



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:27 AM UTC

PDB ID : 3H6F / pdb_00003h6f
Title : Crystal Structure of Mycobacterium Tuberculosis Proteasome Modified by inhibitor HT1171
Authors : Li, D.; Li, H.; Lin, G.
Deposited on : 2009-04-23
Resolution : 2.51 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

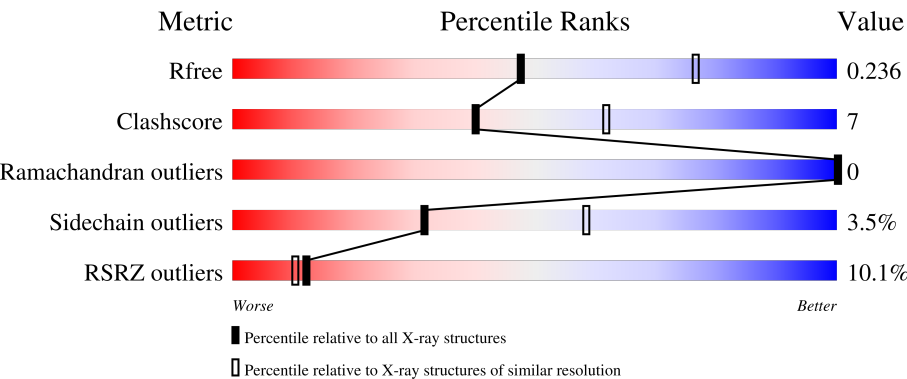
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.51 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	1	248	14% 74% 11% • 13%
1	A	248	13% 72% 13% • 13%
1	B	248	19% 76% 9% • 14%
1	D	248	15% 72% 13% • 14%
1	F	248	16% 76% 10% • 13%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DMF	2	49	-	-	-	X
3	DMF	C	55	-	-	X	-
3	DMF	J	4	-	-	X	-
3	DMF	P	14	-	-	-	X
3	DMF	T	29	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 47697 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	215	Total	C	N	O	S	0	0	0
			1656	1038	303	312	3			
1	B	214	Total	C	N	O	S	0	0	0
			1650	1033	302	312	3			
1	D	214	Total	C	N	O	S	0	0	0
			1648	1032	302	311	3			
1	F	216	Total	C	N	O	S	0	0	0
			1662	1041	304	314	3			
1	I	214	Total	C	N	O	S	0	0	0
			1652	1036	302	311	3			
1	K	215	Total	C	N	O	S	0	0	0
			1656	1038	303	312	3			
1	M	215	Total	C	N	O	S	0	0	0
			1658	1039	303	313	3			
1	O	215	Total	C	N	O	S	0	0	0
			1654	1035	303	313	3			
1	Q	217	Total	C	N	O	S	0	0	0
			1670	1047	305	315	3			
1	S	215	Total	C	N	O	S	0	0	0
			1654	1035	303	313	3			
1	U	214	Total	C	N	O	S	0	0	0
			1650	1033	302	312	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 1593	C 998	N 274	O 317	S 4	0	0	0
2	E	216	Total 1601	C 1004	N 275	O 318	S 4	0	0	0
2	G	216	Total 1601	C 1004	N 275	O 318	S 4	0	0	0
2	H	213	Total 1583	C 992	N 272	O 315	S 4	0	0	0
2	J	216	Total 1601	C 1004	N 275	O 318	S 4	0	0	0
2	L	216	Total 1601	C 1004	N 275	O 318	S 4	0	0	0
2	N	213	Total 1580	C 989	N 272	O 315	S 4	0	0	0
2	P	216	Total 1601	C 1004	N 275	O 318	S 4	0	0	0
2	R	223	Total 1646	C 1031	N 282	O 329	S 4	0	0	0
2	T	216	Total 1601	C 1004	N 275	O 318	S 4	0	0	0
2	V	222	Total 1638	C 1025	N 281	O 328	S 4	0	0	0
2	X	216	Total 1601	C 1004	N 275	O 318	S 4	0	0	0
2	Z	215	Total 1593	C 998	N 274	O 317	S 4	0	0	0
2	2	215	Total 1593	C 998	N 274	O 317	S 4	0	0	0

There are 98 discrepancies between the modelled and reference sequences:

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

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

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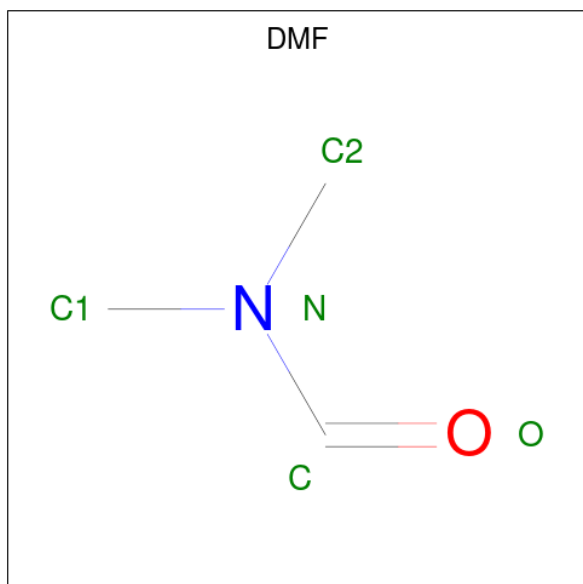
Chain	Residue	Modelled	Actual	Comment	Reference
P	539	HIS	-	expression tag	UNP O33245
P	540	HIS	-	expression tag	UNP O33245
R	301	OZT	-	insertion	UNP O33245
R	535	HIS	-	expression tag	UNP O33245
R	536	HIS	-	expression tag	UNP O33245
R	537	HIS	-	expression tag	UNP O33245
R	538	HIS	-	expression tag	UNP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

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

- Molecule 3 is DIMETHYLFORMAMIDE (CCD ID: DMF) (formula: C_3H_7NO).



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

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

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total	O	0	0
			34	34		
4	B	40	Total	O	0	0
			40	40		
4	C	95	Total	O	0	0
			95	95		
4	D	49	Total	O	0	0
			49	49		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	89	Total 89	O 89	0	0
4	F	40	Total 40	O 40	0	0
4	G	72	Total 72	O 72	0	0
4	H	91	Total 91	O 91	0	0
4	I	38	Total 38	O 38	0	0
4	J	90	Total 90	O 90	0	0
4	K	39	Total 39	O 39	0	0
4	L	90	Total 90	O 90	0	0
4	M	42	Total 42	O 42	0	0
4	N	86	Total 86	O 86	0	0
4	O	40	Total 40	O 40	0	0
4	P	82	Total 82	O 82	0	0
4	Q	34	Total 34	O 34	0	0
4	R	97	Total 97	O 97	0	0
4	S	34	Total 34	O 34	0	0
4	T	78	Total 78	O 78	0	0
4	U	38	Total 38	O 38	0	0
4	V	104	Total 104	O 104	0	0
4	W	27	Total 27	O 27	0	0
4	X	84	Total 84	O 84	0	0
4	Y	24	Total 24	O 24	0	0

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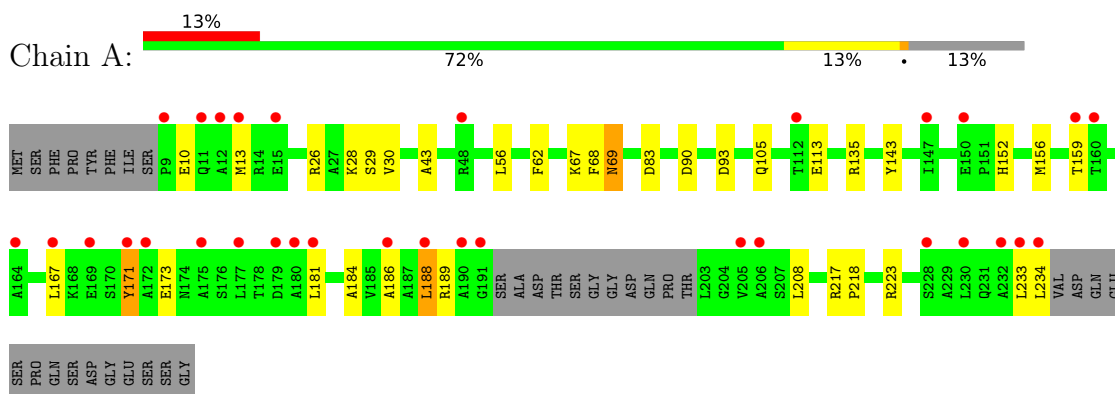
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Z	85	Total 85	O 85	0	0
4	1	34	Total 34	O 34	0	0
4	2	93	Total 93	O 93	0	0

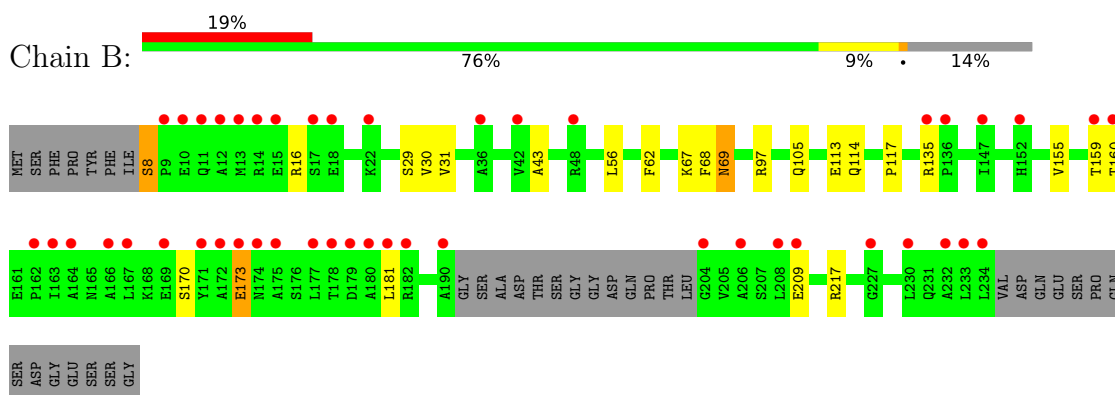
3 Residue-property plots [i](#)

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

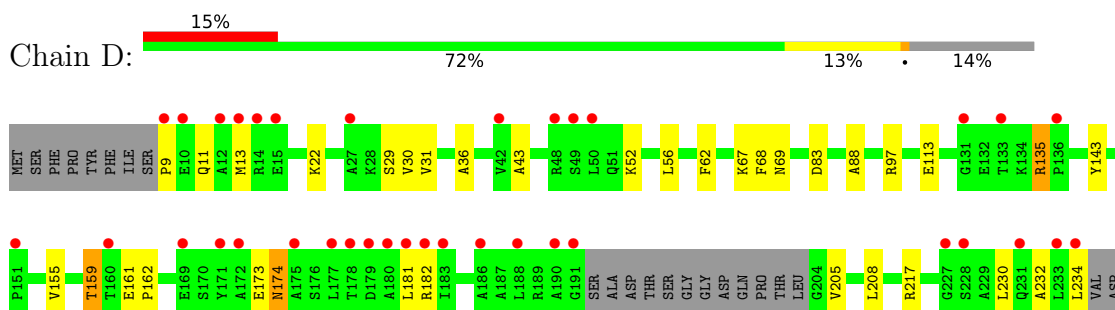
• Molecule 1: Proteasome (Alpha subunit) PrcA



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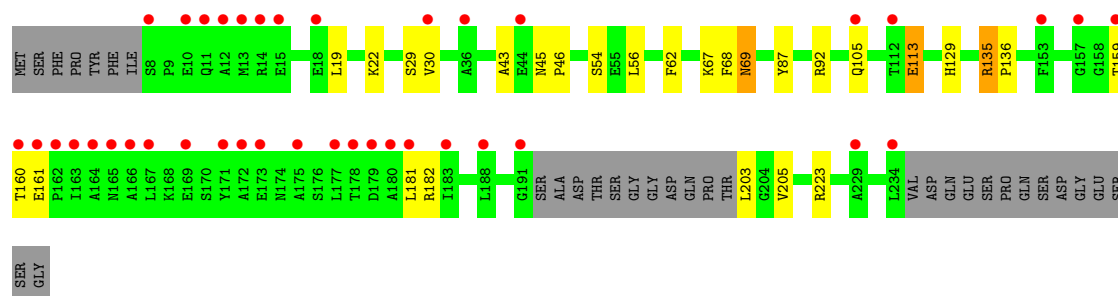
• Molecule 1: Proteasome (Alpha subunit) PrcA



GLN
GLU
SER
PRO
GLN
SER
ASP
GLY
SER
SER
GLY

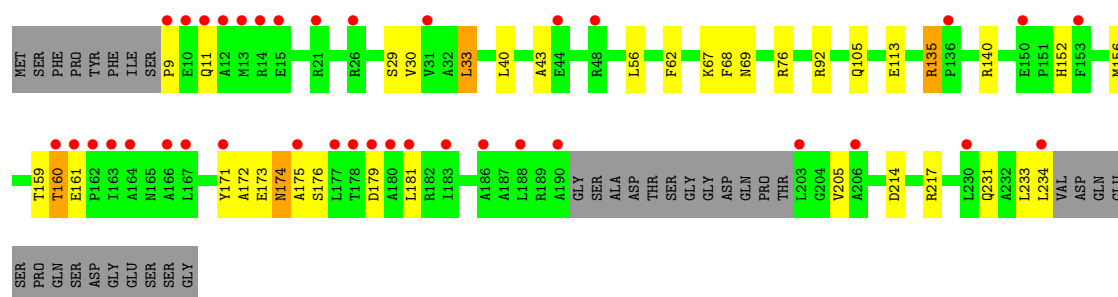
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain F: 16% 76% 10% 13%



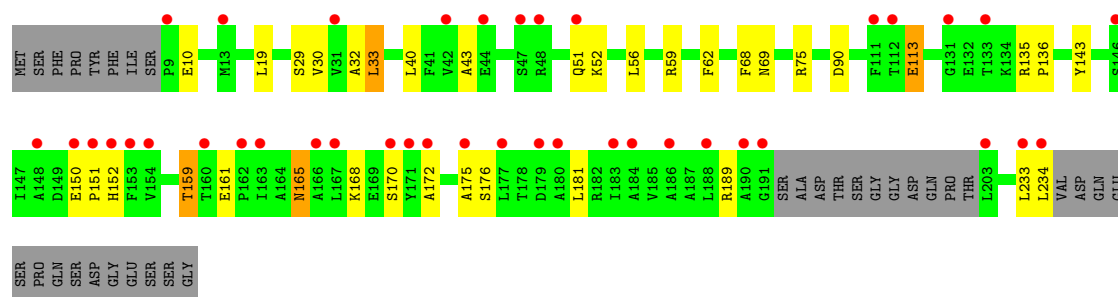
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain I: 15% 71% 13% 14%



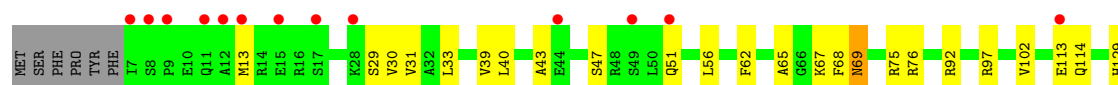
• Molecule 1: Proteasome (Alpha subunit) PrcA

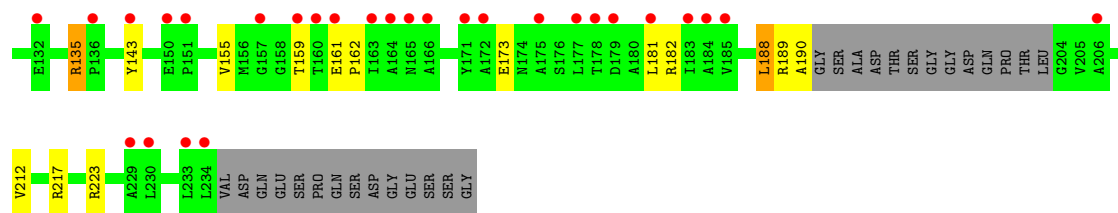
Chain K: 16% 72% 13% 13%



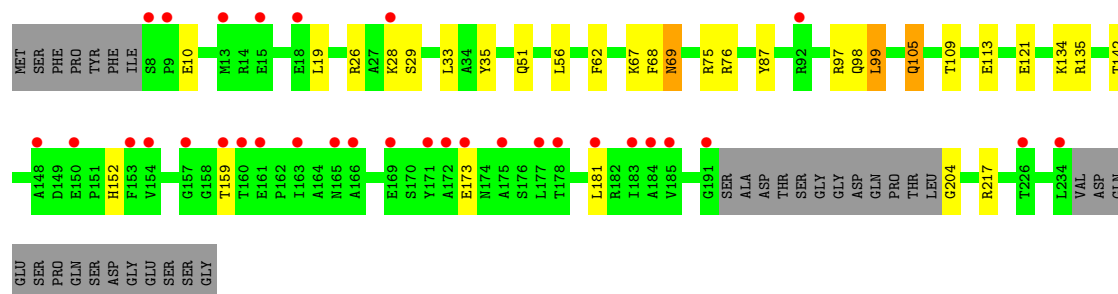
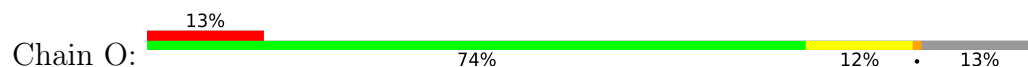
• Molecule 1: Proteasome (Alpha subunit) PrcA

Chain M: 17% 71% 15% 13%

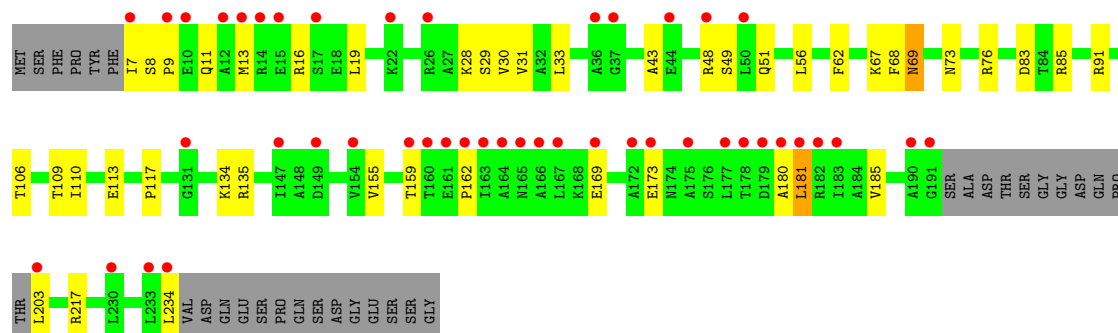




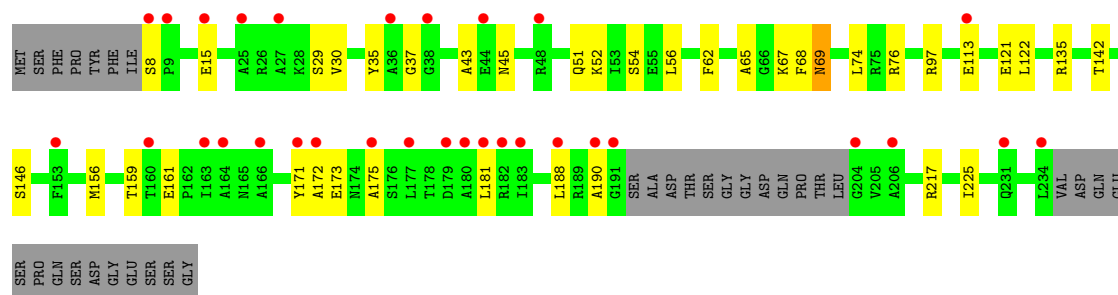
• Molecule 1: Proteasome (Alpha subunit) PrcA



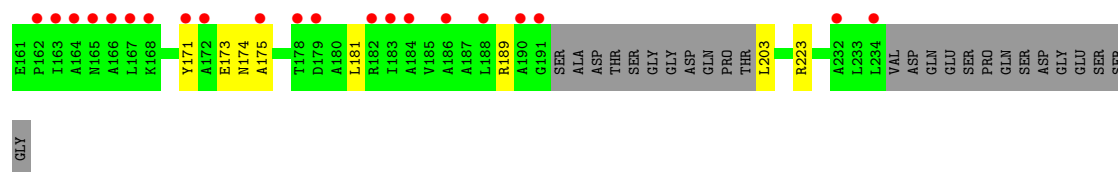
• Molecule 1: Proteasome (Alpha subunit) PrcA



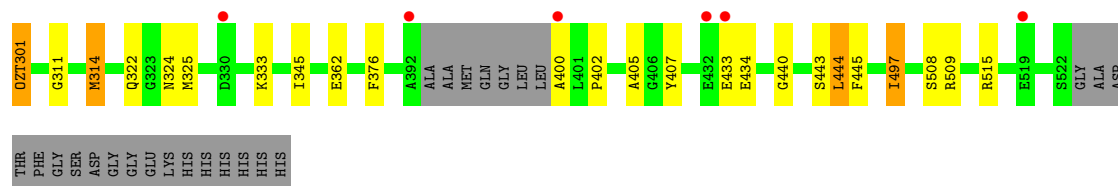
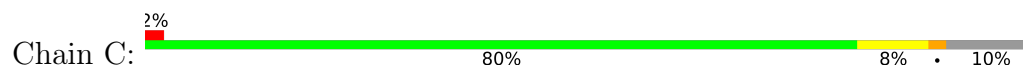
• Molecule 1: Proteasome (Alpha subunit) PrcA



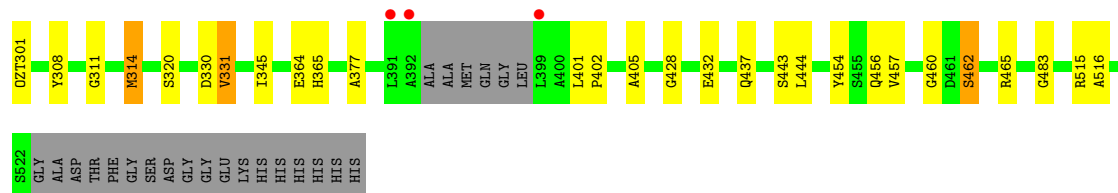
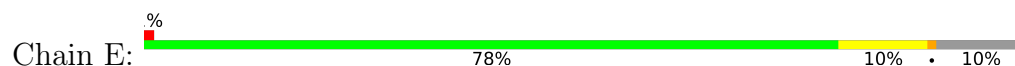
• Molecule 1: Proteasome (Alpha subunit) PrcA



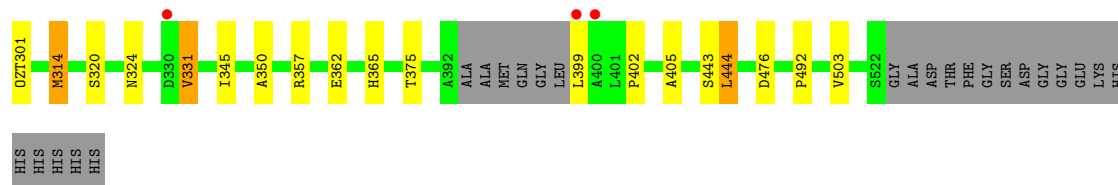
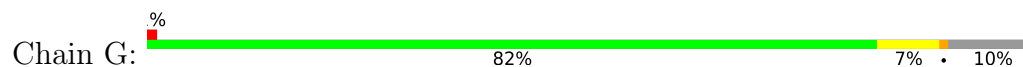
• Molecule 2: Proteasome (Beta subunit) PrcB



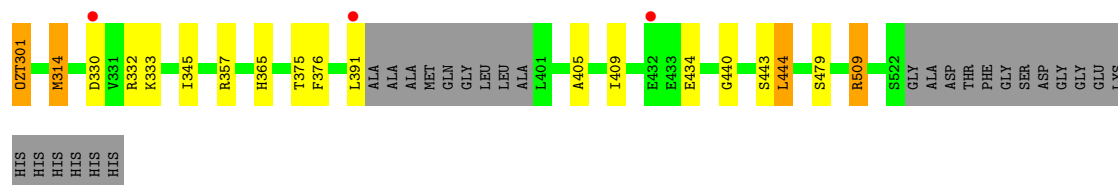
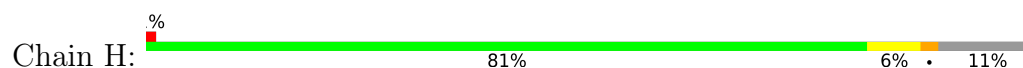
• Molecule 2: Proteasome (Beta subunit) PrcB



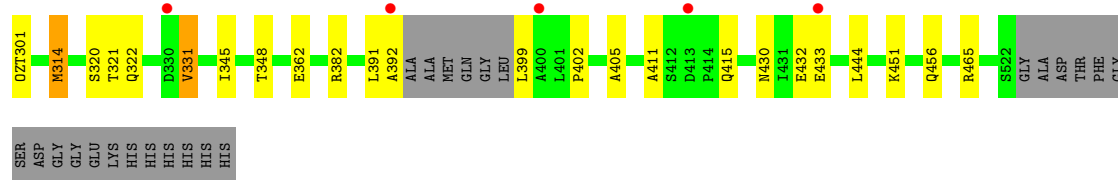
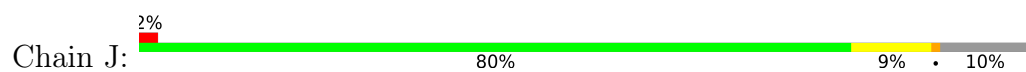
• Molecule 2: Proteasome (Beta subunit) PrcB



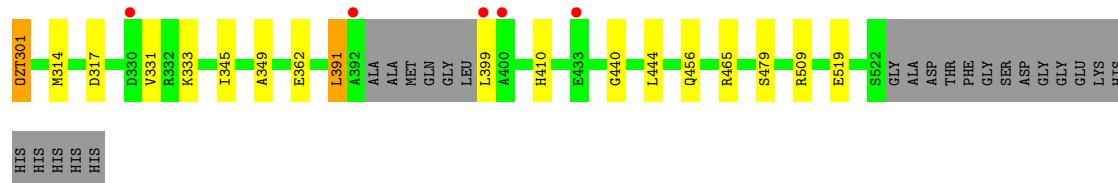
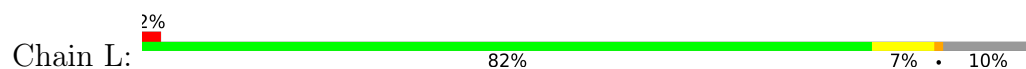
• Molecule 2: Proteasome (Beta subunit) PrcB



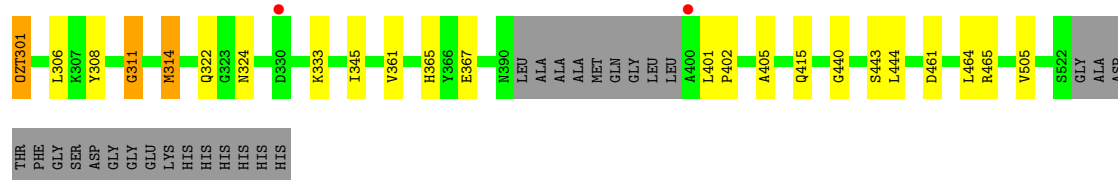
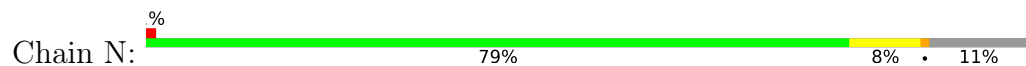
• Molecule 2: Proteasome (Beta subunit) PrcB



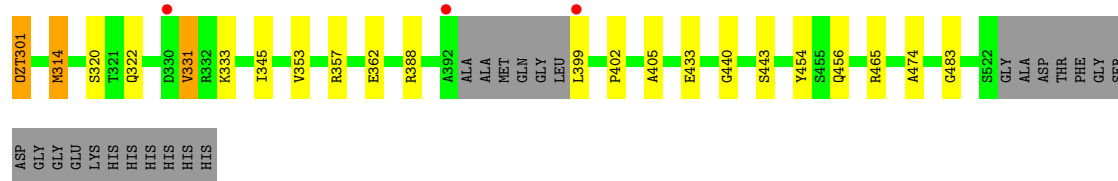
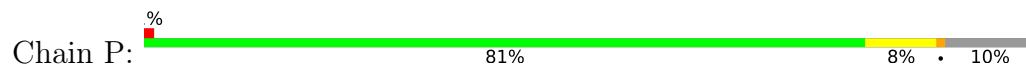
• Molecule 2: Proteasome (Beta subunit) PrcB



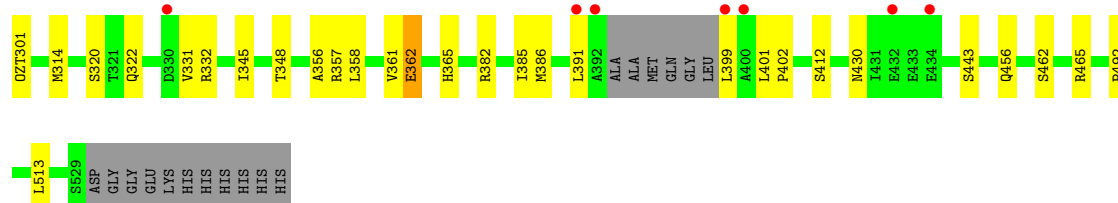
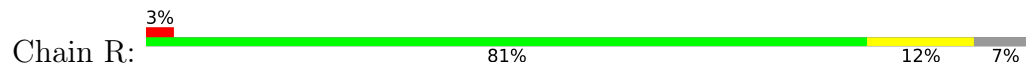
• Molecule 2: Proteasome (Beta subunit) PrcB



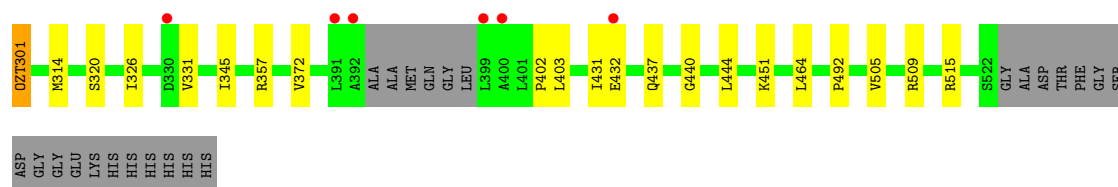
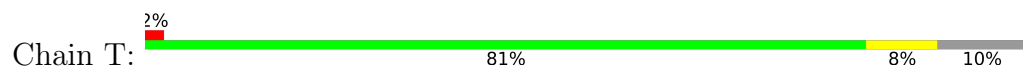
• Molecule 2: Proteasome (Beta subunit) PrcB



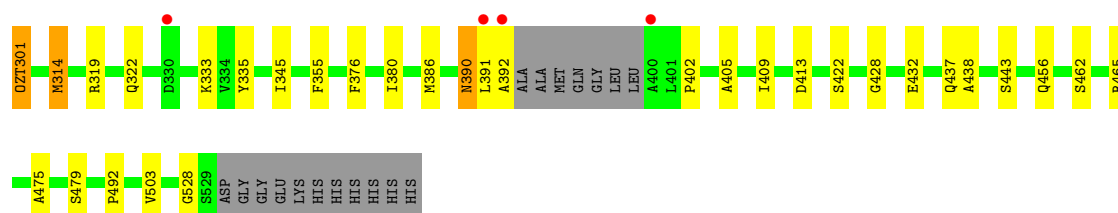
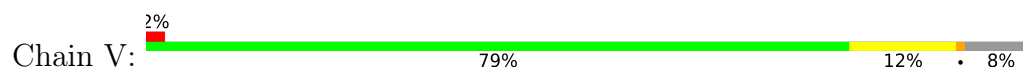
• Molecule 2: Proteasome (Beta subunit) PrcB



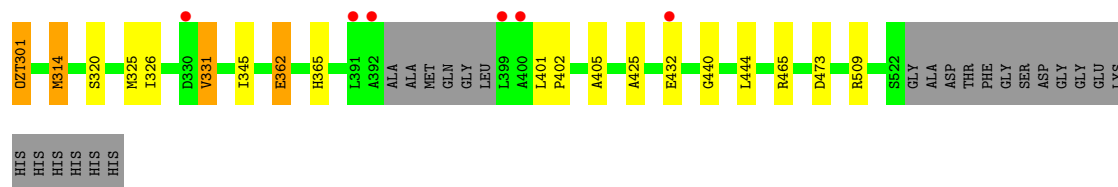
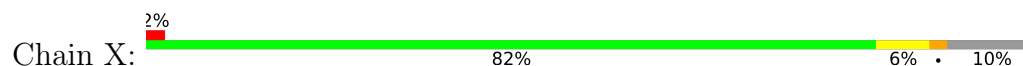
- Molecule 2: Proteasome (Beta subunit) PrcB



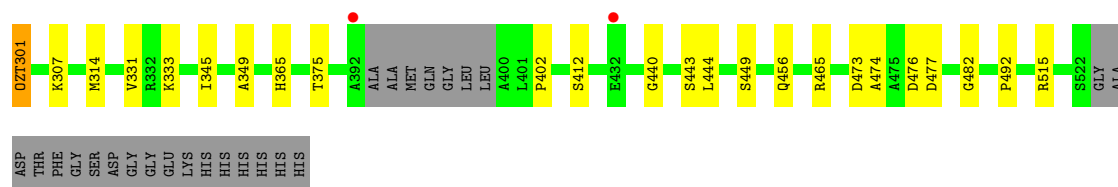
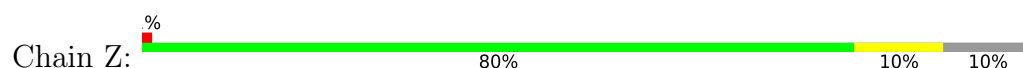
- Molecule 2: Proteasome (Beta subunit) PrcB



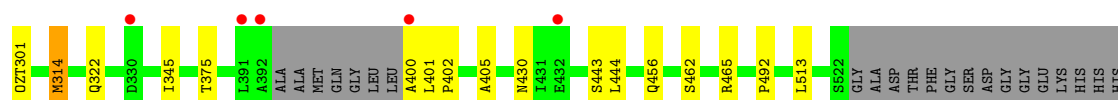
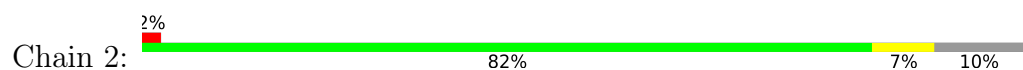
- Molecule 2: Proteasome (Beta subunit) PrcB



- Molecule 2: Proteasome (Beta subunit) PrcB



- Molecule 2: Proteasome (Beta subunit) PrcB



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HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	171.98Å 118.04Å 197.06Å 90.00° 113.62° 90.00°	Depositor
Resolution (Å)	29.83 – 2.51 29.83 – 2.51	Depositor EDS
% Data completeness (in resolution range)	94.2 (29.83-2.51) 94.5 (29.83-2.51)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.216 , 0.238 0.216 , 0.236	Depositor DCC
R_{free} test set	11735 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	47697	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.72	0/1681	1.16	8/2270 (0.4%)
1	A	0.76	0/1681	1.11	7/2270 (0.3%)
1	B	0.69	0/1675	1.13	7/2263 (0.3%)
1	D	0.71	0/1673	1.12	5/2259 (0.2%)
1	F	0.72	0/1687	1.09	5/2279 (0.2%)
1	I	0.78	3/1677 (0.2%)	1.15	8/2265 (0.4%)
1	K	0.72	2/1681 (0.1%)	1.10	5/2270 (0.2%)
1	M	0.76	0/1683	1.15	9/2274 (0.4%)
1	O	0.84	0/1679	1.10	5/2268 (0.2%)
1	Q	0.72	0/1695	1.09	4/2290 (0.2%)
1	S	0.67	0/1679	1.10	5/2268 (0.2%)
1	U	0.86	0/1675	1.08	6/2263 (0.3%)
1	W	0.68	0/1695	1.11	6/2290 (0.3%)
1	Y	0.68	0/1669	1.13	8/2254 (0.4%)
2	2	0.87	1/1607 (0.1%)	1.03	2/2178 (0.1%)
2	C	0.91	2/1607 (0.1%)	1.06	5/2178 (0.2%)
2	E	0.97	3/1615 (0.2%)	1.09	6/2189 (0.3%)
2	G	0.80	1/1615 (0.1%)	1.05	4/2189 (0.2%)
2	H	0.83	1/1597 (0.1%)	1.06	2/2164 (0.1%)
2	J	0.90	1/1615 (0.1%)	1.03	2/2189 (0.1%)
2	L	0.90	1/1615 (0.1%)	1.07	0/2189
2	N	0.88	1/1594 (0.1%)	1.05	3/2160 (0.1%)
2	P	0.88	3/1615 (0.2%)	1.05	4/2189 (0.2%)
2	R	0.94	1/1661 (0.1%)	1.07	4/2251 (0.2%)
2	T	0.96	3/1615 (0.2%)	1.08	2/2189 (0.1%)
2	V	0.92	2/1653 (0.1%)	1.07	7/2240 (0.3%)
2	X	0.87	2/1615 (0.1%)	1.04	1/2189 (0.0%)
2	Z	0.93	3/1607 (0.2%)	1.07	4/2178 (0.2%)
All	All	0.82	30/46161 (0.1%)	1.09	134/62455 (0.2%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	314	MET	SD-CE	-10.12	1.54	1.79
2	T	314	MET	SD-CE	-9.03	1.56	1.79
2	2	314	MET	SD-CE	-8.96	1.57	1.79
2	R	314	MET	SD-CE	-8.91	1.57	1.79
2	V	314	MET	SD-CE	-8.67	1.57	1.79
1	K	165	ASN	C-N	-8.19	1.22	1.33
2	E	314	MET	SD-CE	-8.13	1.59	1.79
2	N	314	MET	SD-CE	-7.81	1.60	1.79
2	H	314	MET	SD-CE	-7.78	1.60	1.79
2	X	314	MET	SD-CE	-7.70	1.60	1.79
2	E	516	ALA	CA-CB	-7.68	1.40	1.53
2	Z	314	MET	SD-CE	-7.61	1.60	1.79
2	C	314	MET	SD-CE	-7.09	1.61	1.79
2	L	314	MET	SD-CE	-6.69	1.62	1.79
1	I	172	ALA	CA-CB	-6.51	1.41	1.53
2	G	314	MET	SD-CE	-6.15	1.64	1.79
1	I	175	ALA	CA-CB	-5.90	1.44	1.53
2	P	314	MET	SD-CE	-5.72	1.65	1.79
1	K	176	SER	C-N	-5.56	1.26	1.33
1	I	174	ASN	CA-C	-5.54	1.45	1.53
2	T	372	VAL	CA-CB	5.53	1.61	1.55
2	E	308	TYR	C-O	-5.51	1.18	1.24
2	T	326	ILE	C-O	-5.45	1.18	1.23
2	V	475	ALA	CA-CB	-5.39	1.44	1.53
2	Z	449	SER	C-O	-5.32	1.17	1.24
2	P	474	ALA	C-O	-5.21	1.18	1.24
2	P	353	VAL	CA-CB	5.15	1.61	1.54
2	X	326	ILE	C-O	-5.14	1.18	1.23
2	Z	474	ALA	C-O	-5.14	1.18	1.24
2	C	407	TYR	C-O	-5.02	1.18	1.23

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	10	GLU	N-CA-C	-12.23	98.53	114.31
1	Y	10	GLU	N-CA-C	-9.40	101.23	112.89
1	I	160	THR	N-CA-C	8.77	120.92	111.36
2	V	528	GLY	N-CA-C	8.35	124.34	112.82
1	B	173	GLU	N-CA-C	8.15	120.97	111.02
1	W	113	GLU	N-CA-C	8.13	121.69	111.69
2	P	402	PRO	N-CA-C	7.42	122.54	111.41
1	F	160	THR	N-CA-C	7.28	119.29	111.36
2	H	443	SER	N-CA-C	7.22	119.16	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	113	GLU	N-CA-C	7.09	120.05	111.40
2	R	443	SER	N-CA-C	7.08	118.99	111.28
1	I	173	GLU	N-CA-C	7.03	118.94	111.28
2	E	311	GLY	N-CA-C	7.00	120.67	110.80
1	Q	173	GLU	N-CA-C	6.87	118.42	111.07
1	A	171	TYR	N-CA-C	6.80	119.83	108.20
1	I	113	GLU	N-CA-C	6.78	120.78	112.23
1	Q	113	GLU	N-CA-C	6.71	119.94	111.69
1	K	170	SER	N-CA-C	6.69	120.42	112.93
2	R	462	SER	N-CA-C	-6.67	103.94	111.14
1	B	113	GLU	N-CA-C	6.65	121.70	112.45
2	R	402	PRO	N-CA-C	6.64	121.94	111.38
2	V	443	SER	N-CA-C	6.64	118.52	111.28
1	M	188	LEU	N-CA-C	-6.63	104.05	111.28
2	Z	402	PRO	N-CA-C	6.62	121.63	111.57
1	I	173	GLU	CA-C-N	-6.57	114.22	123.03
1	I	173	GLU	C-N-CA	-6.57	114.22	123.03
2	C	443	SER	N-CA-C	6.57	118.44	111.28
1	B	8	SER	CA-C-N	6.56	126.80	119.32
1	B	8	SER	C-N-CA	6.56	126.80	119.32
1	O	113	GLU	N-CA-C	6.55	121.55	112.45
1	1	9	PRO	CA-C-N	6.51	132.47	122.24
1	1	9	PRO	C-N-CA	6.51	132.47	122.24
1	F	113	GLU	N-CA-C	6.40	121.12	113.12
2	G	331	VAL	N-CA-C	6.37	117.52	108.93
2	C	402	PRO	N-CA-C	6.26	121.08	111.57
1	D	29	SER	N-CA-C	6.24	120.25	110.32
2	T	402	PRO	N-CA-C	6.20	120.72	111.41
1	M	173	GLU	N-CA-C	6.19	118.54	111.11
2	E	443	SER	N-CA-C	6.18	118.01	111.28
1	1	29	SER	N-CA-C	6.16	120.12	110.32
1	B	170	SER	N-CA-C	6.06	119.98	112.59
1	W	29	SER	N-CA-C	6.01	119.88	110.32
2	2	375	THR	N-CA-C	-5.99	103.04	110.41
1	O	29	SER	N-CA-C	5.97	119.82	110.32
1	M	29	SER	N-CA-C	5.95	119.78	110.32
1	S	68	PHE	N-CA-C	5.93	118.26	111.02
2	N	402	PRO	N-CA-C	5.93	120.58	111.57
1	W	170	SER	N-CA-C	5.93	120.20	113.15
1	U	29	SER	N-CA-C	5.92	119.73	110.32
1	S	29	SER	N-CA-C	5.91	119.71	110.32
1	A	113	GLU	N-CA-C	5.91	118.60	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	68	PHE	N-CA-C	5.89	118.20	111.02
2	E	402	PRO	N-CA-C	5.86	120.20	111.41
1	S	113	GLU	N-CA-C	5.84	120.57	112.45
1	A	29	SER	N-CA-C	5.82	119.57	110.32
2	R	412	SER	N-CA-C	5.81	117.61	111.28
1	K	29	SER	N-CA-C	5.81	119.56	110.32
1	U	173	GLU	N-CA-C	5.79	117.60	111.28
1	W	68	PHE	N-CA-C	5.79	118.08	111.02
1	Y	29	SER	N-CA-C	5.76	119.49	110.32
1	I	29	SER	N-CA-C	5.76	119.47	110.32
1	F	29	SER	N-CA-C	5.74	119.45	110.32
2	N	311	GLY	N-CA-C	5.71	119.47	111.19
2	J	331	VAL	N-CA-C	5.71	116.64	108.93
1	B	29	SER	N-CA-C	5.71	119.40	110.32
1	M	113	GLU	N-CA-C	5.71	120.39	112.45
1	O	217	ARG	CA-C-N	5.70	125.17	119.24
1	O	217	ARG	C-N-CA	5.70	125.17	119.24
2	P	443	SER	N-CA-C	5.65	117.44	111.28
2	V	413	ASP	CA-C-N	5.63	125.48	119.28
2	V	413	ASP	C-N-CA	5.63	125.48	119.28
1	D	68	PHE	N-CA-C	5.60	117.85	111.02
2	E	331	VAL	N-CA-C	5.58	116.21	108.84
1	U	143	TYR	N-CA-C	5.55	118.86	111.75
1	A	68	PHE	N-CA-C	5.55	117.79	111.02
2	C	311	GLY	N-CA-C	5.54	118.33	110.74
1	F	68	PHE	N-CA-C	5.51	117.74	111.02
1	A	143	TYR	N-CA-C	5.50	118.80	111.75
1	A	208	LEU	N-CA-C	5.49	118.05	108.76
1	I	68	PHE	N-CA-C	5.49	117.72	111.02
1	Q	29	SER	N-CA-C	5.45	118.99	110.32
1	O	68	PHE	N-CA-C	5.43	117.64	111.02
2	E	454	TYR	N-CA-C	5.42	117.95	111.71
1	Q	68	PHE	N-CA-C	5.42	117.63	111.02
1	M	217	ARG	CA-C-N	5.41	124.87	119.24
1	M	217	ARG	C-N-CA	5.41	124.87	119.24
1	1	173	GLU	N-CA-C	5.41	117.62	111.02
2	N	443	SER	N-CA-C	5.41	117.17	111.28
2	Z	412	SER	N-CA-C	5.41	117.17	111.28
1	1	143	TYR	N-CA-C	5.40	118.66	111.75
2	E	460	GLY	N-CA-C	5.39	119.20	112.73
1	W	143	TYR	N-CA-C	5.39	118.65	111.75
1	S	8	SER	CA-C-N	5.39	125.06	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	8	SER	C-N-CA	5.39	125.06	119.56
1	K	68	PHE	N-CA-C	5.37	117.58	111.02
1	K	143	TYR	N-CA-C	5.37	118.62	111.75
1	D	208	LEU	N-CA-C	5.37	117.55	109.23
2	G	443	SER	N-CA-C	5.36	117.82	111.33
1	F	205	VAL	N-CA-C	5.36	116.73	110.62
2	T	403	LEU	N-CA-C	-5.32	100.22	108.90
2	V	462	SER	CA-C-N	5.32	125.85	119.94
2	V	462	SER	C-N-CA	5.32	125.85	119.94
1	U	68	PHE	N-CA-C	5.31	117.50	111.02
2	J	402	PRO	N-CA-C	5.30	119.81	111.38
2	C	497	ILE	N-CA-C	5.29	115.60	107.77
1	D	113	GLU	N-CA-C	5.29	121.13	114.31
2	Z	443	SER	N-CA-C	5.29	117.04	111.28
2	V	402	PRO	N-CA-C	5.27	119.76	111.38
1	U	170	SER	N-CA-C	5.26	119.68	113.16
2	Z	375	THR	N-CA-C	-5.25	103.95	110.41
1	I	171	TYR	N-CA-C	5.24	118.15	109.46
1	Y	68	PHE	N-CA-C	5.23	117.41	111.02
2	P	454	TYR	N-CA-C	5.23	117.73	111.71
1	D	143	TYR	N-CA-C	5.22	118.43	111.75
2	C	508	SER	N-CA-C	5.21	116.95	111.28
1	M	161	GLU	N-CA-C	5.19	120.00	113.25
1	B	68	PHE	N-CA-C	5.18	117.34	111.02
1	1	33	LEU	N-CA-C	5.18	117.89	109.24
1	A	10	GLU	N-CA-C	-5.16	106.49	112.89
2	H	375	THR	N-CA-C	-5.14	103.75	110.53
1	U	160	THR	N-CA-C	5.13	116.68	111.14
2	P	331	VAL	N-CA-C	5.12	115.84	108.93
1	M	143	TYR	N-CA-C	5.11	118.29	111.75
1	W	161	GLU	N-CA-C	5.10	119.88	113.25
2	G	402	PRO	N-CA-C	5.09	119.48	111.38
1	Y	9	PRO	CA-C-N	5.09	130.05	121.14
1	Y	9	PRO	C-N-CA	5.09	130.05	121.14
1	Y	161	GLU	N-CA-C	5.08	119.86	113.25
2	2	443	SER	N-CA-C	5.05	116.79	111.28
1	Y	205	VAL	N-CA-C	5.05	115.66	110.36
1	K	113	GLU	N-CA-C	5.03	119.45	112.45
2	G	375	THR	N-CA-C	-5.03	104.22	110.41
2	X	331	VAL	N-CA-C	5.02	115.71	108.93
1	1	68	PHE	N-CA-C	5.02	117.14	111.02

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	25	0
1	A	1656	0	1658	24	0
1	B	1650	0	1648	21	0
1	D	1648	0	1647	39	0
1	F	1662	0	1662	23	0
1	I	1652	0	1655	20	0
1	K	1656	0	1658	32	0
1	M	1658	0	1659	41	0
1	O	1654	0	1651	32	0
1	Q	1670	0	1673	42	0
1	S	1654	0	1651	31	0
1	U	1650	0	1648	26	0
1	W	1670	0	1673	25	0
1	Y	1644	0	1644	38	0
2	2	1593	0	1577	12	0
2	C	1593	0	1577	16	0
2	E	1601	0	1588	16	0
2	G	1601	0	1588	10	0
2	H	1583	0	1567	16	0
2	J	1601	0	1588	18	0
2	L	1601	0	1588	9	0
2	N	1580	0	1561	14	0
2	P	1601	0	1588	12	0
2	R	1646	0	1624	21	0
2	T	1601	0	1588	10	0
2	V	1638	0	1613	23	0
2	X	1601	0	1588	16	0
2	Z	1593	0	1577	14	0
3	1	10	0	14	0	0
3	2	20	0	28	0	0
3	A	5	0	7	0	0
3	B	10	0	14	0	0
3	C	20	0	28	6	0
3	D	5	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	15	0	21	3	0
3	F	5	0	7	0	0
3	G	25	0	35	2	0
3	H	20	0	28	0	0
3	I	10	0	14	0	0
3	J	15	0	21	5	0
3	K	15	0	21	1	0
3	L	15	0	21	2	0
3	M	10	0	14	2	0
3	N	20	0	28	1	0
3	O	5	0	7	0	0
3	P	20	0	28	1	0
3	Q	5	0	7	0	0
3	R	10	0	14	2	0
3	S	5	0	7	0	0
3	T	10	0	14	4	0
3	U	5	0	7	0	0
3	V	10	0	14	1	0
3	W	5	0	7	0	0
3	X	15	0	21	1	0
3	Z	25	0	35	2	0
4	1	34	0	0	9	0
4	2	93	0	0	4	0
4	A	34	0	0	8	0
4	B	40	0	0	13	0
4	C	95	0	0	8	0
4	D	49	0	0	11	0
4	E	89	0	0	5	0
4	F	40	0	0	15	0
4	G	72	0	0	4	0
4	H	91	0	0	11	0
4	I	38	0	0	10	0
4	J	90	0	0	13	0
4	K	39	0	0	18	0
4	L	90	0	0	4	0
4	M	42	0	0	22	0
4	N	86	0	0	4	0
4	O	40	0	0	18	0
4	P	82	0	0	4	0
4	Q	34	0	0	14	0
4	R	97	0	0	5	0
4	S	34	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	T	78	0	0	9	0
4	U	38	0	0	7	0
4	V	104	0	0	4	0
4	W	27	0	0	11	0
4	X	84	0	0	10	0
4	Y	24	0	0	14	0
4	Z	85	0	0	7	0
All	All	47697	0	45866	610	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 7.

All (610) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:GLU:C	1:D:174:ASN:HD22	1.40	1.29
2:J:432:GLU:HG2	4:J:1761:HOH:O	1.37	1.21
1:I:140:ARG:HD2	4:I:1512:HOH:O	1.41	1.19
2:P:399:LEU:HD12	4:P:1556:HOH:O	1.36	1.19
2:E:432:GLU:HG2	4:E:1322:HOH:O	1.42	1.18
1:I:135:ARG:HG2	4:I:1769:HOH:O	1.39	1.17
4:A:1674:HOH:O	1:B:8:SER:HB2	1.45	1.16
1:Y:182:ARG:HD3	4:Y:1675:HOH:O	1.42	1.15
1:O:121:GLU:HG3	4:O:1391:HOH:O	1.41	1.15
2:X:401:LEU:HB2	4:X:1614:HOH:O	1.42	1.14
2:T:515:ARG:HD3	4:T:1499:HOH:O	1.44	1.14
1:Y:233:LEU:O	1:Y:234:LEU:O	1.69	1.11
1:K:168:LYS:HD2	4:K:1705:HOH:O	1.53	1.08
1:K:189:ARG:HD2	4:K:1741:HOH:O	1.51	1.08
1:W:159:THR:HB	4:W:1559:HOH:O	1.53	1.08
2:H:332:ARG:HB2	4:H:1570:HOH:O	1.53	1.07
1:U:9:PRO:HD3	4:U:1536:HOH:O	1.56	1.06
1:B:173:GLU:HG3	4:B:1646:HOH:O	1.52	1.05
2:J:399:LEU:HG	4:J:1403:HOH:O	1.54	1.04
1:Q:134:LYS:HE3	4:Q:1565:HOH:O	1.53	1.03
1:M:223:ARG:HD3	4:M:1627:HOH:O	1.60	1.01
4:F:1688:HOH:O	1:W:9:PRO:HG3	1.58	1.00
1:M:223:ARG:HG2	4:M:1631:HOH:O	1.61	1.00
2:C:400:ALA:HB2	4:C:1575:HOH:O	1.62	1.00
1:A:186:ALA:O	1:A:189:ARG:HG2	1.60	0.99
2:H:332:ARG:HD2	4:H:1570:HOH:O	1.61	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:28:LYS:HE3	4:Y:1700:HOH:O	1.61	0.99
1:D:173:GLU:C	1:D:174:ASN:ND2	2.19	0.99
1:U:92:ARG:HB2	4:U:1709:HOH:O	1.63	0.99
3:X:40:DMF:H22	4:X:1639:HOH:O	1.62	0.98
1:A:152:HIS:HB3	1:A:171:TYR:CE2	2.00	0.97
1:O:26:ARG:HG3	4:O:1474:HOH:O	1.67	0.95
2:V:456:GLN:HE21	2:V:465:ARG:HH22	1.13	0.94
1:A:26:ARG:HD3	4:A:1777:HOH:O	1.69	0.91
1:M:182:ARG:HD3	4:M:1510:HOH:O	1.68	0.91
2:J:456:GLN:HE21	2:J:465:ARG:HH22	1.18	0.89
4:M:1478:HOH:O	2:N:361:VAL:HG23	1.74	0.88
1:U:217:ARG:HD3	4:U:1532:HOH:O	1.74	0.87
4:K:1467:HOH:O	1:M:97:ARG:HD2	1.74	0.87
2:T:357:ARG:HD2	4:T:1567:HOH:O	1.72	0.87
1:O:76:ARG:HD3	4:O:1375:HOH:O	1.74	0.86
2:C:324:ASN:HB2	4:C:1648:HOH:O	1.72	0.86
2:X:465:ARG:HD2	4:X:1379:HOH:O	1.75	0.86
1:D:173:GLU:HG2	1:D:174:ASN:ND2	1.91	0.85
2:J:399:LEU:HD12	4:J:1413:HOH:O	1.75	0.85
2:2:430:ASN:HB2	4:2:1473:HOH:O	1.76	0.85
1:Y:35:TYR:CD2	1:Y:38:GLY:O	2.29	0.85
1:Y:181:LEU:HD12	1:Y:233:LEU:HD22	1.56	0.85
1:S:225:ILE:HA	4:S:1371:HOH:O	1.75	0.84
1:1:14:ARG:HA	4:1:1788:HOH:O	1.77	0.84
1:S:217:ARG:HD2	4:S:1458:HOH:O	1.76	0.84
1:M:182:ARG:HB2	4:M:1510:HOH:O	1.77	0.84
1:B:105:GLN:HG3	4:B:1554:HOH:O	1.78	0.84
1:D:173:GLU:CG	1:D:174:ASN:HD21	1.90	0.84
1:O:26:ARG:CD	4:O:1474:HOH:O	2.25	0.83
2:L:410:HIS:CE1	4:L:1630:HOH:O	2.31	0.83
1:I:9:PRO:HD3	4:I:1373:HOH:O	1.79	0.83
1:1:14:ARG:HG2	4:1:1448:HOH:O	1.76	0.83
1:Q:7:ILE:HG23	1:Q:11:GLN:HB3	1.59	0.83
2:X:432:GLU:HG2	4:X:1310:HOH:O	1.80	0.82
1:I:92:ARG:HD2	4:I:1723:HOH:O	1.77	0.82
1:U:181:LEU:O	1:U:185:VAL:HG23	1.79	0.82
1:U:69:ASN:H	1:U:69:ASN:HD22	1.26	0.81
3:J:4:DMF:C2	4:J:1466:HOH:O	2.28	0.81
1:1:14:ARG:CG	4:1:1788:HOH:O	2.28	0.81
4:M:1478:HOH:O	2:N:361:VAL:CG2	2.28	0.80
1:B:97:ARG:HD2	4:B:1748:HOH:O	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:33:LEU:O	1:K:33:LEU:CD1	2.30	0.80
2:T:509:ARG:HD2	4:T:1578:HOH:O	1.81	0.80
2:V:456:GLN:NE2	2:V:465:ARG:HH22	1.78	0.80
1:D:174:ASN:ND2	1:D:174:ASN:N	2.30	0.79
1:B:97:ARG:CD	4:B:1748:HOH:O	2.29	0.79
1:B:217:ARG:CD	4:B:1475:HOH:O	2.31	0.79
1:D:232:ALA:HB2	4:D:1728:HOH:O	1.81	0.79
2:P:456:GLN:HE21	2:P:465:ARG:HH12	1.27	0.79
1:D:36:ALA:HB3	4:D:1680:HOH:O	1.81	0.79
1:W:231:GLN:HA	4:W:1447:HOH:O	1.82	0.79
1:1:171:TYR:CE1	4:1:1654:HOH:O	2.36	0.79
2:2:444:LEU:CD1	4:2:1592:HOH:O	2.30	0.79
1:K:136:PRO:HD3	4:K:1568:HOH:O	1.82	0.78
1:Y:231:GLN:HA	4:Y:1576:HOH:O	1.83	0.78
2:J:321:THR:H	3:J:4:DMF:HC	1.48	0.78
1:Y:234:LEU:C	1:Y:234:LEU:HD23	2.08	0.78
2:G:444:LEU:HB3	4:G:1370:HOH:O	1.83	0.78
2:2:456:GLN:HE22	2:2:465:ARG:HH22	1.31	0.78
1:A:26:ARG:CD	4:A:1777:HOH:O	2.28	0.77
2:V:456:GLN:HE22	2:V:465:ARG:HH12	1.32	0.77
1:1:223:ARG:CD	4:1:1596:HOH:O	2.32	0.77
1:B:217:ARG:HD3	4:B:1475:HOH:O	1.85	0.77
1:B:160:THR:HG22	4:B:1526:HOH:O	1.84	0.77
1:1:33:LEU:HD12	1:1:40:LEU:HB3	1.67	0.76
1:D:173:GLU:CG	1:D:174:ASN:ND2	2.48	0.76
2:J:444:LEU:HB3	4:J:1376:HOH:O	1.84	0.76
2:V:432:GLU:CD	2:V:437:GLN:HE21	1.95	0.75
1:1:14:ARG:HG3	4:1:1788:HOH:O	1.86	0.75
1:1:223:ARG:HD3	4:1:1596:HOH:O	1.86	0.75
1:O:26:ARG:CG	4:O:1474:HOH:O	2.28	0.75
1:D:173:GLU:CB	1:D:174:ASN:ND2	2.49	0.75
3:T:29:DMF:H22	4:T:1567:HOH:O	1.86	0.75
1:I:92:ARG:CD	4:I:1723:HOH:O	2.34	0.74
1:Y:181:LEU:CD1	1:Y:233:LEU:HD22	2.16	0.74
1:F:54:SER:HA	4:F:1410:HOH:O	1.87	0.74
1:Q:91:ARG:HD2	4:Q:1398:HOH:O	1.88	0.74
2:C:445:PHE:CE2	3:C:55:DMF:H12	2.23	0.73
1:O:56:LEU:HD13	1:O:99:LEU:HD22	1.70	0.73
1:S:121:GLU:HG3	4:S:1386:HOH:O	1.88	0.73
1:K:33:LEU:O	1:K:33:LEU:HD12	1.88	0.73
1:O:134:LYS:HB2	4:O:1785:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:233:LEU:O	1:Y:234:LEU:C	2.30	0.73
1:D:173:GLU:HG2	1:D:174:ASN:HD21	1.49	0.73
1:F:182:ARG:HB2	4:F:1672:HOH:O	1.88	0.73
1:K:136:PRO:HG3	4:K:1568:HOH:O	1.89	0.72
1:A:152:HIS:HB3	1:A:171:TYR:HE2	1.49	0.72
1:U:35:TYR:CE1	1:U:37:GLY:N	2.56	0.72
2:R:456:GLN:HE21	2:R:465:ARG:HH12	1.35	0.72
2:H:376:PHE:HD1	4:H:1358:HOH:O	1.72	0.72
1:U:11:GLN:HG2	4:U:1729:HOH:O	1.89	0.72
1:K:136:PRO:CD	4:K:1568:HOH:O	2.36	0.72
3:J:4:DMF:H21	4:J:1466:HOH:O	1.87	0.72
1:Y:181:LEU:HD12	1:Y:233:LEU:CD2	2.19	0.72
1:S:142:THR:HA	4:S:1386:HOH:O	1.90	0.71
4:D:1754:HOH:O	1:K:10:GLU:HG3	1.91	0.71
1:I:33:LEU:HD11	1:I:40:LEU:HD23	1.73	0.71
1:Q:7:ILE:HG22	1:Q:8:SER:N	2.06	0.70
2:C:434:GLU:HG3	4:J:1791:HOH:O	1.89	0.70
1:O:105:GLN:OE1	1:U:73:ASN:HB2	1.91	0.70
1:Y:233:LEU:C	1:Y:234:LEU:O	2.35	0.70
1:F:92:ARG:CD	4:F:1747:HOH:O	2.39	0.70
1:F:19:LEU:HD21	1:W:13:MET:HE2	1.74	0.70
1:S:97:ARG:CB	4:S:1727:HOH:O	2.38	0.70
1:O:134:LYS:HD2	4:O:1785:HOH:O	1.92	0.69
2:N:324:ASN:HB2	4:N:1388:HOH:O	1.92	0.69
1:Y:159:THR:HG23	4:Y:1427:HOH:O	1.92	0.69
1:Q:106:THR:O	1:Q:110:ILE:HG13	1.92	0.69
1:W:227:GLY:HA3	4:W:1758:HOH:O	1.91	0.68
2:2:444:LEU:HD12	4:2:1592:HOH:O	1.92	0.68
2:V:456:GLN:HE21	2:V:465:ARG:NH2	1.89	0.68
2:X:425:ALA:HB2	4:X:1655:HOH:O	1.93	0.68
1:K:172:ALA:HB3	1:K:175:ALA:HB2	1.76	0.68
1:M:223:ARG:CD	4:M:1627:HOH:O	2.28	0.68
2:2:456:GLN:NE2	2:2:465:ARG:HH22	1.91	0.68
1:D:159:THR:HG22	4:D:1455:HOH:O	1.92	0.68
1:Y:84:THR:HB	4:Y:1479:HOH:O	1.94	0.68
1:I:33:LEU:CD1	1:I:40:LEU:HB3	2.24	0.68
1:M:162:PRO:HB2	1:M:190:ALA:O	1.94	0.67
1:S:15:GLU:OE2	1:I:9:PRO:HB3	1.95	0.67
1:S:35:TYR:CE1	1:S:37:GLY:HA3	2.29	0.67
2:L:410:HIS:ND1	4:L:1630:HOH:O	2.27	0.67
1:Q:73:ASN:ND2	4:Q:1696:HOH:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:176:SER:OG	1:I:179:ASP:HB2	1.95	0.67
2:J:456:GLN:NE2	2:J:465:ARG:HH22	1.90	0.67
1:O:10:GLU:HG3	4:O:1774:HOH:O	1.93	0.67
4:F:1702:HOH:O	2:G:365:HIS:HE1	1.77	0.66
2:R:456:GLN:NE2	2:R:465:ARG:HH22	1.94	0.66
2:C:325:MET:HE3	4:C:1776:HOH:O	1.95	0.66
1:Q:33:LEU:HD11	1:Q:180:ALA:HB1	1.78	0.66
1:M:33:LEU:HD12	1:M:33:LEU:O	1.96	0.66
1:B:97:ARG:NE	4:B:1748:HOH:O	2.29	0.65
1:D:11:GLN:HG2	4:D:1284:HOH:O	1.96	0.65
2:H:357:ARG:HD2	4:H:1224:HOH:O	1.96	0.65
1:A:217:ARG:NH1	4:A:1792:HOH:O	2.30	0.65
1:I:217:ARG:NH1	4:I:1658:HOH:O	2.30	0.65
1:O:33:LEU:C	1:O:33:LEU:HD12	2.22	0.65
2:Z:482:GLY:HA3	4:Z:1417:HOH:O	1.95	0.65
1:K:33:LEU:O	1:K:33:LEU:HD13	1.96	0.65
2:J:399:LEU:CD1	4:J:1413:HOH:O	2.40	0.65
1:Q:7:ILE:HG23	1:Q:11:GLN:CB	2.27	0.65
1:S:156:MET:HA	4:S:1513:HOH:O	1.94	0.65
1:K:33:LEU:CD1	1:K:40:LEU:HB3	2.26	0.65
1:M:223:ARG:CG	4:M:1631:HOH:O	2.32	0.65
1:O:33:LEU:HD12	1:O:33:LEU:O	1.96	0.65
1:Y:105:GLN:NE2	4:Y:1749:HOH:O	2.30	0.65
1:D:9:PRO:HD3	1:Q:7:ILE:CD1	2.27	0.64
1:W:191:GLY:HA3	4:W:1559:HOH:O	1.97	0.64
1:K:152:HIS:CG	4:K:1560:HOH:O	2.50	0.64
2:C:445:PHE:CD2	3:C:55:DMF:H12	2.33	0.64
2:R:456:GLN:HE22	2:R:465:ARG:HH22	1.45	0.64
1:F:92:ARG:HD2	4:F:1747:HOH:O	1.97	0.64
2:R:430:ASN:HB2	4:R:1290:HOH:O	1.98	0.64
2:Z:515:ARG:NE	4:Z:1691:HOH:O	2.30	0.64
4:F:1688:HOH:O	1:W:9:PRO:CG	2.30	0.64
2:J:451:LYS:NZ	2:Z:473:ASP:OD1	2.30	0.64
1:K:136:PRO:CG	4:K:1568:HOH:O	2.46	0.64
3:Z:18:DMF:C	4:Z:1771:HOH:O	2.46	0.64
1:F:161:GLU:N	1:F:161:GLU:OE1	2.30	0.64
1:F:19:LEU:HD11	1:W:13:MET:HG3	1.79	0.63
2:C:325:MET:CE	4:C:1776:HOH:O	2.45	0.63
2:H:444:LEU:HB3	4:H:1361:HOH:O	1.98	0.63
1:U:69:ASN:H	1:U:69:ASN:ND2	1.91	0.63
1:B:114:GLN:NE2	4:B:1389:HOH:O	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:409:ILE:CD1	4:H:1704:HOH:O	2.46	0.62
1:S:172:ALA:HB3	1:S:175:ALA:HB2	1.80	0.62
1:U:35:TYR:CE1	1:U:37:GLY:CA	2.83	0.62
1:Q:83:ASP:OD2	2:R:365:HIS:HD2	1.83	0.62
1:I:11:GLN:HB3	4:I:1368:HOH:O	2.00	0.62
2:H:434:GLU:HG3	4:H:1573:HOH:O	1.99	0.61
1:D:173:GLU:HB3	1:D:174:ASN:ND2	2.14	0.61
1:O:152:HIS:CD2	1:O:173:GLU:OE2	2.52	0.61
1:S:97:ARG:HB3	4:S:1727:HOH:O	1.99	0.61
1:O:28:LYS:HE3	4:O:1486:HOH:O	2.01	0.61
1:Y:172:ALA:HB3	1:Y:175:ALA:HB2	1.82	0.61
3:T:29:DMF:H21	4:T:1461:HOH:O	2.00	0.61
1:M:182:ARG:CG	4:M:1510:HOH:O	2.48	0.61
1:Q:28:LYS:HE3	4:Q:1387:HOH:O	1.99	0.61
1:A:184:ALA:O	1:A:188:LEU:HB2	2.01	0.60
4:M:1390:HOH:O	2:N:365:HIS:HE1	1.82	0.60
2:2:400:ALA:HA	4:2:1459:HOH:O	2.01	0.60
2:P:456:GLN:HE21	2:P:465:ARG:NH1	1.98	0.60
1:Q:7:ILE:CG2	1:Q:11:GLN:HB3	2.31	0.60
1:S:97:ARG:HD3	4:S:1727:HOH:O	2.02	0.60
1:Y:35:TYR:CE1	1:Y:37:GLY:HA3	2.36	0.60
2:N:401:LEU:HB2	4:N:1641:HOH:O	2.01	0.60
1:M:31:VAL:HG12	1:M:155:VAL:HG22	1.83	0.60
2:R:456:GLN:NE2	2:R:465:ARG:HH12	2.00	0.60
1:S:76:ARG:HD3	4:S:1020:HOH:O	2.02	0.60
1:U:217:ARG:CD	4:U:1532:HOH:O	2.39	0.60
1:Q:7:ILE:CG2	1:Q:8:SER:N	2.64	0.60
2:X:425:ALA:CB	4:X:1655:HOH:O	2.47	0.60
2:X:509:ARG:NH1	4:X:1515:HOH:O	2.35	0.59
1:O:26:ARG:HD3	4:O:1474:HOH:O	1.98	0.59
1:D:36:ALA:CB	4:D:1680:HOH:O	2.44	0.59
1:F:56:LEU:HG	1:F:62:PHE:HB2	1.84	0.59
1:U:35:TYR:CD1	1:U:37:GLY:N	2.60	0.59
1:I:33:LEU:HD12	1:I:33:LEU:O	2.02	0.59
2:N:367:GLU:HG2	4:N:1520:HOH:O	2.01	0.59
1:Y:35:TYR:CZ	1:Y:37:GLY:HA3	2.38	0.59
1:1:223:ARG:HD2	4:1:1596:HOH:O	1.99	0.59
1:O:10:GLU:CG	4:O:1774:HOH:O	2.48	0.58
1:Q:48:ARG:CB	4:Q:1636:HOH:O	2.50	0.58
1:1:35:TYR:CE1	1:1:37:GLY:HA3	2.38	0.58
1:K:33:LEU:CD1	1:K:33:LEU:C	2.74	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:456:GLN:HE21	2:2:465:ARG:HH12	1.51	0.58
1:Q:109:THR:HB	4:Q:1637:HOH:O	2.03	0.58
2:R:356:ALA:HB3	3:R:34:DMF:H22	1.86	0.58
1:U:101:ASN:O	1:U:105:GLN:HG2	2.03	0.58
1:Q:7:ILE:N	4:Q:1206:HOH:O	2.36	0.57
2:V:409:ILE:HG22	4:V:1453:HOH:O	2.03	0.57
2:E:456:GLN:HE21	2:E:465:ARG:NH1	2.02	0.57
1:M:33:LEU:HD12	1:M:33:LEU:C	2.28	0.57
1:M:189:ARG:O	1:M:190:ALA:C	2.47	0.57
1:U:35:TYR:CE1	1:U:37:GLY:HA3	2.39	0.57
2:V:456:GLN:NE2	2:V:465:ARG:HH12	2.00	0.57
1:I:161:GLU:OE1	1:I:161:GLU:N	2.30	0.57
1:K:33:LEU:HD11	1:K:40:LEU:HB3	1.86	0.57
1:K:159:THR:HA	4:K:1652:HOH:O	2.05	0.57
3:T:29:DMF:HC	4:T:1461:HOH:O	2.04	0.57
1:A:28:LYS:HE3	4:A:1366:HOH:O	2.04	0.56
1:M:162:PRO:CB	1:M:190:ALA:O	2.53	0.56
1:Q:7:ILE:HG23	1:Q:11:GLN:CG	2.35	0.56
1:M:182:ARG:CD	4:M:1510:HOH:O	2.35	0.56
2:P:456:GLN:NE2	2:P:465:ARG:HH12	2.01	0.56
2:V:301:OZT:H27	2:V:333:LYS:HE2	1.86	0.56
1:B:217:ARG:HD2	4:B:1475:HOH:O	1.98	0.56
2:V:319:ARG:NH1	2:V:479:SER:O	2.38	0.56
2:J:415:GLN:HB3	4:J:1632:HOH:O	2.04	0.56
2:E:444:LEU:HB2	3:E:66:DMF:H12	1.88	0.56
1:Q:13:MET:HG3	1:Y:19:LEU:HD11	1.86	0.56
2:G:324:ASN:HB2	4:G:1736:HOH:O	2.04	0.56
1:Y:28:LYS:HB2	4:Y:1700:HOH:O	2.03	0.56
1:I:152:HIS:HB2	4:I:1601:HOH:O	2.05	0.56
1:B:173:GLU:CG	4:B:1646:HOH:O	2.29	0.55
2:J:348:THR:HG22	3:J:4:DMF:H22	1.88	0.55
1:O:105:GLN:NE2	4:O:1408:HOH:O	2.38	0.55
1:Y:231:GLN:CA	4:Y:1576:HOH:O	2.48	0.55
2:H:376:PHE:CD1	4:H:1358:HOH:O	2.50	0.55
2:X:362:GLU:HG3	4:X:1609:HOH:O	2.06	0.55
1:M:65:ALA:HA	4:M:1412:HOH:O	2.05	0.55
1:D:13:MET:HE2	1:Q:19:LEU:HD21	1.89	0.55
1:S:45:ASN:HA	4:S:1602:HOH:O	2.07	0.55
1:S:161:GLU:OE1	1:S:161:GLU:N	2.30	0.55
2:C:400:ALA:HB1	4:C:1253:HOH:O	2.06	0.55
2:H:409:ILE:HD11	4:H:1704:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:223:ARG:HD3	4:F:1550:HOH:O	2.05	0.54
2:H:301:OZT:H27	2:H:333:LYS:HE2	1.89	0.54
1:O:142:THR:HA	4:O:1391:HOH:O	2.06	0.54
2:C:515:ARG:HD2	4:C:1405:HOH:O	2.07	0.54
2:E:428:GLY:HA2	4:E:1096:HOH:O	2.08	0.54
2:Z:456:GLN:HE21	2:Z:465:ARG:HH12	1.54	0.54
1:Q:7:ILE:CG2	1:Q:8:SER:H	2.21	0.54
2:C:444:LEU:HB2	3:C:55:DMF:H13	1.88	0.54
1:K:165:ASN:HA	4:K:1705:HOH:O	2.07	0.54
1:A:167:LEU:O	1:A:171:TYR:HB2	2.08	0.54
1:D:9:PRO:HD3	1:Q:7:ILE:HD13	1.88	0.54
1:Q:13:MET:HE2	1:Y:19:LEU:HD21	1.88	0.54
3:C:10:DMF:H12	4:C:1638:HOH:O	2.07	0.53
2:G:503:VAL:HA	4:G:1527:HOH:O	2.08	0.53
1:W:15:GLU:OE2	1:Y:9:PRO:HB3	2.08	0.53
2:L:456:GLN:HE21	2:L:465:ARG:HH22	1.55	0.53
1:Y:204:GLY:N	4:Y:1252:HOH:O	2.42	0.53
2:T:451:LYS:NZ	2:X:473:ASP:OD1	2.41	0.53
1:U:36:ALA:HA	1:U:174:ASN:OD1	2.08	0.53
1:F:203:LEU:N	4:F:1740:HOH:O	2.42	0.53
2:R:382:ARG:HH21	2:R:385:ILE:HD13	1.74	0.53
1:W:175:ALA:HB3	1:W:180:ALA:HB2	1.91	0.53
1:I:9:PRO:HB2	1:I:11:GLN:H	1.73	0.52
1:D:173:GLU:CA	1:D:174:ASN:HD22	2.18	0.52
1:Y:159:THR:HA	4:Y:1427:HOH:O	2.08	0.52
1:S:52:LYS:NZ	4:S:1382:HOH:O	2.41	0.52
1:D:135:ARG:HB3	1:Q:48:ARG:HH22	1.75	0.52
2:E:444:LEU:H	3:E:66:DMF:H12	1.73	0.52
4:K:1762:HOH:O	1:M:135:ARG:HB3	2.09	0.52
1:W:230:LEU:C	4:W:1447:HOH:O	2.52	0.52
2:N:306:LEU:C	2:N:306:LEU:HD12	2.35	0.52
4:K:1467:HOH:O	1:M:97:ARG:CD	2.45	0.51
1:M:97:ARG:NH1	4:M:1211:HOH:O	2.37	0.51
2:N:308:TYR:CZ	2:N:311:GLY:HA3	2.45	0.51
2:V:456:GLN:NE2	2:V:465:ARG:NH2	2.53	0.51
1:I:105:GLN:NE2	4:I:1246:HOH:O	2.42	0.51
1:S:97:ARG:NH1	4:S:1727:HOH:O	2.36	0.51
1:W:83:ASP:OD2	2:X:365:HIS:HD2	1.94	0.51
1:Y:231:GLN:C	4:Y:1576:HOH:O	2.53	0.51
1:I:35:TYR:CZ	1:I:37:GLY:HA3	2.44	0.51
2:E:432:GLU:HG3	2:E:437:GLN:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:391:LEU:O	2:J:392:ALA:HB2	2.10	0.51
1:K:59:ARG:HB2	4:K:1392:HOH:O	2.10	0.51
3:N:22:DMF:C1	4:P:1377:HOH:O	2.58	0.51
1:F:136:PRO:HG3	4:F:1598:HOH:O	2.10	0.51
2:R:358:LEU:HD23	2:R:386:MET:HE3	1.91	0.51
1:M:76:ARG:HD3	4:M:647:HOH:O	2.09	0.51
1:Y:9:PRO:HB2	1:Y:11:GLN:H	1.75	0.51
1:D:13:MET:HG3	1:Q:19:LEU:HD11	1.93	0.51
1:M:40:LEU:HD13	1:M:212:VAL:CG1	2.41	0.51
2:2:456:GLN:HE22	2:2:465:ARG:NH2	2.04	0.51
2:J:411:ALA:HB1	4:J:1667:HOH:O	2.11	0.50
1:1:67:LYS:HE3	1:1:69:ASN:HD21	1.76	0.50
1:Q:8:SER:H	1:Q:11:GLN:HB3	1.77	0.50
1:I:205:VAL:HG21	1:I:231:GLN:HG2	1.94	0.50
2:R:348:THR:HG23	4:R:1446:HOH:O	2.11	0.50
2:Z:307:LYS:HD3	4:Z:277:HOH:O	2.11	0.50
1:W:175:ALA:CB	1:W:180:ALA:HB2	2.41	0.50
2:C:445:PHE:CD2	3:C:55:DMF:C1	2.95	0.50
2:E:314:MET:HE3	2:E:405:ALA:HB2	1.93	0.50
1:Q:76:ARG:HD3	4:Q:411:HOH:O	2.12	0.50
2:Z:456:GLN:HE21	2:Z:465:ARG:NH1	2.08	0.50
1:F:135:ARG:NH1	4:F:1640:HOH:O	2.44	0.50
2:L:317:ASP:OD1	2:L:333:LYS:NZ	2.44	0.50
1:W:231:GLN:CA	4:W:1447:HOH:O	2.51	0.50
2:Z:515:ARG:HD2	4:Z:1691:HOH:O	2.12	0.50
1:D:173:GLU:CB	1:D:174:ASN:HD22	2.21	0.49
2:L:391:LEU:HD12	2:L:399:LEU:HD23	1.92	0.49
1:M:40:LEU:CD1	1:M:212:VAL:CG1	2.90	0.49
1:U:69:ASN:ND2	1:U:69:ASN:N	2.59	0.49
1:S:35:TYR:CZ	1:S:37:GLY:HA3	2.47	0.49
1:A:105:GLN:NE2	4:A:1308:HOH:O	2.45	0.49
2:J:314:MET:HE3	2:J:405:ALA:HB2	1.95	0.49
1:M:223:ARG:CD	4:M:1631:HOH:O	2.60	0.49
2:V:409:ILE:CG2	4:V:1453:HOH:O	2.60	0.49
2:R:362:GLU:OE2	2:R:382:ARG:HD3	2.12	0.49
1:F:105:GLN:NE2	4:F:1457:HOH:O	2.46	0.49
1:W:41:PHE:CD1	1:W:63:ALA:HB2	2.48	0.49
1:S:97:ARG:N	4:S:1484:HOH:O	2.34	0.49
1:Q:48:ARG:HB3	4:Q:1636:HOH:O	2.12	0.49
1:1:67:LYS:HG2	1:1:69:ASN:ND2	2.27	0.49
1:A:223:ARG:HD2	4:A:1724:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:GLU:CB	1:D:174:ASN:HD21	2.19	0.49
1:O:204:GLY:N	4:O:1277:HOH:O	2.45	0.48
1:A:90:ASP:OD1	1:A:93:ASP:N	2.46	0.48
1:O:56:LEU:HG	1:O:62:PHE:HB2	1.94	0.48
2:T:432:GLU:O	4:T:1228:HOH:O	2.20	0.48
1:U:54:SER:CB	1:U:75:ARG:HD2	2.43	0.48
1:Y:56:LEU:HG	1:Y:62:PHE:HB2	1.96	0.48
2:2:465:ARG:HG3	2:2:513:LEU:HD22	1.94	0.48
1:U:163:ILE:HG23	1:U:187:ALA:O	2.13	0.48
2:V:390:ASN:HD22	2:V:390:ASN:N	2.11	0.48
2:X:320:SER:HB3	2:X:331:VAL:HG21	1.95	0.48
1:I:56:LEU:HG	1:I:62:PHE:HB2	1.94	0.48
2:G:476:ASP:OD1	3:G:12:DMF:H12	2.13	0.48
2:R:465:ARG:HD3	4:R:1108:HOH:O	2.14	0.48
2:V:355:PHE:CE1	2:V:386:MET:HE2	2.49	0.48
1:M:51:GLN:NE2	1:M:75:ARG:CZ	2.77	0.48
1:O:97:ARG:HG2	1:O:97:ARG:HH11	1.78	0.48
1:S:171:TYR:HE2	1:S:173:GLU:HG2	1.78	0.48
1:A:13:MET:HG3	1:O:19:LEU:HD11	1.94	0.48
1:B:209:GLU:HB2	4:B:1563:HOH:O	2.12	0.48
1:M:102:VAL:HG12	3:M:249:DMF:H22	1.95	0.48
1:M:182:ARG:CB	4:M:1510:HOH:O	2.46	0.48
1:K:51:GLN:NE2	1:K:75:ARG:CZ	2.77	0.48
1:K:52:LYS:NZ	4:K:1439:HOH:O	2.46	0.48
1:Q:51:GLN:HB2	4:Q:851:HOH:O	2.14	0.48
1:1:189:ARG:HH11	1:1:203:LEU:HB2	1.79	0.48
1:D:9:PRO:N	4:D:1284:HOH:O	2.46	0.48
1:1:33:LEU:HD12	1:1:33:LEU:O	2.14	0.48
1:B:56:LEU:HG	1:B:62:PHE:HB2	1.96	0.48
2:C:444:LEU:HB2	3:C:55:DMF:C1	2.44	0.48
2:V:376:PHE:CE2	2:V:380:ILE:HD11	2.49	0.48
1:M:51:GLN:HE21	1:M:75:ARG:CZ	2.26	0.47
1:O:10:GLU:HB2	4:O:1774:HOH:O	2.12	0.47
1:Q:56:LEU:HG	1:Q:62:PHE:HB2	1.96	0.47
1:1:30:VAL:HG13	1:1:43:ALA:HB2	1.96	0.47
1:Y:163:ILE:HG23	1:Y:187:ALA:O	2.13	0.47
2:R:456:GLN:HE22	2:R:465:ARG:NH2	2.11	0.47
2:N:415:GLN:NE2	4:N:541:HOH:O	2.47	0.47
2:N:464:LEU:HD21	2:N:505:VAL:HG11	1.96	0.47
1:S:65:ALA:HA	4:S:1382:HOH:O	2.14	0.47
1:1:41:PHE:CE1	1:1:63:ALA:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:GLU:HG3	4:B:1563:HOH:O	2.13	0.47
1:M:56:LEU:HG	1:M:62:PHE:HB2	1.97	0.47
2:R:465:ARG:HG3	2:R:513:LEU:HD22	1.96	0.47
1:U:92:ARG:NE	4:U:1709:HOH:O	2.46	0.47
1:O:51:GLN:HE21	1:O:75:ARG:CZ	2.28	0.47
2:J:320:SER:HB3	2:J:331:VAL:HG21	1.95	0.47
3:M:249:DMF:H12	4:M:1743:HOH:O	2.15	0.47
2:P:301:OZT:H27	2:P:333:LYS:HE2	1.95	0.47
2:Z:515:ARG:CD	4:Z:1691:HOH:O	2.63	0.47
1:F:161:GLU:N	1:F:161:GLU:CD	2.72	0.47
2:E:456:GLN:HE21	2:E:465:ARG:HH12	1.62	0.47
1:I:30:VAL:HG13	1:I:43:ALA:HB2	1.96	0.47
1:S:56:LEU:HG	1:S:62:PHE:HB2	1.95	0.47
2:V:428:GLY:HA2	4:V:1440:HOH:O	2.14	0.47
1:I:174:ASN:O	1:I:175:ALA:C	2.58	0.47
1:K:56:LEU:HG	1:K:62:PHE:HB2	1.96	0.47
3:J:4:DMF:H23	4:J:1466:HOH:O	2.07	0.46
2:N:314:MET:HE3	2:N:405:ALA:HB2	1.97	0.46
2:V:314:MET:HE3	2:V:405:ALA:HB2	1.97	0.46
1:W:56:LEU:HG	1:W:62:PHE:HB2	1.97	0.46
3:T:29:DMF:C2	4:T:1567:HOH:O	2.55	0.46
1:U:189:ARG:O	1:U:190:ALA:C	2.58	0.46
1:A:56:LEU:HG	1:A:62:PHE:HB2	1.96	0.46
2:L:331:VAL:HG13	2:L:349:ALA:HB2	1.98	0.46
1:S:97:ARG:HB2	4:S:1727:HOH:O	2.05	0.46
2:P:483:GLY:HA2	4:P:38:HOH:O	2.14	0.46
1:K:33:LEU:HD12	1:K:40:LEU:HB3	1.96	0.46
1:F:22:LYS:HE2	4:F:1400:HOH:O	2.15	0.46
2:H:332:ARG:CD	4:H:1570:HOH:O	2.41	0.46
3:L:53:DMF:HC	4:L:1603:HOH:O	2.14	0.46
2:E:377:ALA:HB1	3:L:53:DMF:HC	1.98	0.46
2:N:301:OZT:H27	2:N:333:LYS:HE2	1.97	0.46
1:W:205:VAL:CG2	4:W:1447:HOH:O	2.63	0.46
1:D:30:VAL:HG13	1:D:43:ALA:HB2	1.98	0.46
1:D:217:ARG:NH1	4:D:1496:HOH:O	2.44	0.46
2:V:355:PHE:CZ	2:V:386:MET:HE2	2.51	0.46
1:Y:159:THR:CA	4:Y:1427:HOH:O	2.63	0.46
1:B:67:LYS:HG2	1:B:69:ASN:HD21	1.81	0.46
1:K:51:GLN:HG2	4:K:561:HOH:O	2.15	0.46
2:J:430:ASN:HB2	4:J:1239:HOH:O	2.15	0.45
1:K:51:GLN:HE21	1:K:75:ARG:CZ	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:1478:HOH:O	2:N:361:VAL:HG22	2.06	0.45
1:Q:16:ARG:NH1	1:Q:117:PRO:HD3	2.31	0.45
1:U:35:TYR:CD1	1:U:36:ALA:N	2.84	0.45
1:A:152:HIS:CB	1:A:171:TYR:HE2	2.25	0.45
1:U:56:LEU:HG	1:U:62:PHE:HB2	1.97	0.45
2:Z:331:VAL:HG13	2:Z:349:ALA:HB2	1.98	0.45
1:B:30:VAL:HG13	1:B:43:ALA:HB2	1.97	0.45
1:U:13:MET:HE2	1:1:19:LEU:HD21	1.98	0.45
1:Y:83:ASP:OD2	2:Z:365:HIS:HD2	1.99	0.45
2:C:301:OZT:H27	2:C:333:LYS:HE2	1.97	0.45
2:L:509:ARG:HD3	4:L:1362:HOH:O	2.16	0.45
1:M:40:LEU:CD1	1:M:212:VAL:HG12	2.47	0.45
1:W:231:GLN:N	4:W:1447:HOH:O	2.50	0.45
2:H:509:ARG:HD3	4:H:1309:HOH:O	2.17	0.45
1:1:56:LEU:HG	1:1:62:PHE:HB2	1.99	0.45
1:A:83:ASP:OD2	2:H:365:HIS:HD2	2.00	0.45
1:D:182:ARG:HD3	4:D:1270:HOH:O	2.17	0.45
1:D:9:PRO:CD	1:Q:7:ILE:CD1	2.95	0.45
1:O:51:GLN:CD	4:O:937:HOH:O	2.59	0.45
1:O:87:TYR:O	2:P:357:ARG:NH2	2.49	0.45
1:Y:171:TYR:CE1	4:Y:1692:HOH:O	2.56	0.45
1:1:36:ALA:HB2	1:1:174:ASN:O	2.16	0.45
2:G:320:SER:HB3	2:G:331:VAL:HG21	1.99	0.45
1:I:76:ARG:HD3	4:I:977:HOH:O	2.17	0.45
2:T:515:ARG:HD2	4:T:1505:HOH:O	2.15	0.45
1:M:30:VAL:HG13	1:M:43:ALA:HB2	1.99	0.45
1:S:146:SER:HA	4:S:1501:HOH:O	2.17	0.45
1:M:92:ARG:CG	1:M:92:ARG:O	2.64	0.44
1:A:30:VAL:HG13	1:A:43:ALA:HB2	1.99	0.44
1:D:135:ARG:HB3	1:Q:48:ARG:NH2	2.32	0.44
1:O:51:GLN:NE2	1:O:75:ARG:CZ	2.80	0.44
1:Q:85:ARG:HD3	4:Q:1588:HOH:O	2.16	0.44
1:Y:30:VAL:HG13	1:Y:43:ALA:HB2	1.99	0.44
3:G:12:DMF:H13	4:V:1271:HOH:O	2.17	0.44
1:K:32:ALA:HA	1:K:40:LEU:O	2.16	0.44
1:K:33:LEU:HD13	1:K:33:LEU:C	2.41	0.44
1:M:129:HIS:NE2	4:M:1739:HOH:O	2.35	0.44
2:R:430:ASN:ND2	4:R:1315:HOH:O	2.50	0.44
1:B:67:LYS:HG2	1:B:69:ASN:ND2	2.33	0.44
1:U:11:GLN:CG	4:U:1729:HOH:O	2.57	0.44
2:X:301:OZT:O	2:X:440:GLY:HA3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:35:TYR:HD2	1:Y:38:GLY:O	1.96	0.44
1:S:54:SER:HB2	4:S:1464:HOH:O	2.16	0.44
1:A:67:LYS:HG2	1:A:69:ASN:HD21	1.83	0.44
1:D:56:LEU:HG	1:D:62:PHE:HB2	2.00	0.44
2:C:301:OZT:O	2:C:440:GLY:HA3	2.17	0.44
1:U:30:VAL:HG13	1:U:43:ALA:HB2	1.99	0.44
1:Y:35:TYR:CE1	1:Y:37:GLY:CA	3.00	0.44
1:D:52:LYS:NZ	4:D:1406:HOH:O	2.50	0.44
1:M:40:LEU:HD13	1:M:212:VAL:HG12	2.00	0.44
2:X:401:LEU:HD12	4:X:1614:HOH:O	2.18	0.44
2:E:456:GLN:NE2	2:E:465:ARG:NH1	2.65	0.43
1:F:22:LYS:CE	4:F:1400:HOH:O	2.66	0.43
1:K:19:LEU:HD21	1:M:13:MET:HE2	2.00	0.43
1:Q:162:PRO:HA	4:Q:1424:HOH:O	2.18	0.43
2:R:320:SER:HB3	2:R:331:VAL:HG21	2.00	0.43
1:W:223:ARG:HA	4:W:1590:HOH:O	2.17	0.43
1:B:16:ARG:NH1	1:B:117:PRO:HD3	2.33	0.43
2:G:314:MET:HE3	2:G:405:ALA:HB2	2.00	0.43
1:S:30:VAL:HG13	1:S:43:ALA:HB2	1.98	0.43
2:2:401:LEU:HA	2:2:402:PRO:HD3	1.88	0.43
1:F:67:LYS:HG2	1:F:69:ASN:HD21	1.84	0.43
1:M:65:ALA:CA	4:M:1412:HOH:O	2.64	0.43
1:M:114:GLN:NE2	4:M:1597:HOH:O	2.52	0.43
1:S:74:LEU:HD13	1:S:122:LEU:HD11	2.01	0.43
1:Y:35:TYR:CE1	1:Y:37:GLY:N	2.82	0.43
2:R:356:ALA:CB	3:R:34:DMF:H22	2.49	0.43
1:Y:231:GLN:C	1:Y:233:LEU:H	2.25	0.43
2:C:376:PHE:HD1	4:C:1247:HOH:O	2.02	0.43
2:E:320:SER:HB3	2:E:331:VAL:HG21	2.01	0.43
2:R:357:ARG:O	2:R:361:VAL:HG23	2.19	0.43
1:S:161:GLU:H	1:S:161:GLU:CD	2.21	0.43
2:V:422:SER:OG	2:V:432:GLU:OE2	2.29	0.42
1:W:140:ARG:NH2	4:W:1077:HOH:O	2.45	0.42
2:X:314:MET:HE3	2:X:405:ALA:HB2	2.01	0.42
1:Y:84:THR:CG2	4:Y:1479:HOH:O	2.67	0.42
4:E:1508:HOH:O	1:K:90:ASP:HB2	2.19	0.42
1:K:30:VAL:HG13	1:K:43:ALA:HB2	2.01	0.42
1:O:35:TYR:HE1	4:O:1616:HOH:O	2.02	0.42
1:A:13:MET:HE2	1:O:19:LEU:HD21	2.00	0.42
1:F:30:VAL:HG13	1:F:43:ALA:HB2	2.00	0.42
2:J:415:GLN:CB	4:J:1632:HOH:O	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:250:DMF:C	4:K:1485:HOH:O	2.67	0.42
2:T:301:OZT:O	2:T:440:GLY:HA3	2.18	0.42
2:Z:301:OZT:O	2:Z:440:GLY:HA3	2.20	0.42
1:A:67:LYS:HG2	1:A:69:ASN:ND2	2.35	0.42
1:D:205:VAL:HG13	1:D:230:LEU:HD23	2.00	0.42
2:T:432:GLU:HG3	2:T:437:GLN:HB2	2.01	0.42
2:V:391:LEU:O	2:V:392:ALA:HB2	2.19	0.42
2:E:457:VAL:HA	2:E:462:SER:HB3	2.02	0.42
1:Q:31:VAL:HG12	1:Q:155:VAL:HG22	2.02	0.42
1:Q:69:ASN:HD22	1:Q:69:ASN:H	1.68	0.42
2:T:320:SER:HB3	2:T:331:VAL:HG21	2.00	0.42
1:W:31:VAL:HG12	1:W:155:VAL:HG22	2.02	0.42
1:F:87:TYR:O	2:G:357:ARG:NH2	2.53	0.42
2:V:301:OZT:C7	2:V:333:LYS:HE2	2.50	0.42
2:2:314:MET:HE3	2:2:405:ALA:HB2	2.02	0.42
1:Q:28:LYS:CE	4:Q:1387:HOH:O	2.62	0.42
2:Z:301:OZT:H27	2:Z:333:LYS:HE2	2.01	0.42
2:E:364:GLU:HB3	4:E:1451:HOH:O	2.18	0.42
1:Q:217:ARG:NH2	4:Q:1650:HOH:O	2.52	0.42
1:W:205:VAL:HG22	4:W:1447:HOH:O	2.19	0.42
1:A:69:ASN:H	1:A:69:ASN:HD22	1.68	0.42
1:D:173:GLU:CA	1:D:174:ASN:ND2	2.82	0.42
1:F:129:HIS:CD2	4:F:1726:HOH:O	2.73	0.42
4:K:1467:HOH:O	1:M:97:ARG:NE	2.52	0.42
2:Z:444:LEU:HD12	4:Z:1433:HOH:O	2.20	0.42
1:D:97:ARG:HD2	1:Q:49:SER:O	2.20	0.42
2:E:444:LEU:HD13	3:E:66:DMF:H23	2.02	0.42
2:V:437:GLN:HG3	2:V:438:ALA:N	2.35	0.42
1:A:217:ARG:HA	1:A:218:PRO:HD3	1.85	0.41
1:A:223:ARG:CD	4:A:1724:HOH:O	2.68	0.41
2:J:362:GLU:OE2	2:J:382:ARG:HD3	2.20	0.41
2:2:456:GLN:NE2	2:2:465:ARG:HH12	2.16	0.41
1:B:69:ASN:HD22	1:B:69:ASN:H	1.68	0.41
1:Q:30:VAL:HG13	1:Q:43:ALA:HB2	2.02	0.41
2:T:464:LEU:HD21	2:T:505:VAL:HG11	2.01	0.41
2:Z:476:ASP:OD1	3:Z:18:DMF:H22	2.20	0.41
1:F:69:ASN:H	1:F:69:ASN:HD22	1.68	0.41
2:H:314:MET:HE3	2:H:405:ALA:HB2	2.03	0.41
2:P:320:SER:HB3	2:P:331:VAL:HG21	2.02	0.41
1:Q:181:LEU:O	1:Q:185:VAL:HG23	2.20	0.41
2:X:444:LEU:HD13	4:X:1671:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:VAL:HG12	1:B:155:VAL:HG22	2.02	0.41
1:S:51:GLN:HB2	4:S:1464:HOH:O	2.20	0.41
1:U:42:VAL:HG12	1:U:188:LEU:HD21	2.02	0.41
1:1:14:ARG:HG2	4:1:1788:HOH:O	2.07	0.41
1:D:88:ALA:HB2	4:D:535:HOH:O	2.19	0.41
1:M:67:LYS:HG2	1:M:69:ASN:HD21	1.84	0.41
2:R:332:ARG:NE	4:R:1547:HOH:O	2.35	0.41
2:R:391:LEU:HD12	2:R:399:LEU:HD23	2.03	0.41
1:W:67:LYS:HG2	1:W:69:ASN:HD21	1.86	0.41
1:M:92:ARG:O	1:M:92:ARG:HG3	2.20	0.41
2:P:388:ARG:NH1	4:P:1095:HOH:O	2.53	0.41
2:R:361:VAL:O	2:R:365:HIS:HB2	2.21	0.41
1:D:22:LYS:NZ	1:K:10:GLU:OE1	2.54	0.41
1:D:161:GLU:HB2	1:D:162:PRO:HD3	2.03	0.41
2:E:483:GLY:HA2	4:E:1046:HOH:O	2.20	0.41
1:K:189:ARG:CD	4:K:1741:HOH:O	2.32	0.41
2:L:301:OZT:O	2:L:440:GLY:HA3	2.20	0.41
1:S:67:LYS:HG2	1:S:69:ASN:HD21	1.86	0.41
2:X:401:LEU:HA	2:X:402:PRO:HD3	1.82	0.41
1:A:156:MET:HE3	1:A:156:MET:HB2	2.00	0.41
1:F:67:LYS:HG2	1:F:69:ASN:ND2	2.35	0.41
2:G:444:LEU:HD21	2:X:325:MET:SD	2.61	0.41
1:K:150:GLU:HA	1:K:151:PRO:HD3	1.95	0.41
1:M:47:SER:HA	4:M:1402:HOH:O	2.20	0.41
2:N:301:OZT:O	2:N:440:GLY:HA3	2.21	0.41
2:P:314:MET:HE3	2:P:405:ALA:HB2	2.02	0.41
1:S:35:TYR:CE1	1:S:37:GLY:CA	3.02	0.41
1:W:30:VAL:HG13	1:W:43:ALA:HB2	2.02	0.41
1:D:31:VAL:HG12	1:D:155:VAL:HG22	2.02	0.41
1:D:67:LYS:HG2	1:D:69:ASN:HD21	1.86	0.41
1:D:83:ASP:OD2	2:E:365:HIS:HD2	2.03	0.41
1:S:188:LEU:C	1:S:190:ALA:H	2.28	0.41
2:V:335:TYR:HB3	3:V:27:DMF:H12	2.01	0.41
1:Q:67:LYS:HG2	1:Q:69:ASN:HD21	1.87	0.40
2:H:479:SER:HB2	2:L:479:SER:HB2	2.02	0.40
1:I:67:LYS:HG2	1:I:69:ASN:HD21	1.86	0.40
1:I:156:MET:HE3	1:I:156:MET:HB2	2.02	0.40
1:M:67:LYS:HG2	1:M:69:ASN:ND2	2.35	0.40
1:F:45:ASN:HA	1:F:46:PRO:HD2	2.01	0.40
1:O:51:GLN:NE2	4:O:937:HOH:O	2.54	0.40
2:P:483:GLY:HA3	3:P:14:DMF:H11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:390:ASN:HD22	2:V:390:ASN:H	1.70	0.40
1:Y:67:LYS:HE3	1:Y:69:ASN:HD21	1.85	0.40
2:G:350:ALA:CB	4:G:1411:HOH:O	2.69	0.40
2:H:301:OZT:O	2:H:440:GLY:HA3	2.22	0.40
1:O:33:LEU:C	1:O:33:LEU:CD1	2.91	0.40
2:P:301:OZT:O	2:P:440:GLY:HA3	2.22	0.40
1:W:31:VAL:HG23	1:W:42:VAL:HB	2.02	0.40
2:C:314:MET:HE3	2:C:405:ALA:HB2	2.04	0.40
1:I:214:ASP:O	1:I:217:ARG:HG3	2.22	0.40
1:O:67:LYS:HG2	1:O:69:ASN:ND2	2.37	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%)	205 (97%)	6 (3%)	0	100	100
1	A	211/248 (85%)	204 (97%)	7 (3%)	0	100	100
1	B	210/248 (85%)	205 (98%)	5 (2%)	0	100	100
1	D	210/248 (85%)	205 (98%)	5 (2%)	0	100	100
1	F	212/248 (86%)	207 (98%)	5 (2%)	0	100	100
1	I	210/248 (85%)	204 (97%)	6 (3%)	0	100	100
1	K	211/248 (85%)	206 (98%)	5 (2%)	0	100	100
1	M	211/248 (85%)	205 (97%)	6 (3%)	0	100	100
1	O	211/248 (85%)	207 (98%)	4 (2%)	0	100	100
1	Q	213/248 (86%)	207 (97%)	6 (3%)	0	100	100
1	S	211/248 (85%)	207 (98%)	4 (2%)	0	100	100
1	U	210/248 (85%)	205 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	213/248 (86%)	207 (97%)	6 (3%)	0	100	100
1	Y	209/248 (84%)	202 (97%)	7 (3%)	0	100	100
2	2	211/240 (88%)	209 (99%)	2 (1%)	0	100	100
2	C	211/240 (88%)	209 (99%)	2 (1%)	0	100	100
2	E	212/240 (88%)	210 (99%)	2 (1%)	0	100	100
2	G	212/240 (88%)	208 (98%)	4 (2%)	0	100	100
2	H	209/240 (87%)	206 (99%)	3 (1%)	0	100	100
2	J	212/240 (88%)	209 (99%)	3 (1%)	0	100	100
2	L	212/240 (88%)	210 (99%)	2 (1%)	0	100	100
2	N	209/240 (87%)	208 (100%)	1 (0%)	0	100	100
2	P	212/240 (88%)	209 (99%)	3 (1%)	0	100	100
2	R	219/240 (91%)	217 (99%)	2 (1%)	0	100	100
2	T	212/240 (88%)	210 (99%)	2 (1%)	0	100	100
2	V	218/240 (91%)	216 (99%)	2 (1%)	0	100	100
2	X	212/240 (88%)	208 (98%)	4 (2%)	0	100	100
2	Z	211/240 (88%)	209 (99%)	2 (1%)	0	100	100
All	All	5925/6832 (87%)	5814 (98%)	111 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	164/192 (85%)	159 (97%)	5 (3%)	36	64
1	A	164/192 (85%)	156 (95%)	8 (5%)	22	45
1	B	164/192 (85%)	160 (98%)	4 (2%)	43	70
1	D	163/192 (85%)	158 (97%)	5 (3%)	35	62
1	F	165/192 (86%)	160 (97%)	5 (3%)	36	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	164/192 (85%)	156 (95%)	8 (5%)	22	45
1	K	164/192 (85%)	155 (94%)	9 (6%)	19	40
1	M	165/192 (86%)	159 (96%)	6 (4%)	31	58
1	O	164/192 (85%)	156 (95%)	8 (5%)	22	45
1	Q	166/192 (86%)	158 (95%)	8 (5%)	23	46
1	S	164/192 (85%)	160 (98%)	4 (2%)	43	70
1	U	164/192 (85%)	153 (93%)	11 (7%)	15	31
1	W	166/192 (86%)	159 (96%)	7 (4%)	26	52
1	Y	163/192 (85%)	155 (95%)	8 (5%)	22	45
2	2	160/177 (90%)	156 (98%)	4 (2%)	42	69
2	C	160/177 (90%)	153 (96%)	7 (4%)	25	50
2	E	161/177 (91%)	156 (97%)	5 (3%)	35	62
2	G	161/177 (91%)	156 (97%)	5 (3%)	35	62
2	H	160/177 (90%)	155 (97%)	5 (3%)	35	62
2	J	161/177 (91%)	158 (98%)	3 (2%)	50	76
2	L	161/177 (91%)	156 (97%)	5 (3%)	35	62
2	N	159/177 (90%)	154 (97%)	5 (3%)	35	62
2	P	161/177 (91%)	157 (98%)	4 (2%)	42	69
2	R	165/177 (93%)	160 (97%)	5 (3%)	36	64
2	T	161/177 (91%)	157 (98%)	4 (2%)	42	69
2	V	164/177 (93%)	159 (97%)	5 (3%)	36	64
2	X	161/177 (91%)	159 (99%)	2 (1%)	63	83
2	Z	160/177 (90%)	157 (98%)	3 (2%)	50	76
All	All	4555/5166 (88%)	4397 (96%)	158 (4%)	32	58

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	135	ARG
1	A	159	THR
1	A	173	GLU
1	A	181	LEU
1	A	188	LEU

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Mol	Chain	Res	Type
1	A	233	LEU
1	A	234	LEU
1	B	69	ASN
1	B	135	ARG
1	B	159	THR
1	B	181	LEU
2	C	322	GLN
2	C	345	ILE
2	C	362	GLU
2	C	433	GLU
2	C	444	LEU
2	C	497	ILE
2	C	509	ARG
1	D	135	ARG
1	D	159	THR
1	D	174	ASN
1	D	181	LEU
1	D	234	LEU
2	E	330	ASP
2	E	345	ILE
2	E	401	LEU
2	E	462	SER
2	E	515	ARG
1	F	69	ASN
1	F	113	GLU
1	F	135	ARG
1	F	159	THR
1	F	181	LEU
2	G	345	ILE
2	G	362	GLU
2	G	399	LEU
2	G	444	LEU
2	G	492	PRO
2	H	330	ASP
2	H	345	ILE
2	H	391	LEU
2	H	444	LEU
2	H	509	ARG
1	I	33	LEU
1	I	135	ARG
1	I	159	THR
1	I	160	THR

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Mol	Chain	Res	Type
1	I	174	ASN
1	I	181	LEU
1	I	233	LEU
1	I	234	LEU
2	J	322	GLN
2	J	345	ILE
2	J	433	GLU
1	K	33	LEU
1	K	69	ASN
1	K	113	GLU
1	K	135	ARG
1	K	159	THR
1	K	161	GLU
1	K	181	LEU
1	K	233	LEU
1	K	234	LEU
2	L	345	ILE
2	L	362	GLU
2	L	391	LEU
2	L	444	LEU
2	L	519	GLU
1	M	39	VAL
1	M	69	ASN
1	M	135	ARG
1	M	159	THR
1	M	181	LEU
1	M	188	LEU
2	N	322	GLN
2	N	345	ILE
2	N	444	LEU
2	N	461	ASP
2	N	465	ARG
1	O	69	ASN
1	O	98	GLN
1	O	99	LEU
1	O	105	GLN
1	O	109	THR
1	O	135	ARG
1	O	159	THR
1	O	181	LEU
2	P	322	GLN
2	P	345	ILE

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Mol	Chain	Res	Type
2	P	362	GLU
2	P	433	GLU
1	Q	9	PRO
1	Q	69	ASN
1	Q	135	ARG
1	Q	159	THR
1	Q	169	GLU
1	Q	181	LEU
1	Q	203	LEU
1	Q	234	LEU
2	R	322	GLN
2	R	345	ILE
2	R	362	GLU
2	R	401	LEU
2	R	492	PRO
1	S	69	ASN
1	S	135	ARG
1	S	159	THR
1	S	181	LEU
2	T	345	ILE
2	T	431	ILE
2	T	444	LEU
2	T	492	PRO
1	U	8	SER
1	U	69	ASN
1	U	113	GLU
1	U	135	ARG
1	U	159	THR
1	U	169	GLU
1	U	173	GLU
1	U	181	LEU
1	U	185	VAL
1	U	188	LEU
1	U	217	ARG
2	V	322	GLN
2	V	345	ILE
2	V	390	ASN
2	V	492	PRO
2	V	503	VAL
1	W	113	GLU
1	W	135	ARG
1	W	159	THR

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Mol	Chain	Res	Type
1	W	176	SER
1	W	181	LEU
1	W	203	LEU
1	W	233	LEU
2	X	345	ILE
2	X	362	GLU
1	Y	40	LEU
1	Y	69	ASN
1	Y	113	GLU
1	Y	135	ARG
1	Y	159	THR
1	Y	181	LEU
1	Y	233	LEU
1	Y	234	LEU
2	Z	345	ILE
2	Z	477	ASP
2	Z	492	PRO
1	1	33	LEU
1	1	69	ASN
1	1	135	ARG
1	1	159	THR
1	1	181	LEU
2	2	322	GLN
2	2	345	ILE
2	2	462	SER
2	2	492	PRO

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

Mol	Chain	Res	Type
1	A	51	GLN
1	A	69	ASN
1	A	98	GLN
1	A	114	GLN
1	B	51	GLN
1	B	69	ASN
1	B	98	GLN
1	B	114	GLN
2	C	365	HIS
2	C	430	ASN
2	C	456	GLN
1	D	51	GLN

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Mol	Chain	Res	Type
1	D	69	ASN
1	D	98	GLN
1	D	114	GLN
1	D	174	ASN
2	E	365	HIS
2	E	430	ASN
2	E	456	GLN
1	F	51	GLN
1	F	69	ASN
2	G	365	HIS
2	G	430	ASN
2	H	365	HIS
2	H	430	ASN
2	H	456	GLN
1	I	51	GLN
1	I	69	ASN
1	I	114	GLN
1	I	231	GLN
2	J	365	HIS
2	J	430	ASN
2	J	456	GLN
1	K	51	GLN
1	K	69	ASN
1	K	98	GLN
1	K	114	GLN
2	L	430	ASN
2	L	456	GLN
1	M	51	GLN
1	M	69	ASN
1	M	129	HIS
1	M	174	ASN
2	N	365	HIS
2	N	415	GLN
2	N	430	ASN
1	O	51	GLN
1	O	69	ASN
1	O	98	GLN
1	O	105	GLN
1	O	114	GLN
1	O	174	ASN
2	P	430	ASN
2	P	456	GLN

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Mol	Chain	Res	Type
1	Q	51	GLN
1	Q	69	ASN
1	Q	98	GLN
1	Q	114	GLN
1	Q	231	GLN
2	R	365	HIS
2	R	430	ASN
2	R	456	GLN
1	S	51	GLN
1	S	69	ASN
1	S	98	GLN
1	S	114	GLN
2	T	365	HIS
2	T	430	ASN
1	U	51	GLN
1	U	69	ASN
1	U	105	GLN
1	U	114	GLN
2	V	365	HIS
2	V	390	ASN
2	V	430	ASN
2	V	437	GLN
2	V	456	GLN
1	W	51	GLN
1	W	69	ASN
1	W	80	GLN
1	W	98	GLN
1	W	114	GLN
2	X	322	GLN
2	X	365	HIS
2	X	430	ASN
1	Y	51	GLN
1	Y	69	ASN
1	Y	98	GLN
2	Z	365	HIS
2	Z	430	ASN
2	Z	456	GLN
1	1	51	GLN
1	1	69	ASN
1	1	98	GLN
1	1	114	GLN
1	1	231	GLN

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Mol	Chain	Res	Type
2	2	430	ASN
2	2	456	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	C	301	2	6,9,10	4.56	3 (50%)	9,12,14	5.97	7 (77%)
2	OZT	Z	301	2	6,9,10	4.25	3 (50%)	9,12,14	6.04	6 (66%)
2	OZT	L	301	2	6,9,10	4.52	3 (50%)	9,12,14	6.08	7 (77%)
2	OZT	H	301	2	6,9,10	4.25	3 (50%)	9,12,14	6.11	6 (66%)
2	OZT	X	301	2	6,9,10	4.13	3 (50%)	9,12,14	5.93	6 (66%)
2	OZT	E	301	2	6,9,10	4.57	3 (50%)	9,12,14	5.72	7 (77%)
2	OZT	J	301	2	6,9,10	4.40	3 (50%)	9,12,14	6.09	7 (77%)
2	OZT	R	301	2	6,9,10	4.58	3 (50%)	9,12,14	5.79	7 (77%)
2	OZT	G	301	2	6,9,10	4.17	2 (33%)	9,12,14	5.87	7 (77%)
2	OZT	T	301	2	6,9,10	4.30	3 (50%)	9,12,14	6.12	7 (77%)
2	OZT	V	301	2	6,9,10	4.32	3 (50%)	9,12,14	6.24	7 (77%)
2	OZT	2	301	2	6,9,10	4.05	3 (50%)	9,12,14	6.01	7 (77%)
2	OZT	N	301	2	6,9,10	4.23	3 (50%)	9,12,14	6.01	7 (77%)
2	OZT	P	301	2	6,9,10	4.09	3 (50%)	9,12,14	6.06	7 (77%)

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

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	OZT	O1-C5	10.10	1.49	1.36
2	C	301	OZT	O1-C5	9.91	1.49	1.36
2	R	301	OZT	O1-C5	9.89	1.49	1.36
2	L	301	OZT	O1-C5	9.77	1.49	1.36
2	J	301	OZT	O1-C5	9.52	1.49	1.36
2	T	301	OZT	O1-C5	9.34	1.48	1.36
2	H	301	OZT	O1-C5	9.32	1.48	1.36
2	X	301	OZT	O1-C5	9.18	1.48	1.36
2	G	301	OZT	O1-C5	9.03	1.48	1.36
2	P	301	OZT	O1-C5	8.99	1.48	1.36
2	N	301	OZT	O1-C5	8.99	1.48	1.36
2	Z	301	OZT	O1-C5	8.75	1.48	1.36
2	2	301	OZT	O1-C5	8.66	1.47	1.36
2	V	301	OZT	O1-C5	8.62	1.47	1.36
2	V	301	OZT	C5-N	5.13	1.40	1.33
2	Z	301	OZT	C5-N	4.70	1.40	1.33
2	N	301	OZT	C5-N	4.22	1.39	1.33
2	R	301	OZT	C5-N	4.18	1.39	1.33
2	G	301	OZT	C5-N	4.09	1.39	1.33
2	C	301	OZT	C5-N	4.06	1.39	1.33
2	L	301	OZT	C5-N	3.96	1.39	1.33
2	T	301	OZT	C5-N	3.89	1.38	1.33
2	P	301	OZT	C5-N	3.75	1.38	1.33
2	J	301	OZT	C5-N	3.74	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	301	OZT	C5-N	3.66	1.38	1.33
2	E	301	OZT	C5-N	3.60	1.38	1.33
2	H	301	OZT	C5-N	3.17	1.38	1.33
2	X	301	OZT	O1-C2	-3.13	1.41	1.46
2	H	301	OZT	O1-C2	-3.12	1.41	1.46
2	L	301	OZT	O1-C2	-3.04	1.42	1.46
2	V	301	OZT	O1-C2	-3.00	1.42	1.46
2	2	301	OZT	O1-C2	-2.96	1.42	1.46
2	J	301	OZT	O1-C2	-2.92	1.42	1.46
2	C	301	OZT	O1-C2	-2.91	1.42	1.46
2	R	301	OZT	O1-C2	-2.90	1.42	1.46
2	E	301	OZT	O1-C2	-2.87	1.42	1.46
2	Z	301	OZT	O1-C2	-2.78	1.42	1.46
2	T	301	OZT	O1-C2	-2.70	1.42	1.46
2	X	301	OZT	C5-N	2.62	1.37	1.33
2	N	301	OZT	O1-C2	-2.60	1.42	1.46
2	P	301	OZT	O1-C2	-2.18	1.43	1.46

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	301	OZT	O1-C5-N	10.01	118.03	109.87
2	J	301	OZT	O1-C5-N	9.80	117.86	109.87
2	2	301	OZT	O1-C5-N	9.69	117.77	109.87
2	L	301	OZT	O1-C5-N	9.69	117.76	109.87
2	N	301	OZT	O1-C5-N	9.68	117.75	109.87
2	P	301	OZT	O1-C5-N	9.66	117.74	109.87
2	V	301	OZT	O1-C5-N	9.55	117.65	109.87
2	H	301	OZT	O1-C5-N	9.47	117.58	109.87
2	Z	301	OZT	O1-C5-N	9.46	117.58	109.87
2	X	301	OZT	O1-C5-N	9.40	117.53	109.87
2	C	301	OZT	O1-C5-N	9.35	117.49	109.87
2	G	301	OZT	O1-C5-N	9.22	117.39	109.87
2	R	301	OZT	O1-C5-N	8.81	117.05	109.87
2	Z	301	OZT	CA-N-C5	-8.77	99.20	112.75
2	X	301	OZT	CA-N-C5	-8.71	99.29	112.75
2	E	301	OZT	O1-C5-N	8.67	116.94	109.87
2	L	301	OZT	CA-N-C5	-8.56	99.53	112.75
2	H	301	OZT	CA-N-C5	-8.50	99.61	112.75
2	R	301	OZT	CA-N-C5	-8.49	99.63	112.75
2	2	301	OZT	CA-N-C5	-8.43	99.72	112.75
2	J	301	OZT	CA-N-C5	-8.40	99.76	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	OZT	CA-N-C5	-8.35	99.84	112.75
2	T	301	OZT	CA-N-C5	-8.32	99.89	112.75
2	E	301	OZT	CA-N-C5	-8.28	99.96	112.75
2	P	301	OZT	CA-N-C5	-8.15	100.16	112.75
2	N	301	OZT	CA-N-C5	-8.12	100.20	112.75
2	V	301	OZT	CA-N-C5	-8.06	100.30	112.75
2	V	301	OZT	O1-C2-CA	8.02	111.02	103.72
2	G	301	OZT	CA-N-C5	-8.02	100.36	112.75
2	V	301	OZT	C2-O1-C5	-7.62	99.03	110.33
2	J	301	OZT	O6-C5-N	-7.47	120.35	129.19
2	H	301	OZT	O6-C5-N	-7.34	120.50	129.19
2	T	301	OZT	C2-O1-C5	-7.34	99.46	110.33
2	P	301	OZT	C2-O1-C5	-7.31	99.49	110.33
2	T	301	OZT	O6-C5-N	-7.25	120.61	129.19
2	X	301	OZT	O6-C5-N	-7.25	120.61	129.19
2	L	301	OZT	O6-C5-N	-7.20	120.67	129.19
2	J	301	OZT	C2-O1-C5	-7.19	99.67	110.33
2	L	301	OZT	C2-O1-C5	-7.18	99.69	110.33
2	2	301	OZT	O6-C5-N	-7.14	120.74	129.19
2	H	301	OZT	C2-O1-C5	-7.14	99.75	110.33
2	N	301	OZT	C2-O1-C5	-7.12	99.77	110.33
2	2	301	OZT	C2-O1-C5	-7.08	99.83	110.33
2	C	301	OZT	C2-O1-C5	-7.06	99.86	110.33
2	G	301	OZT	C2-O1-C5	-7.04	99.89	110.33
2	Z	301	OZT	C2-O1-C5	-7.04	99.90	110.33
2	G	301	OZT	O6-C5-N	-6.97	120.94	129.19
2	C	301	OZT	O6-C5-N	-6.92	121.00	129.19
2	N	301	OZT	O6-C5-N	-6.92	121.00	129.19
2	R	301	OZT	C2-O1-C5	-6.91	100.08	110.33
2	P	301	OZT	O6-C5-N	-6.88	121.06	129.19
2	X	301	OZT	C2-O1-C5	-6.86	100.17	110.33
2	E	301	OZT	C2-O1-C5	-6.77	100.29	110.33
2	E	301	OZT	O6-C5-N	-6.77	121.18	129.19
2	Z	301	OZT	O6-C5-N	-6.73	121.23	129.19
2	R	301	OZT	O6-C5-N	-6.53	121.46	129.19
2	V	301	OZT	O6-C5-N	-6.44	121.57	129.19
2	P	301	OZT	O1-C2-CA	6.17	109.33	103.72
2	N	301	OZT	O1-C2-CA	6.02	109.19	103.72
2	C	301	OZT	O1-C2-CA	5.80	108.99	103.72
2	L	301	OZT	O1-C2-CA	5.76	108.96	103.72
2	G	301	OZT	O1-C2-CA	5.75	108.95	103.72
2	J	301	OZT	O1-C2-CA	5.71	108.91	103.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	301	OZT	O1-C2-CA	5.66	108.87	103.72
2	H	301	OZT	C2-CA-C	-5.66	106.29	114.16
2	Z	301	OZT	O1-C2-CA	5.64	108.84	103.72
2	H	301	OZT	O1-C2-CA	5.63	108.84	103.72
2	2	301	OZT	O1-C2-CA	5.58	108.80	103.72
2	Z	301	OZT	C2-CA-C	-5.40	106.65	114.16
2	R	301	OZT	O1-C2-CA	5.39	108.62	103.72
2	E	301	OZT	O1-C2-CA	5.21	108.46	103.72
2	P	301	OZT	C2-CA-C	-5.09	107.09	114.16
2	C	301	OZT	C2-CA-C	-5.07	107.11	114.16
2	E	301	OZT	C2-CA-C	-5.05	107.14	114.16
2	V	301	OZT	C2-CA-C	-4.95	107.28	114.16
2	X	301	OZT	C2-CA-C	-4.93	107.30	114.16
2	N	301	OZT	C2-CA-C	-4.87	107.38	114.16
2	R	301	OZT	C2-CA-C	-4.83	107.44	114.16
2	G	301	OZT	C2-CA-C	-4.80	107.49	114.16
2	T	301	OZT	C2-CA-C	-4.74	107.56	114.16
2	L	301	OZT	C2-CA-C	-4.74	107.57	114.16
2	X	301	OZT	O1-C2-CA	4.72	108.02	103.72
2	J	301	OZT	C2-CA-C	-4.71	107.61	114.16
2	2	301	OZT	C2-CA-C	-4.68	107.65	114.16
2	R	301	OZT	O-C-CA	-2.53	118.17	124.86
2	G	301	OZT	O-C-CA	-2.30	118.78	124.86
2	V	301	OZT	O-C-CA	-2.26	118.89	124.86
2	L	301	OZT	O-C-CA	-2.22	118.99	124.86
2	T	301	OZT	O-C-CA	-2.21	119.01	124.86
2	C	301	OZT	O-C-CA	-2.19	119.07	124.86
2	E	301	OZT	O-C-CA	-2.17	119.11	124.86
2	N	301	OZT	O-C-CA	-2.17	119.11	124.86
2	P	301	OZT	O-C-CA	-2.14	119.20	124.86
2	2	301	OZT	O-C-CA	-2.11	119.29	124.86
2	J	301	OZT	O-C-CA	-2.00	119.56	124.86

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	301	OZT	O-C-CA-C2
2	C	301	OZT	O-C-CA-C2
2	E	301	OZT	O-C-CA-C2
2	G	301	OZT	O-C-CA-C2
2	H	301	OZT	O-C-CA-C2

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Mol	Chain	Res	Type	Atoms
2	J	301	OZT	O-C-CA-C2
2	L	301	OZT	O-C-CA-C2
2	N	301	OZT	O-C-CA-C2
2	P	301	OZT	O-C-CA-C2
2	R	301	OZT	O-C-CA-C2
2	T	301	OZT	O-C-CA-C2
2	V	301	OZT	O-C-CA-C2
2	X	301	OZT	O-C-CA-C2
2	Z	301	OZT	O-C-CA-C2

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	OZT	2	0
2	Z	301	OZT	2	0
2	L	301	OZT	1	0
2	H	301	OZT	2	0
2	X	301	OZT	1	0
2	T	301	OZT	1	0
2	V	301	OZT	2	0
2	N	301	OZT	2	0
2	P	301	OZT	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

67 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	K	251	-	4,4,4	0.48	0	4,4,4	0.32	0
3	DMF	S	249	-	4,4,4	0.54	0	4,4,4	0.29	0
3	DMF	2	63	-	4,4,4	0.61	0	4,4,4	0.39	0
3	DMF	I	250	-	4,4,4	0.56	0	4,4,4	0.30	0
3	DMF	T	29	-	4,4,4	0.55	0	4,4,4	0.33	0
3	DMF	P	65	-	4,4,4	0.64	0	4,4,4	0.34	0
3	DMF	X	40	-	4,4,4	0.64	0	4,4,4	0.33	0
3	DMF	H	32	-	4,4,4	0.69	0	4,4,4	0.37	0
3	DMF	H	33	-	4,4,4	0.63	0	4,4,4	0.39	0
3	DMF	M	250	-	4,4,4	0.75	0	4,4,4	0.38	0
3	DMF	Z	30	-	4,4,4	0.42	0	4,4,4	0.35	0
3	DMF	N	2	-	4,4,4	0.56	0	4,4,4	0.29	0
3	DMF	K	249	-	4,4,4	0.55	0	4,4,4	0.31	0
3	DMF	N	22	-	4,4,4	0.58	0	4,4,4	0.33	0
3	DMF	E	20	-	4,4,4	0.58	0	4,4,4	0.35	0
3	DMF	L	53	-	4,4,4	0.50	0	4,4,4	0.39	0
3	DMF	N	58	-	4,4,4	0.52	0	4,4,4	0.38	0
3	DMF	Q	249	-	4,4,4	0.65	0	4,4,4	0.31	0
3	DMF	E	28	-	4,4,4	0.61	0	4,4,4	0.31	0
3	DMF	R	59	-	4,4,4	0.64	0	4,4,4	0.37	0
3	DMF	C	38	-	4,4,4	0.26	0	4,4,4	0.35	0
3	DMF	F	249	-	4,4,4	0.56	0	4,4,4	0.32	0
3	DMF	L	36	-	4,4,4	0.46	0	4,4,4	0.39	0
3	DMF	2	49	-	4,4,4	0.54	0	4,4,4	0.37	0
3	DMF	G	64	-	4,4,4	0.57	0	4,4,4	0.42	0
3	DMF	B	249	-	4,4,4	0.64	0	4,4,4	0.30	0
3	DMF	G	24	-	4,4,4	0.54	0	4,4,4	0.30	0
3	DMF	J	45	-	4,4,4	0.60	0	4,4,4	0.38	0
3	DMF	Z	18	-	4,4,4	0.45	0	4,4,4	0.37	0
3	DMF	Z	43	-	4,4,4	0.63	0	4,4,4	0.30	0
3	DMF	P	14	-	4,4,4	0.52	0	4,4,4	0.31	0
3	DMF	X	61	-	4,4,4	0.43	0	4,4,4	0.39	0
3	DMF	H	26	-	4,4,4	0.60	0	4,4,4	0.32	0
3	DMF	V	27	-	4,4,4	0.24	0	4,4,4	0.49	0
3	DMF	E	66	-	4,4,4	0.68	0	4,4,4	0.33	0
3	DMF	G	12	-	4,4,4	0.54	0	4,4,4	0.30	0
3	DMF	G	60	-	4,4,4	0.56	0	4,4,4	0.38	0
3	DMF	P	51	-	4,4,4	0.70	0	4,4,4	0.33	0
3	DMF	Z	54	-	4,4,4	0.55	0	4,4,4	0.34	0
3	DMF	J	4	-	4,4,4	0.54	0	4,4,4	0.36	0
3	DMF	P	56	-	4,4,4	0.50	0	4,4,4	0.32	0
3	DMF	U	249	-	4,4,4	0.46	0	4,4,4	0.31	0
3	DMF	H	62	-	4,4,4	0.71	0	4,4,4	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DMF	J	50	-	4,4,4	0.49	0	4,4,4	0.33	0
3	DMF	C	47	-	4,4,4	0.55	0	4,4,4	0.39	0
3	DMF	W	249	-	4,4,4	0.52	0	4,4,4	0.33	0
3	DMF	I	249	-	4,4,4	0.67	0	4,4,4	0.30	0
3	DMF	T	67	-	4,4,4	0.56	0	4,4,4	1.28	0
3	DMF	B	250	-	4,4,4	0.59	0	4,4,4	0.32	0
3	DMF	A	249	-	4,4,4	0.50	0	4,4,4	0.30	0
3	DMF	G	1	-	4,4,4	0.41	0	4,4,4	0.44	0
3	DMF	L	3	-	4,4,4	0.31	0	4,4,4	0.33	0
3	DMF	R	34	-	4,4,4	0.17	0	4,4,4	0.48	0
3	DMF	N	15	-	4,4,4	0.48	0	4,4,4	0.30	0
3	DMF	O	249	-	4,4,4	0.45	0	4,4,4	0.36	0
3	DMF	2	52	-	4,4,4	0.55	0	4,4,4	0.31	0
3	DMF	2	42	-	4,4,4	0.37	0	4,4,4	0.34	0
3	DMF	D	249	-	4,4,4	0.51	0	4,4,4	0.38	0
3	DMF	C	10	-	4,4,4	0.49	0	4,4,4	0.42	0
3	DMF	M	249	-	4,4,4	0.52	0	4,4,4	0.35	0
3	DMF	1	249	-	4,4,4	0.59	0	4,4,4	0.32	0
3	DMF	V	39	-	4,4,4	0.62	0	4,4,4	0.34	0
3	DMF	K	250	-	4,4,4	0.61	0	4,4,4	0.40	0
3	DMF	X	16	-	4,4,4	0.53	0	4,4,4	0.35	0
3	DMF	1	250	-	4,4,4	0.60	0	4,4,4	0.30	0
3	DMF	Z	41	-	4,4,4	0.54	0	4,4,4	0.34	0
3	DMF	C	55	-	4,4,4	0.30	0	4,4,4	0.60	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	K	251	-	-	0/2/2/2	-
3	DMF	S	249	-	-	0/2/2/2	-
3	DMF	2	63	-	-	0/2/2/2	-
3	DMF	I	250	-	-	0/2/2/2	-
3	DMF	T	29	-	-	0/2/2/2	-
3	DMF	P	65	-	-	0/2/2/2	-
3	DMF	X	40	-	-	0/2/2/2	-
3	DMF	H	32	-	-	0/2/2/2	-
3	DMF	H	33	-	-	0/2/2/2	-
3	DMF	M	250	-	-	0/2/2/2	-
3	DMF	Z	30	-	-	0/2/2/2	-
3	DMF	N	2	-	-	0/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	K	249	-	-	0/2/2/2	-
3	DMF	N	22	-	-	0/2/2/2	-
3	DMF	E	20	-	-	0/2/2/2	-
3	DMF	L	53	-	-	0/2/2/2	-
3	DMF	N	58	-	-	0/2/2/2	-
3	DMF	Q	249	-	-	0/2/2/2	-
3	DMF	E	28	-	-	0/2/2/2	-
3	DMF	R	59	-	-	0/2/2/2	-
3	DMF	C	38	-	-	2/2/2/2	-
3	DMF	F	249	-	-	0/2/2/2	-
3	DMF	L	36	-	-	0/2/2/2	-
3	DMF	2	49	-	-	0/2/2/2	-
3	DMF	G	64	-	-	0/2/2/2	-
3	DMF	B	249	-	-	0/2/2/2	-
3	DMF	G	24	-	-	0/2/2/2	-
3	DMF	J	45	-	-	0/2/2/2	-
3	DMF	Z	18	-	-	0/2/2/2	-
3	DMF	Z	43	-	-	0/2/2/2	-
3	DMF	P	14	-	-	0/2/2/2	-
3	DMF	X	61	-	-	0/2/2/2	-
3	DMF	H	26	-	-	0/2/2/2	-
3	DMF	V	27	-	-	2/2/2/2	-
3	DMF	E	66	-	-	0/2/2/2	-
3	DMF	G	12	-	-	0/2/2/2	-
3	DMF	G	60	-	-	0/2/2/2	-
3	DMF	P	51	-	-	0/2/2/2	-
3	DMF	Z	54	-	-	0/2/2/2	-
3	DMF	J	4	-	-	0/2/2/2	-
3	DMF	P	56	-	-	0/2/2/2	-
3	DMF	U	249	-	-	0/2/2/2	-
3	DMF	H	62	-	-	0/2/2/2	-
3	DMF	J	50	-	-	0/2/2/2	-
3	DMF	C	47	-	-	0/2/2/2	-
3	DMF	W	249	-	-	0/2/2/2	-
3	DMF	I	249	-	-	0/2/2/2	-
3	DMF	T	67	-	-	2/2/2/2	-
3	DMF	B	250	-	-	0/2/2/2	-
3	DMF	A	249	-	-	0/2/2/2	-
3	DMF	G	1	-	-	0/2/2/2	-
3	DMF	L	3	-	-	0/2/2/2	-
3	DMF	R	34	-	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	N	15	-	-	0/2/2/2	-
3	DMF	O	249	-	-	0/2/2/2	-
3	DMF	2	52	-	-	0/2/2/2	-
3	DMF	2	42	-	-	0/2/2/2	-
3	DMF	D	249	-	-	0/2/2/2	-
3	DMF	C	10	-	-	0/2/2/2	-
3	DMF	M	249	-	-	0/2/2/2	-
3	DMF	1	249	-	-	0/2/2/2	-
3	DMF	V	39	-	-	0/2/2/2	-
3	DMF	K	250	-	-	0/2/2/2	-
3	DMF	X	16	-	-	0/2/2/2	-
3	DMF	1	250	-	-	0/2/2/2	-
3	DMF	Z	41	-	-	0/2/2/2	-
3	DMF	C	55	-	-	2/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	38	DMF	O-C-N-C2
3	C	38	DMF	O-C-N-C1
3	R	34	DMF	O-C-N-C2
3	R	34	DMF	O-C-N-C1
3	C	55	DMF	O-C-N-C1
3	T	67	DMF	O-C-N-C1
3	V	27	DMF	O-C-N-C1
3	T	67	DMF	O-C-N-C2
3	V	27	DMF	O-C-N-C2
3	C	55	DMF	O-C-N-C2

There are no ring outliers.

15 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	29	DMF	4	0
3	X	40	DMF	1	0
3	N	22	DMF	1	0
3	L	53	DMF	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Z	18	DMF	2	0
3	P	14	DMF	1	0
3	V	27	DMF	1	0
3	E	66	DMF	3	0
3	G	12	DMF	2	0
3	J	4	DMF	5	0
3	R	34	DMF	2	0
3	C	10	DMF	1	0
3	M	249	DMF	2	0
3	K	250	DMF	1	0
3	C	55	DMF	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	215/248 (86%)	1.02	35 (16%) 4 3	19, 54, 89, 99	0
1	A	215/248 (86%)	1.04	32 (14%) 5 4	18, 54, 91, 98	0
1	B	214/248 (86%)	1.13	46 (21%) 2 2	19, 55, 89, 97	0
1	D	214/248 (86%)	1.14	36 (16%) 4 3	17, 55, 91, 98	0
1	F	216/248 (87%)	0.99	39 (18%) 3 3	19, 55, 87, 95	0
1	I	214/248 (86%)	1.03	37 (17%) 4 3	18, 54, 88, 94	0
1	K	215/248 (86%)	1.12	40 (18%) 3 2	18, 56, 89, 98	0
1	M	215/248 (86%)	1.11	41 (19%) 3 2	19, 53, 88, 98	0
1	O	215/248 (86%)	1.00	32 (14%) 5 4	19, 53, 89, 94	0
1	Q	217/248 (87%)	1.13	45 (20%) 2 2	18, 53, 87, 95	0
1	S	215/248 (86%)	1.01	31 (14%) 6 5	18, 55, 93, 100	0
1	U	214/248 (86%)	1.03	40 (18%) 3 2	18, 54, 91, 96	0
1	W	217/248 (87%)	1.12	38 (17%) 4 3	20, 55, 92, 97	0
1	Y	213/248 (85%)	1.37	59 (27%) 1 1	20, 56, 94, 105	0
2	2	214/240 (89%)	-0.21	5 (2%) 61 57	4, 20, 45, 67	0
2	C	214/240 (89%)	-0.19	6 (2%) 55 50	6, 20, 48, 73	0
2	E	215/240 (89%)	-0.25	3 (1%) 73 70	6, 20, 47, 72	0
2	G	215/240 (89%)	-0.19	3 (1%) 73 70	8, 22, 48, 74	0
2	H	212/240 (88%)	-0.22	3 (1%) 73 70	8, 21, 44, 64	0
2	J	215/240 (89%)	-0.20	5 (2%) 61 57	7, 20, 48, 64	0
2	L	215/240 (89%)	-0.16	5 (2%) 61 57	5, 21, 48, 71	0
2	N	212/240 (88%)	-0.23	2 (0%) 81 78	4, 20, 44, 64	0
2	P	215/240 (89%)	-0.21	3 (1%) 73 70	6, 22, 49, 72	0
2	R	222/240 (92%)	-0.26	7 (3%) 50 46	7, 20, 48, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
2	T	215/240 (89%)	-0.18	6 (2%)	55	50	8, 22, 49, 77	0
2	V	221/240 (92%)	-0.30	4 (1%)	67	64	3, 20, 44, 69	0
2	X	215/240 (89%)	-0.20	6 (2%)	55	50	8, 22, 49, 75	0
2	Z	214/240 (89%)	-0.19	2 (0%)	81	78	9, 23, 48, 64	0
All	All	6023/6832 (88%)	0.44	611 (10%)	12	10	3, 34, 86, 105	0

All (611) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	9	PRO	7.0
1	M	7	ILE	6.3
1	B	234	LEU	5.6
1	Y	233	LEU	5.0
1	W	7	ILE	4.9
1	Q	7	ILE	4.8
1	A	9	PRO	4.7
1	A	172	ALA	4.7
1	D	234	LEU	4.6
1	1	234	LEU	4.6
1	Y	234	LEU	4.5
1	O	234	LEU	4.4
1	Y	188	LEU	4.4
1	M	12	ALA	4.4
1	W	234	LEU	4.4
1	K	9	PRO	4.3
1	Y	184	ALA	4.3
1	S	175	ALA	4.3
1	Q	234	LEU	4.2
1	Y	9	PRO	4.1
1	O	13	MET	4.1
1	B	160	THR	4.1
1	Q	169	GLU	4.1
2	N	330	ASP	4.1
1	1	191	GLY	4.1
1	D	9	PRO	4.0
1	A	190	ALA	4.0
1	D	172	ALA	4.0
1	S	172	ALA	4.0
1	Y	172	ALA	4.0
1	I	9	PRO	4.0
1	W	175	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	190	ALA	3.9
1	Y	180	ALA	3.9
1	Y	131	GLY	3.9
1	I	234	LEU	3.9
1	S	188	LEU	3.9
2	R	392	ALA	3.9
1	O	165	ASN	3.8
1	Q	191	GLY	3.8
1	B	12	ALA	3.8
1	F	15	GLU	3.8
1	Q	160	THR	3.8
1	B	206	ALA	3.8
1	M	172	ALA	3.8
1	A	234	LEU	3.8
1	M	234	LEU	3.8
1	D	180	ALA	3.7
1	K	191	GLY	3.7
1	D	12	ALA	3.7
1	U	15	GLU	3.7
1	D	183	ILE	3.7
1	O	172	ALA	3.6
2	L	400	ALA	3.6
1	F	160	THR	3.6
1	K	175	ALA	3.6
1	U	234	LEU	3.6
2	R	400	ALA	3.6
1	U	9	PRO	3.6
1	F	162	PRO	3.6
1	O	161	GLU	3.5
1	Y	171	TYR	3.5
1	I	13	MET	3.5
1	M	8	SER	3.5
1	S	8	SER	3.5
1	U	160	THR	3.5
1	K	172	ALA	3.5
2	T	392	ALA	3.5
1	F	11	GLN	3.5
1	W	11	GLN	3.5
1	K	190	ALA	3.5
1	Q	166	ALA	3.5
1	1	172	ALA	3.5
1	W	13	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	S	234	LEU	3.5
1	F	166	ALA	3.5
1	Y	179	ASP	3.4
1	A	177	LEU	3.4
1	F	234	LEU	3.4
1	B	232	ALA	3.4
1	K	234	LEU	3.4
1	Y	12	ALA	3.4
2	J	400	ALA	3.4
2	L	392	ALA	3.4
1	A	171	TYR	3.4
2	G	330	ASP	3.4
1	U	206	ALA	3.4
2	X	400	ALA	3.4
1	Q	179	ASP	3.3
1	I	162	PRO	3.3
1	Q	165	ASN	3.3
1	Q	162	PRO	3.3
1	Q	181	LEU	3.3
1	D	48	ARG	3.3
1	D	179	ASP	3.3
1	K	150	GLU	3.3
1	S	191	GLY	3.3
1	D	177	LEU	3.3
1	F	12	ALA	3.3
1	Y	11	GLN	3.2
1	D	13	MET	3.2
1	M	160	THR	3.2
1	Y	166	ALA	3.2
1	U	166	ALA	3.2
1	I	166	ALA	3.2
1	I	178	THR	3.2
1	Q	177	LEU	3.2
1	D	191	GLY	3.2
2	Z	392	ALA	3.1
1	Q	10	GLU	3.1
1	B	171	TYR	3.1
1	Q	37	GLY	3.1
1	M	113	GLU	3.1
1	I	181	LEU	3.1
1	B	159	THR	3.1
1	O	160	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	1	182	ARG	3.1
1	B	11	GLN	3.1
1	I	180	ALA	3.1
1	B	13	MET	3.1
1	Q	13	MET	3.1
1	F	171	TYR	3.1
1	W	160	THR	3.1
1	D	175	ALA	3.1
1	Q	175	ALA	3.1
1	U	190	ALA	3.1
1	Y	175	ALA	3.1
1	B	10	GLU	3.1
1	U	13	MET	3.1
1	Q	203	LEU	3.1
1	K	183	ILE	3.1
1	B	175	ALA	3.0
1	I	190	ALA	3.0
1	M	175	ALA	3.0
1	Q	173	GLU	3.0
1	S	160	THR	3.0
1	1	160	THR	3.0
1	A	180	ALA	3.0
2	T	400	ALA	3.0
1	A	13	MET	3.0
1	U	10	GLU	3.0
1	M	136	PRO	3.0
1	K	180	ALA	3.0
1	S	25	ALA	3.0
1	U	18	GLU	3.0
1	Y	13	MET	3.0
2	C	433	GLU	3.0
2	P	392	ALA	3.0
1	Y	147	ILE	3.0
1	Y	190	ALA	3.0
1	S	171	TYR	3.0
1	A	188	LEU	3.0
1	D	182	ARG	3.0
1	Y	167	LEU	3.0
1	Y	111	PHE	3.0
1	F	163	ILE	2.9
1	U	48	ARG	2.9
1	U	181	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	179	ASP	2.9
1	A	191	GLY	2.9
1	D	169	GLU	2.9
1	Q	172	ALA	2.9
1	S	166	ALA	2.9
1	1	175	ALA	2.9
2	N	400	ALA	2.9
1	W	181	LEU	2.9
1	A	228	SER	2.9
1	I	10	GLU	2.9
1	K	42	VAL	2.9
1	M	178	THR	2.9
1	I	166	ALA	2.9
2	V	330	ASP	2.9
1	S	153	PHE	2.9
1	M	13	MET	2.9
1	D	10	GLU	2.9
1	M	163	ILE	2.9
1	Q	14	ARG	2.9
1	A	206	ALA	2.9
1	U	12	ALA	2.9
1	K	13	MET	2.9
1	Y	150	GLU	2.9
1	Q	182	ARG	2.8
1	Y	163	ILE	2.8
1	Y	174	ASN	2.8
1	D	27	ALA	2.8
1	O	166	ALA	2.8
1	1	148	ALA	2.8
2	H	391	LEU	2.8
1	A	150	GLU	2.8
1	F	14	ARG	2.8
1	U	8	SER	2.8
1	U	233	LEU	2.8
2	L	399	LEU	2.8
1	D	227	GLY	2.8
1	Y	29	SER	2.8
1	I	136	PRO	2.8
1	K	188	LEU	2.8
1	Y	177	LEU	2.8
1	Q	22	LYS	2.8
1	F	183	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	171	TYR	2.8
1	1	163	ILE	2.8
1	W	151	PRO	2.8
1	D	178	THR	2.8
1	K	112	THR	2.8
1	K	167	LEU	2.8
1	U	177	LEU	2.8
1	D	14	ARG	2.8
1	Y	14	ARG	2.8
1	F	181	LEU	2.7
1	Q	233	LEU	2.7
1	Y	160	THR	2.7
2	P	399	LEU	2.7
1	B	172	ALA	2.7
1	W	172	ALA	2.7
1	I	44	GLU	2.7
1	F	191	GLY	2.7
1	Y	38	GLY	2.7
1	Y	136	PRO	2.7
1	F	8	SER	2.7
1	F	36	ALA	2.7
1	O	159	THR	2.7
1	U	232	ALA	2.7
1	Y	178	THR	2.7
1	S	15	GLU	2.7
1	U	11	GLN	2.7
1	F	153	PHE	2.7
1	W	9	PRO	2.7
1	M	165	ASN	2.7
1	A	205	VAL	2.7
1	Y	30	VAL	2.7
1	B	177	LEU	2.7
1	I	177	LEU	2.7
1	B	166	ALA	2.7
1	Q	164	ALA	2.7
1	Y	148	ALA	2.7
1	F	169	GLU	2.7
1	W	183	ILE	2.7
1	D	160	THR	2.7
1	I	15	GLU	2.7
1	U	175	ALA	2.7
1	K	153	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	181	LEU	2.6
1	B	181	LEU	2.6
1	O	181	LEU	2.6
1	W	10	GLU	2.6
1	Y	170	SER	2.6
1	F	172	ALA	2.6
1	F	178	THR	2.6
1	O	148	ALA	2.6
1	S	190	ALA	2.6
1	U	231	GLN	2.6
2	E	392	ALA	2.6
1	D	131	GLY	2.6
1	S	9	PRO	2.6
1	B	167	LEU	2.6
1	K	203	LEU	2.6
1	M	181	LEU	2.6
2	X	391	LEU	2.6
1	F	10	GLU	2.6
1	S	44	GLU	2.6
2	2	432	GLU	2.6
1	O	8	SER	2.6
1	O	175	ALA	2.6
1	Q	36	ALA	2.6
1	W	12	ALA	2.6
1	D	171	TYR	2.6
1	M	179	ASP	2.6
1	Y	183	ILE	2.6
1	D	181	LEU	2.6
1	Q	167	LEU	2.6
1	1	167	LEU	2.6
2	R	432	GLU	2.6
1	A	160	THR	2.6
1	O	178	THR	2.6
1	W	190	ALA	2.6
1	1	186	ALA	2.6
1	B	136	PRO	2.6
1	O	9	PRO	2.6
1	S	204	GLY	2.6
2	T	330	ASP	2.6
1	Q	183	ILE	2.6
1	A	230	LEU	2.6
1	B	18	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	177	LEU	2.6
2	V	391	LEU	2.6
1	B	17	SER	2.6
1	K	170	SER	2.6
1	F	159	THR	2.6
1	M	229	ALA	2.6
2	C	392	ALA	2.6
1	M	143	TYR	2.6
1	1	13	MET	2.5
2	J	330	ASP	2.5
2	L	330	ASP	2.5
1	M	161	GLU	2.5
1	S	177	LEU	2.5
1	1	152	HIS	2.5
1	S	206	ALA	2.5
2	V	392	ALA	2.5
2	2	392	ALA	2.5
1	K	133	THR	2.5
1	1	159	THR	2.5
1	K	171	TYR	2.5
2	X	330	ASP	2.5
1	S	163	ILE	2.5
1	F	173	GLU	2.5
1	K	111	PHE	2.5
1	O	154	VAL	2.5
1	A	12	ALA	2.5
1	F	164	ALA	2.5
1	I	12	ALA	2.5
1	I	164	ALA	2.5
1	1	25	ALA	2.5
2	G	400	ALA	2.5
2	2	400	ALA	2.5
1	I	160	THR	2.5
1	B	162	PRO	2.5
1	Y	130	TYR	2.5
1	A	147	ILE	2.5
1	B	163	ILE	2.5
1	U	163	ILE	2.5
1	B	230	LEU	2.5
1	S	181	LEU	2.5
2	X	399	LEU	2.5
1	B	152	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	1	178	THR	2.5
1	Q	44	GLU	2.5
1	O	163	ILE	2.5
1	Y	149	ASP	2.5
1	1	183	ILE	2.5
1	1	188	LEU	2.5
2	2	391	LEU	2.5
1	I	31	VAL	2.5
1	Q	26	ARG	2.5
1	A	175	ALA	2.5
1	Y	164	ALA	2.5
1	1	190	ALA	2.5
1	W	162	PRO	2.4
1	U	44	GLU	2.4
1	Q	147	ILE	2.4
2	R	330	ASP	2.4
1	F	167	LEU	2.4
2	E	399	LEU	2.4
1	S	182	ARG	2.4
1	K	154	VAL	2.4
1	Y	185	VAL	2.4
1	K	184	ALA	2.4
1	K	186	ALA	2.4
1	K	160	THR	2.4
1	1	112	THR	2.4
1	D	136	PRO	2.4
1	B	209	GLU	2.4
1	Y	168	LYS	2.4
1	K	179	ASP	2.4
1	B	233	LEU	2.4
1	B	14	ARG	2.4
1	F	175	ALA	2.4
1	Y	128	ALA	2.4
2	J	392	ALA	2.4
1	W	161	GLU	2.4
2	C	432	GLU	2.4
1	B	147	ILE	2.4
1	O	183	ILE	2.4
2	2	330	ASP	2.4
1	F	105	GLN	2.4
1	M	51	GLN	2.4
1	M	233	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	R	391	LEU	2.4
2	T	399	LEU	2.4
1	I	26	ARG	2.4
1	Q	48	ARG	2.4
1	I	171	TYR	2.4
1	B	42	VAL	2.4
1	Q	154	VAL	2.4
1	K	166	ALA	2.4
1	I	150	GLU	2.4
1	M	9	PRO	2.4
1	U	162	PRO	2.4
1	B	204	GLY	2.4
1	A	11	GLN	2.4
1	A	179	ASP	2.4
1	F	177	LEU	2.4
2	R	399	LEU	2.4
1	W	143	TYR	2.4
1	M	166	ALA	2.4
1	O	184	ALA	2.4
1	Y	206	ALA	2.4
1	I	184	ALA	2.4
1	B	169	GLU	2.4
1	I	161	GLU	2.4
1	O	150	GLU	2.4
1	O	173	GLU	2.4
2	L	433	GLU	2.4
1	D	49	SER	2.3
1	D	50	LEU	2.3
2	C	330	ASP	2.3
1	Y	205	VAL	2.3
1	D	190	ALA	2.3
1	I	175	ALA	2.3
1	M	150	GLU	2.3
1	O	15	GLU	2.3
1	W	180	ALA	2.3
1	W	184	ALA	2.3
2	H	432	GLU	2.3
1	D	228	SER	2.3
1	M	11	GLN	2.3
1	I	188	LEU	2.3
1	M	230	LEU	2.3
1	U	153	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	Y	154	VAL	2.3
1	O	18	GLU	2.3
2	J	433	GLU	2.3
1	F	165	ASN	2.3
1	A	232	ALA	2.3
1	I	162	PRO	2.3
1	Q	9	PRO	2.3
1	Y	187	ALA	2.3
1	B	227	GLY	2.3
1	K	152	HIS	2.3
1	1	147	ILE	2.3
2	T	391	LEU	2.3
1	1	149	ASP	2.3
1	B	15	GLU	2.3
1	D	42	VAL	2.3
1	Q	15	GLU	2.3
1	U	31	VAL	2.3
1	K	162	PRO	2.3
1	W	14	ARG	2.3
1	D	233	LEU	2.3
1	K	163	ILE	2.3
1	O	177	LEU	2.3
1	S	183	ILE	2.3
1	Y	181	LEU	2.3
2	E	391	LEU	2.3
2	G	399	LEU	2.3
1	B	179	ASP	2.3
1	F	44	GLU	2.3
1	1	111	PHE	2.3
1	K	31	VAL	2.3
1	B	48	ARG	2.3
1	I	48	ARG	2.3
1	B	36	ALA	2.2
1	O	171	TYR	2.3
1	S	27	ALA	2.2
1	S	180	ALA	2.2
1	1	171	TYR	2.3
2	X	392	ALA	2.2
1	B	178	THR	2.2
1	Y	133	THR	2.2
1	O	191	GLY	2.2
1	Q	131	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	S	38	GLY	2.2
1	F	13	MET	2.2
1	M	17	SER	2.2
1	W	225	ILE	2.2
1	I	179	ASP	2.2
1	D	15	GLU	2.2
1	A	48	ARG	2.2
1	I	14	ARG	2.2
1	M	184	ALA	2.2
1	Y	186	ALA	2.2
1	W	171	TYR	2.2
1	Q	159	THR	2.2
1	O	28	LYS	2.2
1	I	168	LYS	2.2
1	I	203	LEU	2.2
1	K	177	LEU	2.2
1	W	233	LEU	2.2
1	M	49	SER	2.2
1	Q	17	SER	2.2
1	O	169	GLU	2.2
1	W	169	GLU	2.2
2	T	432	GLU	2.2
2	Z	432	GLU	2.2
1	I	21	ARG	2.2
1	U	21	ARG	2.2
1	W	153	PHE	2.2
1	M	185	VAL	2.2
1	A	164	ALA	2.2
1	F	229	ALA	2.2
1	S	36	ALA	2.2
1	I	165	ASN	2.2
1	F	188	LEU	2.2
1	W	203	LEU	2.2
1	M	183	ILE	2.2
2	H	330	ASP	2.2
2	J	413	ASP	2.2
1	S	113	GLU	2.2
1	W	119	GLU	2.2
1	Y	44	GLU	2.2
2	C	519	GLU	2.2
1	B	182	ARG	2.2
1	O	153	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	Y	162	PRO	2.2
1	Y	210	VAL	2.2
1	B	164	ALA	2.2
1	D	186	ALA	2.2
1	S	164	ALA	2.2
1	W	174	ASN	2.2
1	Y	232	ALA	2.2
1	1	164	ALA	2.2
2	V	400	ALA	2.2
1	K	51	GLN	2.2
1	Q	178	THR	2.2
1	U	159	THR	2.2
1	A	167	LEU	2.2
1	A	233	LEU	2.2
1	F	157	GLY	2.2
1	K	131	GLY	2.2
1	Y	37	GLY	2.2
1	Y	204	GLY	2.2
1	W	176	SER	2.2
1	M	44	GLU	2.2
1	Q	161	GLU	2.2
1	O	92	ARG	2.2
1	B	9	PRO	2.2
1	K	151	PRO	2.2
1	D	231	GLN	2.1
1	F	180	ALA	2.1
1	Q	180	ALA	2.1
1	U	172	ALA	2.1
1	W	25	ALA	2.1
1	A	112	THR	2.1
1	F	112	THR	2.1
1	U	230	LEU	2.1
1	U	171	TYR	2.1
1	B	173	GLU	2.1
1	K	44	GLU	2.1
1	Y	137	GLU	2.1
2	X	432	GLU	2.1
1	U	49	SER	2.1
1	F	30	VAL	2.1
1	D	133	THR	2.1
1	M	159	THR	2.1
1	O	157	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	163	ILE	2.1
1	I	183	ILE	2.1
1	Q	163	ILE	2.1
1	A	15	GLU	2.1
1	B	135	ARG	2.1
1	K	48	ARG	2.1
2	R	434	GLU	2.1
1	M	28	LYS	2.1
1	Y	28	LYS	2.1
1	U	46	PRO	2.1
1	1	153	PHE	2.1
1	S	231	GLN	2.1
1	I	206	ALA	2.1
1	K	148	ALA	2.1
1	Q	12	ALA	2.1
1	U	164	ALA	2.1
1	B	174	ASN	2.1
1	S	48	ARG	2.1
1	U	189	ARG	2.1
1	A	169	GLU	2.1
1	F	18	GLU	2.1
1	F	161	GLU	2.1
1	M	132	GLU	2.1
1	W	147	ILE	2.1
1	Y	10	GLU	2.1
1	1	137	GLU	2.1
1	B	22	LYS	2.1
1	W	168	LYS	2.1
1	K	47	SER	2.1
1	I	11	GLN	2.1
1	O	185	VAL	2.1
1	A	186	ALA	2.1
1	M	164	ALA	2.1
1	W	148	ALA	2.1
1	W	187	ALA	2.1
1	1	12	ALA	2.1
1	1	232	ALA	2.1
1	M	157	GLY	2.1
1	A	159	THR	2.1
1	M	15	GLU	2.1
1	W	137	GLU	2.1
1	Q	149	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	179	ASP	2.1
1	U	93	ASP	2.1
1	1	179	ASP	2.1
2	P	330	ASP	2.1
1	K	146	SER	2.1
1	Y	49	SER	2.1
1	D	151	PRO	2.1
1	M	151	PRO	2.1
1	I	153	PHE	2.0
1	B	180	ALA	2.0
1	I	186	ALA	2.0
1	Q	190	ALA	2.0
1	U	148	ALA	2.0
2	C	400	ALA	2.0
1	D	188	LEU	2.0
1	Q	230	LEU	2.0
1	W	167	LEU	2.0
1	U	178	THR	2.0
1	U	143	TYR	2.0
1	Y	151	PRO	2.0
1	Y	228	SER	2.0
1	B	208	LEU	2.0
1	I	167	LEU	2.0
1	I	230	LEU	2.0
1	K	233	LEU	2.0
1	M	206	ALA	2.0
1	Q	50	LEU	2.0
1	U	186	ALA	2.0
1	O	226	THR	2.0
1	W	178	THR	2.0
1	U	151	PRO	2.0
1	Y	156	MET	2.0
1	W	49	SER	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	OZT	L	301	9/10	0.93	0.08	19,24,26,27	0
2	OZT	X	301	9/10	0.93	0.08	19,21,23,26	0
2	OZT	J	301	9/10	0.94	0.07	19,23,27,31	0
2	OZT	G	301	9/10	0.94	0.07	21,24,29,32	0
2	OZT	P	301	9/10	0.94	0.07	23,28,30,33	0
2	OZT	V	301	9/10	0.94	0.08	20,22,27,31	0
2	OZT	H	301	9/10	0.94	0.08	22,24,25,28	0
2	OZT	R	301	9/10	0.95	0.07	20,23,27,28	0
2	OZT	2	301	9/10	0.95	0.08	25,31,33,35	0
2	OZT	N	301	9/10	0.96	0.06	21,24,27,31	0
2	OZT	Z	301	9/10	0.96	0.06	19,21,23,24	0
2	OZT	C	301	9/10	0.96	0.06	18,23,26,29	0
2	OZT	T	301	9/10	0.97	0.05	22,22,24,25	0
2	OZT	E	301	9/10	0.98	0.04	20,23,25,27	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DMF	H	32	5/5	0.45	0.29	73,74,75,76	0
3	DMF	X	40	5/5	0.55	0.34	92,93,93,93	0
3	DMF	P	51	5/5	0.60	0.31	76,76,76,76	0
3	DMF	1	250	5/5	0.68	0.31	61,62,63,63	0
3	DMF	2	49	5/5	0.69	0.43	93,93,94,94	0
3	DMF	P	14	5/5	0.70	0.42	90,91,92,92	0
3	DMF	V	39	5/5	0.71	0.28	72,72,72,72	0
3	DMF	G	64	5/5	0.71	0.29	56,57,58,58	0
3	DMF	J	45	5/5	0.73	0.36	85,85,85,85	0
3	DMF	E	20	5/5	0.74	0.34	84,84,85,85	0
3	DMF	K	250	5/5	0.74	0.24	57,59,59,60	0
3	DMF	E	66	5/5	0.75	0.28	65,65,66,67	0
3	DMF	Z	41	5/5	0.75	0.34	93,93,93,93	0
3	DMF	G	12	5/5	0.76	0.24	66,67,67,67	0
3	DMF	Z	54	5/5	0.77	0.34	85,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DMF	N	58	5/5	0.77	0.25	54,56,58,59	0
3	DMF	C	47	5/5	0.77	0.27	71,71,71,72	0
3	DMF	J	4	5/5	0.78	0.21	60,61,61,62	0
3	DMF	C	38	5/5	0.78	0.23	63,64,64,65	0
3	DMF	R	59	5/5	0.78	0.25	58,59,60,60	0
3	DMF	K	251	5/5	0.79	0.20	60,62,62,62	0
3	DMF	M	250	5/5	0.79	0.16	39,40,41,41	0
3	DMF	I	249	5/5	0.80	0.23	55,56,58,59	0
3	DMF	N	22	5/5	0.80	0.35	91,92,92,92	0
3	DMF	2	52	5/5	0.80	0.27	75,75,76,76	0
3	DMF	B	249	5/5	0.81	0.17	47,47,48,48	0
3	DMF	H	26	5/5	0.82	0.23	64,64,65,65	0
3	DMF	D	249	5/5	0.82	0.18	53,53,53,54	0
3	DMF	L	53	5/5	0.83	0.27	84,84,85,86	0
3	DMF	C	10	5/5	0.83	0.17	42,45,46,48	0
3	DMF	N	2	5/5	0.83	0.23	69,69,70,70	0
3	DMF	G	24	5/5	0.83	0.29	80,80,81,82	0
3	DMF	L	3	5/5	0.83	0.22	57,58,59,60	0
3	DMF	C	55	5/5	0.85	0.23	74,74,74,74	0
3	DMF	F	249	5/5	0.85	0.22	70,71,71,71	0
3	DMF	P	56	5/5	0.85	0.24	64,64,64,65	0
3	DMF	X	61	5/5	0.85	0.17	55,56,58,60	0
3	DMF	Z	18	5/5	0.85	0.35	97,98,98,99	0
3	DMF	B	250	5/5	0.86	0.23	77,78,78,79	0
3	DMF	T	67	5/5	0.86	0.21	51,51,53,53	0
3	DMF	1	249	5/5	0.86	0.16	49,51,51,52	0
3	DMF	P	65	5/5	0.87	0.17	50,51,52,52	0
3	DMF	W	249	5/5	0.88	0.29	76,76,77,78	0
3	DMF	G	60	5/5	0.88	0.18	50,52,52,52	0
3	DMF	Z	43	5/5	0.89	0.17	48,48,49,49	0
3	DMF	R	34	5/5	0.89	0.22	68,69,70,71	0
3	DMF	M	249	5/5	0.89	0.15	54,54,55,56	0
3	DMF	T	29	5/5	0.89	0.18	63,63,63,63	0
3	DMF	O	249	5/5	0.89	0.16	46,47,48,50	0
3	DMF	H	62	5/5	0.89	0.17	42,43,45,47	0
3	DMF	N	15	5/5	0.90	0.13	44,46,47,47	0
3	DMF	Z	30	5/5	0.90	0.16	56,56,57,57	0
3	DMF	Q	249	5/5	0.90	0.13	49,49,50,50	0
3	DMF	G	1	5/5	0.91	0.14	42,44,45,46	0
3	DMF	H	33	5/5	0.91	0.14	39,40,41,41	0
3	DMF	X	16	5/5	0.91	0.14	46,46,47,48	0
3	DMF	E	28	5/5	0.91	0.16	45,47,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DMF	S	249	5/5	0.91	0.23	79,80,81,81	0
3	DMF	J	50	5/5	0.91	0.16	57,58,58,58	0
3	DMF	K	249	5/5	0.91	0.14	51,53,54,55	0
3	DMF	U	249	5/5	0.92	0.15	51,51,52,52	0
3	DMF	V	27	5/5	0.92	0.27	77,77,78,79	0
3	DMF	2	42	5/5	0.92	0.17	54,54,55,55	0
3	DMF	A	249	5/5	0.92	0.17	60,61,62,62	0
3	DMF	L	36	5/5	0.92	0.14	57,57,58,58	0
3	DMF	2	63	5/5	0.92	0.12	43,45,45,46	0
3	DMF	I	250	5/5	0.93	0.14	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.