wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:44 AM GMT

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

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

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

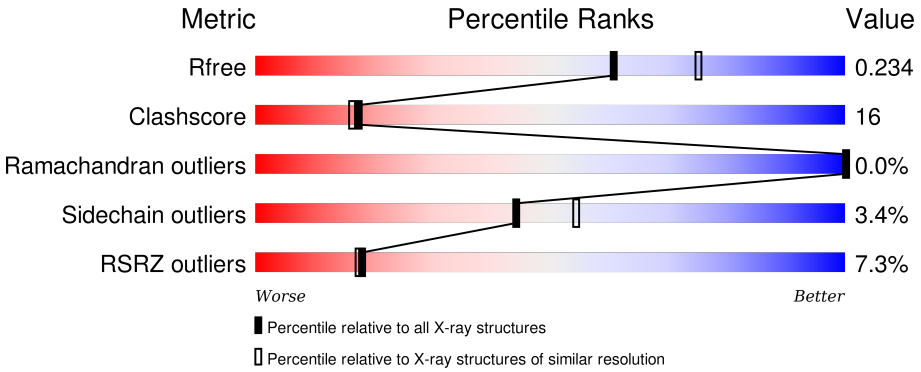
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	1	248	8% 64% 21% • 13%
1	A	248	13% 60% 24% • 13%
1	B	248	8% 59% 24% • 14%
1	D	248	25% 50% 34% • 14%
1	F	248	7% 60% 27% • 11%

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Mol	Chain	Length	Quality of chain
1	I	248	12% 54% 31% • 13%
1	K	248	9% 60% 24% • 13%
1	M	248	14% 54% 29% • 13%
1	O	248	10% 60% 26% • 13%
1	Q	248	9% 56% 29% • 13%
1	S	248	15% 55% 30% • 13%
1	U	248	11% 63% 23% • 13%
1	W	248	19% 54% 31% • 13%
1	Y	248	15% 56% 30% • 13%
2	2	240	80% 11% • 7%
2	C	240	% 78% 14% 8%
2	E	240	% 76% 16% • 7%
2	G	240	78% 14% 8%
2	H	240	82% 11% 8%
2	J	240	80% 12% • 8%
2	L	240	80% 12% • 7%
2	N	240	76% 16% 8%
2	P	240	82% 10% 8%
2	R	240	2% 84% 14% •
2	T	240	81% 12% 7%
2	V	240	% 85% 13% •
2	X	240	2% 82% 11% 7%
2	Z	240	% 81% 11% • 7%

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	1	249	-	-	-	X
3	DMF	2	101	-	-	-	X
3	DMF	2	108	-	-	X	X
3	DMF	2	112	-	-	X	X
3	DMF	2	4	-	-	X	X
3	DMF	2	49	-	-	-	X
3	DMF	2	52	-	-	-	X
3	DMF	2	57	-	-	-	X
3	DMF	2	87	-	-	-	X
3	DMF	A	249	-	-	-	X
3	DMF	A	250	-	-	-	X
3	DMF	B	249	-	-	-	X
3	DMF	B	250	-	-	-	X
3	DMF	C	103	-	-	X	X
3	DMF	C	47	-	-	-	X
3	DMF	C	63	-	-	-	X
3	DMF	C	88	-	-	-	X
3	DMF	D	249	-	-	-	X
3	DMF	D	250	-	-	-	X
3	DMF	D	251	-	-	X	X
3	DMF	D	252	-	-	-	X
3	DMF	D	253	-	-	-	X
3	DMF	E	20	-	-	X	X
3	DMF	E	28	-	-	-	X
3	DMF	E	53	-	-	-	X
3	DMF	E	75	-	-	X	X
3	DMF	F	249	-	-	-	X
3	DMF	F	250	-	-	-	X
3	DMF	F	251	-	-	-	X
3	DMF	G	111	-	-	-	X
3	DMF	G	119	-	-	X	X
3	DMF	G	12	-	-	X	X
3	DMF	G	24	-	-	-	X
3	DMF	G	62	-	-	-	X
3	DMF	G	64	-	-	X	X
3	DMF	G	70	-	-	-	X
3	DMF	G	77	-	-	-	X
3	DMF	G	98	-	-	-	X
3	DMF	H	117	-	-	-	X
3	DMF	H	43	-	-	X	X
3	DMF	H	72	-	-	-	X
3	DMF	I	249	-	-	-	X
3	DMF	I	250	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DMF	J	110	-	-	-	X
3	DMF	J	123	-	-	X	X
3	DMF	J	45	-	-	-	X
3	DMF	K	249	-	-	-	X
3	DMF	K	250	-	-	X	X
3	DMF	K	251	-	-	-	X
3	DMF	L	36	-	-	-	X
3	DMF	L	81	-	-	-	X
3	DMF	L	97	-	-	X	X
3	DMF	M	249	-	-	-	X
3	DMF	M	250	-	-	-	X
3	DMF	M	251	-	-	-	X
3	DMF	M	252	-	-	-	X
3	DMF	N	104	-	-	X	X
3	DMF	N	118	-	-	X	X
3	DMF	N	22	-	-	X	-
3	DMF	N	90	-	-	X	X
3	DMF	N	93	-	-	X	X
3	DMF	O	249	-	-	-	X
3	DMF	O	250	-	-	-	X
3	DMF	O	251	-	-	-	X
3	DMF	P	107	-	-	X	X
3	DMF	P	14	-	-	X	X
3	DMF	P	2	-	-	-	X
3	DMF	P	56	-	-	-	X
3	DMF	P	60	-	-	-	X
3	DMF	Q	249	-	-	-	X
3	DMF	Q	250	-	-	X	X
3	DMF	Q	251	-	-	-	X
3	DMF	R	59	-	-	X	X
3	DMF	R	89	-	-	-	X
3	DMF	R	95	-	-	-	X
3	DMF	S	249	-	-	-	X
3	DMF	S	250	-	-	-	X
3	DMF	T	10	-	-	-	X
3	DMF	T	102	-	-	-	X
3	DMF	T	113	-	-	X	X
3	DMF	T	115	-	-	-	X
3	DMF	T	29	-	-	-	X
3	DMF	T	84	-	-	-	X
3	DMF	U	249	-	-	-	X
3	DMF	U	250	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DMF	V	109	-	-	-	X
3	DMF	V	116	-	-	X	-
3	DMF	V	120	-	-	X	X
3	DMF	V	27	-	-	X	X
3	DMF	V	32	-	-	X	X
3	DMF	V	39	-	-	-	X
3	DMF	V	42	-	-	X	X
3	DMF	V	82	-	-	-	X
3	DMF	V	83	-	-	X	X
3	DMF	W	249	-	-	-	X
3	DMF	W	250	-	-	X	X
3	DMF	X	122	-	-	-	X
3	DMF	X	15	-	-	-	X
3	DMF	X	16	-	-	-	X
3	DMF	X	41	-	-	-	X
3	DMF	Y	249	-	-	-	X
3	DMF	Y	250	-	-	-	X
3	DMF	Y	251	-	-	-	X
3	DMF	Z	114	-	-	-	X
3	DMF	Z	18	-	-	-	X
3	DMF	Z	54	-	-	-	X
3	DMF	Z	94	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 50080 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit alpha.

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

- Molecule 2 is a protein called Proteasome subunit beta.

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

There are 84 discrepancies between the modelled and reference sequences:

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

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

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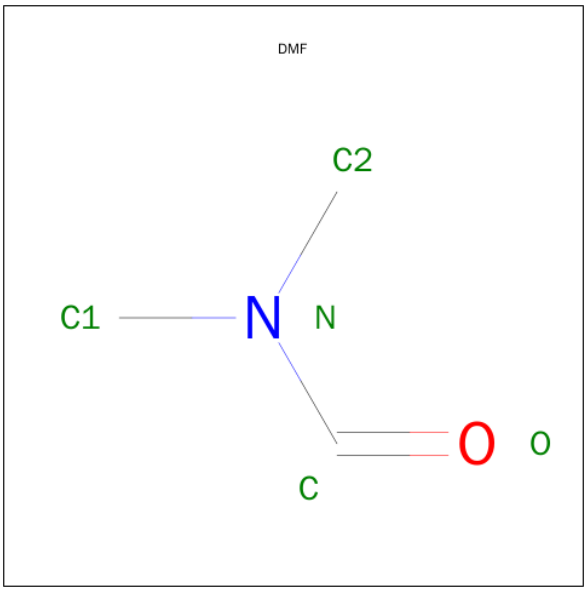
Chain	Residue	Modelled	Actual	Comment	Reference
T	535	HIS	-	EXPRESSION TAG	UNP O33245
T	536	HIS	-	EXPRESSION TAG	UNP O33245
T	537	HIS	-	EXPRESSION TAG	UNP O33245
T	538	HIS	-	EXPRESSION TAG	UNP O33245
T	539	HIS	-	EXPRESSION TAG	UNP O33245
T	540	HIS	-	EXPRESSION TAG	UNP O33245
V	535	HIS	-	EXPRESSION TAG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

- Molecule 3 is DIMETHYLFORMAMIDE (three-letter code: 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	A	1	Total	C	N	O	0	0
			5	3	1	1		
3	B	1	Total	C	N	O	0	0
			5	3	1	1		
3	B	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	D	1	Total	C	N	O	0	0
			5	3	1	1		
3	D	1	Total	C	N	O	0	0
			5	3	1	1		
3	D	1	Total	C	N	O	0	0
			5	3	1	1		

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

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

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

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

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

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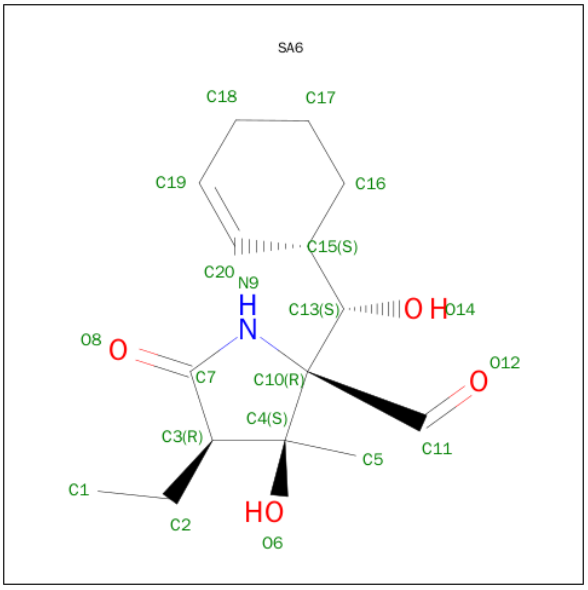
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	2	1	Total C N O 5 3 1 1	0	0
3	2	1	Total C N O 5 3 1 1	0	0
3	2	1	Total C N O 5 3 1 1	0	0
3	2	1	Total C N O 5 3 1 1	0	0

- Molecule 4 is (2R,3S,4R)-2-[(S)-(1S)-CYCLOHEX-2-EN-1-YL(HYDROXY)METHYL]-4-ETHYL-3-HYDROXY-3-METHYL-5-OXOPYRROLIDINE-2-CARBALDEHYDE (three-letter code: SA6) (formula: $C_{15}H_{23}NO_4$).



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

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

- Molecule 5 is water.

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

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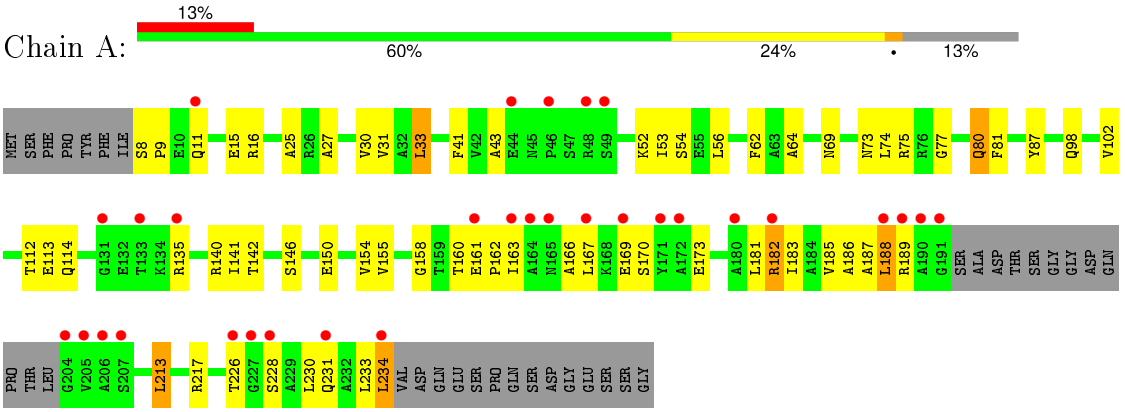
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	153	Total O 153 153	0	0
5	M	40	Total O 40 40	0	0
5	N	154	Total O 154 154	0	0
5	O	47	Total O 47 47	0	0
5	P	139	Total O 139 139	0	0
5	Q	38	Total O 38 38	0	0
5	R	170	Total O 170 170	0	0
5	S	42	Total O 42 42	0	0
5	T	116	Total O 116 116	0	0
5	U	49	Total O 49 49	0	0
5	V	177	Total O 177 177	0	0
5	W	35	Total O 35 35	0	0
5	X	150	Total O 150 150	0	0
5	Y	28	Total O 28 28	0	0
5	Z	123	Total O 123 123	0	0
5	1	47	Total O 47 47	0	0
5	2	143	Total O 143 143	0	0

3 Residue-property plots (i)

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

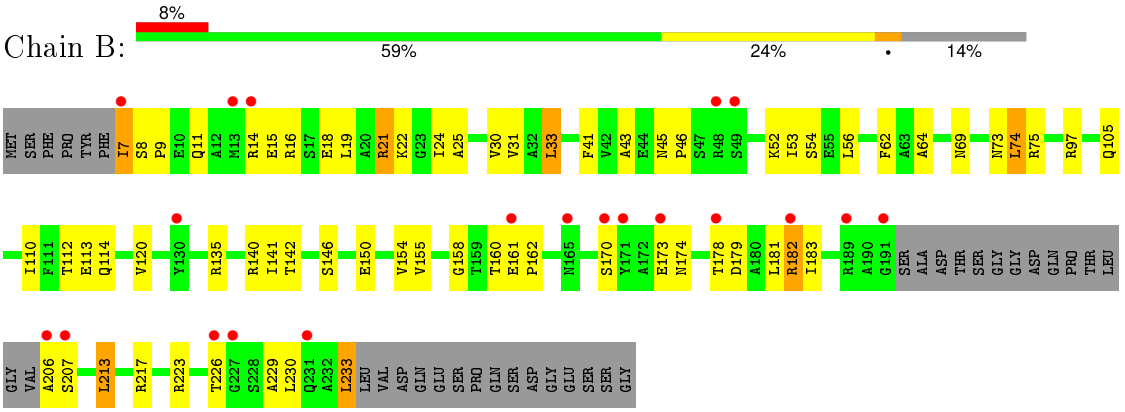
- Molecule 1: Proteasome subunit alpha

Chain A:



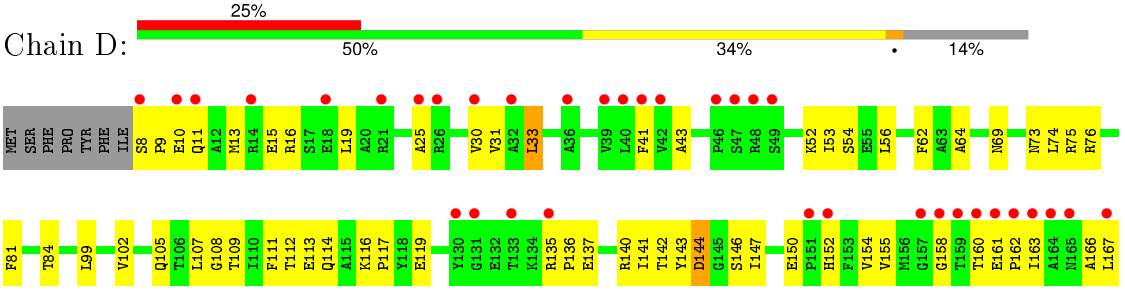
- Molecule 1: Proteasome subunit alpha

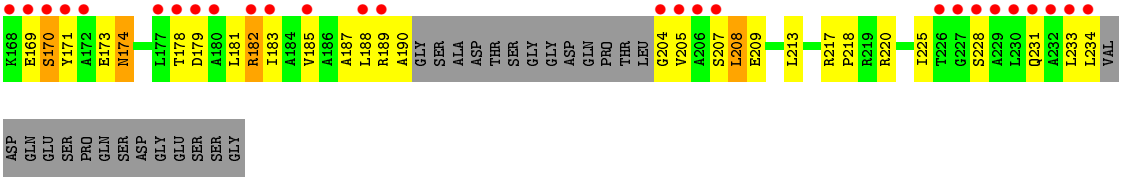
Chain B:



- Molecule 1: Proteasome subunit alpha

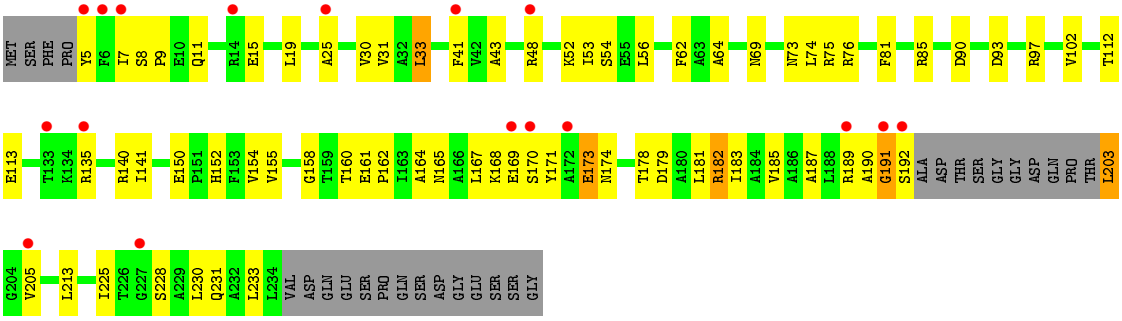
Chain D:





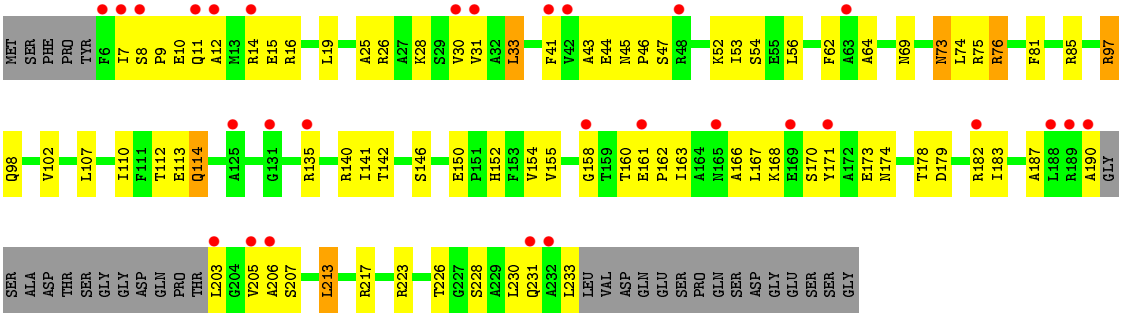
• Molecule 1: Proteasome subunit alpha

Chain F:



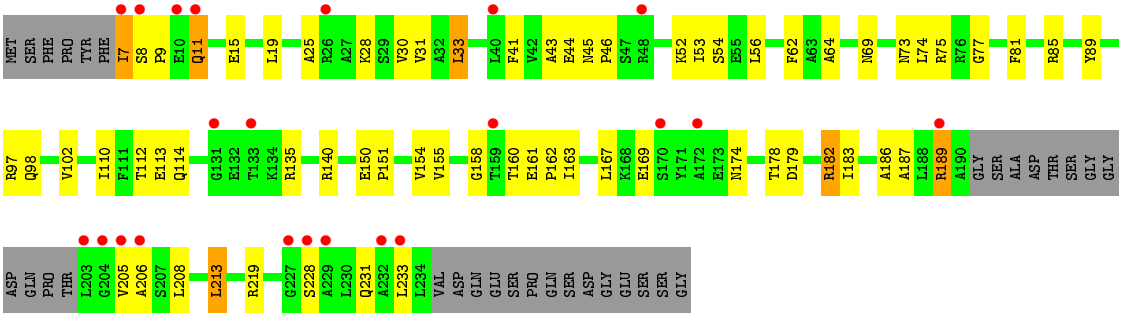
• Molecule 1: Proteasome subunit alpha

Chain I:



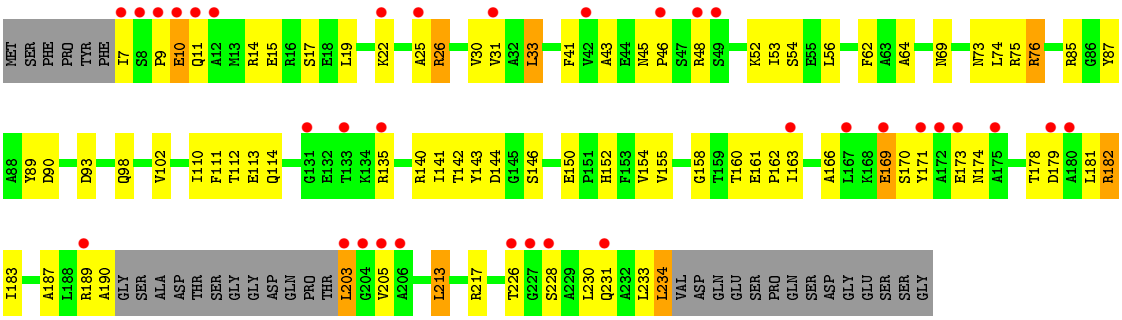
• Molecule 1: Proteasome subunit alpha

Chain K:



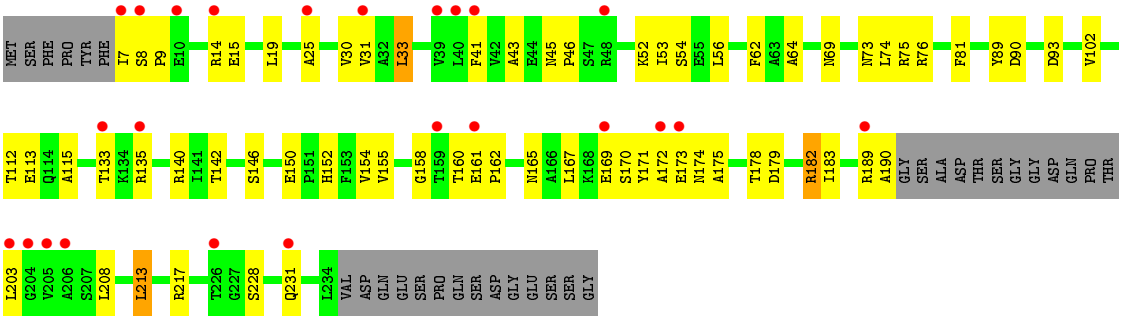
• Molecule 1: Proteasome subunit alpha

Chain M:



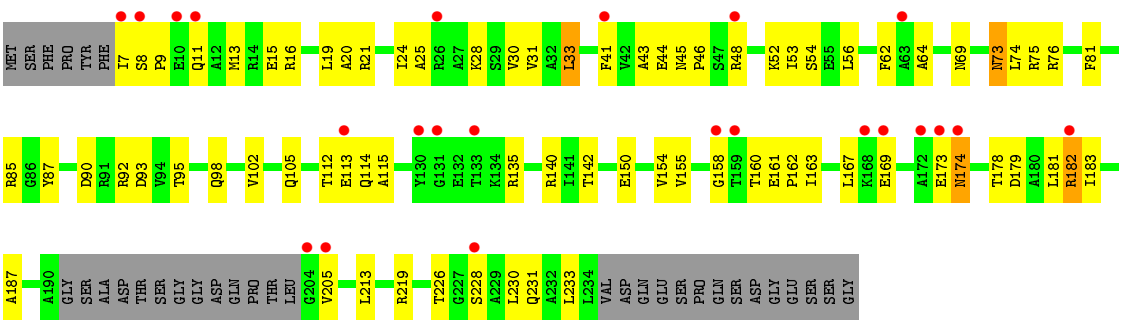
• Molecule 1: Proteasome subunit alpha

Chain O:



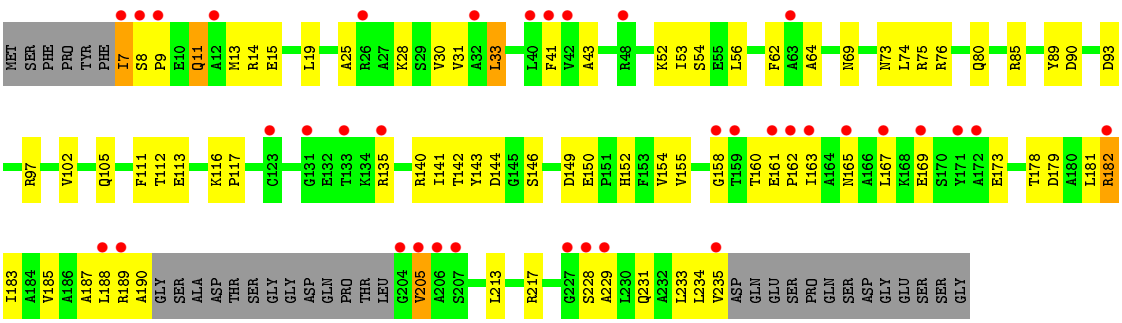
• Molecule 1: Proteasome subunit alpha

Chain Q:



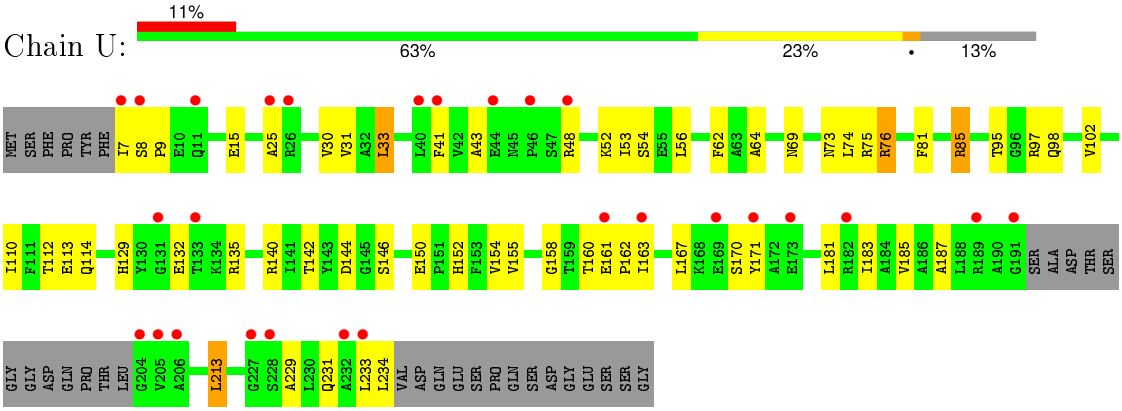
• Molecule 1: Proteasome subunit alpha

Chain S:



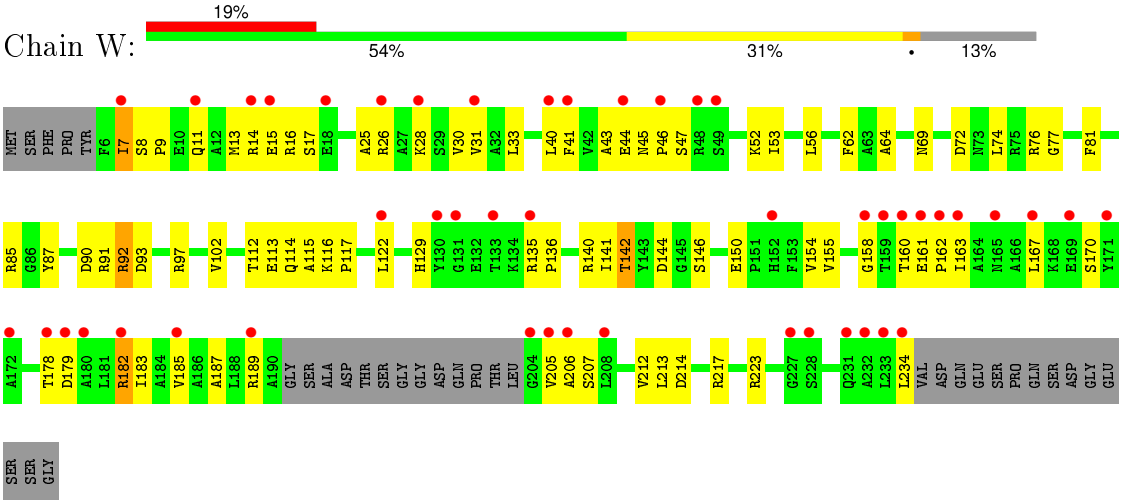
- Molecule 1: Proteasome subunit alpha

Chain U:



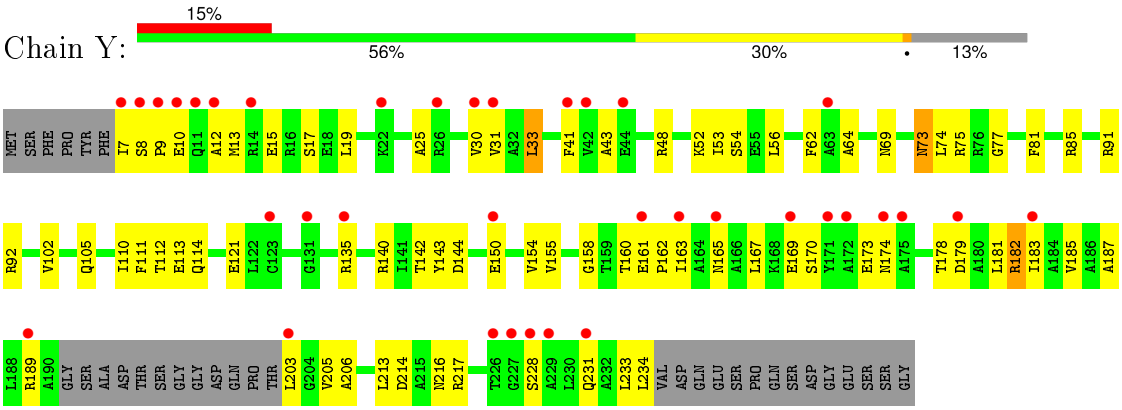
- Molecule 1: Proteasome subunit alpha

Chain W:



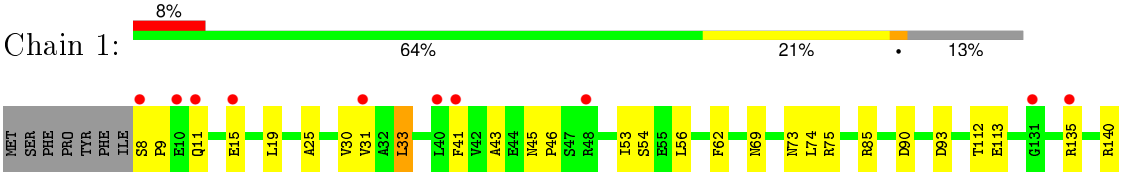
- Molecule 1: Proteasome subunit alpha

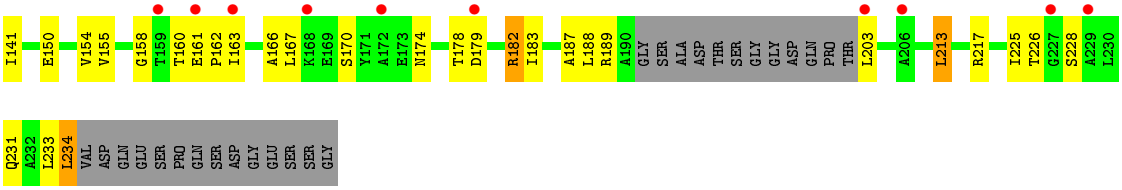
Chain Y:



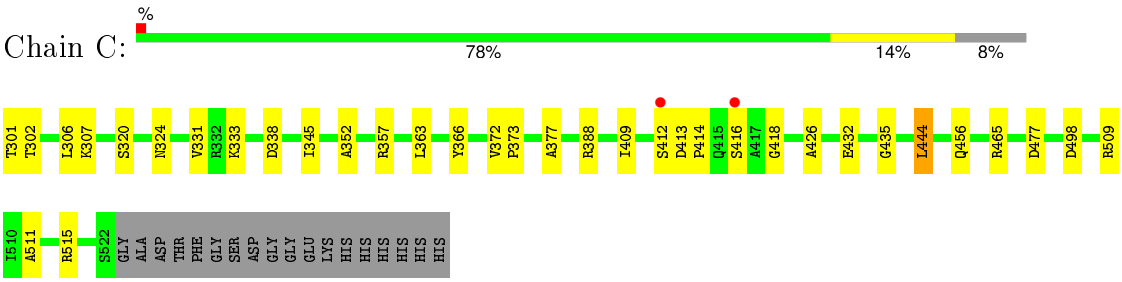
- Molecule 1: Proteasome subunit alpha

Chain 1:

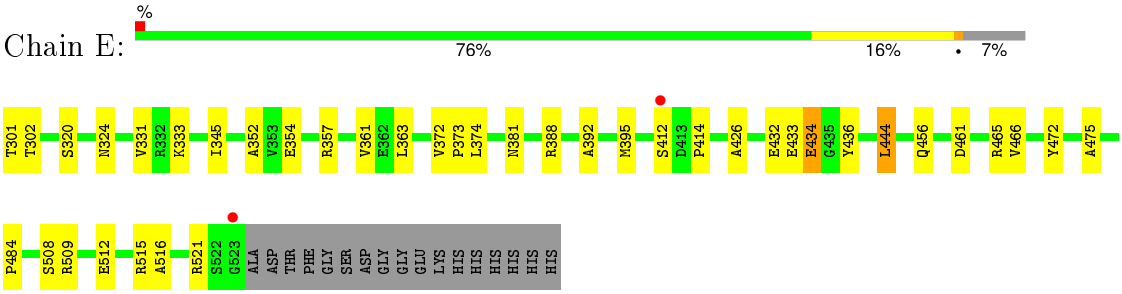




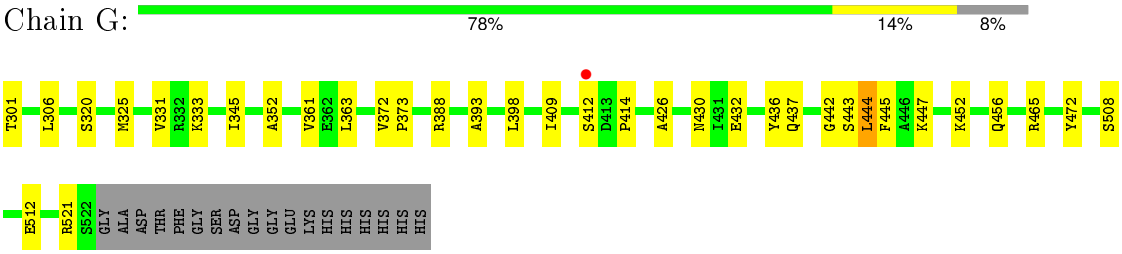
• Molecule 2: Proteasome subunit beta



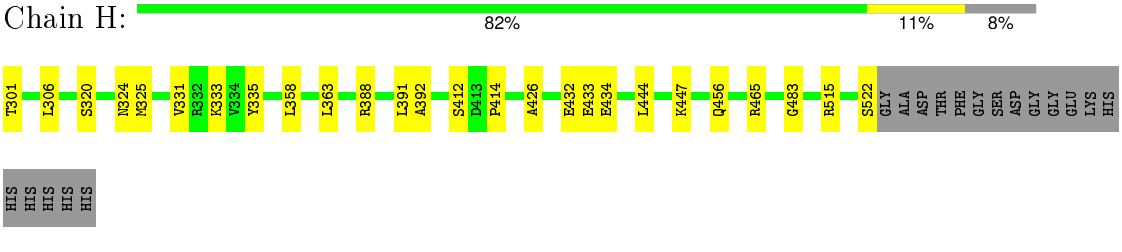
• Molecule 2: Proteasome subunit beta



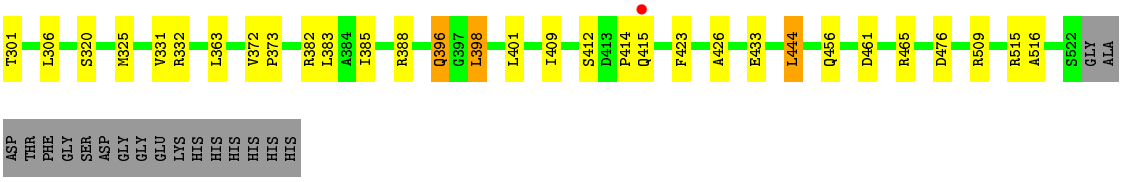
• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta

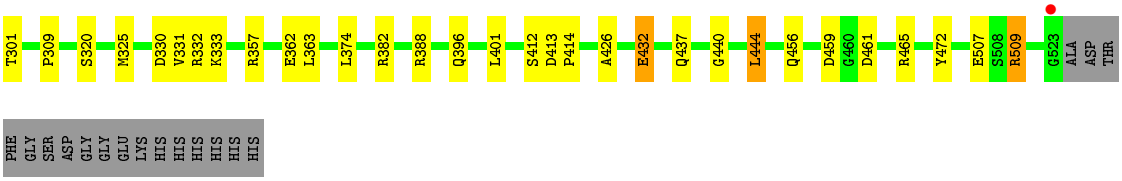


• Molecule 2: Proteasome subunit beta



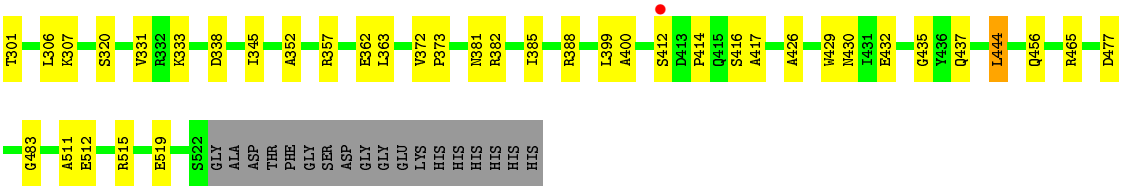
• Molecule 2: Proteasome subunit beta

Chain L:



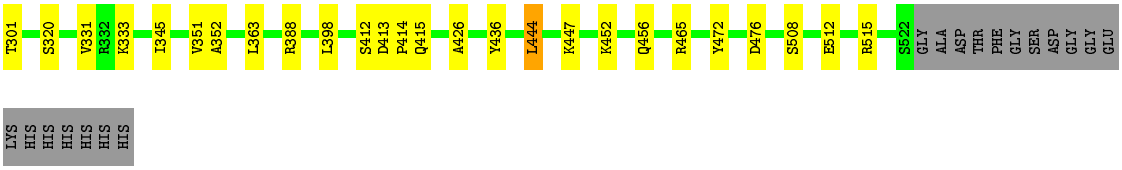
• Molecule 2: Proteasome subunit beta

Chain N:



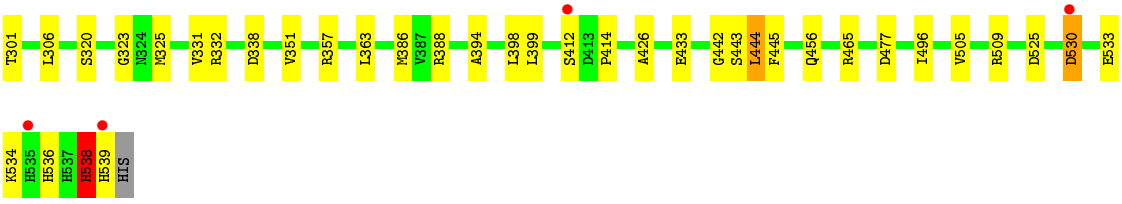
• Molecule 2: Proteasome subunit beta

Chain P:



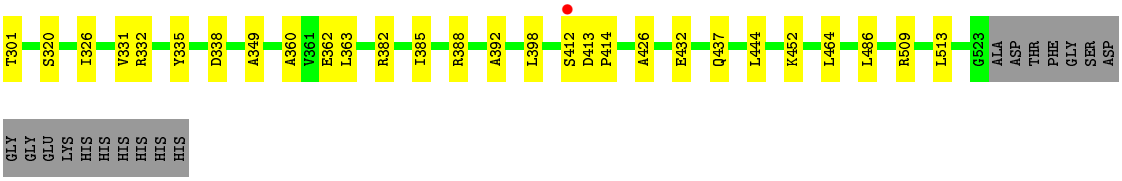
• Molecule 2: Proteasome subunit beta

Chain R:



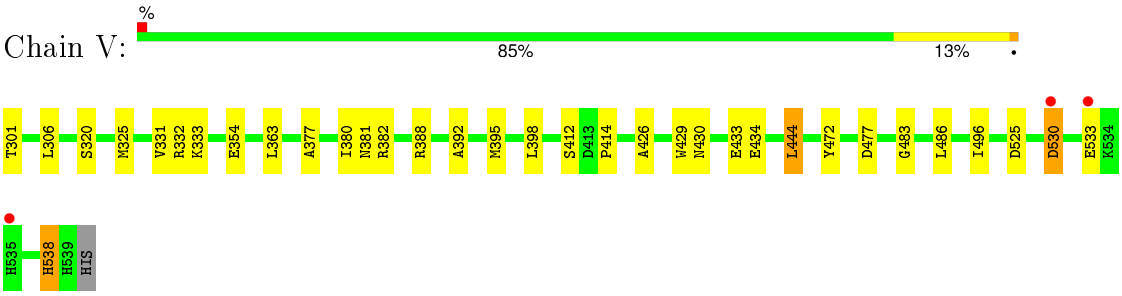
• Molecule 2: Proteasome subunit beta

Chain T:



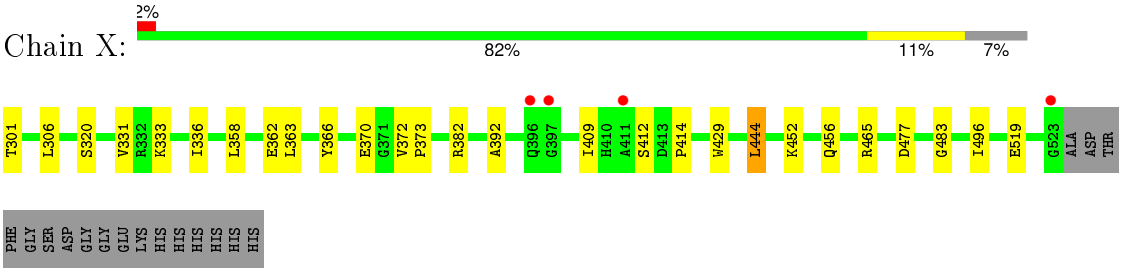
- Molecule 2: Proteasome subunit beta

Chain V:



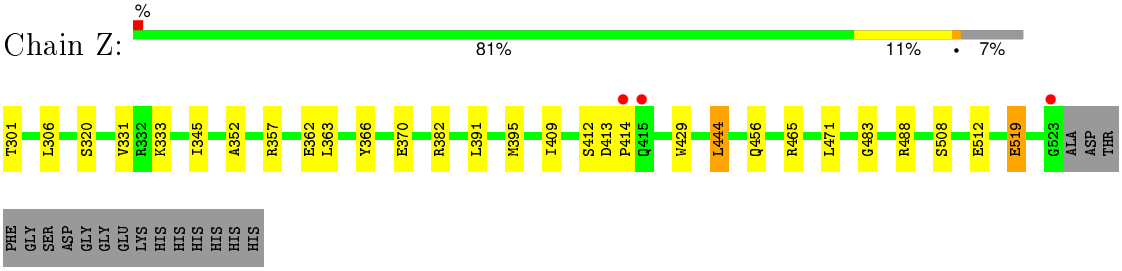
- Molecule 2: Proteasome subunit beta

Chain X:



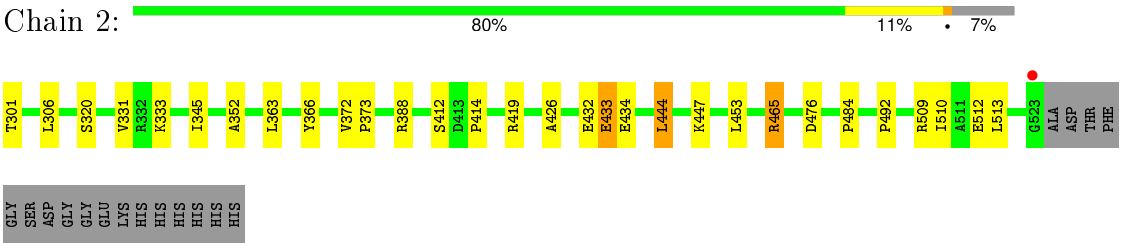
- Molecule 2: Proteasome subunit beta

Chain Z:



- Molecule 2: Proteasome subunit beta

Chain 2:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	170.37Å 118.44Å 195.25Å 90.00° 113.02° 90.00°	Depositor
Resolution (Å)	24.95 – 2.20 25.11 – 2.12	Depositor EDS
% Data completeness (in resolution range)	92.0 (24.95-2.20) 89.2 (25.11-2.12)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.11Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.205 , 0.234 0.205 , 0.234	Depositor DCC
R_{free} test set	16561 reflections (4.98%)	DCC
Wilson B-factor (Å^2)	22.6	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 56.1	EDS
Estimated twinning fraction	0.008 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	3 of 378893 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	50080	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1	0.53	0/1683	0.73	1/2274 (0.0%)
1	A	0.49	0/1679	0.72	1/2268 (0.0%)
1	B	0.52	0/1668	0.71	1/2253 (0.0%)
1	D	0.46	0/1675	0.69	1/2263 (0.0%)
1	F	0.51	0/1726	0.74	2/2332 (0.1%)
1	I	0.51	0/1695	0.73	4/2290 (0.2%)
1	K	0.51	0/1691	0.71	1/2285 (0.0%)
1	M	0.51	0/1691	0.74	2/2285 (0.1%)
1	O	0.51	0/1691	0.72	1/2285 (0.0%)
1	Q	0.47	0/1683	0.69	1/2274 (0.0%)
1	S	0.50	0/1690	0.72	2/2284 (0.1%)
1	U	0.49	0/1687	0.71	3/2279 (0.1%)
1	W	0.44	0/1695	0.68	1/2290 (0.0%)
1	Y	0.48	0/1691	0.72	1/2285 (0.0%)
2	2	0.65	0/1666	0.79	0/2259
2	C	0.71	0/1662	0.84	2/2254 (0.1%)
2	E	0.73	0/1666	0.81	0/2259
2	G	0.66	0/1662	0.77	0/2254
2	H	0.70	0/1662	0.79	0/2254
2	J	0.71	0/1662	0.81	0/2254
2	L	0.70	0/1666	0.80	0/2259
2	N	0.69	0/1662	0.81	1/2254 (0.0%)
2	P	0.69	0/1662	0.79	0/2254
2	R	0.71	0/1797	0.81	3/2435 (0.1%)
2	T	0.66	0/1666	0.77	1/2259 (0.0%)
2	V	0.70	0/1797	0.78	1/2435 (0.0%)
2	X	0.64	0/1666	0.78	0/2259
2	Z	0.62	0/1666	0.75	0/2259
All	All	0.60	0/47207	0.76	30/63895 (0.0%)

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	213	LEU	N-CA-C	-5.99	94.82	111.00
2	R	338	ASP	CB-CG-OD1	5.80	123.52	118.30
1	M	76	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	I	213	LEU	N-CA-C	-5.71	95.60	111.00
1	K	213	LEU	N-CA-C	-5.70	95.61	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1658	0	1659	55	0
1	A	1654	0	1651	68	0
1	B	1643	0	1639	82	0
1	D	1650	0	1648	99	0
1	F	1699	0	1696	70	0
1	I	1669	0	1668	96	0
1	K	1666	0	1670	67	0
1	M	1666	0	1670	78	0
1	O	1666	0	1670	67	0
1	Q	1658	0	1659	82	0
1	S	1665	0	1668	86	0
1	U	1662	0	1662	51	0
1	W	1669	0	1668	70	0
1	Y	1666	0	1670	80	0
2	2	1642	0	1632	39	0
2	C	1638	0	1629	33	0
2	E	1642	0	1632	47	0
2	G	1638	0	1629	43	0
2	H	1638	0	1629	33	0
2	J	1638	0	1629	43	0
2	L	1642	0	1632	31	0
2	N	1638	0	1629	44	0
2	P	1638	0	1629	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	1767	0	1729	46	0
2	T	1642	0	1632	21	0
2	V	1767	0	1729	40	0
2	X	1642	0	1632	25	0
2	Z	1642	0	1632	26	0
3	1	5	0	7	0	0
3	2	40	0	56	27	0
3	A	10	0	14	1	0
3	B	10	0	14	2	0
3	C	35	0	49	15	0
3	D	25	0	35	6	0
3	E	30	0	42	16	0
3	F	15	0	21	1	0
3	G	45	0	63	31	0
3	H	30	0	42	12	0
3	I	10	0	14	2	0
3	J	15	0	21	7	0
3	K	20	0	28	11	0
3	L	20	0	28	5	0
3	M	20	0	28	0	0
3	N	25	0	35	26	0
3	O	15	0	21	1	0
3	P	40	0	56	14	0
3	Q	15	0	21	9	0
3	R	25	0	35	13	0
3	S	10	0	14	1	0
3	T	30	0	42	15	0
3	U	10	0	14	8	0
3	V	45	0	63	48	0
3	W	10	0	14	7	0
3	X	25	0	35	7	0
3	Y	15	0	21	4	0
3	Z	20	0	28	8	0
4	2	20	0	22	4	0
4	C	20	0	22	3	0
4	E	20	0	22	3	0
4	G	20	0	22	3	0
4	H	20	0	22	5	0
4	J	20	0	22	2	0
4	L	20	0	22	3	0
4	N	20	0	22	3	0
4	P	20	0	22	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	20	0	22	3	0
4	T	20	0	22	3	0
4	V	20	0	22	4	0
4	X	20	0	22	4	0
4	Z	20	0	22	3	0
5	1	47	0	0	1	0
5	2	143	0	0	7	0
5	A	43	0	0	4	0
5	B	41	0	0	6	0
5	C	163	0	0	10	0
5	D	40	0	0	8	0
5	E	166	0	0	9	0
5	F	58	0	0	5	0
5	G	131	0	0	2	0
5	H	148	0	0	7	0
5	I	52	0	0	10	0
5	J	142	0	0	10	0
5	K	45	0	0	5	0
5	L	153	0	0	12	0
5	M	40	0	0	5	0
5	N	154	0	0	5	0
5	O	47	0	0	5	0
5	P	139	0	0	6	0
5	Q	38	0	0	9	0
5	R	170	0	0	7	0
5	S	42	0	0	8	0
5	T	116	0	0	7	0
5	U	49	0	0	4	0
5	V	177	0	0	14	0
5	W	35	0	0	4	0
5	X	150	0	0	7	0
5	Y	28	0	0	6	0
5	Z	123	0	0	4	0
All	All	50080	0	47491	1521	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 1521 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ILE:HG21	1:B:11:GLN:CG	1.63	1.27
1:F:7:ILE:CG2	1:F:11:GLN:HB3	1.65	1.27
3:R:92:DMF:H21	5:R:1869:HOH:O	1.30	1.23
1:O:9:PRO:HD2	1:U:15:GLU:CG	1.69	1.21
1:A:80:GLN:HE21	1:A:80:GLN:C	1.45	1.20

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	211/248 (85%)	199 (94%)	12 (6%)	0	100	100
1	A	211/248 (85%)	203 (96%)	8 (4%)	0	100	100
1	B	209/248 (84%)	201 (96%)	8 (4%)	0	100	100
1	D	210/248 (85%)	201 (96%)	9 (4%)	0	100	100
1	F	216/248 (87%)	209 (97%)	6 (3%)	1 (0%)	34	35
1	I	212/248 (86%)	201 (95%)	11 (5%)	0	100	100
1	K	212/248 (86%)	202 (95%)	10 (5%)	0	100	100
1	M	212/248 (86%)	201 (95%)	11 (5%)	0	100	100
1	O	212/248 (86%)	199 (94%)	13 (6%)	0	100	100
1	Q	211/248 (85%)	198 (94%)	13 (6%)	0	100	100
1	S	212/248 (86%)	203 (96%)	9 (4%)	0	100	100
1	U	212/248 (86%)	200 (94%)	12 (6%)	0	100	100
1	W	212/248 (86%)	199 (94%)	13 (6%)	0	100	100
1	Y	212/248 (86%)	202 (95%)	10 (5%)	0	100	100
2	2	221/240 (92%)	220 (100%)	1 (0%)	0	100	100
2	C	220/240 (92%)	219 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	221/240 (92%)	219 (99%)	2 (1%)	0	100	100
2	G	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	H	220/240 (92%)	219 (100%)	1 (0%)	0	100	100
2	J	220/240 (92%)	219 (100%)	1 (0%)	0	100	100
2	L	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
2	N	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	P	220/240 (92%)	218 (99%)	2 (1%)	0	100	100
2	R	237/240 (99%)	236 (100%)	1 (0%)	0	100	100
2	T	221/240 (92%)	220 (100%)	1 (0%)	0	100	100
2	V	237/240 (99%)	234 (99%)	3 (1%)	0	100	100
2	X	221/240 (92%)	219 (99%)	2 (1%)	0	100	100
2	Z	221/240 (92%)	218 (99%)	3 (1%)	0	100	100
All	All	6084/6832 (89%)	5913 (97%)	170 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	191	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	165/192 (86%)	158 (96%)	7 (4%)	36	44
1	A	164/192 (85%)	155 (94%)	9 (6%)	27	30
1	B	163/192 (85%)	154 (94%)	9 (6%)	27	30
1	D	164/192 (85%)	152 (93%)	12 (7%)	17	18
1	F	169/192 (88%)	161 (95%)	8 (5%)	32	39
1	I	166/192 (86%)	161 (97%)	5 (3%)	48	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	166/192 (86%)	157 (95%)	9 (5%)	27	31
1	M	166/192 (86%)	155 (93%)	11 (7%)	21	22
1	O	166/192 (86%)	161 (97%)	5 (3%)	48	60
1	Q	165/192 (86%)	158 (96%)	7 (4%)	36	44
1	S	166/192 (86%)	158 (95%)	8 (5%)	31	37
1	U	165/192 (86%)	160 (97%)	5 (3%)	48	60
1	W	166/192 (86%)	160 (96%)	6 (4%)	42	52
1	Y	166/192 (86%)	159 (96%)	7 (4%)	36	44
2	2	165/178 (93%)	160 (97%)	5 (3%)	48	60
2	C	165/178 (93%)	163 (99%)	2 (1%)	78	88
2	E	165/178 (93%)	161 (98%)	4 (2%)	57	69
2	G	165/178 (93%)	163 (99%)	2 (1%)	78	88
2	H	165/178 (93%)	162 (98%)	3 (2%)	66	79
2	J	165/178 (93%)	161 (98%)	4 (2%)	57	69
2	L	165/178 (93%)	160 (97%)	5 (3%)	48	60
2	N	165/178 (93%)	162 (98%)	3 (2%)	66	79
2	P	165/178 (93%)	163 (99%)	2 (1%)	78	88
2	R	177/178 (99%)	173 (98%)	4 (2%)	58	71
2	T	165/178 (93%)	160 (97%)	5 (3%)	48	60
2	V	177/178 (99%)	173 (98%)	4 (2%)	58	71
2	X	165/178 (93%)	162 (98%)	3 (2%)	66	79
2	Z	165/178 (93%)	162 (98%)	3 (2%)	66	79
All	All	4651/5180 (90%)	4494 (97%)	157 (3%)	44	54

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	509	ARG
1	O	69	ASN
1	1	33	LEU
1	M	26	ARG
1	M	182	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	129	HIS
1	Q	73	ASN
2	Z	456	GLN
2	N	430	ASN
1	O	80	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

137 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	DMF	1	249	-	4,4,4	0.28	0	4,4,4	0.34	0
3	DMF	2	101	-	4,4,4	0.32	0	4,4,4	0.39	0
3	DMF	2	108	-	4,4,4	0.30	0	4,4,4	0.41	0
3	DMF	2	112	-	4,4,4	0.18	0	4,4,4	0.36	0
4	SA6	2	300	2	16,21,21	2.59	5 (31%)	21,32,32	1.92	8 (38%)
3	DMF	2	4	-	4,4,4	0.30	0	4,4,4	0.43	0
3	DMF	2	49	-	4,4,4	0.24	0	4,4,4	0.46	0
3	DMF	2	52	-	4,4,4	0.30	0	4,4,4	0.40	0
3	DMF	2	57	-	4,4,4	0.29	0	4,4,4	0.30	0
3	DMF	2	87	-	4,4,4	0.29	0	4,4,4	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	DMF	A	249	-	4,4,4	0.55	0	4,4,4	0.26	0
3	DMF	A	250	-	4,4,4	0.44	0	4,4,4	0.49	0
3	DMF	B	249	-	4,4,4	0.27	0	4,4,4	0.39	0
3	DMF	B	250	-	4,4,4	0.28	0	4,4,4	0.33	0
3	DMF	C	103	-	4,4,4	0.30	0	4,4,4	0.33	0
3	DMF	C	121	-	4,4,4	0.29	0	4,4,4	0.40	0
4	SA6	C	300	2	16,21,21	3.08	6 (37%)	21,32,32	1.92	5 (23%)
3	DMF	C	38	-	4,4,4	0.17	0	4,4,4	0.48	0
3	DMF	C	47	-	4,4,4	0.52	0	4,4,4	0.22	0
3	DMF	C	63	-	4,4,4	0.27	0	4,4,4	0.48	0
3	DMF	C	69	-	4,4,4	0.27	0	4,4,4	0.42	0
3	DMF	C	88	-	4,4,4	0.31	0	4,4,4	0.46	0
3	DMF	D	249	-	4,4,4	0.55	0	4,4,4	0.34	0
3	DMF	D	250	-	4,4,4	0.31	0	4,4,4	0.36	0
3	DMF	D	251	-	4,4,4	0.29	0	4,4,4	0.39	0
3	DMF	D	252	-	4,4,4	0.28	0	4,4,4	0.36	0
3	DMF	D	253	-	4,4,4	0.25	0	4,4,4	0.31	0
3	DMF	E	100	-	4,4,4	0.29	0	4,4,4	0.43	0
3	DMF	E	20	-	4,4,4	0.29	0	4,4,4	0.42	0
3	DMF	E	28	-	4,4,4	0.28	0	4,4,4	0.19	0
4	SA6	E	300	2	16,21,21	2.88	6 (37%)	21,32,32	1.81	5 (23%)
3	DMF	E	53	-	4,4,4	0.28	0	4,4,4	0.37	0
3	DMF	E	73	-	4,4,4	0.27	0	4,4,4	0.40	0
3	DMF	E	75	-	4,4,4	0.26	0	4,4,4	0.39	0
3	DMF	F	249	-	4,4,4	0.26	0	4,4,4	0.35	0
3	DMF	F	250	-	4,4,4	0.28	0	4,4,4	0.33	0
3	DMF	F	251	-	4,4,4	0.20	0	4,4,4	0.37	0
3	DMF	G	111	-	4,4,4	0.24	0	4,4,4	0.32	0
3	DMF	G	119	-	4,4,4	0.27	0	4,4,4	0.33	0
3	DMF	G	12	-	4,4,4	0.28	0	4,4,4	0.40	0
3	DMF	G	24	-	4,4,4	0.29	0	4,4,4	0.38	0
4	SA6	G	300	2	16,21,21	3.22	7 (43%)	21,32,32	1.53	3 (14%)
3	DMF	G	62	-	4,4,4	0.29	0	4,4,4	0.39	0
3	DMF	G	64	-	4,4,4	0.30	0	4,4,4	0.35	0
3	DMF	G	70	-	4,4,4	0.67	0	4,4,4	0.29	0
3	DMF	G	77	-	4,4,4	0.42	0	4,4,4	0.39	0
3	DMF	G	98	-	4,4,4	0.30	0	4,4,4	0.39	0
3	DMF	H	117	-	4,4,4	0.39	0	4,4,4	0.75	0
4	SA6	H	300	2	16,21,21	3.10	7 (43%)	21,32,32	1.66	6 (28%)
3	DMF	H	43	-	4,4,4	0.35	0	4,4,4	0.68	0
3	DMF	H	66	-	4,4,4	0.29	0	4,4,4	0.39	0
3	DMF	H	71	-	4,4,4	0.48	0	4,4,4	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	DMF	H	72	-	4,4,4	0.30	0	4,4,4	0.38	0
3	DMF	H	91	-	4,4,4	0.27	0	4,4,4	0.43	0
3	DMF	I	249	-	4,4,4	0.30	0	4,4,4	0.37	0
3	DMF	I	250	-	4,4,4	0.26	0	4,4,4	0.31	0
3	DMF	J	110	-	4,4,4	0.32	0	4,4,4	0.55	0
3	DMF	J	123	-	4,4,4	0.29	0	4,4,4	0.38	0
4	SA6	J	300	2	16,21,21	3.14	8 (50%)	21,32,32	1.58	4 (19%)
3	DMF	J	45	-	4,4,4	0.28	0	4,4,4	0.29	0
3	DMF	K	249	-	4,4,4	0.27	0	4,4,4	0.36	0
3	DMF	K	250	-	4,4,4	0.26	0	4,4,4	0.31	0
3	DMF	K	251	-	4,4,4	0.30	0	4,4,4	0.16	0
3	DMF	K	252	-	4,4,4	0.27	0	4,4,4	0.34	0
4	SA6	L	300	2	16,21,21	3.15	7 (43%)	21,32,32	1.87	5 (23%)
3	DMF	L	36	-	4,4,4	0.31	0	4,4,4	0.43	0
3	DMF	L	50	-	4,4,4	0.22	0	4,4,4	0.27	0
3	DMF	L	81	-	4,4,4	0.28	0	4,4,4	0.31	0
3	DMF	L	97	-	4,4,4	0.28	0	4,4,4	0.41	0
3	DMF	M	249	-	4,4,4	0.29	0	4,4,4	0.40	0
3	DMF	M	250	-	4,4,4	0.30	0	4,4,4	0.33	0
3	DMF	M	251	-	4,4,4	0.30	0	4,4,4	0.30	0
3	DMF	M	252	-	4,4,4	0.31	0	4,4,4	0.35	0
3	DMF	N	104	-	4,4,4	0.32	0	4,4,4	0.37	0
3	DMF	N	118	-	4,4,4	0.36	0	4,4,4	0.62	0
3	DMF	N	22	-	4,4,4	0.30	0	4,4,4	0.33	0
4	SA6	N	300	2	16,21,21	2.83	7 (43%)	21,32,32	1.70	5 (23%)
3	DMF	N	90	-	4,4,4	0.29	0	4,4,4	0.42	0
3	DMF	N	93	-	4,4,4	0.31	0	4,4,4	0.37	0
3	DMF	O	249	-	4,4,4	0.24	0	4,4,4	0.49	0
3	DMF	O	250	-	4,4,4	0.33	0	4,4,4	0.37	0
3	DMF	O	251	-	4,4,4	0.38	0	4,4,4	0.75	0
3	DMF	P	107	-	4,4,4	0.22	0	4,4,4	0.42	0
3	DMF	P	14	-	4,4,4	0.26	0	4,4,4	0.38	0
3	DMF	P	2	-	4,4,4	0.26	0	4,4,4	0.49	0
4	SA6	P	300	2	16,21,21	2.93	6 (37%)	21,32,32	1.74	5 (23%)
3	DMF	P	33	-	4,4,4	0.26	0	4,4,4	0.23	0
3	DMF	P	51	-	4,4,4	0.25	0	4,4,4	0.33	0
3	DMF	P	56	-	4,4,4	0.29	0	4,4,4	0.42	0
3	DMF	P	60	-	4,4,4	0.27	0	4,4,4	0.37	0
3	DMF	P	86	-	4,4,4	0.28	0	4,4,4	0.38	0
3	DMF	Q	249	-	4,4,4	0.29	0	4,4,4	0.38	0
3	DMF	Q	250	-	4,4,4	0.26	0	4,4,4	0.50	0
3	DMF	Q	251	-	4,4,4	0.30	0	4,4,4	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SA6	R	300	2	16,21,21	3.80	7 (43%)	21,32,32	1.71	5 (23%)
3	DMF	R	59	-	4,4,4	0.30	0	4,4,4	0.38	0
3	DMF	R	80	-	4,4,4	0.28	0	4,4,4	0.35	0
3	DMF	R	89	-	4,4,4	0.38	0	4,4,4	0.64	0
3	DMF	R	92	-	4,4,4	0.28	0	4,4,4	0.37	0
3	DMF	R	95	-	4,4,4	0.32	0	4,4,4	0.36	0
3	DMF	S	249	-	4,4,4	0.27	0	4,4,4	0.34	0
3	DMF	S	250	-	4,4,4	0.64	0	4,4,4	0.34	0
3	DMF	T	10	-	4,4,4	0.33	0	4,4,4	0.48	0
3	DMF	T	102	-	4,4,4	0.15	0	4,4,4	0.12	0
3	DMF	T	113	-	4,4,4	0.23	0	4,4,4	0.40	0
3	DMF	T	115	-	4,4,4	0.30	0	4,4,4	0.46	0
3	DMF	T	29	-	4,4,4	0.28	0	4,4,4	0.37	0
4	SA6	T	300	2	16,21,21	3.26	7 (43%)	21,32,32	1.90	5 (23%)
3	DMF	T	84	-	4,4,4	0.08	0	4,4,4	0.15	0
3	DMF	U	249	-	4,4,4	0.27	0	4,4,4	0.32	0
3	DMF	U	250	-	4,4,4	0.65	0	4,4,4	0.31	0
3	DMF	V	109	-	4,4,4	0.21	0	4,4,4	0.29	0
3	DMF	V	116	-	4,4,4	0.42	0	4,4,4	0.98	0
3	DMF	V	120	-	4,4,4	0.32	0	4,4,4	0.41	0
3	DMF	V	27	-	4,4,4	0.28	0	4,4,4	0.32	0
4	SA6	V	300	2	16,21,21	3.25	8 (50%)	21,32,32	1.43	3 (14%)
3	DMF	V	32	-	4,4,4	0.29	0	4,4,4	0.45	0
3	DMF	V	39	-	4,4,4	0.31	0	4,4,4	0.35	0
3	DMF	V	42	-	4,4,4	0.28	0	4,4,4	0.44	0
3	DMF	V	82	-	4,4,4	0.32	0	4,4,4	0.39	0
3	DMF	V	83	-	4,4,4	0.23	0	4,4,4	0.40	0
3	DMF	W	249	-	4,4,4	0.29	0	4,4,4	0.38	0
3	DMF	W	250	-	4,4,4	0.28	0	4,4,4	0.41	0
3	DMF	X	122	-	4,4,4	0.29	0	4,4,4	0.33	0
3	DMF	X	15	-	4,4,4	0.30	0	4,4,4	0.43	0
3	DMF	X	16	-	4,4,4	0.27	0	4,4,4	0.37	0
4	SA6	X	300	2	16,21,21	3.14	8 (50%)	21,32,32	1.65	2 (9%)
3	DMF	X	40	-	4,4,4	0.30	0	4,4,4	0.38	0
3	DMF	X	41	-	4,4,4	0.52	0	4,4,4	0.33	0
3	DMF	Y	249	-	4,4,4	0.30	0	4,4,4	0.40	0
3	DMF	Y	250	-	4,4,4	0.62	0	4,4,4	0.30	0
3	DMF	Y	251	-	4,4,4	0.29	0	4,4,4	0.39	0
3	DMF	Z	114	-	4,4,4	0.32	0	4,4,4	0.42	0
3	DMF	Z	18	-	4,4,4	0.22	0	4,4,4	0.40	0
4	SA6	Z	300	2	16,21,21	3.36	9 (56%)	21,32,32	1.64	4 (19%)
3	DMF	Z	54	-	4,4,4	0.33	0	4,4,4	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	DMF	Z	94	-	4,4,4	0.26	0	4,4,4	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	1	249	-	-	0/2/2/2	0/0/0/0
3	DMF	2	101	-	-	0/2/2/2	0/0/0/0
3	DMF	2	108	-	-	0/2/2/2	0/0/0/0
3	DMF	2	112	-	-	0/2/2/2	0/0/0/0
4	SA6	2	300	2	-	0/6/47/47	0/2/2/2
3	DMF	2	4	-	-	0/2/2/2	0/0/0/0
3	DMF	2	49	-	-	0/2/2/2	0/0/0/0
3	DMF	2	52	-	-	0/2/2/2	0/0/0/0
3	DMF	2	57	-	-	0/2/2/2	0/0/0/0
3	DMF	2	87	-	-	0/2/2/2	0/0/0/0
3	DMF	A	249	-	-	0/2/2/2	0/0/0/0
3	DMF	A	250	-	-	0/2/2/2	0/0/0/0
3	DMF	B	249	-	-	0/2/2/2	0/0/0/0
3	DMF	B	250	-	-	0/2/2/2	0/0/0/0
3	DMF	C	103	-	-	0/2/2/2	0/0/0/0
3	DMF	C	121	-	-	0/2/2/2	0/0/0/0
4	SA6	C	300	2	-	0/6/47/47	0/2/2/2
3	DMF	C	38	-	-	0/2/2/2	0/0/0/0
3	DMF	C	47	-	-	0/2/2/2	0/0/0/0
3	DMF	C	63	-	-	0/2/2/2	0/0/0/0
3	DMF	C	69	-	-	0/2/2/2	0/0/0/0
3	DMF	C	88	-	-	0/2/2/2	0/0/0/0
3	DMF	D	249	-	-	0/2/2/2	0/0/0/0
3	DMF	D	250	-	-	0/2/2/2	0/0/0/0
3	DMF	D	251	-	-	0/2/2/2	0/0/0/0
3	DMF	D	252	-	-	0/2/2/2	0/0/0/0
3	DMF	D	253	-	-	0/2/2/2	0/0/0/0
3	DMF	E	100	-	-	0/2/2/2	0/0/0/0
3	DMF	E	20	-	-	0/2/2/2	0/0/0/0
3	DMF	E	28	-	-	0/2/2/2	0/0/0/0
4	SA6	E	300	2	-	0/6/47/47	0/2/2/2
3	DMF	E	53	-	-	0/2/2/2	0/0/0/0
3	DMF	E	73	-	-	0/2/2/2	0/0/0/0
3	DMF	E	75	-	-	0/2/2/2	0/0/0/0
3	DMF	F	249	-	-	0/2/2/2	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	F	250	-	-	0/2/2/2	0/0/0/0
3	DMF	F	251	-	-	0/2/2/2	0/0/0/0
3	DMF	G	111	-	-	0/2/2/2	0/0/0/0
3	DMF	G	119	-	-	0/2/2/2	0/0/0/0
3	DMF	G	12	-	-	0/2/2/2	0/0/0/0
3	DMF	G	24	-	-	0/2/2/2	0/0/0/0
4	SA6	G	300	2	-	0/6/47/47	0/2/2/2
3	DMF	G	62	-	-	0/2/2/2	0/0/0/0
3	DMF	G	64	-	-	0/2/2/2	0/0/0/0
3	DMF	G	70	-	-	0/2/2/2	0/0/0/0
3	DMF	G	77	-	-	0/2/2/2	0/0/0/0
3	DMF	G	98	-	-	0/2/2/2	0/0/0/0
3	DMF	H	117	-	-	0/2/2/2	0/0/0/0
4	SA6	H	300	2	-	0/6/47/47	0/2/2/2
3	DMF	H	43	-	-	0/2/2/2	0/0/0/0
3	DMF	H	66	-	-	0/2/2/2	0/0/0/0
3	DMF	H	71	-	-	0/2/2/2	0/0/0/0
3	DMF	H	72	-	-	0/2/2/2	0/0/0/0
3	DMF	H	91	-	-	0/2/2/2	0/0/0/0
3	DMF	I	249	-	-	0/2/2/2	0/0/0/0
3	DMF	I	250	-	-	0/2/2/2	0/0/0/0
3	DMF	J	110	-	-	0/2/2/2	0/0/0/0
3	DMF	J	123	-	-	0/2/2/2	0/0/0/0
4	SA6	J	300	2	-	0/6/47/47	0/2/2/2
3	DMF	J	45	-	-	0/2/2/2	0/0/0/0
3	DMF	K	249	-	-	0/2/2/2	0/0/0/0
3	DMF	K	250	-	-	0/2/2/2	0/0/0/0
3	DMF	K	251	-	-	0/2/2/2	0/0/0/0
3	DMF	K	252	-	-	0/2/2/2	0/0/0/0
4	SA6	L	300	2	-	0/6/47/47	0/2/2/2
3	DMF	L	36	-	-	0/2/2/2	0/0/0/0
3	DMF	L	50	-	-	0/2/2/2	0/0/0/0
3	DMF	L	81	-	-	0/2/2/2	0/0/0/0
3	DMF	L	97	-	-	0/2/2/2	0/0/0/0
3	DMF	M	249	-	-	0/2/2/2	0/0/0/0
3	DMF	M	250	-	-	0/2/2/2	0/0/0/0
3	DMF	M	251	-	-	0/2/2/2	0/0/0/0
3	DMF	M	252	-	-	0/2/2/2	0/0/0/0
3	DMF	N	104	-	-	0/2/2/2	0/0/0/0
3	DMF	N	118	-	-	0/2/2/2	0/0/0/0
3	DMF	N	22	-	-	0/2/2/2	0/0/0/0
4	SA6	N	300	2	-	0/6/47/47	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	N	90	-	-	0/2/2/2	0/0/0/0
3	DMF	N	93	-	-	0/2/2/2	0/0/0/0
3	DMF	O	249	-	-	0/2/2/2	0/0/0/0
3	DMF	O	250	-	-	0/2/2/2	0/0/0/0
3	DMF	O	251	-	-	0/2/2/2	0/0/0/0
3	DMF	P	107	-	-	0/2/2/2	0/0/0/0
3	DMF	P	14	-	-	0/2/2/2	0/0/0/0
3	DMF	P	2	-	-	0/2/2/2	0/0/0/0
4	SA6	P	300	2	-	0/6/47/47	0/2/2/2
3	DMF	P	33	-	-	0/2/2/2	0/0/0/0
3	DMF	P	51	-	-	0/2/2/2	0/0/0/0
3	DMF	P	56	-	-	0/2/2/2	0/0/0/0
3	DMF	P	60	-	-	0/2/2/2	0/0/0/0
3	DMF	P	86	-	-	0/2/2/2	0/0/0/0
3	DMF	Q	249	-	-	0/2/2/2	0/0/0/0
3	DMF	Q	250	-	-	0/2/2/2	0/0/0/0
3	DMF	Q	251	-	-	0/2/2/2	0/0/0/0
4	SA6	R	300	2	-	0/6/47/47	0/2/2/2
3	DMF	R	59	-	-	0/2/2/2	0/0/0/0
3	DMF	R	80	-	-	0/2/2/2	0/0/0/0
3	DMF	R	89	-	-	0/2/2/2	0/0/0/0
3	DMF	R	92	-	-	0/2/2/2	0/0/0/0
3	DMF	R	95	-	-	0/2/2/2	0/0/0/0
3	DMF	S	249	-	-	0/2/2/2	0/0/0/0
3	DMF	S	250	-	-	0/2/2/2	0/0/0/0
3	DMF	T	10	-	-	0/2/2/2	0/0/0/0
3	DMF	T	102	-	-	0/2/2/2	0/0/0/0
3	DMF	T	113	-	-	0/2/2/2	0/0/0/0
3	DMF	T	115	-	-	0/2/2/2	0/0/0/0
3	DMF	T	29	-	-	0/2/2/2	0/0/0/0
4	SA6	T	300	2	-	0/6/47/47	0/2/2/2
3	DMF	T	84	-	-	0/2/2/2	0/0/0/0
3	DMF	U	249	-	-	0/2/2/2	0/0/0/0
3	DMF	U	250	-	-	0/2/2/2	0/0/0/0
3	DMF	V	109	-	-	0/2/2/2	0/0/0/0
3	DMF	V	116	-	-	0/2/2/2	0/0/0/0
3	DMF	V	120	-	-	0/2/2/2	0/0/0/0
3	DMF	V	27	-	-	0/2/2/2	0/0/0/0
4	SA6	V	300	2	-	0/6/47/47	0/2/2/2
3	DMF	V	32	-	-	0/2/2/2	0/0/0/0
3	DMF	V	39	-	-	0/2/2/2	0/0/0/0
3	DMF	V	42	-	-	0/2/2/2	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMF	V	82	-	-	0/2/2/2	0/0/0/0
3	DMF	V	83	-	-	0/2/2/2	0/0/0/0
3	DMF	W	249	-	-	0/2/2/2	0/0/0/0
3	DMF	W	250	-	-	0/2/2/2	0/0/0/0
3	DMF	X	122	-	-	0/2/2/2	0/0/0/0
3	DMF	X	15	-	-	0/2/2/2	0/0/0/0
3	DMF	X	16	-	-	0/2/2/2	0/0/0/0
4	SA6	X	300	2	-	0/6/47/47	0/2/2/2
3	DMF	X	40	-	-	0/2/2/2	0/0/0/0
3	DMF	X	41	-	-	0/2/2/2	0/0/0/0
3	DMF	Y	249	-	-	0/2/2/2	0/0/0/0
3	DMF	Y	250	-	-	0/2/2/2	0/0/0/0
3	DMF	Y	251	-	-	0/2/2/2	0/0/0/0
3	DMF	Z	114	-	-	0/2/2/2	0/0/0/0
3	DMF	Z	18	-	-	0/2/2/2	0/0/0/0
4	SA6	Z	300	2	-	0/6/47/47	0/2/2/2
3	DMF	Z	54	-	-	0/2/2/2	0/0/0/0
3	DMF	Z	94	-	-	0/2/2/2	0/0/0/0

The worst 5 of 98 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	300	SA6	C7-N9	-4.49	1.29	1.34
4	L	300	SA6	C7-N9	-3.83	1.29	1.34
4	C	300	SA6	C7-N9	-3.35	1.30	1.34
4	Z	300	SA6	C7-N9	-3.09	1.30	1.34
4	H	300	SA6	C7-N9	-2.70	1.31	1.34

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	X	300	SA6	C4-C3-C7	-5.22	99.79	104.25
4	T	300	SA6	C4-C3-C7	-5.03	99.95	104.25
4	R	300	SA6	C4-C3-C7	-4.59	100.32	104.25
4	C	300	SA6	C4-C3-C7	-4.57	100.34	104.25
4	P	300	SA6	C4-C3-C7	-4.56	100.35	104.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

105 monomers are involved in 314 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	2	101	DMF	2	0
3	2	108	DMF	5	0
3	2	112	DMF	7	0
4	2	300	SA6	4	0
3	2	4	DMF	8	0
3	2	49	DMF	1	0
3	2	52	DMF	2	0
3	2	87	DMF	2	0
3	A	249	DMF	1	0
3	B	249	DMF	2	0
3	C	103	DMF	8	0
4	C	300	SA6	3	0
3	C	38	DMF	3	0
3	C	47	DMF	1	0
3	C	63	DMF	1	0
3	C	69	DMF	1	0
3	C	88	DMF	1	0
3	D	251	DMF	4	0
3	D	253	DMF	2	0
3	E	100	DMF	2	0
3	E	20	DMF	4	0
3	E	28	DMF	1	0
4	E	300	SA6	3	0
3	E	53	DMF	2	0
3	E	73	DMF	3	0
3	E	75	DMF	4	0
3	F	250	DMF	1	0
3	G	111	DMF	1	0
3	G	119	DMF	11	0
3	G	12	DMF	4	0
3	G	24	DMF	2	0
4	G	300	SA6	3	0
3	G	62	DMF	1	0
3	G	64	DMF	9	0
3	G	70	DMF	1	0
3	G	98	DMF	2	0
3	H	117	DMF	2	0
4	H	300	SA6	5	0
3	H	43	DMF	4	0
3	H	66	DMF	3	0
3	H	71	DMF	1	0
3	H	91	DMF	2	0
3	I	250	DMF	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	123	DMF	6	0
4	J	300	SA6	2	0
3	J	45	DMF	1	0
3	K	249	DMF	1	0
3	K	250	DMF	4	0
3	K	251	DMF	3	0
3	K	252	DMF	3	0
4	L	300	SA6	3	0
3	L	81	DMF	1	0
3	L	97	DMF	4	0
3	N	104	DMF	7	0
3	N	118	DMF	4	0
3	N	22	DMF	4	0
4	N	300	SA6	3	0
3	N	90	DMF	7	0
3	N	93	DMF	4	0
3	O	250	DMF	1	0
3	P	107	DMF	5	0
3	P	14	DMF	5	0
3	P	2	DMF	1	0
4	P	300	SA6	4	0
3	P	33	DMF	3	0
3	Q	249	DMF	2	0
3	Q	250	DMF	6	0
3	Q	251	DMF	1	0
4	R	300	SA6	3	0
3	R	59	DMF	9	0
3	R	80	DMF	1	0
3	R	92	DMF	2	0
3	R	95	DMF	1	0
3	S	249	DMF	1	0
3	T	102	DMF	3	0
3	T	113	DMF	5	0
3	T	115	DMF	1	0
3	T	29	DMF	3	0
4	T	300	SA6	3	0
3	T	84	DMF	3	0
3	U	250	DMF	8	0
3	V	116	DMF	6	0
3	V	120	DMF	8	0
3	V	27	DMF	8	0
4	V	300	SA6	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	V	32	DMF	5	0
3	V	39	DMF	1	0
3	V	42	DMF	7	0
3	V	82	DMF	2	0
3	V	83	DMF	11	0
3	W	249	DMF	2	0
3	W	250	DMF	5	0
3	X	122	DMF	1	0
3	X	15	DMF	1	0
3	X	16	DMF	3	0
4	X	300	SA6	4	0
3	X	40	DMF	1	0
3	X	41	DMF	1	0
3	Y	249	DMF	1	0
3	Y	250	DMF	1	0
3	Y	251	DMF	2	0
3	Z	18	DMF	2	0
4	Z	300	SA6	3	0
3	Z	54	DMF	3	0
3	Z	94	DMF	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1	215/248 (86%)	0.46	20 (9%) 11 10	19, 48, 88, 109	0
1	A	215/248 (86%)	0.75	31 (14%) 3 3	20, 54, 91, 107	0
1	B	213/248 (85%)	0.52	20 (9%) 11 10	20, 49, 88, 106	0
1	D	214/248 (86%)	1.33	62 (28%) 1 0	20, 65, 98, 110	0
1	F	220/248 (88%)	0.53	17 (7%) 16 16	17, 48, 86, 104	0
1	I	216/248 (87%)	0.64	29 (13%) 4 4	18, 52, 92, 108	0
1	K	216/248 (87%)	0.60	22 (10%) 9 8	21, 55, 92, 107	0
1	M	216/248 (87%)	0.77	34 (15%) 3 2	18, 53, 92, 104	0
1	O	216/248 (87%)	0.63	24 (11%) 7 7	17, 49, 87, 102	0
1	Q	215/248 (86%)	0.56	23 (10%) 8 7	22, 50, 86, 99	0
1	S	216/248 (87%)	0.78	36 (16%) 2 2	20, 56, 91, 104	0
1	U	216/248 (87%)	0.54	27 (12%) 5 5	16, 49, 86, 102	0
1	W	216/248 (87%)	1.05	47 (21%) 1 1	20, 63, 94, 107	0
1	Y	216/248 (87%)	0.88	36 (16%) 2 2	22, 58, 94, 123	0
2	2	223/240 (92%)	-0.42	1 (0%) 93 93	11, 21, 45, 65	0
2	C	222/240 (92%)	-0.47	2 (0%) 85 85	8, 20, 48, 79	0
2	E	223/240 (92%)	-0.44	2 (0%) 85 85	8, 20, 46, 63	0
2	G	222/240 (92%)	-0.43	1 (0%) 91 91	10, 23, 53, 75	0
2	H	222/240 (92%)	-0.46	0 100 100	9, 23, 50, 71	0
2	J	222/240 (92%)	-0.44	1 (0%) 91 91	9, 21, 49, 70	0
2	L	223/240 (92%)	-0.40	1 (0%) 93 93	8, 21, 46, 66	0
2	N	222/240 (92%)	-0.43	1 (0%) 91 91	8, 21, 47, 79	0
2	P	222/240 (92%)	-0.45	0 100 100	10, 23, 49, 73	0
2	R	239/240 (99%)	-0.46	4 (1%) 73 72	8, 20, 55, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	T	223/240 (92%)	-0.34	1 (0%) 93 93	10, 24, 53, 72	0
2	V	239/240 (99%)	-0.44	3 (1%) 79 78	8, 20, 63, 91	0
2	X	223/240 (92%)	-0.42	4 (1%) 71 70	10, 24, 56, 73	0
2	Z	223/240 (92%)	-0.38	3 (1%) 79 78	11, 24, 52, 69	0
All	All	6168/6832 (90%)	0.13	452 (7%) 18 17	8, 33, 84, 123	0

The worst 5 of 452 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	6	PHE	8.7
1	M	203	LEU	7.7
1	S	7	ILE	7.2
1	I	203	LEU	7.1
1	Y	8	SER	7.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
3	DMF	P	2	5/5	0.82	0.31	35.44	62,62,64,64	0
3	DMF	N	118	5/5	0.92	0.37	27.20	20,20,20,20	0
3	DMF	G	24	5/5	0.80	0.40	25.36	65,67,68,68	0
3	DMF	T	84	5/5	0.68	0.45	25.34	59,59,60,62	0
3	DMF	C	63	5/5	0.80	0.23	21.50	58,59,59,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	DMF	V	27	5/5	0.87	0.32	20.52	63,63,64,64	0
3	DMF	E	20	5/5	0.84	0.44	20.44	76,77,77,78	0
3	DMF	G	111	5/5	0.86	0.40	20.15	20,20,20,20	0
3	DMF	D	252	5/5	0.86	0.33	17.30	20,20,20,20	0
3	DMF	N	93	5/5	0.88	0.32	17.16	20,20,20,20	0
3	DMF	2	87	5/5	0.96	0.37	16.59	20,20,20,20	0
3	DMF	L	81	5/5	0.61	0.51	16.24	59,60,61,62	0
3	DMF	V	120	5/5	0.84	0.39	15.58	20,20,20,20	0
3	DMF	T	102	5/5	0.80	0.43	15.45	20,20,20,20	0
3	DMF	R	59	5/5	0.77	0.43	14.81	54,55,57,57	0
3	DMF	2	108	5/5	0.83	0.45	14.76	20,20,20,20	0
3	DMF	2	112	5/5	0.79	0.48	14.41	20,20,20,20	0
3	DMF	Z	18	5/5	0.80	0.28	14.41	55,55,55,55	0
3	DMF	D	253	5/5	0.52	0.45	14.21	20,20,20,20	0
3	DMF	C	88	5/5	0.88	0.43	14.12	20,20,20,20	0
3	DMF	Z	114	5/5	0.80	0.45	14.09	20,20,20,20	0
3	DMF	H	117	5/5	0.76	0.42	13.64	20,20,20,20	0
3	DMF	V	82	5/5	0.78	0.36	13.62	45,47,47,48	0
3	DMF	F	249	5/5	0.64	0.43	13.62	90,91,91,91	0
3	DMF	Z	94	5/5	0.87	0.45	13.61	20,20,20,20	0
3	DMF	V	109	5/5	0.85	0.42	13.37	20,20,20,20	0
3	DMF	X	122	5/5	0.65	0.33	13.18	20,20,20,20	0
3	DMF	R	95	5/5	0.77	0.43	13.15	20,20,20,20	0
3	DMF	R	89	5/5	0.85	0.39	13.13	20,20,20,20	0
3	DMF	M	252	5/5	0.89	0.29	13.12	20,20,20,20	0
3	DMF	C	103	5/5	0.82	0.42	13.07	20,20,20,20	0
3	DMF	T	113	5/5	0.86	0.48	13.06	20,20,20,20	0
3	DMF	J	123	5/5	0.87	0.53	13.01	20,20,20,20	0
3	DMF	G	64	5/5	0.79	0.40	12.93	66,68,68,69	0
3	DMF	G	119	5/5	0.85	0.44	12.72	20,20,20,20	0
3	DMF	V	42	5/5	0.90	0.27	12.71	58,58,59,61	0
3	DMF	J	110	5/5	0.84	0.44	12.44	20,20,20,20	0
3	DMF	N	104	5/5	0.74	0.48	12.22	20,20,20,20	0
3	DMF	N	90	5/5	0.93	0.32	12.13	20,20,20,20	0
3	DMF	G	70	5/5	0.81	0.28	12.06	37,38,41,41	0
3	DMF	P	107	5/5	0.89	0.34	12.02	20,20,20,20	0
3	DMF	O	249	5/5	0.89	0.19	11.89	39,40,41,41	0
3	DMF	E	28	5/5	0.58	0.34	11.58	61,61,63,64	0
3	DMF	T	115	5/5	0.92	0.39	11.57	20,20,20,20	0
3	DMF	C	47	5/5	0.82	0.26	11.40	61,62,62,62	0
3	DMF	G	98	5/5	0.88	0.45	11.38	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	DMF	J	45	5/5	0.52	0.43	11.11	41,43,45,46	0
3	DMF	2	57	5/5	0.71	0.34	11.07	54,56,57,57	0
3	DMF	A	250	5/5	0.85	0.27	10.98	39,41,42,44	0
3	DMF	Y	249	5/5	0.93	0.22	10.83	62,64,64,65	0
3	DMF	P	14	5/5	0.86	0.28	10.78	56,58,58,59	0
3	DMF	2	52	5/5	0.74	0.27	10.68	77,77,78,78	0
3	DMF	2	49	5/5	0.76	0.33	10.29	57,57,57,58	0
3	DMF	Y	251	5/5	0.84	0.53	9.94	20,20,20,20	0
3	DMF	O	251	5/5	0.73	0.35	9.60	20,20,20,20	0
3	DMF	V	39	5/5	0.74	0.29	9.10	60,60,61,61	0
3	DMF	H	43	5/5	0.90	0.27	8.99	82,82,83,83	0
3	DMF	B	250	5/5	0.76	0.30	8.98	53,53,55,55	0
3	DMF	H	72	5/5	0.86	0.44	8.93	20,20,20,20	0
3	DMF	X	41	5/5	0.81	0.26	8.71	61,61,62,62	0
3	DMF	K	250	5/5	0.85	0.33	8.29	77,78,79,79	0
3	DMF	F	251	5/5	0.82	0.26	8.06	54,54,55,55	0
3	DMF	M	251	5/5	0.55	0.34	8.04	64,64,66,66	0
3	DMF	X	16	5/5	0.83	0.22	7.93	86,86,86,86	0
3	DMF	2	101	5/5	0.87	0.38	7.76	20,20,20,20	0
3	DMF	K	251	5/5	0.71	0.37	7.52	63,63,64,64	0
3	DMF	G	77	5/5	0.87	0.24	7.32	49,50,50,51	0
3	DMF	W	250	5/5	0.91	0.22	7.22	63,63,64,64	0
3	DMF	G	12	5/5	0.88	0.33	7.20	60,61,62,63	0
3	DMF	Z	54	5/5	0.75	0.24	7.12	58,59,60,61	0
3	DMF	G	62	5/5	0.75	0.29	6.93	72,73,73,74	0
3	DMF	A	249	5/5	0.84	0.27	6.88	44,44,44,44	0
3	DMF	L	97	5/5	0.91	0.28	6.82	20,20,20,20	0
3	DMF	P	56	5/5	0.92	0.19	6.77	59,60,60,61	0
3	DMF	2	4	5/5	0.88	0.22	6.73	62,62,62,62	0
3	DMF	L	36	5/5	0.84	0.21	6.52	41,42,43,43	0
3	DMF	E	53	5/5	0.77	0.25	6.10	56,57,58,59	0
3	DMF	I	250	5/5	0.92	0.22	6.09	41,41,42,42	0
3	DMF	P	60	5/5	0.81	0.24	5.88	68,69,69,69	0
3	DMF	D	249	5/5	0.86	0.24	5.83	53,53,53,54	0
3	DMF	O	250	5/5	0.87	0.21	5.75	44,45,46,48	0
3	DMF	F	250	5/5	0.86	0.24	5.67	56,56,58,59	0
3	DMF	T	10	5/5	0.80	0.33	5.47	71,72,72,74	0
3	DMF	T	29	5/5	0.88	0.22	5.36	76,76,76,76	0
3	DMF	S	250	5/5	0.81	0.19	5.10	59,59,60,61	0
3	DMF	D	251	5/5	0.86	0.27	5.07	94,95,96,96	0
3	DMF	M	250	5/5	0.78	0.26	5.05	60,61,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	DMF	U	249	5/5	0.83	0.24	5.03	40,40,44,45	0
3	DMF	B	249	5/5	0.88	0.21	5.01	50,51,51,53	0
3	DMF	S	249	5/5	0.91	0.25	4.88	54,54,55,56	0
3	DMF	Q	249	5/5	0.92	0.22	4.82	48,48,49,49	0
3	DMF	W	249	5/5	0.83	0.25	4.61	69,70,71,72	0
3	DMF	V	83	5/5	0.88	0.22	4.57	58,59,60,62	0
3	DMF	V	32	5/5	0.93	0.18	4.39	73,74,74,74	0
3	DMF	U	250	5/5	0.88	0.21	4.22	49,50,51,51	0
3	DMF	E	75	5/5	0.89	0.23	3.82	64,64,64,65	0
3	DMF	K	249	5/5	0.80	0.21	3.78	49,50,51,52	0
3	DMF	X	15	5/5	0.85	0.23	3.73	66,67,68,70	0
3	DMF	Y	250	5/5	0.88	0.20	3.55	42,42,44,44	0
3	DMF	M	249	5/5	0.84	0.18	3.50	46,47,48,48	0
3	DMF	D	250	5/5	0.87	0.21	3.12	61,63,64,65	0
3	DMF	Q	250	5/5	0.84	0.28	3.06	84,85,85,86	0
3	DMF	Q	251	5/5	0.91	0.19	2.67	53,53,56,57	0
3	DMF	1	249	5/5	0.91	0.14	2.66	45,47,48,49	0
3	DMF	I	249	5/5	0.93	0.18	2.45	40,42,42,43	0
3	DMF	R	92	5/5	0.94	0.33	1.56	20,20,20,20	0
3	DMF	L	50	5/5	0.82	0.20	1.14	55,56,57,57	0
4	SA6	L	300	20/20	0.93	0.10	0.60	16,19,26,27	0
4	SA6	H	300	20/20	0.92	0.11	0.56	16,21,23,24	0
3	DMF	R	80	5/5	0.88	0.19	0.48	74,75,76,76	0
4	SA6	R	300	20/20	0.95	0.10	0.44	12,21,24,31	0
4	SA6	C	300	20/20	0.96	0.10	0.30	16,19,24,24	0
4	SA6	Z	300	20/20	0.94	0.10	0.26	17,19,22,25	0
4	SA6	V	300	20/20	0.94	0.10	0.24	15,17,21,22	0
4	SA6	N	300	20/20	0.94	0.10	0.22	13,18,23,26	0
4	SA6	2	300	20/20	0.95	0.11	0.19	17,20,28,29	0
4	SA6	P	300	20/20	0.96	0.09	0.12	16,20,28,29	0
4	SA6	J	300	20/20	0.96	0.08	0.04	12,19,24,27	0
4	SA6	E	300	20/20	0.95	0.09	-0.02	12,18,21,24	0
4	SA6	X	300	20/20	0.96	0.09	-0.14	15,17,23,25	0
4	SA6	T	300	20/20	0.94	0.10	-0.17	17,22,28,29	0
4	SA6	G	300	20/20	0.94	0.09	-0.20	11,19,22,24	0
3	DMF	P	33	5/5	0.82	0.20	-	65,66,66,66	0
3	DMF	H	71	5/5	0.91	0.28	-	54,55,55,56	0
3	DMF	E	100	5/5	0.88	0.46	-	20,20,20,20	0
3	DMF	V	116	5/5	0.92	0.21	-	20,20,20,20	0
3	DMF	E	73	5/5	0.64	0.52	-	120,120,121,121	0
3	DMF	C	69	5/5	0.92	0.25	-	48,48,50,50	0
3	DMF	K	252	5/5	0.78	0.37	-	80,81,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	DMF	H	66	5/5	0.80	0.31	-	69,69,69,70	0
3	DMF	P	86	5/5	0.83	0.50	-	20,20,20,20	0
3	DMF	C	121	5/5	0.88	0.24	-	20,20,20,20	0
3	DMF	H	91	5/5	0.86	0.31	-	20,20,20,20	0
3	DMF	N	22	5/5	0.88	0.29	-	44,45,49,50	0
3	DMF	P	51	5/5	0.81	0.23	-	75,76,76,77	0
3	DMF	X	40	5/5	0.73	0.29	-	84,85,85,85	0
3	DMF	C	38	5/5	0.92	0.24	-	64,64,65,65	0

6.5 Other polymers

There are no such residues in this entry.