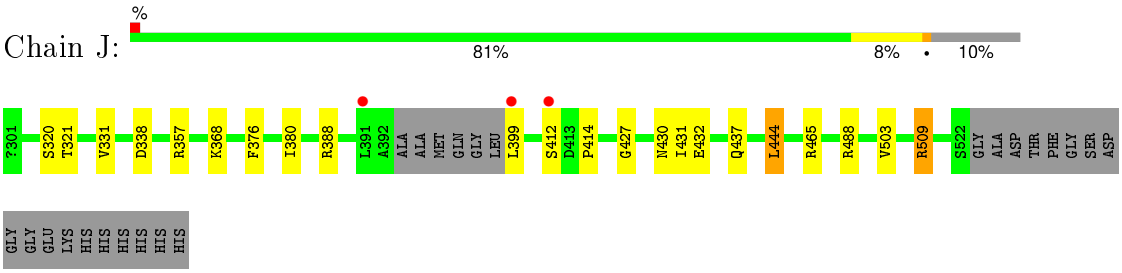
Chain G:



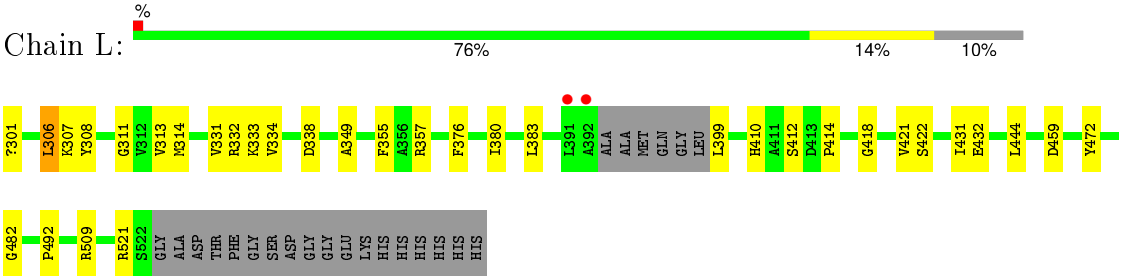
• Molecule 2: Proteasome (Beta subunit) PrcB



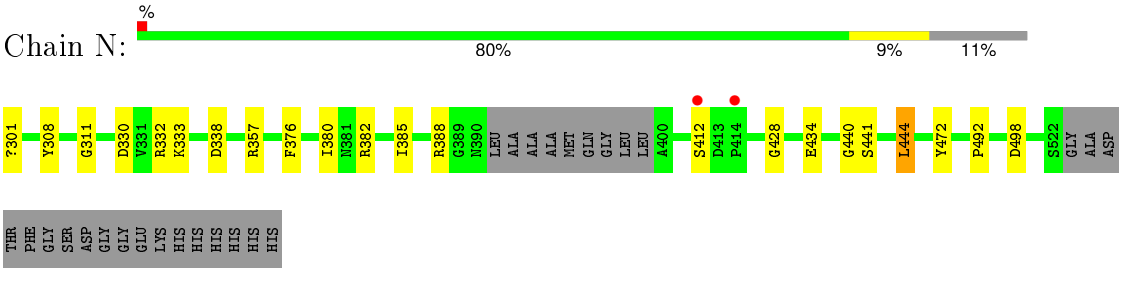
• Molecule 2: Proteasome (Beta subunit) PrcB



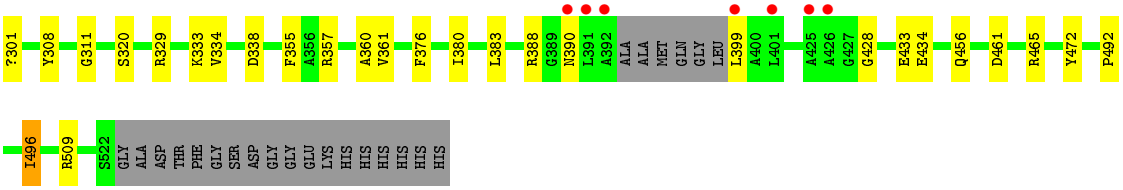
• Molecule 2: Proteasome (Beta subunit) PrcB



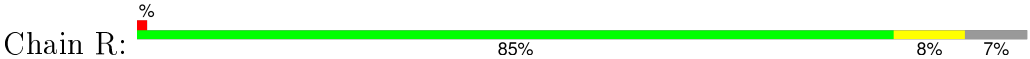
• Molecule 2: Proteasome (Beta subunit) PrcB

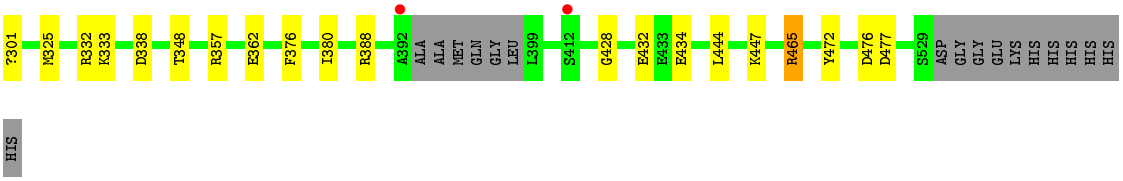


• Molecule 2: Proteasome (Beta subunit) PrcB

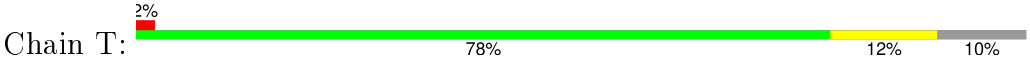


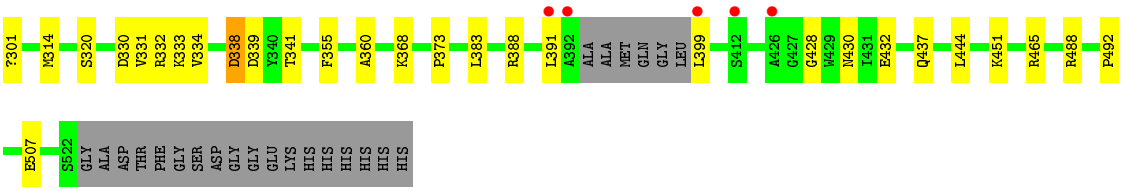
• Molecule 2: Proteasome (Beta subunit) PrcB



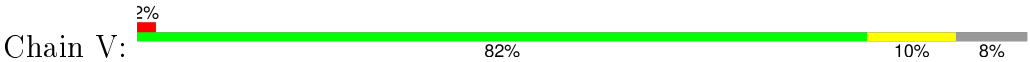


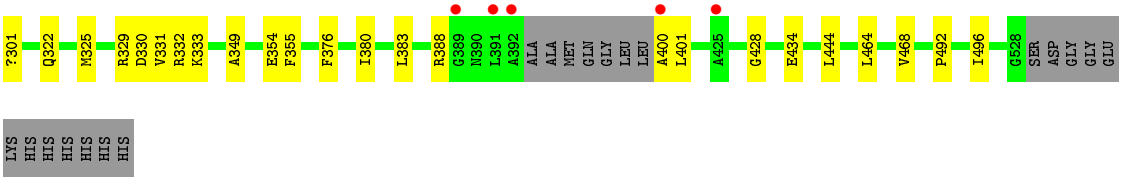
• Molecule 2: Proteasome (Beta subunit) PrcB



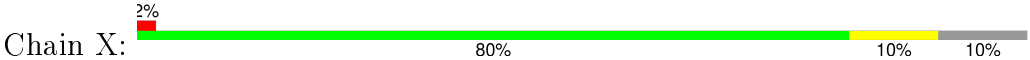


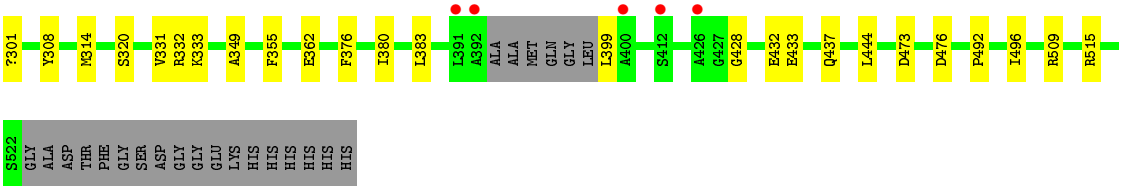
• Molecule 2: Proteasome (Beta subunit) PrcB



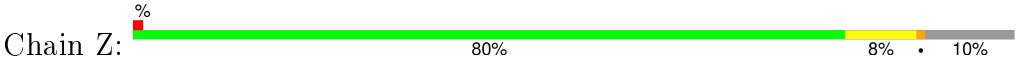


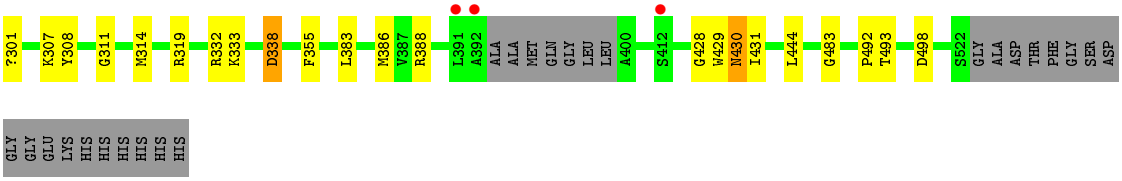
• Molecule 2: Proteasome (Beta subunit) PrcB



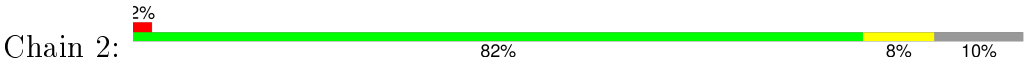


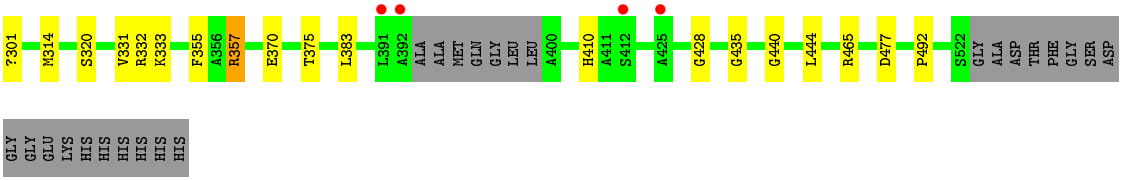
• Molecule 2: Proteasome (Beta subunit) PrcB





- Molecule 2: Proteasome (Beta subunit) PrcB





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	171.62Å 117.67Å 196.34Å 90.00° 113.65° 90.00°	Depositor
Resolution (Å)	29.75 – 2.43 30.57 – 2.44	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.75-2.43) 97.9 (30.57-2.44)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.82 (at 2.45Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.204 , 0.232 0.203 , 0.230	Depositor DCC
R_{free} test set	12991 reflections (4.97%)	DCC
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.2	EDS
Estimated twinning fraction	0.003 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	4 of 265904 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	48540	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1	0.76	0/1681	0.85	0/2270
1	A	0.75	0/1687	0.83	1/2279 (0.0%)
1	B	0.76	0/1675	0.85	2/2263 (0.1%)
1	D	0.75	0/1669	0.84	1/2254 (0.0%)
1	F	0.76	0/1694	0.84	1/2289 (0.0%)
1	I	0.73	0/1681	0.87	2/2270 (0.1%)
1	K	0.74	0/1695	0.85	2/2290 (0.1%)
1	M	0.77	0/1687	0.86	0/2279
1	O	0.78	0/1679	0.84	1/2268 (0.0%)
1	Q	0.76	0/1702	0.81	2/2300 (0.1%)
1	S	0.74	0/1679	0.85	1/2268 (0.0%)
1	U	0.77	0/1679	0.85	2/2268 (0.1%)
1	W	0.76	0/1695	0.86	0/2290
1	Y	0.75	0/1669	0.85	2/2254 (0.1%)
2	2	0.89	1/1607 (0.1%)	0.84	1/2178 (0.0%)
2	C	0.87	1/1607 (0.1%)	0.88	2/2178 (0.1%)
2	E	0.91	0/1615	0.88	0/2189
2	G	0.89	0/1615	0.88	3/2189 (0.1%)
2	H	0.91	0/1597	0.87	2/2164 (0.1%)
2	J	0.92	1/1615 (0.1%)	0.87	1/2189 (0.0%)
2	L	0.91	0/1615	0.87	0/2189
2	N	0.89	0/1594	0.87	1/2160 (0.0%)
2	P	0.86	1/1615 (0.1%)	0.85	1/2189 (0.0%)
2	R	0.88	0/1661	0.86	0/2251
2	T	0.86	0/1615	0.86	1/2189 (0.0%)
2	V	0.92	0/1647	0.83	0/2232
2	X	0.91	1/1615 (0.1%)	0.88	1/2189 (0.0%)
2	Z	0.88	1/1607 (0.1%)	0.87	2/2178 (0.1%)
All	All	0.83	6/46197 (0.0%)	0.86	32/62506 (0.1%)

All (6) bond length outliers are listed below:

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

All (32) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

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

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

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

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

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:400:ALA:HA	4:V:2033:HOH:O	1.27	1.32
2:C:430:ASN:HB2	4:C:2190:HOH:O	1.33	1.26
2:C:447:LYS:CD	3:C:5:DMF:H12	1.66	1.26
2:V:332:ARG:HB3	4:V:2317:HOH:O	1.32	1.25
1:U:160:THR:HG22	4:U:2365:HOH:O	1.34	1.24
2:C:447:LYS:HD2	3:C:5:DMF:C1	1.64	1.24
1:S:121:GLU:HG3	4:S:2023:HOH:O	1.34	1.23
1:A:162:PRO:HB2	4:A:2159:HOH:O	1.36	1.21
1:Y:18:GLU:OE1	1:Y:22:LYS:HE3	1.43	1.19
2:G:402:PRO:HD3	4:G:2237:HOH:O	1.41	1.18
2:X:332:ARG:HD2	4:X:2151:HOH:O	1.44	1.16
2:C:447:LYS:CD	3:C:5:DMF:C1	2.22	1.15
1:1:11:GLN:HA	1:1:14:ARG:HG2	1.21	1.12
1:W:134:LYS:HE2	4:W:2357:HOH:O	1.49	1.11
2:C:447:LYS:HD3	3:C:5:DMF:H12	1.13	1.10
1:S:76:ARG:HD3	4:S:2370:HOH:O	1.52	1.09
2:C:447:LYS:HD2	3:C:5:DMF:H11	1.29	1.08
1:1:11:GLN:HG3	1:1:14:ARG:NE	1.68	1.08
1:O:229:ALA:O	1:O:233:LEU:HD23	1.55	1.06
1:1:11:GLN:HG3	1:1:14:ARG:HE	0.93	1.06
2:H:332:ARG:HD2	4:H:2352:HOH:O	1.55	1.06
2:L:306:LEU:CD1	2:L:313:VAL:CG1	2.33	1.05
2:R:357:ARG:HD2	4:Z:2095:HOH:O	1.56	1.05
2:T:388:ARG:HG2	4:T:2215:HOH:O	1.57	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:428:GLY:HA2	4:E:2161:HOH:O	1.57	1.04
1:D:104:ALA:HB2	4:D:2360:HOH:O	1.58	1.04
2:L:306:LEU:HD12	2:L:313:VAL:CG1	1.89	1.03
1:U:51:GLN:HB2	4:U:2105:HOH:O	1.59	1.01
1:B:52:LYS:HD3	4:B:2129:HOH:O	1.58	1.01
2:G:351:VAL:HG13	4:G:2353:HOH:O	1.59	1.01
1:M:231:GLN:HG3	4:M:2387:HOH:O	1.58	1.01
1:Q:14:ARG:HH11	1:Q:14:ARG:HB3	1.24	1.00
2:L:306:LEU:HD12	2:L:313:VAL:HG13	1.40	1.00
2:2:465:ARG:HD3	4:2:2340:HOH:O	1.61	1.00
2:L:306:LEU:CD1	2:L:313:VAL:HG13	1.91	1.00
3:Z:91:DMF:HC	4:Z:1148:HOH:O	1.59	1.00
2:X:432:GLU:HB3	4:X:2235:HOH:O	1.62	1.00
3:U:252:DMF:H13	4:2:2315:HOH:O	1.62	0.99
1:F:28:LYS:HE2	4:F:2298:HOH:O	1.60	0.99
1:U:9:PRO:HD2	1:1:15:GLU:OE1	1.63	0.99
2:C:496:ILE:HD13	3:C:64:DMF:HC	1.43	0.99
1:O:76:ARG:HD3	4:O:2287:HOH:O	1.61	0.98
2:E:386:MET:SD	4:E:2398:HOH:O	2.21	0.97
1:D:54:SER:HB3	4:D:2426:HOH:O	1.63	0.97
3:E:55:DMF:HC	4:K:2288:HOH:O	1.65	0.96
1:Q:14:ARG:NH1	1:Q:14:ARG:HB3	1.81	0.95
2:J:388:ARG:HG2	4:J:2405:HOH:O	1.67	0.94
2:P:433:GLU:HG3	4:P:2308:HOH:O	1.67	0.92
2:G:509:ARG:HG3	4:G:2167:HOH:O	1.69	0.92
1:Q:97:ARG:HD2	1:Y:49:SER:OG	1.66	0.92
1:O:21:ARG:HD3	4:O:2361:HOH:O	1.69	0.92
1:Y:18:GLU:CD	1:Y:21:ARG:HH21	1.73	0.91
2:X:428:GLY:HA2	4:X:2092:HOH:O	1.71	0.91
2:T:399:LEU:HA	4:T:2342:HOH:O	1.71	0.90
3:L:60:DMF:H12	4:N:2035:HOH:O	1.71	0.90
1:D:147:ILE:HB	4:D:2360:HOH:O	1.70	0.90
1:D:11:GLN:HG2	1:D:14:ARG:NH2	1.87	0.89
2:J:509:ARG:HG2	4:J:2068:HOH:O	1.71	0.89
1:I:92:ARG:HB2	4:I:2214:HOH:O	1.73	0.88
1:A:76:ARG:HD3	4:A:2166:HOH:O	1.72	0.88
1:1:11:GLN:HA	1:1:14:ARG:CG	2.04	0.88
2:R:428:GLY:HA2	4:R:2208:HOH:O	1.72	0.88
2:Z:493:THR:HB	4:Z:2402:HOH:O	1.72	0.88
1:1:11:GLN:CA	1:1:14:ARG:HG2	2.03	0.88
2:R:447:LYS:HD3	4:R:2181:HOH:O	1.72	0.87

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

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

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

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

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:30:VAL:HG13	1:Y:43:ALA:HB2	1.92	0.51
1:Q:8:SER:HB2	1:Q:9:PRO:HD2	1.91	0.51
1:B:21:ARG:NH2	1:B:22:LYS:CG	2.74	0.51
3:O:250:DMF:H12	2:P:361:VAL:HA	1.92	0.51
1:S:177:LEU:HG	1:S:233:LEU:HD11	1.93	0.51
1:Y:31:VAL:HG22	1:Y:155:VAL:HG22	1.92	0.51
1:W:31:VAL:HG22	1:W:155:VAL:HG22	1.93	0.51
1:O:217:ARG:NH2	1:O:223:ARG:HG3	2.26	0.51
3:C:43:DMF:HC	1:I:88:ALA:HA	1.92	0.51
2:Z:308:TYR:CZ	2:Z:311:GLY:HA3	2.46	0.51
1:B:21:ARG:NH2	1:B:22:LYS:HG2	2.26	0.51
1:K:69:ASN:H	1:K:69:ASN:HD22	1.58	0.51
2:J:431:ILE:CD1	4:J:2185:HOH:O	2.50	0.50
4:U:2295:HOH:O	1:1:48:ARG:NH2	2.44	0.50
3:Z:91:DMF:C	4:Z:1148:HOH:O	2.37	0.50
1:U:75:ARG:HD3	4:U:2058:HOH:O	2.09	0.50
2:L:355:PHE:HE1	2:L:383:LEU:HD11	1.76	0.50
1:Y:76:ARG:HD3	4:Y:1321:HOH:O	2.10	0.50
1:K:217:ARG:NH2	1:K:223:ARG:HG3	2.24	0.50
1:K:169:GLU:O	1:K:169:GLU:OE1	2.30	0.50
1:K:170:SER:O	1:K:183:ILE:HD13	2.11	0.50
1:W:185:VAL:HG21	1:W:234:LEU:HD11	1.93	0.50
3:C:64:DMF:C	4:C:2195:HOH:O	2.60	0.50
2:P:355:PHE:HE2	4:P:2412:HOH:O	1.95	0.50
1:A:69:ASN:HD22	1:A:69:ASN:H	1.60	0.50
2:C:496:ILE:CD1	3:C:64:DMF:HC	2.28	0.50
1:Y:10:GLU:O	1:Y:13:MET:HB3	2.11	0.50
1:F:13:MET:HE2	1:F:13:MET:HA	1.94	0.50
1:S:163:ILE:CG1	1:S:191:GLY:HA3	2.42	0.50
2:R:376:PHE:CE2	2:R:380:ILE:HD11	2.46	0.50
2:H:362:GLU:HG3	4:H:1702:HOH:O	2.12	0.50
1:S:69:ASN:H	1:S:69:ASN:HD22	1.59	0.50
2:C:410:HIS:CE1	4:C:2344:HOH:O	2.64	0.50
1:A:111:PHE:CE1	1:A:143:TYR:CD2	2.96	0.50
1:B:115:ALA:HB3	1:I:112:THR:HG23	1.93	0.50
2:L:472:TYR:CE1	3:L:9:DMF:C1	2.95	0.50
1:Q:31:VAL:HG22	1:Q:155:VAL:HG22	1.94	0.50
1:U:101:ASN:HB3	3:U:250:DMF:HC	1.94	0.50
1:K:97:ARG:HG2	1:K:97:ARG:NH1	2.27	0.50
2:R:301:OZT:H27	2:R:333:LYS:HE2	1.94	0.49
2:G:476:ASP:O	2:V:329:ARG:NH2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LYS:NZ	1:I:10:GLU:OE2	2.38	0.49
2:T:373:PRO:HG2	3:T:35:DMF:C1	2.42	0.49
2:R:432:GLU:HB2	4:R:2012:HOH:O	2.12	0.49
2:L:472:TYR:CE1	3:L:9:DMF:H13	2.48	0.49
2:N:301:OZT:H17	2:N:333:LYS:NZ	2.27	0.49
2:P:329:ARG:HD2	2:V:434:GLU:OE2	2.12	0.49
1:B:102:VAL:HG12	3:B:249:DMF:H12	1.93	0.49
1:A:30:VAL:HG13	1:A:43:ALA:HB2	1.95	0.49
2:J:432:GLU:HG2	2:J:437:GLN:HB2	1.95	0.49
2:J:368:LYS:NZ	4:J:2318:HOH:O	2.39	0.49
2:Z:332:ARG:NH2	4:Z:2163:HOH:O	2.45	0.49
1:D:56:LEU:HG	1:D:62:PHE:HB2	1.94	0.49
1:Y:173:GLU:O	1:Y:174:ASN:HB2	2.13	0.49
1:S:142:THR:HA	4:S:2023:HOH:O	2.12	0.49
1:K:8:SER:OG	1:K:11:GLN:HB2	2.12	0.49
2:2:320:SER:HB3	2:2:331:VAL:HG21	1.94	0.49
1:O:76:ARG:NH1	4:O:2287:HOH:O	2.30	0.49
1:Y:204:GLY:O	1:Y:208:LEU:HG	2.12	0.49
2:P:376:PHE:CE2	2:P:380:ILE:HD11	2.48	0.49
2:H:320:SER:HB3	2:H:331:VAL:HG21	1.94	0.49
1:A:97:ARG:HD3	1:O:49:SER:HB2	1.95	0.49
1:F:11:GLN:O	1:F:15:GLU:HG3	2.13	0.49
2:N:472:TYR:CZ	3:N:36:DMF:H22	2.48	0.48
4:O:2280:HOH:O	2:P:357:ARG:NH1	2.34	0.48
2:T:430:ASN:HA	3:T:92:DMF:HC	1.94	0.48
2:R:301:OZT:H17	2:R:333:LYS:NZ	2.28	0.48
2:R:388:ARG:NH1	4:R:2208:HOH:O	2.47	0.48
1:U:136:PRO:HG3	4:U:2145:HOH:O	2.13	0.48
1:I:176:SER:OG	1:I:179:ASP:HB2	2.13	0.48
1:U:51:GLN:CB	4:U:2105:HOH:O	2.38	0.48
1:Y:92:ARG:CB	4:Y:2307:HOH:O	2.61	0.48
2:Z:429:TRP:CZ3	2:Z:431:ILE:HG13	2.48	0.48
1:F:30:VAL:HG22	1:F:52:LYS:NZ	2.28	0.48
1:S:163:ILE:CG1	1:S:191:GLY:CA	2.92	0.48
2:L:376:PHE:CE2	2:L:380:ILE:HD11	2.48	0.48
1:1:205:VAL:HG21	1:1:231:GLN:HG2	1.95	0.48
1:D:10:GLU:HG2	1:Q:15:GLU:HG3	1.95	0.48
1:I:152:HIS:HB3	1:I:171:TYR:CZ	2.49	0.48
2:G:376:PHE:CE2	2:G:380:ILE:HD11	2.49	0.47
1:F:52:LYS:HE2	1:F:52:LYS:HB3	1.56	0.47
2:P:388:ARG:NH1	4:P:1465:HOH:O	2.46	0.47

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

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

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

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

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

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

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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

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

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

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	164/192 (85%)	156 (95%)	8 (5%)	31	43
1	A	165/192 (86%)	161 (98%)	4 (2%)	57	72
1	B	164/192 (85%)	158 (96%)	6 (4%)	41	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	163/192 (85%)	154 (94%)	9 (6%)	27 37
1	F	166/192 (86%)	162 (98%)	4 (2%)	57 72
1	I	164/192 (85%)	160 (98%)	4 (2%)	57 72
1	K	166/192 (86%)	155 (93%)	11 (7%)	21 27
1	M	165/192 (86%)	160 (97%)	5 (3%)	48 65
1	O	164/192 (85%)	160 (98%)	4 (2%)	57 72
1	Q	167/192 (87%)	161 (96%)	6 (4%)	42 58
1	S	164/192 (85%)	158 (96%)	6 (4%)	41 57
1	U	164/192 (85%)	159 (97%)	5 (3%)	48 65
1	W	166/192 (86%)	163 (98%)	3 (2%)	66 79
1	Y	163/192 (85%)	159 (98%)	4 (2%)	55 71
2	2	160/177 (90%)	159 (99%)	1 (1%)	90 94
2	C	160/177 (90%)	157 (98%)	3 (2%)	65 78
2	E	161/177 (91%)	155 (96%)	6 (4%)	41 57
2	G	161/177 (91%)	158 (98%)	3 (2%)	65 78
2	H	160/177 (90%)	156 (98%)	4 (2%)	55 71
2	J	161/177 (91%)	158 (98%)	3 (2%)	65 78
2	L	161/177 (91%)	154 (96%)	7 (4%)	35 50
2	N	159/177 (90%)	155 (98%)	4 (2%)	55 71
2	P	161/177 (91%)	158 (98%)	3 (2%)	65 78
2	R	165/177 (93%)	162 (98%)	3 (2%)	66 79
2	T	161/177 (91%)	156 (97%)	5 (3%)	47 64
2	V	163/177 (92%)	158 (97%)	5 (3%)	47 64
2	X	161/177 (91%)	157 (98%)	4 (2%)	55 71
2	Z	160/177 (90%)	157 (98%)	3 (2%)	65 78
All	All	4559/5166 (88%)	4426 (97%)	133 (3%)	50 66

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

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

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

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

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

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

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

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

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

14 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	OZT	2	301	2	8,9,10	4.47	6 (75%)	7,12,14	4.15	4 (57%)
2	OZT	C	301	2	8,9,10	4.38	4 (50%)	7,12,14	4.44	4 (57%)
2	OZT	E	301	2	8,9,10	4.08	4 (50%)	7,12,14	4.42	5 (71%)
2	OZT	G	301	2	8,9,10	3.91	4 (50%)	7,12,14	4.60	5 (71%)
2	OZT	H	301	2	8,9,10	4.26	4 (50%)	7,12,14	4.50	4 (57%)
2	OZT	J	301	2	8,9,10	4.54	3 (37%)	7,12,14	4.60	4 (57%)
2	OZT	L	301	2	8,9,10	4.48	4 (50%)	7,12,14	4.58	4 (57%)
2	OZT	N	301	2	8,9,10	4.09	3 (37%)	7,12,14	4.26	4 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	OZT	P	301	2	8,9,10	3.73	4 (50%)	7,12,14	4.46	4 (57%)
2	OZT	R	301	2	8,9,10	4.67	5 (62%)	7,12,14	4.10	4 (57%)
2	OZT	T	301	2	8,9,10	4.15	4 (50%)	7,12,14	4.64	4 (57%)
2	OZT	V	301	2	8,9,10	4.15	4 (50%)	7,12,14	4.56	5 (71%)
2	OZT	X	301	2	8,9,10	4.65	5 (62%)	7,12,14	4.56	5 (71%)
2	OZT	Z	301	2	8,9,10	4.28	4 (50%)	7,12,14	4.43	4 (57%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OZT	2	301	2	-	0/1/14/16	0/1/1/1
2	OZT	C	301	2	-	0/1/14/16	0/1/1/1
2	OZT	E	301	2	-	0/1/14/16	0/1/1/1
2	OZT	G	301	2	-	0/1/14/16	0/1/1/1
2	OZT	H	301	2	-	0/1/14/16	0/1/1/1
2	OZT	J	301	2	-	0/1/14/16	0/1/1/1
2	OZT	L	301	2	-	0/1/14/16	0/1/1/1
2	OZT	N	301	2	-	0/1/14/16	0/1/1/1
2	OZT	P	301	2	-	0/1/14/16	0/1/1/1
2	OZT	R	301	2	-	0/1/14/16	0/1/1/1
2	OZT	T	301	2	-	0/1/14/16	0/1/1/1
2	OZT	V	301	2	-	0/1/14/16	0/1/1/1
2	OZT	X	301	2	-	0/1/14/16	0/1/1/1
2	OZT	Z	301	2	-	0/1/14/16	0/1/1/1

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	301	OZT	O1-C2	-4.80	1.38	1.46
2	N	301	OZT	O1-C2	-4.47	1.39	1.46
2	2	301	OZT	O1-C2	-4.33	1.39	1.46
2	R	301	OZT	O1-C2	-4.16	1.40	1.46
2	Z	301	OZT	O1-C2	-4.13	1.40	1.46
2	L	301	OZT	O1-C2	-4.01	1.40	1.46
2	X	301	OZT	O1-C2	-3.79	1.40	1.46
2	Z	301	OZT	C2-CA	-3.78	1.46	1.54
2	T	301	OZT	O1-C2	-3.53	1.41	1.46
2	V	301	OZT	C2-CA	-3.50	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	301	OZT	O1-C2	-3.50	1.41	1.46
2	J	301	OZT	O1-C2	-3.46	1.41	1.46
2	C	301	OZT	O1-C2	-3.45	1.41	1.46
2	E	301	OZT	O1-C2	-3.40	1.41	1.46
2	H	301	OZT	O1-C2	-3.35	1.41	1.46
2	G	301	OZT	O1-C2	-3.30	1.41	1.46
2	2	301	OZT	C2-CA	-3.06	1.47	1.54
2	R	301	OZT	C2-CA	-3.00	1.48	1.54
2	E	301	OZT	C2-CA	-2.94	1.48	1.54
2	H	301	OZT	C2-CA	-2.57	1.48	1.54
2	X	301	OZT	C2-CA	-2.51	1.49	1.54
2	T	301	OZT	C2-CA	-2.41	1.49	1.54
2	C	301	OZT	C2-CA	-2.40	1.49	1.54
2	G	301	OZT	C2-CA	-2.34	1.49	1.54
2	P	301	OZT	C2-CA	-2.33	1.49	1.54
2	X	301	OZT	C7-C2	-2.26	1.46	1.51
2	L	301	OZT	C2-CA	-2.25	1.49	1.54
2	2	301	OZT	C7-C2	-2.22	1.46	1.51
2	2	301	OZT	O6-C5	2.24	1.26	1.21
2	R	301	OZT	O6-C5	2.29	1.26	1.21
2	T	301	OZT	C5-N	3.66	1.39	1.33
2	E	301	OZT	C5-N	4.03	1.39	1.33
2	G	301	OZT	C5-N	4.22	1.39	1.33
2	P	301	OZT	C5-N	4.39	1.40	1.33
2	V	301	OZT	C5-N	4.49	1.40	1.33
2	J	301	OZT	C5-N	4.66	1.40	1.33
2	L	301	OZT	C5-N	4.81	1.40	1.33
2	Z	301	OZT	C5-N	4.89	1.40	1.33
2	H	301	OZT	C5-N	5.29	1.41	1.33
2	X	301	OZT	C5-N	5.32	1.41	1.33
2	2	301	OZT	C5-N	5.71	1.42	1.33
2	N	301	OZT	C5-N	5.98	1.42	1.33
2	C	301	OZT	C5-N	6.08	1.42	1.33
2	R	301	OZT	C5-N	6.48	1.43	1.33
2	P	301	OZT	O1-C5	8.41	1.47	1.36
2	N	301	OZT	O1-C5	8.58	1.47	1.36
2	V	301	OZT	O1-C5	8.69	1.47	1.36
2	Z	301	OZT	O1-C5	9.25	1.48	1.36
2	G	301	OZT	O1-C5	9.31	1.48	1.36
2	2	301	OZT	O1-C5	9.42	1.48	1.36
2	E	301	OZT	O1-C5	9.45	1.48	1.36
2	C	301	OZT	O1-C5	9.58	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	301	OZT	O1-C5	9.73	1.49	1.36
2	R	301	OZT	O1-C5	9.77	1.49	1.36
2	T	301	OZT	O1-C5	10.15	1.49	1.36
2	L	301	OZT	O1-C5	10.57	1.50	1.36
2	X	301	OZT	O1-C5	10.84	1.50	1.36
2	J	301	OZT	O1-C5	11.11	1.51	1.36

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	301	OZT	O6-C5-N	-6.99	120.67	129.16
2	J	301	OZT	O6-C5-N	-6.85	120.84	129.16
2	G	301	OZT	O6-C5-N	-6.45	121.32	129.16
2	L	301	OZT	O6-C5-N	-6.38	121.41	129.16
2	E	301	OZT	O6-C5-N	-6.22	121.60	129.16
2	H	301	OZT	O6-C5-N	-6.11	121.73	129.16
2	P	301	OZT	O6-C5-N	-6.06	121.79	129.16
2	X	301	OZT	O6-C5-N	-6.06	121.80	129.16
2	Z	301	OZT	O6-C5-N	-5.90	122.00	129.16
2	C	301	OZT	O6-C5-N	-5.85	122.05	129.16
2	V	301	OZT	O6-C5-N	-5.65	122.30	129.16
2	N	301	OZT	O6-C5-N	-5.37	122.63	129.16
2	2	301	OZT	O6-C5-N	-5.31	122.72	129.16
2	V	301	OZT	C7-C2-CA	-5.02	107.67	114.67
2	R	301	OZT	O6-C5-N	-4.95	123.14	129.16
2	L	301	OZT	C7-C2-CA	-4.95	107.76	114.67
2	X	301	OZT	C7-C2-CA	-4.92	107.81	114.67
2	Z	301	OZT	C7-C2-CA	-4.91	107.82	114.67
2	E	301	OZT	C7-C2-CA	-4.85	107.89	114.67
2	C	301	OZT	C7-C2-CA	-4.63	108.20	114.67
2	J	301	OZT	C7-C2-CA	-4.56	108.30	114.67
2	H	301	OZT	C7-C2-CA	-4.54	108.33	114.67
2	G	301	OZT	C7-C2-CA	-4.53	108.34	114.67
2	T	301	OZT	C7-C2-CA	-4.35	108.59	114.67
2	R	301	OZT	C7-C2-CA	-4.31	108.65	114.67
2	P	301	OZT	C7-C2-CA	-4.28	108.70	114.67
2	2	301	OZT	C7-C2-CA	-4.25	108.74	114.67
2	N	301	OZT	C7-C2-CA	-3.48	109.82	114.67
2	G	301	OZT	O-C-CA	-2.29	118.69	125.74
2	E	301	OZT	O-C-CA	-2.27	118.76	125.74
2	X	301	OZT	O-C-CA	-2.20	118.98	125.74
2	V	301	OZT	O-C-CA	-2.11	119.25	125.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	301	OZT	O1-C2-CA	4.07	109.84	103.42
2	T	301	OZT	O1-C2-CA	4.25	110.12	103.42
2	Z	301	OZT	O1-C2-CA	4.26	110.14	103.42
2	E	301	OZT	O1-C2-CA	4.29	110.19	103.42
2	J	301	OZT	O1-C2-CA	4.38	110.33	103.42
2	C	301	OZT	O1-C2-CA	4.40	110.36	103.42
2	R	301	OZT	O1-C2-CA	4.41	110.37	103.42
2	N	301	OZT	O1-C2-CA	4.48	110.49	103.42
2	P	301	OZT	O1-C2-CA	4.56	110.61	103.42
2	X	301	OZT	O1-C2-CA	4.62	110.71	103.42
2	2	301	OZT	O1-C2-CA	4.64	110.73	103.42
2	H	301	OZT	O1-C2-CA	4.70	110.84	103.42
2	L	301	OZT	O1-C2-CA	5.01	111.33	103.42
2	V	301	OZT	O1-C2-CA	5.47	112.05	103.42
2	2	301	OZT	O1-C5-N	7.01	116.61	109.84
2	E	301	OZT	O1-C5-N	7.02	116.62	109.84
2	R	301	OZT	O1-C5-N	7.02	116.63	109.84
2	V	301	OZT	O1-C5-N	7.32	116.91	109.84
2	L	301	OZT	O1-C5-N	7.34	116.93	109.84
2	Z	301	OZT	O1-C5-N	7.45	117.04	109.84
2	J	301	OZT	O1-C5-N	7.57	117.15	109.84
2	X	301	OZT	O1-C5-N	7.57	117.15	109.84
2	C	301	OZT	O1-C5-N	7.59	117.17	109.84
2	H	301	OZT	O1-C5-N	7.64	117.22	109.84
2	P	301	OZT	O1-C5-N	7.72	117.31	109.84
2	N	301	OZT	O1-C5-N	7.79	117.37	109.84
2	T	301	OZT	O1-C5-N	7.84	117.41	109.84
2	G	301	OZT	O1-C5-N	7.92	117.50	109.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	301	OZT	3	0
2	C	301	OZT	2	0
2	H	301	OZT	2	0
2	L	301	OZT	1	0
2	N	301	OZT	3	0
2	P	301	OZT	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	301	OZT	3	0
2	T	301	OZT	1	0
2	V	301	OZT	2	0
2	X	301	OZT	1	0
2	Z	301	OZT	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

102 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	DMF	1	249	-	4,4,4	0.49	0	4,4,4	0.38	0
3	DMF	1	250	-	4,4,4	0.32	0	4,4,4	0.26	0
3	DMF	1	251	-	4,4,4	0.42	0	4,4,4	0.59	0
3	DMF	2	58	-	4,4,4	0.72	0	4,4,4	0.29	0
3	DMF	2	66	-	4,4,4	0.67	0	4,4,4	0.25	0
3	DMF	2	78	-	4,4,4	0.19	0	4,4,4	0.37	0
3	DMF	A	249	-	4,4,4	0.52	0	4,4,4	0.33	0
3	DMF	A	250	-	4,4,4	0.59	0	4,4,4	0.43	0
3	DMF	B	249	-	4,4,4	0.19	0	4,4,4	0.38	0
3	DMF	B	250	-	4,4,4	0.80	0	4,4,4	0.27	0
3	DMF	B	251	-	4,4,4	0.63	0	4,4,4	0.21	0
3	DMF	C	15	-	4,4,4	0.36	0	4,4,4	0.40	0
3	DMF	C	17	-	4,4,4	0.24	0	4,4,4	0.39	0
3	DMF	C	28	-	4,4,4	0.51	0	4,4,4	0.28	0
3	DMF	C	43	-	4,4,4	0.86	0	4,4,4	0.34	0
3	DMF	C	48	-	4,4,4	0.44	0	4,4,4	0.27	0
3	DMF	C	5	-	4,4,4	0.30	0	4,4,4	0.52	0
3	DMF	C	64	-	4,4,4	0.26	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	C	73	-	4,4,4	0.25	0	4,4,4	0.32	0
3	DMF	D	249	-	4,4,4	0.27	0	4,4,4	0.30	0
3	DMF	D	250	-	4,4,4	0.62	0	4,4,4	0.31	0
3	DMF	D	251	-	4,4,4	0.42	0	4,4,4	0.45	0
3	DMF	D	252	-	4,4,4	0.23	0	4,4,4	0.34	0
3	DMF	E	32	-	4,4,4	0.65	0	4,4,4	0.32	0
3	DMF	E	44	-	4,4,4	0.27	0	4,4,4	0.48	0
3	DMF	E	55	-	4,4,4	0.40	0	4,4,4	0.32	0
3	DMF	E	70	-	4,4,4	0.31	0	4,4,4	0.49	0
3	DMF	E	83	-	4,4,4	0.27	0	4,4,4	0.69	0
3	DMF	E	95	-	4,4,4	1.01	0	4,4,4	0.40	0
3	DMF	F	249	-	4,4,4	0.50	0	4,4,4	0.42	0
3	DMF	F	250	-	4,4,4	0.31	0	4,4,4	0.38	0
3	DMF	G	1	-	4,4,4	0.34	0	4,4,4	0.55	0
3	DMF	G	20	-	4,4,4	0.47	0	4,4,4	0.32	0
3	DMF	G	39	-	4,4,4	0.66	0	4,4,4	0.32	0
3	DMF	G	96	-	4,4,4	0.73	0	4,4,4	0.30	0
3	DMF	H	102	-	4,4,4	0.44	0	4,4,4	0.37	0
3	DMF	H	14	-	4,4,4	0.54	0	4,4,4	0.29	0
3	DMF	H	19	-	4,4,4	0.45	0	4,4,4	0.27	0
3	DMF	H	31	-	4,4,4	0.79	0	4,4,4	0.30	0
3	DMF	H	41	-	4,4,4	0.51	0	4,4,4	0.33	0
3	DMF	H	52	-	4,4,4	0.34	0	4,4,4	0.50	0
3	DMF	H	53	-	4,4,4	0.31	0	4,4,4	0.34	0
3	DMF	I	249	-	4,4,4	0.68	0	4,4,4	0.35	0
3	DMF	I	250	-	4,4,4	0.43	0	4,4,4	0.25	0
3	DMF	J	59	-	4,4,4	0.22	0	4,4,4	0.35	0
3	DMF	J	6	-	4,4,4	0.25	0	4,4,4	0.39	0
3	DMF	J	82	-	4,4,4	0.48	0	4,4,4	0.32	0
3	DMF	K	249	-	4,4,4	0.66	0	4,4,4	0.26	0
3	DMF	K	250	-	4,4,4	0.53	0	4,4,4	0.34	0
3	DMF	L	4	-	4,4,4	0.39	0	4,4,4	0.27	0
3	DMF	L	60	-	4,4,4	0.43	0	4,4,4	0.28	0
3	DMF	L	9	-	4,4,4	0.20	0	4,4,4	0.42	0
3	DMF	M	249	-	4,4,4	0.53	0	4,4,4	0.38	0
3	DMF	M	250	-	4,4,4	0.67	0	4,4,4	0.49	0
3	DMF	N	2	-	4,4,4	0.16	0	4,4,4	0.39	0
3	DMF	N	21	-	4,4,4	0.24	0	4,4,4	0.39	0
3	DMF	N	24	-	4,4,4	0.43	0	4,4,4	0.31	0
3	DMF	N	36	-	4,4,4	0.31	0	4,4,4	0.42	0
3	DMF	N	37	-	4,4,4	0.62	0	4,4,4	0.38	0
3	DMF	N	97	-	4,4,4	0.83	0	4,4,4	0.42	0
3	DMF	N	99	-	4,4,4	0.84	0	4,4,4	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	DMF	O	249	-	4,4,4	0.25	0	4,4,4	0.61	0
3	DMF	O	250	-	4,4,4	0.28	0	4,4,4	0.42	0
3	DMF	P	100	-	4,4,4	0.45	0	4,4,4	0.31	0
3	DMF	P	23	-	4,4,4	0.20	0	4,4,4	0.33	0
3	DMF	P	61	-	4,4,4	0.69	0	4,4,4	0.28	0
3	DMF	P	74	-	4,4,4	0.36	0	4,4,4	0.17	0
3	DMF	P	85	-	4,4,4	0.77	0	4,4,4	0.36	0
3	DMF	Q	249	-	4,4,4	0.41	0	4,4,4	0.33	0
3	DMF	Q	250	-	4,4,4	0.28	0	4,4,4	0.49	0
3	DMF	R	3	-	4,4,4	0.25	0	4,4,4	0.41	0
3	DMF	R	54	-	4,4,4	0.35	0	4,4,4	0.39	0
3	DMF	R	68	-	4,4,4	0.24	0	4,4,4	0.48	0
3	DMF	R	89	-	4,4,4	0.28	0	4,4,4	0.52	0
3	DMF	S	249	-	4,4,4	0.54	0	4,4,4	0.20	0
3	DMF	S	250	-	4,4,4	0.27	0	4,4,4	0.39	0
3	DMF	S	251	-	4,4,4	0.29	0	4,4,4	0.38	0
3	DMF	T	35	-	4,4,4	0.32	0	4,4,4	0.35	0
3	DMF	T	46	-	4,4,4	0.49	0	4,4,4	0.34	0
3	DMF	T	62	-	4,4,4	0.43	0	4,4,4	0.29	0
3	DMF	T	92	-	4,4,4	0.78	0	4,4,4	0.34	0
3	DMF	T	94	-	4,4,4	0.49	0	4,4,4	0.34	0
3	DMF	U	249	-	4,4,4	0.48	0	4,4,4	0.21	0
3	DMF	U	250	-	4,4,4	0.28	0	4,4,4	0.44	0
3	DMF	U	251	-	4,4,4	0.81	0	4,4,4	0.26	0
3	DMF	U	252	-	4,4,4	0.78	0	4,4,4	0.34	0
3	DMF	V	16	-	4,4,4	0.33	0	4,4,4	0.52	0
3	DMF	V	65	-	4,4,4	0.82	0	4,4,4	0.26	0
3	DMF	V	86	-	4,4,4	0.26	0	4,4,4	0.45	0
3	DMF	V	90	-	4,4,4	0.24	0	4,4,4	0.32	0
3	DMF	W	249	-	4,4,4	0.32	0	4,4,4	0.35	0
3	DMF	W	250	-	4,4,4	0.65	0	4,4,4	0.30	0
3	DMF	X	25	-	4,4,4	0.54	0	4,4,4	0.43	0
3	DMF	X	67	-	4,4,4	0.66	0	4,4,4	0.29	0
3	DMF	X	88	-	4,4,4	0.43	0	4,4,4	0.44	0
3	DMF	Y	249	-	4,4,4	0.60	0	4,4,4	0.42	0
3	DMF	Z	27	-	4,4,4	0.15	0	4,4,4	0.35	0
3	DMF	Z	50	-	4,4,4	0.22	0	4,4,4	0.39	0
3	DMF	Z	69	-	4,4,4	0.54	0	4,4,4	0.28	0
3	DMF	Z	71	-	4,4,4	0.44	0	4,4,4	0.32	0
3	DMF	Z	79	-	4,4,4	0.81	0	4,4,4	0.44	0
3	DMF	Z	91	-	4,4,4	0.29	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	1	249	-	-	0/2/2/2	0/0/0/0
3	DMF	1	250	-	-	0/2/2/2	0/0/0/0
3	DMF	1	251	-	-	0/2/2/2	0/0/0/0
3	DMF	2	58	-	-	0/2/2/2	0/0/0/0
3	DMF	2	66	-	-	0/2/2/2	0/0/0/0
3	DMF	2	78	-	-	0/2/2/2	0/0/0/0
3	DMF	A	249	-	-	0/2/2/2	0/0/0/0
3	DMF	A	250	-	-	0/2/2/2	0/0/0/0
3	DMF	B	249	-	-	0/2/2/2	0/0/0/0
3	DMF	B	250	-	-	0/2/2/2	0/0/0/0
3	DMF	B	251	-	-	0/2/2/2	0/0/0/0
3	DMF	C	15	-	-	0/2/2/2	0/0/0/0
3	DMF	C	17	-	-	0/2/2/2	0/0/0/0
3	DMF	C	28	-	-	0/2/2/2	0/0/0/0
3	DMF	C	43	-	-	0/2/2/2	0/0/0/0
3	DMF	C	48	-	-	0/2/2/2	0/0/0/0
3	DMF	C	5	-	-	0/2/2/2	0/0/0/0
3	DMF	C	64	-	-	0/2/2/2	0/0/0/0
3	DMF	C	73	-	-	0/2/2/2	0/0/0/0
3	DMF	D	249	-	-	0/2/2/2	0/0/0/0
3	DMF	D	250	-	-	0/2/2/2	0/0/0/0
3	DMF	D	251	-	-	0/2/2/2	0/0/0/0
3	DMF	D	252	-	-	0/2/2/2	0/0/0/0
3	DMF	E	32	-	-	0/2/2/2	0/0/0/0
3	DMF	E	44	-	-	0/2/2/2	0/0/0/0
3	DMF	E	55	-	-	0/2/2/2	0/0/0/0
3	DMF	E	70	-	-	0/2/2/2	0/0/0/0
3	DMF	E	83	-	-	0/2/2/2	0/0/0/0
3	DMF	E	95	-	-	0/2/2/2	0/0/0/0
3	DMF	F	249	-	-	0/2/2/2	0/0/0/0
3	DMF	F	250	-	-	0/2/2/2	0/0/0/0
3	DMF	G	1	-	-	0/2/2/2	0/0/0/0
3	DMF	G	20	-	-	0/2/2/2	0/0/0/0
3	DMF	G	39	-	-	0/2/2/2	0/0/0/0
3	DMF	G	96	-	-	0/2/2/2	0/0/0/0
3	DMF	H	102	-	-	0/2/2/2	0/0/0/0
3	DMF	H	14	-	-	0/2/2/2	0/0/0/0
3	DMF	H	19	-	-	0/2/2/2	0/0/0/0
3	DMF	H	31	-	-	0/2/2/2	0/0/0/0
3	DMF	H	41	-	-	0/2/2/2	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	H	52	-	-	0/2/2/2	0/0/0/0
3	DMF	H	53	-	-	0/2/2/2	0/0/0/0
3	DMF	I	249	-	-	0/2/2/2	0/0/0/0
3	DMF	I	250	-	-	0/2/2/2	0/0/0/0
3	DMF	J	59	-	-	0/2/2/2	0/0/0/0
3	DMF	J	6	-	-	0/2/2/2	0/0/0/0
3	DMF	J	82	-	-	0/2/2/2	0/0/0/0
3	DMF	K	249	-	-	0/2/2/2	0/0/0/0
3	DMF	K	250	-	-	0/2/2/2	0/0/0/0
3	DMF	L	4	-	-	0/2/2/2	0/0/0/0
3	DMF	L	60	-	-	0/2/2/2	0/0/0/0
3	DMF	L	9	-	-	0/2/2/2	0/0/0/0
3	DMF	M	249	-	-	0/2/2/2	0/0/0/0
3	DMF	M	250	-	-	0/2/2/2	0/0/0/0
3	DMF	N	2	-	-	0/2/2/2	0/0/0/0
3	DMF	N	21	-	-	0/2/2/2	0/0/0/0
3	DMF	N	24	-	-	0/2/2/2	0/0/0/0
3	DMF	N	36	-	-	0/2/2/2	0/0/0/0
3	DMF	N	37	-	-	0/2/2/2	0/0/0/0
3	DMF	N	97	-	-	0/2/2/2	0/0/0/0
3	DMF	N	99	-	-	0/2/2/2	0/0/0/0
3	DMF	O	249	-	-	0/2/2/2	0/0/0/0
3	DMF	O	250	-	-	0/2/2/2	0/0/0/0
3	DMF	P	100	-	-	0/2/2/2	0/0/0/0
3	DMF	P	23	-	-	0/2/2/2	0/0/0/0
3	DMF	P	61	-	-	0/2/2/2	0/0/0/0
3	DMF	P	74	-	-	0/2/2/2	0/0/0/0
3	DMF	P	85	-	-	0/2/2/2	0/0/0/0
3	DMF	Q	249	-	-	0/2/2/2	0/0/0/0
3	DMF	Q	250	-	-	0/2/2/2	0/0/0/0
3	DMF	R	3	-	-	0/2/2/2	0/0/0/0
3	DMF	R	54	-	-	0/2/2/2	0/0/0/0
3	DMF	R	68	-	-	0/2/2/2	0/0/0/0
3	DMF	R	89	-	-	0/2/2/2	0/0/0/0
3	DMF	S	249	-	-	0/2/2/2	0/0/0/0
3	DMF	S	250	-	-	0/2/2/2	0/0/0/0
3	DMF	S	251	-	-	0/2/2/2	0/0/0/0
3	DMF	T	35	-	-	0/2/2/2	0/0/0/0
3	DMF	T	46	-	-	0/2/2/2	0/0/0/0
3	DMF	T	62	-	-	0/2/2/2	0/0/0/0
3	DMF	T	92	-	-	0/2/2/2	0/0/0/0
3	DMF	T	94	-	-	0/2/2/2	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	U	249	-	-	0/2/2/2	0/0/0/0
3	DMF	U	250	-	-	0/2/2/2	0/0/0/0
3	DMF	U	251	-	-	0/2/2/2	0/0/0/0
3	DMF	U	252	-	-	0/2/2/2	0/0/0/0
3	DMF	V	16	-	-	0/2/2/2	0/0/0/0
3	DMF	V	65	-	-	0/2/2/2	0/0/0/0
3	DMF	V	86	-	-	0/2/2/2	0/0/0/0
3	DMF	V	90	-	-	0/2/2/2	0/0/0/0
3	DMF	W	249	-	-	0/2/2/2	0/0/0/0
3	DMF	W	250	-	-	0/2/2/2	0/0/0/0
3	DMF	X	25	-	-	0/2/2/2	0/0/0/0
3	DMF	X	67	-	-	0/2/2/2	0/0/0/0
3	DMF	X	88	-	-	0/2/2/2	0/0/0/0
3	DMF	Y	249	-	-	0/2/2/2	0/0/0/0
3	DMF	Z	27	-	-	0/2/2/2	0/0/0/0
3	DMF	Z	50	-	-	0/2/2/2	0/0/0/0
3	DMF	Z	69	-	-	0/2/2/2	0/0/0/0
3	DMF	Z	71	-	-	0/2/2/2	0/0/0/0
3	DMF	Z	79	-	-	0/2/2/2	0/0/0/0
3	DMF	Z	91	-	-	0/2/2/2	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

57 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1	250	DMF	1	0
3	1	251	DMF	2	0
3	2	78	DMF	1	0
3	A	250	DMF	2	0
3	B	249	DMF	1	0
3	B	250	DMF	1	0
3	C	17	DMF	1	0
3	C	43	DMF	1	0
3	C	5	DMF	5	0
3	C	64	DMF	6	0
3	C	73	DMF	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	251	DMF	1	0
3	D	252	DMF	1	0
3	E	32	DMF	1	0
3	E	55	DMF	1	0
3	E	70	DMF	2	0
3	E	95	DMF	1	0
3	F	250	DMF	1	0
3	G	1	DMF	1	0
3	G	20	DMF	3	0
3	G	39	DMF	1	0
3	G	96	DMF	3	0
3	H	19	DMF	4	0
3	H	31	DMF	1	0
3	H	41	DMF	1	0
3	H	53	DMF	2	0
3	J	6	DMF	4	0
3	J	82	DMF	1	0
3	K	250	DMF	2	0
3	L	4	DMF	1	0
3	L	60	DMF	1	0
3	L	9	DMF	3	0
3	M	249	DMF	1	0
3	N	2	DMF	2	0
3	N	36	DMF	2	0
3	N	97	DMF	3	0
3	O	249	DMF	2	0
3	O	250	DMF	4	0
3	P	23	DMF	1	0
3	P	61	DMF	1	0
3	R	68	DMF	1	0
3	R	89	DMF	1	0
3	S	250	DMF	1	0
3	T	35	DMF	5	0
3	T	92	DMF	1	0
3	T	94	DMF	3	0
3	U	250	DMF	1	0
3	U	251	DMF	2	0
3	U	252	DMF	1	0
3	V	16	DMF	1	0
3	W	249	DMF	1	0
3	X	67	DMF	1	0
3	Z	27	DMF	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Z	69	DMF	3	0
3	Z	71	DMF	1	0
3	Z	79	DMF	1	0
3	Z	91	DMF	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.49	22 (10%) 9 7	20, 55, 92, 101	0
1	A	216/248 (87%)	0.74	37 (17%) 2 1	21, 56, 100, 109	0
1	B	214/248 (86%)	0.50	20 (9%) 11 9	22, 56, 98, 108	0
1	D	213/248 (85%)	0.72	30 (14%) 4 2	21, 56, 96, 105	0
1	F	217/248 (87%)	0.51	15 (6%) 20 18	22, 55, 91, 102	0
1	I	215/248 (86%)	0.54	21 (9%) 10 8	23, 56, 98, 107	0
1	K	217/248 (87%)	0.61	25 (11%) 6 5	19, 57, 94, 109	0
1	M	216/248 (87%)	0.47	15 (6%) 20 18	21, 55, 92, 99	0
1	O	215/248 (86%)	0.56	20 (9%) 11 9	21, 56, 92, 102	0
1	Q	218/248 (87%)	0.46	17 (7%) 16 14	21, 55, 90, 101	0
1	S	215/248 (86%)	0.69	34 (15%) 3 1	21, 57, 102, 112	0
1	U	215/248 (86%)	0.52	17 (7%) 15 14	22, 55, 96, 106	0
1	W	217/248 (87%)	0.56	21 (9%) 10 9	22, 56, 93, 99	0
1	Y	213/248 (85%)	0.82	36 (16%) 2 1	23, 57, 99, 111	0
2	2	214/240 (89%)	-0.47	4 (1%) 70 69	10, 20, 43, 73	0
2	C	214/240 (89%)	-0.33	6 (2%) 56 56	8, 20, 46, 76	0
2	E	215/240 (89%)	-0.46	4 (1%) 70 69	10, 20, 45, 76	0
2	G	215/240 (89%)	-0.54	1 (0%) 91 92	10, 21, 47, 75	0
2	H	212/240 (88%)	-0.45	2 (0%) 85 87	11, 22, 45, 70	0
2	J	215/240 (89%)	-0.32	3 (1%) 78 79	10, 21, 46, 70	0
2	L	215/240 (89%)	-0.40	2 (0%) 85 87	10, 21, 45, 72	0
2	N	212/240 (88%)	-0.45	2 (0%) 85 87	9, 21, 43, 67	0
2	P	215/240 (89%)	-0.37	7 (3%) 50 48	10, 23, 47, 73	0
2	R	222/240 (92%)	-0.46	2 (0%) 85 87	8, 19, 44, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	T	215/240 (89%)	-0.30	5 (2%) 64 63	9, 22, 47, 80	0
2	V	220/240 (91%)	-0.53	5 (2%) 64 63	8, 20, 44, 74	0
2	X	215/240 (89%)	-0.44	5 (2%) 64 63	10, 22, 46, 79	0
2	Z	214/240 (89%)	-0.39	3 (1%) 78 79	10, 23, 46, 68	0
All	All	6029/6832 (88%)	0.08	381 (6%) 23 21	8, 34, 89, 112	0

All (381) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	12	ALA	9.9
1	F	202	THR	7.6
1	S	188	LEU	7.6
1	B	205	VAL	7.4
1	U	204	GLY	6.8
1	S	8	SER	6.4
1	U	206	ALA	6.4
1	B	204	GLY	6.0
1	A	172	ALA	5.9
1	D	169	GLU	5.9
1	U	205	VAL	5.7
1	Y	10	GLU	5.6
1	D	131	GLY	5.4
1	Y	11	GLN	5.4
2	T	392	ALA	5.3
1	Y	231	GLN	5.2
1	U	231	GLN	5.2
1	Y	188	LEU	5.1
1	Q	7	ILE	5.0
1	D	48	ARG	5.0
1	B	206	ALA	4.9
1	K	7	ILE	4.8
1	W	7	ILE	4.8
1	O	172	ALA	4.8
1	M	10	GLU	4.7
1	F	169	GLU	4.5
1	Y	131	GLY	4.5
1	K	169	GLU	4.4
1	Y	184	ALA	4.4
1	Y	186	ALA	4.4
1	1	179	ASP	4.4
1	A	131	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
2	L	392	ALA	4.3
1	D	206	ALA	4.3
2	P	425	ALA	4.3
1	O	161	GLU	4.2
1	1	232	ALA	4.2
1	Q	14	ARG	4.2
1	A	10	GLU	4.2
1	Y	169	GLU	4.2
2	R	412	SER	4.2
1	S	232	ALA	4.1
1	O	14	ARG	4.1
2	T	391	LEU	4.1
2	X	391	LEU	4.1
2	H	425	ALA	4.1
1	B	231	GLN	4.0
1	Q	202	THR	4.0
1	S	172	ALA	4.0
1	A	191	GLY	3.9
1	D	10	GLU	3.9
1	O	168	LYS	3.9
1	U	232	ALA	3.9
1	D	228	SER	3.9
1	Y	9	PRO	3.9
1	A	168	LYS	3.9
1	O	8	SER	3.9
1	F	179	ASP	3.9
1	Q	172	ALA	3.9
1	K	179	ASP	3.9
1	Y	179	ASP	3.9
1	Y	234	LEU	3.9
1	D	207	SER	3.9
1	D	165	ASN	3.8
1	K	232	ALA	3.8
2	2	392	ALA	3.8
1	A	227	GLY	3.8
1	B	234	LEU	3.8
1	B	232	ALA	3.8
1	M	206	ALA	3.7
1	D	231	GLN	3.7
1	D	227	GLY	3.7
1	W	161	GLU	3.7
1	D	168	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	206	ALA	3.6
1	Y	44	GLU	3.6
1	O	234	LEU	3.6
2	Z	391	LEU	3.6
1	O	13	MET	3.6
1	I	203	LEU	3.6
1	O	169	GLU	3.5
1	S	205	VAL	3.5
1	D	159	THR	3.5
1	D	27	ALA	3.5
1	1	165	ASN	3.4
1	Y	14	ARG	3.4
2	V	400	ALA	3.4
2	N	412	SER	3.4
1	A	161	GLU	3.4
2	X	392	ALA	3.4
1	Y	165	ASN	3.4
1	K	205	VAL	3.4
1	K	186	ALA	3.3
1	S	11	GLN	3.3
1	S	14	ARG	3.3
1	I	11	GLN	3.3
1	F	205	VAL	3.3
1	M	113	GLU	3.3
1	U	8	SER	3.3
1	1	133	THR	3.3
1	O	11	GLN	3.3
1	O	182	ARG	3.3
1	O	206	ALA	3.3
1	Q	11	GLN	3.3
1	A	207	SER	3.2
1	B	14	ARG	3.2
1	O	189	ARG	3.2
2	E	392	ALA	3.2
1	1	159	THR	3.2
2	E	391	LEU	3.2
1	Y	13	MET	3.2
1	1	160	THR	3.2
1	I	205	VAL	3.2
1	K	131	GLY	3.2
1	A	231	GLN	3.2
1	S	227	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
2	R	392	ALA	3.1
1	S	191	GLY	3.1
1	K	148	ALA	3.1
2	E	426	ALA	3.1
1	A	169	GLU	3.1
1	A	163	ILE	3.1
1	S	153	PHE	3.0
1	K	10	GLU	3.0
1	I	188	LEU	3.0
1	S	160	THR	3.0
1	I	161	GLU	3.0
1	I	206	ALA	3.0
1	A	165	ASN	3.0
1	S	44	GLU	3.0
1	1	152	HIS	3.0
2	T	412	SER	2.9
1	K	161	GLU	2.9
1	W	178	THR	2.9
1	S	36	ALA	2.9
2	X	426	ALA	2.9
1	A	8	SER	2.9
1	B	227	GLY	2.9
1	M	11	GLN	2.9
1	B	10	GLU	2.9
1	1	205	VAL	2.9
1	U	171	TYR	2.9
2	C	416	SER	2.9
1	K	203	LEU	2.9
1	Q	36	ALA	2.9
1	Q	204	GLY	2.9
1	Q	203	LEU	2.9
1	F	172	ALA	2.9
1	U	169	GLU	2.8
1	B	173	GLU	2.8
1	Y	15	GLU	2.8
1	S	186	ALA	2.8
1	K	147	ILE	2.8
1	1	11	GLN	2.8
1	F	165	ASN	2.8
1	A	133	THR	2.8
1	W	48	ARG	2.8
2	L	391	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	O	153	PHE	2.8
1	S	131	GLY	2.8
1	W	165	ASN	2.8
1	D	133	THR	2.8
1	Q	131	GLY	2.8
1	D	229	ALA	2.8
1	W	135	ARG	2.8
1	1	203	LEU	2.8
1	S	169	GLU	2.8
1	O	231	GLN	2.7
1	Q	10	GLU	2.7
1	1	161	GLU	2.7
1	I	10	GLU	2.7
1	W	14	ARG	2.7
1	Q	169	GLU	2.7
1	W	228	SER	2.7
1	W	231	GLN	2.7
1	A	232	ALA	2.7
1	A	53	ILE	2.7
1	F	10	GLU	2.7
1	S	161	GLU	2.7
1	K	188	LEU	2.7
1	U	228	SER	2.7
1	W	162	PRO	2.7
1	K	206	ALA	2.7
1	S	10	GLU	2.7
1	Y	172	ALA	2.7
1	S	135	ARG	2.7
1	W	46	PRO	2.7
2	C	412	SER	2.7
1	I	26	ARG	2.6
1	U	173	GLU	2.6
1	W	15	GLU	2.6
1	B	228	SER	2.6
1	F	133	THR	2.6
1	D	179	ASP	2.6
1	B	171	TYR	2.6
1	I	182	ARG	2.6
1	S	15	GLU	2.6
1	A	203	LEU	2.6
2	P	391	LEU	2.6
2	J	412	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	161	GLU	2.6
1	W	182	ARG	2.6
1	K	130	TYR	2.6
1	1	231	GLN	2.6
1	I	189	ARG	2.6
1	O	165	ASN	2.6
1	A	171	TYR	2.6
1	S	231	GLN	2.6
2	2	391	LEU	2.6
1	I	204	GLY	2.6
1	1	48	ARG	2.6
1	A	31	VAL	2.6
1	A	205	VAL	2.6
1	W	26	ARG	2.6
1	S	179	ASP	2.6
1	A	173	GLU	2.6
2	Z	392	ALA	2.6
1	D	205	VAL	2.5
1	S	182	ARG	2.5
1	M	46	PRO	2.5
1	M	231	GLN	2.5
1	I	184	ALA	2.5
1	W	12	ALA	2.5
1	Y	161	GLU	2.5
1	Y	228	SER	2.5
1	1	228	SER	2.5
2	J	399	LEU	2.5
1	A	11	GLN	2.5
2	C	425	ALA	2.5
1	M	228	SER	2.5
1	S	159	THR	2.5
2	T	426	ALA	2.5
1	U	131	GLY	2.5
1	S	28	LYS	2.5
1	A	48	ARG	2.5
1	W	207	SER	2.5
1	M	234	LEU	2.5
1	W	233	LEU	2.5
1	B	152	HIS	2.5
1	S	171	TYR	2.5
1	A	135	ARG	2.5
2	C	392	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	V	392	ALA	2.5
2	X	400	ALA	2.5
1	Q	8	SER	2.5
1	U	233	LEU	2.5
1	W	188	LEU	2.5
1	I	135	ARG	2.5
1	Q	168	LYS	2.4
1	Y	135	ARG	2.4
1	D	160	THR	2.4
1	S	12	ALA	2.4
2	P	426	ALA	2.4
1	F	162	PRO	2.4
1	O	10	GLU	2.4
1	K	149	ASP	2.4
1	A	28	LYS	2.4
1	1	163	ILE	2.4
1	I	15	GLU	2.4
2	P	399	LEU	2.4
1	K	135	ARG	2.4
2	P	392	ALA	2.4
2	2	425	ALA	2.4
1	M	161	GLU	2.4
2	V	389	GLY	2.4
1	M	179	ASP	2.4
2	H	412	SER	2.4
2	V	425	ALA	2.4
1	O	48	ARG	2.4
2	2	412	SER	2.4
1	M	44	GLU	2.4
1	Y	22	LYS	2.3
1	D	21	ARG	2.3
1	D	37	GLY	2.3
1	F	14	ARG	2.3
1	I	191	GLY	2.3
1	1	9	PRO	2.3
1	D	161	GLU	2.3
1	Q	113	GLU	2.3
1	S	133	THR	2.3
1	B	190	ALA	2.3
1	S	27	ALA	2.3
2	G	392	ALA	2.3
1	K	165	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	U	227	GLY	2.3
1	D	49	SER	2.3
1	F	161	GLU	2.3
1	Y	233	LEU	2.3
1	A	162	PRO	2.3
2	J	391	LEU	2.3
1	Q	189	ARG	2.3
1	A	190	ALA	2.2
1	D	11	GLN	2.2
1	Y	207	SER	2.2
1	B	230	LEU	2.2
1	A	159	THR	2.2
1	K	31	VAL	2.2
1	K	189	ARG	2.2
1	Y	111	PHE	2.2
1	Y	189	ARG	2.2
1	M	12	ALA	2.2
1	K	152	HIS	2.2
1	Y	149	ASP	2.2
2	C	391	LEU	2.2
1	I	231	GLN	2.2
1	A	130	TYR	2.2
1	I	190	ALA	2.2
1	S	165	ASN	2.2
1	A	182	ARG	2.2
1	K	204	GLY	2.2
1	W	23	GLY	2.2
1	Y	204	GLY	2.2
1	A	177	LEU	2.2
1	D	234	LEU	2.2
2	V	391	LEU	2.2
1	I	133	THR	2.2
1	1	178	THR	2.2
1	Y	168	LYS	2.2
1	1	135	ARG	2.2
1	O	173	GLU	2.2
2	P	401	LEU	2.2
1	A	180	ALA	2.2
1	S	13	MET	2.2
1	F	173	GLU	2.2
1	Q	44	GLU	2.2
1	W	203	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	T	399	LEU	2.2
1	U	46	PRO	2.2
1	U	11	GLN	2.1
1	A	189	ARG	2.1
1	O	135	ARG	2.1
1	A	188	LEU	2.1
1	D	188	LEU	2.1
1	I	177	LEU	2.1
1	S	233	LEU	2.1
2	P	390	ASN	2.1
1	D	152	HIS	2.1
1	M	172	ALA	2.1
1	1	172	ALA	2.1
1	D	130	TYR	2.1
1	K	26	ARG	2.1
1	M	163	ILE	2.1
1	F	203	LEU	2.1
1	W	153	PHE	2.1
1	Y	19	LEU	2.1
1	F	11	GLN	2.1
1	O	131	GLY	2.1
1	K	228	SER	2.1
1	1	206	ALA	2.1
1	I	163	ILE	2.1
1	1	233	LEU	2.1
1	A	228	SER	2.1
1	B	8	SER	2.1
2	E	425	ALA	2.1
1	U	15	GLU	2.1
1	M	7	ILE	2.1
1	B	48	ARG	2.1
1	S	152	HIS	2.1
1	F	36	ALA	2.1
1	Y	205	VAL	2.1
1	Y	139	TYR	2.1
1	Y	147	ILE	2.1
2	X	412	SER	2.1
1	K	22	LYS	2.1
1	Y	16	ARG	2.1
1	D	46	PRO	2.1
1	I	37	GLY	2.0
1	U	152	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	Y	227	GLY	2.0
2	N	414	PRO	2.0
1	B	179	ASP	2.0
1	A	179	ASP	2.0
1	S	177	LEU	2.0
2	C	415	GLN	2.0
1	Q	182	ARG	2.0
1	Y	113	GLU	2.0
1	1	10	GLU	2.0
1	D	164	ALA	2.0
1	B	31	VAL	2.0
1	D	51	GLN	2.0
2	Z	412	SER	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	OZT	L	301	9/10	0.92	0.13	-	25,29,34,35	0
2	OZT	Z	301	9/10	0.95	0.12	-	25,28,32,33	0
2	OZT	X	301	9/10	0.92	0.14	-	28,31,35,36	0
2	OZT	R	301	9/10	0.87	0.20	-	23,29,35,38	0
2	OZT	C	301	9/10	0.91	0.15	-	19,28,34,37	0
2	OZT	V	301	9/10	0.90	0.15	-	23,30,35,36	0
2	OZT	E	301	9/10	0.94	0.13	-	25,31,33,36	0
2	OZT	P	301	9/10	0.92	0.15	-	25,29,34,39	0
2	OZT	2	301	9/10	0.91	0.16	-	23,30,34,35	0
2	OZT	J	301	9/10	0.92	0.16	-	24,30,34,38	0
2	OZT	T	301	9/10	0.96	0.11	-	26,29,32,34	0
2	OZT	N	301	9/10	0.92	0.13	-	23,28,35,38	0
2	OZT	H	301	9/10	0.94	0.12	-	24,30,33,33	0
2	OZT	G	301	9/10	0.96	0.11	-	24,30,34,37	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	DMF	H	31	5/5	0.61	0.55	24.02	64,66,68,68	0
3	DMF	N	36	5/5	0.80	0.31	22.52	50,53,54,57	0
3	DMF	G	20	5/5	0.75	0.35	22.09	46,50,51,53	0
3	DMF	E	32	5/5	0.72	0.43	21.62	60,62,63,65	0
3	DMF	C	15	5/5	0.88	0.29	21.21	51,53,54,56	0
3	DMF	D	252	5/5	0.60	0.33	18.14	50,50,54,55	0
3	DMF	R	89	5/5	0.88	0.26	17.74	52,53,53,54	0
3	DMF	H	41	5/5	0.84	0.27	15.99	62,63,63,64	0
3	DMF	K	250	5/5	0.84	0.29	15.53	59,61,62,63	0
3	DMF	L	9	5/5	0.88	0.28	15.07	61,63,64,65	0
3	DMF	O	250	5/5	0.81	0.32	14.44	59,60,60,61	0
3	DMF	J	82	5/5	0.80	0.30	14.08	50,52,54,57	0
3	DMF	G	39	5/5	0.70	0.31	13.68	55,57,59,60	0
3	DMF	P	74	5/5	0.90	0.30	12.50	72,73,74,74	0
3	DMF	2	66	5/5	0.79	0.33	12.35	69,70,70,71	0
3	DMF	A	250	5/5	0.82	0.24	12.00	52,54,56,59	0
3	DMF	S	250	5/5	0.75	0.28	11.87	48,49,51,51	0
3	DMF	U	251	5/5	0.87	0.22	10.31	45,45,46,48	0
3	DMF	R	54	5/5	0.77	0.32	10.16	46,48,49,51	0
3	DMF	V	65	5/5	0.81	0.27	9.88	60,60,61,61	0
3	DMF	T	35	5/5	0.58	0.37	9.48	75,75,76,77	0
3	DMF	S	249	5/5	0.76	0.33	9.37	63,64,65,66	0
3	DMF	Z	91	5/5	0.91	0.24	9.06	54,55,55,56	0
3	DMF	V	86	5/5	0.93	0.23	8.85	44,44,45,48	0
3	DMF	T	62	5/5	0.84	0.30	8.02	56,58,58,60	0
3	DMF	X	25	5/5	0.86	0.24	7.56	47,49,50,51	0
3	DMF	R	68	5/5	0.90	0.23	7.49	53,56,57,57	0
3	DMF	Z	71	5/5	0.92	0.26	7.40	52,52,54,56	0
3	DMF	G	1	5/5	0.93	0.24	7.30	38,42,43,46	0
3	DMF	B	250	5/5	0.82	0.19	7.27	39,39,43,45	0
3	DMF	X	88	5/5	0.88	0.24	7.17	46,48,50,51	0
3	DMF	1	251	5/5	0.83	0.26	7.11	45,48,49,49	0
3	DMF	Z	50	5/5	0.91	0.21	6.87	48,49,50,52	0
3	DMF	Q	250	5/5	0.73	0.32	6.87	69,70,70,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	DMF	W	250	5/5	0.70	0.35	6.33	61,62,64,64	0
3	DMF	N	21	5/5	0.90	0.26	6.29	75,76,76,76	0
3	DMF	P	100	5/5	0.86	0.23	6.29	53,54,54,55	0
3	DMF	N	97	5/5	0.83	0.27	6.29	31,36,38,38	0
3	DMF	E	44	5/5	0.93	0.19	6.16	42,44,46,46	0
3	DMF	E	83	5/5	0.90	0.24	5.90	64,65,65,66	0
3	DMF	E	70	5/5	0.90	0.26	5.80	77,77,78,78	0
3	DMF	S	251	5/5	0.87	0.21	5.56	69,70,70,70	0
3	DMF	T	46	5/5	0.94	0.18	5.36	45,46,47,48	0
3	DMF	2	78	5/5	0.89	0.20	5.32	43,44,46,48	0
3	DMF	G	96	5/5	0.80	0.29	5.18	79,80,80,81	0
3	DMF	H	102	5/5	0.90	0.27	5.14	73,73,74,74	0
3	DMF	D	251	5/5	0.81	0.27	5.11	51,53,54,56	0
3	DMF	C	48	5/5	0.76	0.31	4.70	68,69,70,70	0
3	DMF	F	250	5/5	0.70	0.28	4.63	68,69,71,71	0
3	DMF	T	94	5/5	0.68	0.45	4.46	104,104,104,104	0
3	DMF	D	250	5/5	0.90	0.25	4.35	67,67,67,68	0
3	DMF	B	249	5/5	0.91	0.23	4.28	49,52,53,55	0
3	DMF	U	249	5/5	0.94	0.22	4.08	46,47,48,49	0
3	DMF	D	249	5/5	0.56	0.45	4.08	83,83,84,84	0
3	DMF	M	250	5/5	0.92	0.19	3.78	35,37,37,38	0
3	DMF	T	92	5/5	0.90	0.29	3.72	41,44,45,46	0
3	DMF	J	6	5/5	0.93	0.23	3.47	53,54,55,57	0
3	DMF	N	99	5/5	0.78	0.25	3.45	50,52,53,54	0
3	DMF	B	251	5/5	0.74	0.27	3.44	61,64,64,64	0
3	DMF	V	90	5/5	0.92	0.20	3.41	66,66,68,71	0
3	DMF	O	249	5/5	0.89	0.21	3.40	42,46,47,49	0
3	DMF	F	249	5/5	0.88	0.27	3.27	55,55,56,56	0
3	DMF	C	73	5/5	0.87	0.24	3.26	53,54,54,55	0
3	DMF	N	24	5/5	0.93	0.15	3.25	41,42,44,46	0
3	DMF	1	249	5/5	0.92	0.19	3.09	56,57,58,59	0
3	DMF	C	43	5/5	0.77	0.25	3.04	57,57,59,59	0
3	DMF	I	249	5/5	0.92	0.19	2.97	42,43,44,45	0
3	DMF	1	250	5/5	0.83	0.20	2.92	60,60,61,61	0
3	DMF	C	5	5/5	0.85	0.33	2.87	77,77,78,78	0
3	DMF	L	60	5/5	0.89	0.22	2.86	57,57,58,59	0
3	DMF	W	249	5/5	0.86	0.26	2.84	77,77,78,78	0
3	DMF	C	17	5/5	0.90	0.17	2.49	37,38,41,42	0
3	DMF	M	249	5/5	0.94	0.17	2.31	43,43,44,46	0
3	DMF	N	37	5/5	0.87	0.29	2.25	63,64,65,67	0
3	DMF	L	4	5/5	0.94	0.13	2.20	47,47,47,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	DMF	H	53	5/5	0.93	0.21	2.07	63,64,65,65	0
3	DMF	Y	249	5/5	0.85	0.20	2.05	58,59,61,62	0
3	DMF	E	95	5/5	0.82	0.26	2.03	46,49,51,55	0
3	DMF	P	85	5/5	0.91	0.23	1.99	52,53,54,54	0
3	DMF	U	252	5/5	0.89	0.19	1.88	60,60,61,61	0
3	DMF	I	250	5/5	0.92	0.15	1.82	48,51,51,52	0
3	DMF	Q	249	5/5	0.93	0.21	1.80	52,52,53,54	0
3	DMF	V	16	5/5	0.92	0.23	1.69	48,50,51,52	0
3	DMF	J	59	5/5	0.96	0.16	1.24	65,65,66,66	0
3	DMF	A	249	5/5	0.94	0.15	1.23	54,55,55,56	0
3	DMF	E	55	5/5	0.97	0.16	1.08	41,41,42,42	0
3	DMF	K	249	5/5	0.93	0.17	1.06	37,40,41,41	0
3	DMF	Z	79	5/5	0.93	0.18	1.06	38,38,39,40	0
3	DMF	U	250	5/5	0.89	0.14	-0.49	71,71,72,72	0
3	DMF	Z	27	5/5	0.84	0.34	-	57,62,64,65	0
3	DMF	C	64	5/5	0.90	0.26	-	60,60,60,61	0
3	DMF	H	14	5/5	0.92	0.24	-	63,63,64,64	0
3	DMF	R	3	5/5	0.83	0.33	-	63,63,65,65	0
3	DMF	X	67	5/5	0.83	0.25	-	58,59,60,60	0
3	DMF	P	61	5/5	0.83	0.27	-	58,59,61,62	0
3	DMF	2	58	5/5	0.73	0.38	-	60,62,64,64	0
3	DMF	C	28	5/5	0.91	0.21	-	53,54,56,57	0
3	DMF	H	52	5/5	0.87	0.27	-	65,66,66,67	0
3	DMF	H	19	5/5	0.85	0.27	-	52,53,55,58	0
3	DMF	Z	69	5/5	0.90	0.28	-	69,70,71,71	0
3	DMF	P	23	5/5	0.91	0.31	-	60,60,61,63	0
3	DMF	N	2	5/5	0.92	0.23	-	44,45,48,50	0

6.5 Other polymers (i)

There are no such residues in this entry.